Mathematical results on quantum many-body physics

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ABSTRACT

The collective behavior exhibited by a large number of microscopic quantum particles is at the heart of some of the most striking phenomena in condensed-matter physics such as Bose-Einstein condensation and superconductivity. Physicists and mathematicians have made great progress in understanding when and how these collective phenomena emerge through the interplay of particle statistics, particle interaction and the value of thermodynamic parameters like the temperature or the chemical potential. Due to the extreme complexity of realistic many-body systems, it is natural to introduce appropriate simplifications to render their analysis feasible. Three examples of such simplifications which have proven themselves as viable starting points for a fruitful and mathematically rigorous analysis of many-body systems are the following: (a) the study of integrable models; (b) the derivation of effective theories, valid on a macroscopic scale, from more fundamental microscopic theories under appropriate coarse-graining; and (c) the use of quantum information theory to understand general connections between correlation, entanglement and particle statistics.

In this thesis, we present mathematically rigorous results that were obtained in these three directions. (1) We prove anomalous quantum many-body transport in XY quantum spin chains for certain choices of the external magnetic field. The anomalous transport is described via new kinds of anomalous Lieb-Robinson bounds, including one of power-law type. We note that the XY spin chain is integrable as it can be mapped to free fermions via the non-local Jordan-Wigner transformation. (2) We derive effective macroscopic theories of Ginzburg-Landau type from the microscopic BCS theory of superconductivity in certain circumstances. We study the case of a multi-component order parameter for translation-invariant systems and the condensation of fermion pairs at zero temperature in a domain with a hard boundary. (3) We use techniques from quantum information-theory to derive bounds on the entropy of fermionic reduced density matrices, a measure of the entanglement inherent to a fermionic quantum state.

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Chapter 1

INTRODUCTION

This thesis is devoted to a mathematical study of aspects pertaining to the quantum many-body problem. Chapter I is a general introduction to the topic. It is purposefully kept rather informal and mainly serves to illustrate the big picture. Chapter II contains an overview of the results presented in Chapters III-VII. These chapters contain specific results that were obtained during my Ph.D. studies. They belong to the following three general avenues of investigation into the quantum many-body problem.

(a) **Integrable toy models.** Chapters III and IV treat anomalous quantum many-body transport in certain quantum XY spin chains.

(b) **Emergence of effective macroscopic theories from microscopic ones.** Chapters V and VI are concerned with the emergence of effective Ginzburg-Landau type theories from the BCS theory of superconductivity, in particular for a system with a hard boundary.

(c) **Quantum information theory and the study of many-body entanglement.** Chapter VII contains bounds on the entropy of fermionic reduced density matrices which quantify the entanglement inherent to fermionic states.

We now begin the general introduction. The quantum many body problem refers to a variety of phenomena that are associated with systems comprised of a large number of interacting microscopic quantum particles. First we review the mathematical framework that is used to define and study quantum many-body systems. Then we continue with an overview of the kind of questions that one commonly asks about these systems, followed by an explanation of why their analysis is difficult. Next, we survey ways to approach and simplify the quantum many-body problem in various contexts and we describe how the results of this thesis fit into this landscape.

1.1 The definition of a quantum many-body system

We have in mind a system consisting of N indistinguishable quantum particles, where N is a fixed large number. In defining such a system, we specify the following three ingredients.

- **One-body Hilbert space** $\mathcal{H}_1$. In many applications, this is an $L^2(X)$ space of complex-valued functions, where X is the configuration space (the set of allowed positions) of a single particle. For example, if a particle can sit anywhere in three-dimensional Euclidean space, one takes $\mathcal{H}_1 = L^2(\mathbb{R}^3)$ with Lebesgue measure; if a particle is placed on a one-dimensional lattice, one takes $\mathcal{H}_1 = \ell^2(\mathbb{Z})$.

- **Particle statistics**. The usual rule in quantum mechanics is that the composition of two Hilbert spaces $\mathcal{H}_A$ and $\mathcal{H}_B$ is described by their tensor product $\mathcal{H}_A \otimes \mathcal{H}_B$. For example, when we combine N copies of the one-body Hilbert space $\mathcal{H}_1$, we obtain $\mathcal{H}_1^{\otimes N}$. To obtain from this tensor power the true *many-body Hilbert space*, we take into account the indistinguishability of the particles. Namely, we project $\mathcal{H}_1^{\otimes N}$ onto the subspace that is appropriate for the *particle statistics*. It is a fundamental fact of Nature that only two kinds of statistics can occur for elementary particles (we ignore the possibility of emergent anyonic statistics here and in the following). These two kinds of statistics give rise to the bosonic and fermionic Hilbert spaces

$$\mathcal{H}_N^{\text{bos}} = \mathcal{S}(\mathcal{H}_1^{\otimes N}), \qquad \mathcal{H}_N^{\text{fer}} = \mathcal{A}(\mathcal{H}_1^{\otimes N}), \tag{1.1}$$

  where $\mathcal{S}$ (respectively $\mathcal{A}$) denotes the projection onto symmetric (respectively antisymmetric) tensors.

- **Hamiltonian**. To complete the definition of a quantum many-body system, the final ingredient is a choice of *many-body Hamiltonian*, denoted H_N. This is a (potentially unbounded) self-adjoint operator defined on the many-body Hilbert space from (1.1). The Hamiltonian determines the physical effects that contribute to the energy of the system and so there is a great variety of Hamiltonians that can be considered.

It is often the case that $\mathcal{H}_1$ is an $L^2(X)$ space and so its N-fold tensor power is isomorphic to $L^2(X^N)$. In this way, one can identify the many-body Hilbert space (1.1) with the subspace of $L^2(X^N)$ corresponding to either symmetric or antisymmetric functions as in (1.2) below. The elements of this space are called *many-body wave functions*.

We now give an *example* of a many-body quantum system that can be defined according to the above procedure.

The example is that of *interacting fermions in three dimensions*. For this, we take the one-body Hilbert space to be $\mathcal{H}_1 = L^2(\mathbb{R}^3)$ with Lebesgue measure. Since the particles have fermionic statistics, the many-body Hilbert space is

$$\mathcal{H}_N^{\text{fer}} = \mathcal{A}((L^2(\mathbb{R}^3))^{\otimes N}) \cong \mathcal{A}(L^2(\mathbb{R}^{3N})).$$

(We ignore spin variables here.) Equivalently, the many-body wave functions are those $\Psi_N \in L^2(\mathbb{R}^{3N})$ satisfying

$$\Psi_N(x_1, x_2, \dots, x_N) = \text{sgn}(\pi)\Psi_N(x_{\pi(1)}, x_{\pi(2)} \dots, x_{\pi(N)}), \quad \forall \pi \in S_N, \tag{1.2}$$

for almost every $(x_1, \dots, x_N) \in \mathbb{R}^{3N}$. Here, $x_i \in \mathbb{R}^3$ describes the position of the ith particle, $\text{sgn}(\pi)$ is the sign of a permutation and S_N denotes the permutation group of N elements.

To complete the example, we define a many-body Hamiltonian H_N. We take H_N to be a sum of one-body terms (acting only on a single x_i) and of a two-body local interaction (a multiplication operator $V(x_i - x_j)$ for every pair of particles). Namely, we take

$$H_N = \sum_{i=1}^{N} (-\Delta_{x_i} + W(x_i)) + \sum_{1 \le i < j \le N} V(x_i - x_j). \tag{1.3}$$

The i-th term in the first sum represents the energy of a single quantum particle in an external potential $W : \mathbb{R}^3 \to \mathbb{R}$ ($-\Delta_{x_i}$ is the kinetic energy of a non-relativistic particle in appropriate units). The second sum ascribes the potential energy $V(x_i - x_j)$ to each pair of particles. The potentials V and W can be specified further depending on the physical system under study. Common specifications are that $W(x) = x^2$ is a harmonic trapping potential and that V depends only on the distance $|x_i - x_j|$.

The above example is the kind of system that we have in mind when we speak of a quantum many-body system. In the next section, we discuss the general questions that are of interest for these systems.

We close the introduction with two remarks concerning alternative formalisms for quantum many-body systems.

For the sake of simplicity, we have focused the above presentation to the case when the total number of particles N is fixed. For systems where N is not fixed, one employs the *Fock space formalism* [70]. The data specifying a quantum many-body system in this formalism is unchanged: One fixes a one-body Hilbert space, the particle statistics and the system Hamiltonian. The idea of the Fock space formalism, in a nutshell, is that in order to define the system state, it suffices to keep track of which elements of the one-body Hilbert space are "occupied" by the many-body system (and the multiplicity of their occupation). This leads to the definition of creation and annihilation operators whose commutation properties implement the particle statistics. The Fock space formalism is important, both from a conceptual and technical standpoint. However, in order to keep the introduction brief, we have opted not to give a detailed definition of the Fock space formalism here.

The above discussion focused on systems in which the *positions* of spinless particles constitute are free to vary. Another important class of quantum many-body systems are *quantum spin systems*, in which conversely the particles are localized to fixed lattice sites but their spin can vary. For example, the many-body Hilbert space of a system of spin 1/2 particles located at the sites j of a finite graph Γ is given by

$$\bigotimes_{j\in\Gamma} \mathbb{C}^2.$$

Common examples of many-body Hamiltonians that are considered on this Hilbert space are the quantum Ising, XY and Heisenberg Hamiltonians with nearest-neighbor couplings. Note that there is no symmetrization or antisymmetrization involved in this definition, in contrast to (1.1). Implicitly, quantum spin systems are bosonic models because operators that act on different tensor copies of the local Hilbert space $\mathbb{C}^2$ automatically commute. The bosonic nature of these models can be made apparent by mapping them to *lattice gas models* in the Fock space formalism via the introduction of spin raising and lowering operators. We will discuss these ideas in detail in Chapters III and IV.

1.2 Questions of interest

In this section, we present the questions that are generally of interest when studying quantum many-body systems.

There are two broad categories: (1) questions that concern the static/time-independent behavior of the system; these are often associated with variational formulations; (2) questions that concern the dynamical/time-dependent behavior of the system; these are often associated with partial differential equations.

Common questions in the static case

We begin with some background concerning quadratic forms. In the static setting, many questions concern the ground state, i.e., the wave function of minimal energy. One commonly studies this in a variational framework, using the quadratic form associated to the Hamiltonian H_N. For the example from the previous section, which had H_N given by (1.3), this quadratic form is obtained from the L^2 scalar product $\langle \Psi_N, H_N \Psi_N \rangle$ by formally integrating by parts, and it reads

$$\begin{aligned} &q[\Psi_N] \\ &:= \sum_{i=1}^N \int_{\mathbb{R}^{3N}} \left(|\nabla_{x_i} \Psi_N|^2 + \left(W(x_i) + \sum_{j>i} V(x_i - x_j) \right) |\Psi_N|^2 \right) \mathrm{d}x_1 \dots \mathrm{d}x_N. \end{aligned}$$

Assuming that V and W are sufficiently nice functions, this quadratic form is well-defined and bounded from below when the input varies over all $\Psi_N \in H^1(\mathbb{R}^{3N})$. (Note that we only need one derivative of Ψ_N to define $q[\Psi_N]$, this is the virtue of working with quadratic forms instead of operators.)

Quadratic forms that are *bounded from below* are the central object of study for static questions. Lower boundedness is essential because it renders the problem of finding the ground state and ground state energy well-defined. Moreover, if one has a slightly stronger condition than lower-boundedness, one can use the KLMN theorem to recover the self-adjoint operator H_N from the quadratic form [159]. (In this context, we mention the related concept of stability of the second kind, the fact that one can obtain a lower bound on the quadratic form that is linear in the number of particles for atomic Hamiltonians [126].)

We now list some of the questions that are commonly asked in the *static* case.

- What is the ground state energy $\inf_{\Psi_N} q[\Psi_N]$? If the infimum is attained, consider the minimizers of q, the ground states. What is their functional form? Are they unique? What are their symmetry properties? How entangled are they?

- Can we describe minimizing sequences in an analogous way? (This is a sensible question also if ground states exist, since it gives a way to establish the stability of certain properties of ground states.)

- Are there macroscopically observable effects that are a consequence of the quantum nature of the microscopic particles? Examples of such macroscopic effects are Bose-Einstein condensation and superconductivity. More generally, does the system display markedly different behavior on different length or energy scales?

- How do the system properties described so far behave in the thermodynamic limit, as the system size and particle number N go to infinity? In particular, are there any phase transitions? I.e., do any of the above answers depend discontinuously on the value of some thermodynamic parameters, like density or temperature? The discontinuity may present itself in a derivative, in that case one speaks of a higher-order phase transition.

- For a system defined on a finite domain, do its properties depend on the boundary conditions or on the topology of that domain?

Common questions in the dynamic case

We come to the *dynamic* (or time-dependent) case. The dynamics are generated by the many-body Schrödinger equation

$$i\frac{d}{dt}\Psi_N(t) = H_N\Psi_N(t).$$

It is sometimes convenient to discuss a dual notion of dynamics, the Heisenberg dynamics that are generated on bounded operators via

$$i\frac{d}{dt}A(t) = [A(t), H_N].$$

These two notions of dynamics are dual in the sense that they yield the same expectation values $\langle\Psi_N(t), A(0)\Psi_N(t)\rangle = \langle\Psi_N(0), A(t)\Psi_N(0)\rangle$ for all t.

The following kinds of questions are commonly asked in the dynamic case.

- Is there transport in the system? Transport can refer for example to the propagation of particles (perhaps understood as wave packets), information and entanglement. The complete absence of transport and ergodic behavior indicates the occurrence of the special "many-body localized" phase.

- If there is transport in any of the above senses, one can ask how fast it is. Is the propagation diffusive, does it occur at a positive ballistic speed, or is it anomalous?

- Suppose we have an efficient description of the system at an initial time (say in form of a tensor product state). For how long is this description valid, at least approximately?

- Is there return to equilibrium? For instance, is there a mechanism that ensures that the time-evolution of some or all initial states converges to a ground state? (A common way to generate such a mechanism is to couple the system to a large environment.) If so, what is the asymptotic rate of equilibration?

- As in the static case: How do the properties described above behave in the thermodynamic limit? Are there phase transitions? What roles do boundary conditions and topology play?

This completes our list of general questions that are commonly asked about quantum many-body systems.

1.3 The difficulty in analyzing quantum many-body systems

Recall formula (1.3) that gave an example of a quantum many-body Hamiltonian. The difficulty in studying such systems comes from the *interaction* term

$$\sum_{1\leq i<j\leq N} V(x_i - x_j),$$

since it creates *correlations* between the different particles. Correlation can occur both in the classical sense (as for correlated random variables) and in the quantum sense (realized e.g. as entanglement).

In particular the quantum correlations pose difficulties. They can be highly non-local and it is not always clear how they manifest themselves. For instance, the antisymmetry of a fermionic wave function Ψ_N as described by the relation (1.2) is an instance of a "quantum correlation" that is inherent to all the available states of a fermionic system but its effects are not easily quantifiable. It is an ongoing quest to understand what kind of reduced density matrices can arise from an antisymmetric N-body wave function Ψ_N. This is called the *N-representability problem* and its solution would have great bearing on quantum chemistry.

The difficulty with controlling entanglement is also related to the fact that the number of possible system states grows exponentially in the system size for quantum systems, due to the built-in tensor product structure. For instance, consider a lattice of N spin 1/2 particles. Its Hilbert space is $(\mathbb{C}^2)^{\otimes N}$, which has complex dimension 2^N and this grows exponentially with N.

Another issue is that the particle number N is often quite large in applications to real-world systems. (An exception are experiments with cold quantum gases. For these, the particle number can be comparatively small, say of the order 10^2.)

To summarize, the quantum aspects and the large numbers of particles involved in quantum many-body systems allow for extensive and intricate correlations within the system state. For interacting systems, these correlations play an important role and cannot be ignored. Consequently, one cannot solve a quantum many-body system analytically, or even numerically, in general.

Since the early days of quantum mechanics, extensive efforts have been made to find approaches to the quantum many-body problem that circumvent these issues. These approaches should be simple enough to allow for conclusive theoretical and numerical investigations, but complex enough to describe the relevant aspects of the true system to good accuracy, at least in certain regimes. This will be the topic of the next section.

1.4 Approaches to the quantum many-body problem

We present a number of the different approaches that have been invented to study the quantum many-body problem. We focus on topics that have been studied mathematically as well.

(1) Integrable models. In special cases, the quantum many-body Hamiltonian under consideration possesses additional algebraic structure that allows one to *solve the system exactly*. Here, "solving a system exactly" does not have a unique meaning. Typically, it means that one can write down the exact eigenstates and eigenvalues for the Hamiltonian, or that one can derive an exact and computable formula for the partition function of the system. Highlights in this context were Bethe's solution of the one-dimensional Heisenberg antiferromagnet [25], Onsager's solution of the two-dimensional Ising model [142] and Lieb's solution of the square ice model [122].

While integrable systems are very special, one can study them in detail and they serve as a testbed for theories and conjectures about more general systems. This is particularly true for system properties that are believed to be the same in an entire *universality class*.

(2) Effective theories. Soon after the advent of quantum mechanics, in 1927, Thomas and Fermi [167, 69] invented the first version of density functional theory to simplify the quantum theory of atomic physics to a more amenable theory. Their simplified theory is in fact correct in the limit of large atomic number [129].

There exist a great number of similar theories that describe the static or dynamical behavior of a quantum many-body system *in some parameter limit*. Three particularly prevalent examples are the *semiclassical limit*, the *dilute limit* and the *mean-field limit*. Justifying the validity of these effective theories in the appropriate parameter limit has been an active field of research in mathematical physics in the last decades. An important example was the derivation of the Gross-Pitaevskii theory describing a Bose-Einstein condensate in the static [127, 128] and in the dynamical case [67]. A common feature of effective theories is that one starts from a quantum many-body Hamiltonian, i.e., a *linear theory of $O(N)$ degrees of freedom* and then, upon coarse-graining the appropriate microscopic degrees of freedom, one derives an *effective non-linear theory of $O(1)$ degrees of freedom.*

(3) Renormalization group methods. Assume that the interaction term, e.g. $\sum_{i<j} V(x_i - x_j)$, is multiplied by a small parameter $\lambda > 0$. Then, for some systems one can obtain convergent power series expansions of physically relevant quantities in λ; a rigorous approach has been developed, e.g. by Benfatto and Gallavotti [18]. In some cases, one can obtain power series that do not converge but that provide valid asymptotic series.

(4) Quantum information theory and the role of entanglement. It can be very useful for studying a quantum many-body system if one can restrict to studying states that are only *mildly entangled* (for example when searching for the ground state of a many-body Hamiltonian). Small entanglement may yield a representation of the state which is more efficient for computation and theoretical investigation. For example, a state satisfying the *area law for the entanglement entropy* (e.g. the ground state of a gapped one-dimensional lattice Hamiltonian [98] or one-dimensional many-body localized states [26]), can be expressed as a *matrix product state* with small bond dimension [13, 77].

It is therefore important to understand both (a) which Hamiltonians have ground states of small entanglement and (b) how small entanglement constrains the structure of a many-body state. In particular the latter issue belongs to the realm of quantum information theory and can be studied using entropy inequalities.

This concludes our discussion of the various approaches to the quantum many-body problem.

We finish this part with an explanation of how the mathematical results in this thesis fit into the landscape that was just discussed.

Chapters III and IV concern the *dynamics of an integrable toy model*, the isotropic XY spin chain in an external magnetic field. We are interested in how its Heisenberg dynamics propagate information. More precisely, we are interested in the *dynamical propagation rate of quantum correlations*, which are expressed as commutators of initially localized observables.

Chapters V and VI concern the *ground state properties of certain effective theories*. We consider the relation between the microscopic BCS theory and macroscopic Ginzburg-Landau type theories. We are interested in the relation between energy minimizing sequences in these two theories, in particular in terms of *degeneracy*, *symmetry* and *boundary conditions*.

Chapter VII concerns the implications that *fermionic statistics* have on the *entanglement structure* of quantum states. This vein of research is loosely motivated by the N-representability problem and thus ultimately by the goal of understanding the ground-state properties of large molecular systems.

Chapter 2

OVERVIEW OF THE RESULTS

In this chapter, we give an overview of the results presented in Chapters III-VII of this thesis. For the overview, the results are grouped as follows: *anomalous Lieb-Robinson bounds* (Chapters III and IV); *effective theories derived from BCS theory* (Chapters V and VI); *entanglement of fermionic states* (Chapter VII).

2.1 Anomalous Lieb-Robinson bounds

Review of the standard Lieb-Robinson bounds

The standard Lieb-Robinson (LR) bounds are *propagation bounds for many-body systems* defined on a lattice via a local Hamiltonian. They control the spread of quantum correlations (expressed as the commutators of initially localized observables) under the Heisenberg dynamics. One may interpret LR bounds as saying that under the many-body dynamics information propagates *at most ballistically*, namely up to exponentially small errors that leak out of a certain spacetime light cone. LR bounds were first proved by Lieb and Robinson [124] in 1972 and they were generalized to a larger class of systems by Nachtergaele and Sims [138]. Hastings and collaborators have found many uses for LR bounds, e.g., for studying the ground states of gapped Hamiltonians [29, 13, 98].

Let us state the standard LR bound (in a slightly simplified version), so that we can compare our results with it. We may consider any system defined on a lattice via a Hamiltonian that has local and bounded interactions. For definiteness, we restrict to *quantum spin systems* defined on the lattice $\mathbb{Z}^d$. The local Hilbert space of a spin 1/2 site is simply $\mathbb{C}^2$. The total Hilbert space of a box $\Lambda_L \subset \mathbb{Z}^d$ of sidelength $2L+1$ is then

$$\mathcal{H}_L = \bigotimes_{j\in\Lambda_L} \mathbb{C}^2.$$

The Hamiltonian H_L is taken to be a self-adjoint operator on this Hilbert space with bounded and finite-range interaction terms. Common and important examples include the nearest-neighbor quantum Heisenberg, XY and Ising models.

To state the LR bound, we introduce a notion of locality for observables. Since $\mathcal{H}_L$ is a finite-dimensional Hilbert space, the set of viable observables is just the set of all matrices on $\mathcal{H}_L$, which we denote by $\mathrm{Mat}(\mathcal{H}_L)$ (we do not require self-adjointness here). We define the local algebra of observables at a site $j \in \Lambda_L$ by

$$\mathcal{O}_j := \left\{ A \in \mathrm{Mat}(\mathcal{H}_L) \ : \ A = A_j \otimes I_{\Lambda_L \setminus \{j\}} \text{ for some } A_j \in \mathrm{Mat}(\mathbb{C}^2) \right\}.$$

In other words, a local observable at site $j \in \Lambda_L$ is one that acts non-trivially exactly at j. For any observable $A \in \mathrm{Mat}(\mathcal{H}_L)$, we define its Heisenberg dynamics at time $t \in \mathbb{R}$ by

$$A(t) := e^{itH_N} A e^{-itH_N}.$$

Theorem 2.1.1 (LR bound)**.** *Let H_L be a Hamiltonian on $\mathcal{H}_L$ that has local and bounded interactions. There exist constants $C, \xi > 0$ and $v \geq 0$ such that the following holds. For all $j, k \in \Lambda_L$ with $j \neq k$, we have the bound*

$$\|[A(t), B]\| \leq C\|A\|\|B\|e^{\xi(vt - |j-k|)}, \tag{2.1}$$

for all observables $A \in \mathcal{O}_j$ and $B \in \mathcal{O}_k$.

Here we wrote $|| \cdot \|$ for the standard operator norm on $\mathrm{Mat}(\mathcal{H}_L)$ and $| \cdot |$ for graph distance on $\mathbb{Z}^d$.

Let us make some comments about this theorem.

The left-hand side in (2.1) vanishes at $t = 0$. Indeed, $A(0) = A$ and $[A, B] = 0$ since the two operators only act non-trivially at different sites $j \neq k$. In other words, A and B are uncorrelated observables at time $t = 0$. For any arbitrarily small positive time $t > 0$, $A(t)$ will be supported on the whole box Λ_L, so the above argument breaks down immediately. Nonetheless, the LR bound (2.1) quantifies the extent to which the correlation (commutator) between $A(t)$ and B remains small under the Heisenberg dynamics.

The LR bound is useful when the right-hand side is small and this is the case precisely *outside of the spacetime light cone* $vt = |j-k|$, namely for $vt < |j-k|$. The slope of the cone is v, the so-called *Lieb-Robinson velocity*. (The name "light cone" is of course used in reference to relativistic systems which possess a light cone of slope c, the speed of light, outside of which correlations vanish identically; in LR bounds the slope is v and correlations are only exponentially suppressed outside of the cone.)

We also remark on the thermodynamic limit $L \to \infty$. The constants C, ξ and v depend on the dimension d and the operator norm of the local interaction terms. Therefore, if the individual interaction terms that are added as L grows are all identical (e.g. if H_L describes a quantum Heisenberg, XY or Ising model at fixed coupling), then the constants C, ξ and v are uniform in the thermodynamic limit $L \to \infty$.

Our results on anomalous LR bounds

We are now ready to discuss our results in Chapters III and IV. In both of these chapters, we consider an isotropic XY quantum spin chain. The Hilbert space of a one-dimensional chain of L quantum spins reads

$$\mathcal{H}_L = \bigotimes_{j=1}^{L} \mathbb{C}^2.$$

On this Hilbert space, we consider the Hamiltonian

$$H_L = -\sum_{j=1}^{L-1} \left(\sigma_j^1 \sigma_{j+1}^1 + \sigma_j^2 \sigma_{j+1}^2\right) + \sum_{j=1}^{L} h_j \sigma_j^3. \tag{2.2}$$

Here $\sigma^1, \sigma^2, \sigma^3$ denote the standard Pauli matrices; they are embedded into $\mathrm{Mat}(\mathcal{H}_L)$ by tensoring them with the identity, i.e. $\sigma_j^a = \sigma^a \otimes I_{\{1,\ldots,L\}\setminus\{j\}}$ for $a = 1, 2, 3$. The remaining free parameters in the model are the local magnetic fields $h_j \in \mathbb{R}$.

The model (2.2) is an integrable toy model for truly interacting systems. It is unitarily equivalent to a system of free fermions via the Jordan-Wigner transformation. This allows to relate its many-body transport properties, expressed in terms of LR bounds, to the transport properties of a one-dimensional discrete Schrödinger operator describing a single electron, a topic that has been studied extensively in the past. The magnetic field h_j becomes the on-site potential felt by the single electron under the Jordan-Wigner transformation. In this way, one can vary h_j to obtain many-body models (2.2) showing various different kinds of transport behavior. We mention that relating the transport properties of the Schrödinger operator back to the many-body system is non-trivial because the Jordan-Wigner transformation is *non-local* (and transport bounds of course depend inherently on the notion of locality that is being used).

Previous results concerning LR bounds in the model (2.2) (and its anisotropic generalization) considered the following two extreme cases.

- Hamza, Sims and Stolz [96] proved that if the $\{h_j\}$ are i.i.d. random variables sampled according to a distribution with bounded probability density, then the LR bound (2.1) holds with velocity $v = 0$. This may be understood as a version of many-body localization.
- Damanik, Lukic and Yessen [50] proved that if the $\{h_j\}$ are periodic, then the LR bound (2.1) can only hold for $v \geq v_* > 0$, where the minimal velocity v_* can be characterized explicitly in terms of a certain propagation operator. This may be understood as saying that for periodic potentials, many-body transport is precisely ballistic. The result was later generalized to quasi-periodic potentials admitting a Floquet decomposition [105].

Given these two results, it is natural to ask if one can derive intermediate transport behavior by selecting a different magnetic field. This is the content of our joint works [48, 47] with David Damanik, Milivoje Lukic and William Yessen. The main result of these works reads as follows. We write χ_I for the indicator function of an interval I.

Theorem 2.1.2. *Let h_j be given by the Fibonacci external potential, i.e.,*

$$h_j = \lambda \chi_{[1-\phi^{-1},1)}(j\phi^{-1} \text{mod} 1),$$

where $\lambda \geq 8$ is a coupling constant and $\phi = (1+\sqrt{5})/2$ is the golden mean. Then, there exists $0 < \alpha < 1$ and constants $C, \xi > 0$, $v \geq 0$ such that for all $1 \leq j < k \leq L$, we have

$$\|[A(t), B]\| \leq C\|A\|\|B\| e^{\xi(vt^\alpha - |j-k|)}, \tag{2.3}$$

for all observables $A \in \mathcal{O}_j$ and $B \in \mathcal{O}_k$.

The key here is the occurrence of the exponent $0 < \alpha < 1$ in (2.3). It signifies anomalous quantum many-body transport because it "bends" the light cone where the LR bound is effective. The new "light cone" is now the set $\{vt^\alpha = |j-k|\}$.

Our results in [48, 47] also give an explicit characterization of the optimal value of α such that (2.3) holds. Namely, α has to be greater or equal to the one-body transport exponent α_u^+ of the discrete Schrödinger operator obtained via the Jordan-Wigner transformation. (This statement holds for all $\lambda > 0$, but we only know that $0 < \alpha_u^+ < 1$ for $\lambda > 8$.) Roughly speaking, α_u^+ is the propagation rate of the fastest part of an initially localized wave packet under the one-body dynamics. That is, if one starts with an initially localized wave packet at the origin, then after time t the fastest part of the wave packet has traveled a distance $O(t^{\alpha_u^+})$ if one ignores exponential tails (exponential tails usually cannot be avoided in quantum theory). The precise definition of α_u^+ and further details are discussed in Chapter III.

Let us explain why the bound (2.3) is indeed a qualitative improvement over the standard LR bound (2.1). (We do not track the numerical values of the constants C, ξ and v, so we cannot make quantitative statements.) Let $j = 1$, fix a far away site k and start the dynamics at $t = 0$. Then the bound (2.3) is informative for times of the order $|k|^{1/\alpha}$, while the original bound (2.1) is informative for times of the order $|k|$. Since $0 < \alpha < 1$, we have $|k|^{1/\alpha} \gg |k|$ for large k and so the new bound (2.3) is useful for substantially longer times.

Lieb-Robinson bounds of power-law type

We now come to the results of Chapter IV, which were obtained in collaboration with Martin Gebert. To motivate these, we mention that there exist other discrete Schödinger operators which display intermediate transport behavior in a different sense than the Schödinger operator with Fibonacci potential considered above.

For the discrete Schrödinger operator with Fibonacci potential, one quantifies the one-body quantum transport on an *exponential scale* in terms of the transport exponent α_u^+ described above. It is then natural that the anomalous LR bound (2.3) for the Fibonacci model also features an exponentially small error term.

However, for some other models, like the random dimer model of Dunlap, Wu and Philips [63], the one-body quantum transport looks ballistic on the exponential scale, but it is *anomalously slow if power-law errors are allowed.*

For such models, $\alpha_u^+ = 1$ and so a bound like (2.3) will only hold with $\alpha = 1$, meaning that there is no improvement over the original LR bound. However, one may take the perspective that this is the case only because one is asking for a lot by requiring *exponential* decay away from the light cone. These considerations led us to attempt to prove LR bounds with *power-law error terms* for the random dimer model in [48, 47], but it turns out that the method breaks down for this model. (In a nutshell, the reason is that the Jordan-Wigner transformation allows one to bound $\|[A(t), B]\|$ by a sum of one-body transport quantities. These can be bounded by objects that decay like a power law for the random dimer model, but the power-law decay decreases by one order under summation. This decrease by one renders the method inconclusive for the random dimer model.)

A year after the works [48, 47] were completed, in a collaboration with Martin Gebert [79], we found a different model to which the idea of power-law type LR bounds could be applied. The model is one with decaying randomness, i.e.,

$$h_j = \lambda \frac{\omega_j}{\sqrt{j}}, \tag{2.4}$$

where $\lambda > 0$ is a coupling constant and $\{\omega_j\}$ are i.i.d. random variables of mean zero, variance one and distributed according to a bounded probability density. The decaying envelope $j^{-1/2}$ is critical in the sense that it is just barely not square-summable. The corresponding one-body Schrödinger operator was studied extensively by Delyon, Simon and Souillard [56] and by Kiselev, Last and Simon [111].

Our first result with M. Gebert, which is discussed in more detail in Chapter IV of this thesis, says that one has a zero-velocity power-law LR bound on average when the disorder strength λ is sufficiently large.

Theorem 2.1.3. *Let H_L be given by (2.2) with h_j as in (2.4). Then, there exist constants $C, \kappa > 0$ such that for all $\lambda > 0$ with $\kappa\lambda^2 > 5/4$ and for all $1 \leq j < k \leq L$, we have*

$$\mathbf{E}\left(\sup_{t\in\mathbb{R}} \|[A(t), B]\|\right) \leq C\|A\|\|B\|(jk)^{5/4}\left(\frac{j}{k}\right)^{\kappa\lambda^2}, \tag{2.5}$$

for all observables $A \in \mathcal{O}_j$ and $B \in \mathcal{O}_k$.

We comment on the form of the right-hand side in (2.5). The model is not translation-invariant, so there is no direct dependence on $|j-k|$. For simplicity, set $j = 1$. Then, the bound says that the commutator $[A(t), B]$ decays like a power-law in k, with a power that is determined by the disorder strength. The bound holds uniformly in time, making it a *zero-velocity* LR bound.

In [79], we also prove a converse statement: For *small* disorder ($\lambda < 2$), there are signs of transport in the model. Namely, the *anomalous power-law LR bound*

$$\|[A(t), B]\| \leq C\|A\|\|B\| \left(\frac{vt^a}{k}\right)^b$$

will fail (for some $A \in \mathcal{O}_1$ and $B \in \mathcal{O}_k$) if a is small and b is large. (The precise condition is $1 + 1/(2b-1) < a^{-1}$.) The failure of such a propagation bound to hold *suggests* that the model exhibits a *phase transition*, as the disorder strength is varied, from a phase with many-body localization in the sense of (2.5) to a phase with many-body transport.

A breakdown of the delicate many-body localized (MBL) phase is indeed expected to occur in more realistic systems [144, 171]. The MBL phase should break down as interactions get too strong, which is equivalent to λ getting smaller in our model. The fact that the present model might exhibit a breakdown of the MBL phase is an advantage it holds compared to another popular toy model, the XY chain with ordinary i.i.d. (non-decaying) disorder. The latter model is fully localized for arbitrarily small disorder strength.

This concludes our discussion of anomalous Lieb-Robinson bounds. Further details are provided in Chapters III and IV. An interesting open problem in this context is whether one can establish analogously anomalous dynamical behavior for the *entanglement entropy* in the systems discussed above. A static variant of this question is whether the many-body ground states of these systems violate the area law for the entanglement entropy (and if so, in which way).

2.2 Effective theories derived from BCS theory

Translation-invariant multi-component systems

In Chapter V, we describe joint work with Rupert L. Frank. We consider a system of interacting fermions in d dimensions ($d = 1, 2, 3$) at chemical potential $\mu \in \mathbb{R}$ and temperature $T \geq 0$. The particles have a tendency to form pairs due to some underlying physical mechanism which is expressed by a local interaction potential $V(x)$. There are no external fields and therefore the system is translation-invariant.

The system is described using a variational formulation of BCS theory in which system states are described by quasi-free states. Thanks to translation-invariance, a BCS state is fully characterized by the following multiplication operator on $L^2(\mathbb{R}^d) \oplus L^2(\mathbb{R}^d)$. For any value of the momentum $p \in \mathbb{R}^d$, the operator is defined by

$$\widehat{\Gamma}(p) = \begin{pmatrix} \widehat{\gamma}(p) & \widehat{\alpha}(p) \\ \overline{\widehat{\alpha}}(p) & 1 - \widehat{\gamma}(p) \end{pmatrix}. \tag{2.6}$$

The physical meaning of the functions appearing here is that $\widehat{\gamma}(p)$ is the Fourier transform of the one-body density matrix and $\widehat{\alpha}(p)$ is the Fourier transform of the Cooper pair wave function. Since $\widehat{\Gamma}$ describes a fermionic quantum state, it must satisfy the constraint $0 \leq \widehat{\Gamma}(p) \leq 1$ for every $p \in \mathbb{R}^d$. The variational theory is defined via the *BCS free energy* of a system state $\widehat{\Gamma}$

$$\mathcal{F}^{BCS}(\widehat{\Gamma}) = \int_{\mathbb{R}^d} (p^2 - \mu)\widehat{\gamma}(p)\mathrm{d}p - TS[\widehat{\Gamma}] + \iint_{\mathbb{R}^d \times \mathbb{R}^d} V(x)|\alpha(x)|^2 \mathrm{d}x. \tag{2.7}$$

Here we introduced the entropy

$$S[\widehat{\Gamma}] = -\int_{\mathbb{R}^d} \mathrm{Tr}[\widehat{\Gamma}(p) \log \widehat{\Gamma}(p)]\mathrm{d}p.$$

This variational formulation of BCS theory is due to [11, 57]. For a heuristic derivation of the free energy functional (2.7) from an appropriate many-body Hamiltonian, see, e.g., Appendix A in [89].

To get a better grasp of the free energy, (2.7), let us consider the terms separately. The first term describes unpaired electrons and would be minimal for $\widehat{\gamma}(p) = \mathbb{1}_{p^2<\mu}$, which is the indicator function of the Fermi sphere (the constraint $0 \leq \widehat{\Gamma}(p) \leq 1$ implies that $0 \leq \widehat{\gamma}(p) \leq 1$ as well). The third term in (2.7) describes the energetic gain of pair formation and would be minimal when $\alpha(x)$ is large where $V(x)$ is negative. While the third term could be made arbitrarily large, its size is constrained by the estimate $|\widehat{\alpha}(p)|^2 \leq \widehat{\gamma}(p)(1-\widehat{\gamma}(p))$ which follows from $0 \leq \widehat{\Gamma}(p) \leq 1$. In particular, if $\widehat{\gamma}(p)$ is an indicator function, then $\alpha = 0$. The difficulty in analyzing the free energy functional (2.7) stems from the constraint $|\widehat{\alpha}(p)|^2 \leq \widehat{\gamma}(p)(1 - \widehat{\gamma}(p))$ and the entropy term in (2.7), which couples $\widehat{\gamma}$ and $\widehat{\alpha}$ in a nonlinear way.

The BCS free energy is a microscopic model for superconductivity or superfluidity (depending on the physical context). These are macroscopic quantum effects which stem from the existence of a Cooper pair wave function that is coherent over the system. In the variational framework considered here, we say that pair formation (and therefore superconductivity, respectively superfluidity) occurs if any BCS state $\widehat{\Gamma}$ minimizing the BCS free energy has a non-zero Cooper pair wave function $\widehat{\alpha} \neq 0$.

It turns out that in the translation-invariant model considered here, there exists a unique critical temperature T_c such that pair formation occurs iff $T < T_c$. In 2008, Hainzl, Hamza, Seiringer and Solovej [89] characterized the critical temperature by the following linear criterion. To state it, we introduce the linear operator

$$K_T := \frac{-\Delta - \mu}{\tanh\left(\frac{-\Delta-\mu}{2T}\right)}$$

on the space of even functions

$$L^2_{\mathrm{symm}}(\mathbb{R}^d) = \left\{ f \in L^2(\mathbb{R}^d) \ : \ f(x) = f(-x) \text{ a.e.} \right\}.$$

The operator K_T can be defined as a multiplication operator in Fourier space. Elementary considerations inform us that the operator $K_T + V$ (which may be thought of as a variant of a Schrödinger operator) has essential spectrum starting at $2T > 0$. The following theorem is proved in [89].

Theorem 2.2.1. *The system exhibits pair formation (i.e. any minimizer of $\mathcal{F}^{BCS}$ has $\widehat{\alpha} \neq 0$) iff $K_T + V$ has at least one negative eigenvalue. There exists a unique critical temperature $T_c \geq 0$ such that $K_T + V$ has a negative eigenvalue iff $T < T_c$.*

The basic idea behind this linear criterion describing T_c is that it checks whether the Hessian $K_T + V$ of the "normal state" Γ_0 is positive definite. (The normal state Γ_0 is the minimizer of $\mathcal{F}^{BCS}$ for $\alpha = 0$; its $\widehat{\gamma}(p)$ is just the Fermi-Dirac distribution.) The reason for this is that the normal state is the prime competitor for the presence of non-trivial α and therefore its instability signifies the onset of pair formation. What is remarkable about this theorem is that it proves that in the nonlinear theory under consideration, the local instability of the normal state is equivalent to global instability. The uniqueness of T_c follows from the monotonicity properties of K_T (note that tanh is a monotone function).

Given the definition of the critical temperature, one may ask if one can derive an effective Ginzburg-Landau description of the superconductivity (or superfluidity) for T close to T_c, in the spirit of Gorkov's argument [85] for the original BCS model (which featured a very particular choice of V, an indicator function in Fourier space). This question was asked and answered in a breakthrough paper by Frank, Hainzl, Seiringer and Solovej [73] who considered the technically more challenging situation with weak and slowly varying external fields (so that one loses translation-invariance). However, they work under a non-degeneracy assumption that we explain now.

At the critical temperature, the operator $K_{T_c} + V$ has a zero eigenvalue. The key parameter for us is the dimension of this eigenspace

$$n := \dim \ker(K_{T_c} + V).$$

We know that $1 \leq n < \infty$, since zero belongs to the discrete spectrum. The assumption in [73] is that $n = 1$ and our contribution is to drop this assumption for translation-invariant systems. The physical meaning of the case $n > 1$ is that superconductivity, respectively superfluidity, may occur in different "channels". Indeed, the elements of $\ker(K_{T_c} + V)$ are precisely the microscopically realized Cooper pair wave functions.

The first main result of Chapter V is that one obtains a multi-component Ginzburg-Landau (GL) theory from the microscopic BCS free energy close to the critical temperature. The degeneracy parameter n gives exactly the number of order parameters in the GL theory.

To state the theorem, we recall that Γ_0 denotes the normal state. We restrict the BCS free energy to an appropriate set of admissible states $\mathcal{D}$ in order to ensure that the corresponding minimization problem is well-defined. The detailed definition of this set is of no further importance and we refer the interested reader to Chapter V for the details.

Theorem 2.2.2. *As $T \uparrow T_c$, we have*

$$\inf_{\Gamma \in \mathcal{D}} \mathcal{F}^{BCS}(\Gamma) - \mathcal{F}^{BCS}(\Gamma) = \left(\frac{T_c - T}{T_c} \right)^2 \inf_{\mathfrak{a} \in \ker(K_{T_c}+V)} \mathcal{E}^{GP}(\mathfrak{a}) + O\left(\frac{T_c - T}{T_c} \right)^3 \tag{2.8}$$

with the Ginzburg-Landau energy

$$\mathcal{E}^{GP}(\mathfrak{a}) = \int_{\mathbb{R}^d} F(p)|\mathfrak{a}(p)|^4 \mathrm{d}p - \int_{\mathbb{R}^d} G(p)|\mathfrak{a}(p)|^2 \mathrm{d}p \tag{2.9}$$

for certain explicit functions $F, G : \mathbb{R}^d \to \mathbb{R}_+$.

This theorem expresses an energetic "derivation" of GL theory from BCS theory. One may also establish the convergence of approximate minimizers. We discuss this in Chapter V as well.

This theorem establishes the naturality of the "Mexican hat shape" in the GL description of translation-invariant systems. The usual Mexican hat potential emerges when $n = 1$, in which case we have $\ker(K_{T_c} + V) = \operatorname{span}\{\mathfrak{a}_0\}$ and so we can rewrite the minimization over $\mathfrak{a} \in \ker(K_{T_c} + V)$ as one over coefficients $\psi \in \mathbb{C}$ where $\mathfrak{a} = \psi \mathfrak{a}_0$. Then (2.9) becomes

$$\begin{aligned} \mathcal{E}^{GP}(\psi) =& |\psi|^4 \left(\int_{\mathbb{R}^d} F(p) |\mathfrak{a}_0(p)|^4 \mathrm{d}p \right) - |\psi|^2 \left(\int_{\mathbb{R}^d} G(p) |\mathfrak{a}_0(p)|^2 \mathrm{d}p \right) \\ =& c_1 |\psi|^4 - c_2 |\psi|^2. \end{aligned}$$

In Chapter V, we compute and study examples of microscopically derived GL theories with multi-component order parameters: a pure d-wave order parameter and a mixed $(s + d)$-wave order parameter. One of our findings is that the emergent symmetry group in the case of a pure d-wave order parameter is rather large, $O(5)$, as compared to the $O(3)$ that could be expected.

Moreover, in Chapter V, we construct radial potentials of the form

$$V(x) = -\lambda \delta(|x| - R),$$

which produce eigenspaces $\ker(K_{T_c} + V)$ of *arbitrary angular momentum*, for open sets of parameter values. This is in stark contrast to the Schrödinger case $\ker(-\Delta + V)$ for which ground states are non-degenerate (and therefore have angular momentum zero in the radial case). This is a consequence of the Perron-Frobenius theorem which holds under weak assumptions on V. The construction of these potentials is based on a new fact about the maxima of half-integer Bessel functions which is discussed in the appendix to Chapter V.

The macroscopic persistence of boundary conditions

In Chapter VI, we describe joint work with Rupert L. Frank and Barry Simon in which we consider a zero-temperature and low-density version of the BCS theory in which particles are confined to a domain $\Omega \subset \mathbb{R}^d$ and are subjected to a weak external field $W : \Omega \to \mathbb{R}$. Clearly, the model is then no longer translation-invariant. Consequently, we need to make some changes in the setup of the theory.

First, the system states are now described by an operator $0 \leq \Gamma \leq 1$ on $L^2(\Omega) \oplus L^2(\Omega)$ of the form

$$\Gamma = \begin{pmatrix} \gamma & \alpha \\ \overline{\alpha} & 1 - \overline{\gamma} \end{pmatrix},$$

which is no longer a multiplication operator in Fourier space. Here γ and α are operators on $L^2(\Omega)$ and we can describe them via their operator kernels $\gamma(x, y)$ and $\alpha(x, y)$.

We introduce a small parameter $h > 0$ that describes the ratio between the microscopic and macroscopic lengthscales. The BCS energy is defined as

$$\mathcal{E}_\mu^{BCS}(\Gamma) = \mathrm{Tr}[(-h^2\Delta_\Omega + h^2 W - \mu)\gamma] + \iint_{\Omega\times\Omega} V\left(\frac{x-y}{h}\right)|\alpha(x,y)|^2 \mathrm{d}x\mathrm{d}y. \tag{2.10}$$

Here $-\Delta_\Omega$ is the Dirichlet Laplacian on Ω; it indicates the confinement of the particles to the domain Ω. The bounded function $W : \Omega \to \mathbb{R}$ describes the external potential; it is weak because it comes with the h^2 prefactor. We emphasize that there is no entropy term in (2.10) because we consider the system at zero temperature.

We will consider this energy at choices of the chemical potential $\mu \in \mathbb{R}$ that correspond to small particle density. The physical picture that we have in mind is the following: the system will be composed mostly of tightly bound fermion pairs. At low density, these pairs are on average far apart and thus look like bosons to one another. Since we are at zero temperature, the pairs should then form a Bose-Einstein condensate. In analogy to the derivation of Ginzburg-Landau theory in the previous section, we can then derive an effective Gross-Pitaevskii theory describing the condensate of fermion pairs. The fact that BCS theory can be used to describe this physical regime was noticed in the early 80s and is commonly called the BCS-BEC crossover.

To implement the idea of tightly bound fermion pairs, we make the key assumption that the potential V is indeed strong enough to form a bound state.

Assumption 2.2.3. *$V : \mathbb{R}^d \to \mathbb{R}$ is such that $-E_b := \inf \mathrm{spec}(-\Delta_{\mathbb{R}^d} + V) < 0$.*

The following theorem derives Gross-Pitaevskii (GP) theory from the BCS energy (2.10) in a regime of low density (it is proved in Chapter VI by a duality argument that the choice of chemical potential $\mu = -E_b + O(h^2)$

below indeed corresponds to low density). The GP energy is defined similarly to the Ginzburg-Landau energy from the previous section as

$$\mathcal{E}_D^{GP}(\psi) := \int \left(\frac{1}{4}|\nabla\psi|^2 + (W-D)|\psi|^2 + g|\psi|^4\right) \mathrm{d}x,$$

where $D \in \mathbb{R}$ and $g > 0$ are parameters. As before, $\mathcal{D}$ represents some admissible class of BCS states Γ that renders the minimization problem $\mathcal{E}_\mu^{BCS}$ well-defined. The detailed definition of $\mathcal{D}$ can be found in Chapter VI.

Theorem 2.2.4. *Assume that $\Omega \subset \mathbb{R}^d$ is a bounded Lipschitz domain and that V satisfies the assumption above. Then, there exists $c_\Omega > 0$ so that, as $h \downarrow 0$, we have*

$$\inf_{\Gamma\in\mathcal{D}} \mathcal{E}_{-E_b+Dh^2}^{BCS}(\Gamma) = h^{4-d} \inf_{\psi\in H_0^1(\Omega)} \mathcal{E}_D^{GP}(\psi) + O(h^{4-d+c_\Omega}), \tag{2.11}$$

for some explicit $g > 0$.

We remark that the constant $c_\Omega > 0$ in the error term depends on the regularity of Ω. For example, one can choose $c_\Omega = 1 - \varepsilon$ for any $\varepsilon > 0$ if Ω is convex.

This theorem is not the first in this context. Similar results were proved on the torus [94] and on the full space with bounded W [28]. A time-dependent analogue was proved in [91]. The difference between all of these results and ours is that they consider a *system without boundary.* We consider instead a system with a sharp boundary, modeled by the Dirichlet condition.

On the right-hand side of (2.11), observe that the minimization takes place over the Sobolev space $H_0^1(\Omega)$. In other words, the *Dirichlet boundary conditions are preserved* under the limit $h \downarrow 0$. This is not a priori clear. We are integrating out microscopic scales to arrive at the GP energy and one might think that the boundary condition is a subleading effect as one integrates out small scales. The result says that the boundary in fact plays a role on the macroscopic scale to leading order. To see that this is a subtle question, we mention that de Gennes [58] predicted that, at positive temperature and density, the sharp boundary conditions should be forgotten (i.e. a Dirichlet BCS energy should yield a Neumann Ginzburg-Landau energy).

This concludes our presentation of the results concerning effective theories derived from BCS theory in Chapters V and VI.

2.3 The entanglement inherent to fermionic states

In Chapter VII, we describe a recent result concerning the entropy of the reduced density matrices of any permutation-invariant quantum state. These entropies can be viewed as a way to quantify the entanglement that is inherent to a quantum state.

To make this more precise, let us define the quantities under consideration. We consider the many-body Hilbert space $\bigotimes_{m=1}^{N} \mathbb{C}^d$, where d is the dimension of the one-body Hilbert space. We will take $d \geq N$ which is necessary for having fermionic states. (We have $d \geq N$ e.g. for a tight-binding model of N spin-polarized electrons hopping on d lattice sites.) Given any quantum state ρ_N on the many-body Hilbert space, we obtain its k-body reduced reduced density matrix by tracing out $N-k$ of the particles, i.e.,

$$\gamma_k = \mathrm{Tr}_{k+1,\ldots,N}[\rho_N].$$

Here we use the convention for the partial trace that gives $\mathrm{Tr}[\gamma_k] = \mathrm{Tr}[\rho_N] = 1$. We are interested in the following entropies

$$S_k := S(\gamma_k) := -\mathrm{Tr}[\gamma_k \log \gamma_k].$$

These entropies quantify the entanglement of the state ρ_N with respect to the Hilbert space decomposition

$$\bigotimes_{m=1}^{N} \mathbb{C}^d = \bigotimes_{m=1}^{k} \mathbb{C}^d \otimes \bigotimes_{m=1}^{N-k} \mathbb{C}^d,$$

i.e., they quantify the extent to which k particles are entangled with the remaining $N-k$ particles in the state ρ_N. We are interested in finding *lower bounds* on the entropies S_k. In other words, we are interested in finding the states that are the *least entangled* in this sense.

For bosonic states, one can make all $S_k = 0$. This is achieved by taking ρ_N to be a pure condensate wave function, namely

$$\rho_N = |\phi^{\otimes N}\rangle\langle\phi^{\otimes N}|.$$

Indeed, then we have for every k that $\gamma_k = |\phi^{\otimes k}\rangle\langle\phi^{\otimes k}|$ is still a pure state and so its entropy vanishes.

The situation is markedly different for fermions. The entropies S_k can not all be made zero and therefore fermionic states are always non-trivially entangled in this sense. A natural question is then which fermionic states minimize the entropies S_k. By concavity of the entropy, one may restrict to pure fermionic states $|\Psi_N\rangle\langle\Psi_N|$.

In 1976, Coleman [39] solved this problem in the $k = 1$ case.

Theorem 2.3.1 (Coleman)**.** *$S(\gamma_1) \geq \log N$ and the minimum is achieved if Ψ_N is a Slater determinant.*

Coleman's result was generalized to the following conjecture by Carlen, Lieb and Reuvers (CLR) in 2016 [33].

Conjecture 2.3.2. *$S(\gamma_2) \geq \log \binom{N}{2}$ and the minimum is achieved if Ψ_N is a Slater determinant.*

The fact that $S(\gamma_2) = \log \binom{N}{2}$ for Slater determinants follows from an elementary computation. CLR also put forward a weaker, asymptotic form of their conjecture that $S(\gamma_2) \geq 2 \log N + o(1)$ as $N \to \infty$. They prove in their paper that

$$S(\gamma_2) \geq \log N + o(1) \tag{2.12}$$

by using a strengthened form of the strong subadditivity of the quantum entropy. (Alternatively, this fact can be proved by using Yang's bound on the largest eigenvalue of γ_2, as is also mentioned in [33].)

One of the observations put forward in Chapter VII are general properties of the map $k \mapsto S_k$ that yield an improvement of (2.12) as a corollary.

Theorem 2.3.3. *Let γ_k be the k-body density matrix of any permutation-invariant pure state $|\Psi_N\rangle\langle\Psi_N|$. Then the map $k \mapsto S_k$ has the following properties.*

(i) ***Monotonicity.*** *For every $1 \leq k \leq \frac{N}{2} - 1$,*

$$S_k \leq S_{k+1}. \tag{2.13}$$

(ii) ***Concavity.*** *For every $2 \leq k \leq N - 1$,*

$$S_k \geq \frac{S_{k+1} + S_{k-1}}{2}. \tag{2.14}$$

These properties follow directly from applications of the monotonicity of the relative entropy and the symmetry property $S_k = S_{N-k}$ which holds for any permutation-invariant state. (Note that if Ψ_N is a fermionic wave function, then $|\Psi_N\rangle\langle\Psi_N|$ is a permutation-invariant state.)

Combining the monotonicity property with Coleman's theorem yields

$$S_2 \geq S_1 \geq \log N,$$

so as a corollary we obtain a new proof of (2.12).

Chapter VII contains the proof of this result as well as another theorem that establishes the bound $S(\gamma_2) \geq 2\log N + \log(d - N)$. This bound also follows from Yang's bound on ther largest eigenvalue of γ_2, but we give an entropic proof of it that is is inspired by a joint work on approximate quantum cloning with Mark M. Wilde [121]. We note that the bound $S(\gamma_2) \geq 2\log N + \log(d - N)$ implies the conjecture by CLR if $d - N = O(1)$.

This finishes our overview of the results in Chapters III-VII. The remainder of this thesis contains further details and proofs of the statements that we presented in this overview.

Chapter 3

NEW ANOMALOUS LIEB-ROBINSON BOUNDS IN QUASI-PERIODIC XY CHAINS

David Damanik, Marius Lemm, Milivoje Lukic and William Yessen

3.1 Introduction

Relativistic systems are local in the sense that information propagates at most at the speed of light. In their seminal paper [124], Lieb and Robinson found that non-relativistic quantum spin systems described by local Hamiltonians satisfy a similar "quasi-locality" under the Heisenberg dynamics. Their *Lieb-Robinson bound* and its recent generalizations [97, 138] implies the existence of a "light cone" $|x| \leq v|t|$ in space-time, outside of which quantum correlations (concretely: commutators of local observables) are exponentially small. In other words, the LR bound shows that, to a good approximation, quantum correlations *propagate at most ballistically*, with a system-dependent "Lieb-Robinson velocity" v.

About ten years ago, the general interest in LR bounds re-surged when Hastings and co-workers realized that they are the key tool to derive exponential clustering, a higher-dimensional Lieb-Schultz-Mattis theorem and the celebrated *area law for the entanglement entropy* in one-dimensional systems with a spectral gap [99, 97, 98]. These results highlight the role of entanglement in constraining the structure of ground states in gapped systems and yield many applications to quantum information theory, e.g. in developing algorithms to simulate quantum systems on a classical computer [29, 13].

In this paper, we announce and sketch the rigorous proof of a new kind of *anomalous (or sub-ballistic) Lieb-Robinson bound* for an isotropic XY chain in a quasi-periodic transversal magnetic field. The LR bound is anomalous in the sense that the forward half of the ordinary light cone is changed to the region $|x| \leq v|t|^\alpha$ for some $0 < \alpha < 1$.

Previous study has focused on the dependence of the Lieb-Robinson velocity v on the system details [138], with particular interest in the case $v = 0$, since it may be interpreted as dynamical localization [96]. In a very recent paper [82], a logarithmic light-cone was obtained for long-range, i.e. power-law decaying, interactions. The anomalous LR bound we find yields a *qualitatively completely different*, anomalously slow many-body transport.

We expect that if one has an anomalous LR bound for a system with a spectral gap, the arguments of [99, 138] will yield anomalously strong exponential clustering (see the discussion after Def. 1).

We actually have an exact characterization of the values of α for which the anomalous LR bound holds, namely whenever α exceeds α_u^+, the upper transport exponent of the one-body discrete Schrödinger operator with potential given exactly by the quasi-periodic field. Thanks to extensive study, there exist both rigorous and numerical upper and lower bounds on α_u^+ [3, 42, 43, 45, 46, 51, 52].

We mention that quasi-periodic sequences serve as models for one-dimensional quasi-crystals and their sometimes exotic transport properties. Especially the discrete one-body Schrödinger operator with Fibonacci potential, see (3.5), has been considered [113, 143, 3, 35, 165, 86, 166, 49, 46, 51, 52, 44, 43, 45]. Quasi-periodic spin chains (in particular with Fibonacci disorder) have also been studied extensively, with a focus on spectral properties and critical phenomena [21, 22, 23, 59, 100, 36, 153, 130].

While we give the full statements below, we only give a rough sketch of the proof; a detailed version will appear elsewhere [48].

3.2 Setup and main result

For any integer N, we consider the isotropic XY chain defined by the Hamiltonian

$$H_N = -\sum_{x=1}^{N-1} \left(\sigma_x^1\sigma_{x+1}^1 + \sigma_x^2\sigma_{x+1}^2\right) + \sum_{x=1}^{N} h_x\sigma_x^3, \tag{3.1}$$

where $\sigma^1, \sigma^2, \sigma^3$ are the usual Pauli matrices. We scaled out the usual J factor in front of the first term and chose zero boundary conditions for convenience. For definiteness, we let h_x be the *Fibonacci magnetic field*

$$h_x = \lambda\chi_{[1-\phi,1)}(x\phi + \omega \mod 1), \tag{3.2}$$

where $\lambda > 0$ is a coupling constant, $\omega \in [0, 1)$ is an arbitrary phase offset, and ϕ is the inverse of the golden mean, i.e.

$$\phi = \frac{\sqrt{5}-1}{2}.$$

The Fibonacci field (3.2) is prototypical in the study of one-dimensional quasi-crystals, but in fact ϕ can be replaced by an arbitrary irrational number in $(0,1)$ here ("Sturmian class"); compare [113, 143, 154, 17, 43]. We let $\mathcal{O}_x$ denote the set of observables at site x, which is of course just the set of Hermitian 2×2 matrices, and for an observable A, we let

$$A(t) \equiv e^{itH_N} A e^{-itH_N} \tag{3.3}$$

be its image under the Heisenberg evolution after time t. Note that $A(t)$ implicitly depends on N as well.

Definition 3.2.1 (anomalous LR bound)**.** *We say that* $\mathbf{LR}(\alpha)$ *holds if there exist positive constants* C, ξ, v *such that for all integers* x, x', N *with* $1 \le x < x' \le N$ *and all times* $t > 0$*, the bound*

$$\|[A(t), B]\| \le C\|A\|\|B\| e^{-\xi(|x-x'|-vt^{\alpha})} \tag{3.4}$$

holds for all observables $A \in \mathcal{O}_x$ *and* $B \in \mathcal{O}_{x'}$*.*

Let us make a few remarks about this: Firstly, the usual Lieb-Robinson bound corresponds to $\mathbf{LR(1)}$ and is known to hold by general considerations [124]. When comparing $\mathbf{LR}(\alpha)$ with $\mathbf{LR(1)}$ in the particularly relevant regime of small times, it is important to keep in mind that $|x-x'| \ge 1$ by definition and consequently $|x-x'|^{1/\alpha} > |x-x'|$ for $0 < \alpha < 1$. Hence, for fixed t, $\mathbf{LR}(\alpha)$ is effective at smaller distances than $\mathbf{LR(1)}$. Secondly, (3.4) can be extended to a much wider class of observables, provided that their supports are a non-zero distance apart [48, 50]. Thirdly, we emphasize that the constants above do not depend on the system size N, so that the estimate (3.4) is stable in the thermodynamic limit $N \to \infty$. Finally, as mentioned in the introduction, if one can prove $\mathbf{LR}(\alpha)$ for a system with a spectral gap, we expect that ground-state correlations will decay anomalously fast, i.e. the usual exponential decay in $d(X,Y)$ is replaced by decay in $d(X,Y)^{1/\alpha}$ (see e.g. Theorem 2 in [138]). Essentially, this should follow from the proofs in [99, 138], by using $\mathbf{LR}(\alpha)$ instead of $\mathbf{LR(1)}$, which only changes the optimization problem in the time cutoff parameter (called s in [138]).

Our first main result is:

Theorem 3.2.2. *Let* $\lambda \ge 8$*. There exists* $0 < \alpha < 1$ *such that* $\mathbf{LR}(\alpha)$ *holds.*

As mentioned in the introduction, we actually have a characterization of the values of α for which $\mathbf{LR}(\alpha)$ holds for all $\lambda > 0$. This characterization is in terms of the upper transport exponent α_u^+ of the one-body discrete Schrödinger operator $\mathfrak{h}$ with Fibonacci potential. It acts on a square-summable sequence $\{\psi_x\}_{x\geq 1}$ by

$$(\mathfrak{h}\psi)_x = \psi_{x+1} + \psi_{x-1} + h_x\psi_x, \tag{3.5}$$

with $\psi_0 \equiv 0$ and h_x given by (3.2). α_u^+ is then the propagation rate of the fastest part of an initially localized wave-packet. Since exponential tails cannot be evaded in quantum mechanics, α_u^+ is, roughly, the largest exponent β for which the probability of an initially localized wavepacket to travel a distance t^β in time t is *not* exponentially small.

More formally: For any integer $x \geq 1$ and any positive real number β, let

$$P(x,t) = \sum_{x'>x} |\langle \delta_{x'}|e^{-it\mathfrak{h}}|\delta_1\rangle|^2, \tag{3.6}$$

$$R^+(\beta) = -\limsup_{t\to\infty} \frac{\log P(t^\beta, t)}{\log t}. \tag{3.7}$$

Then, we define

$$\alpha_u^+ = \sup_{\beta\geq 0} \left\{ R^+(\beta) < \infty \right\}. \tag{3.8}$$

Note that $\alpha_u^+ = \alpha_u^+(\lambda)$. We mention that α_u^+ is just one of several transport exponents commonly associated to anomalous one-body dynamics [51, 52], but as it turns out it is the only one relevant for LR bounds.

As anticipated before, we have the following characterization:

Theorem 3.2.3. *Let $\lambda > 0$. If $\alpha > \alpha_u^+$, then $\mathbf{LR}(\alpha)$ holds. Conversely, if $\alpha < \alpha_u^+$, then $\mathbf{LR}(\alpha)$ does not hold.*

In words, $\mathbf{LR}(\alpha)$ is a precise way to state that tails are exponentially decaying beyond a modified light-cone of the form $|x| \leq vt^\alpha$, and our theorem states that this is true for $\alpha > \alpha_u^+$ and false for $\alpha < \alpha_u^+$. In fact, the second statement holds for completely general transversal magnetic fields (e.g. periodic ones, where $\alpha_u^+ = 1$). At first sight, it may be surprising that the quantity α_u^+, which describes large-time asymptotics, characterizes the LR bound. Intuitively, this is due to the fact that the asymptotics capture precisely the fastest moving part of the one-body dynamics.

We also obtain an explicit expression for the LR velocity v, see (38) in [48]. Appropriately, v is a decreasing function of α.

Let us discuss α_u^+ from a quantitative viewpoint. Since Theorem 2 holds for arbitrary coupling constant $\lambda > 0$, we see that the restriction to $\lambda \geq 8$ in Theorem 1 is due to the fact that we do not know rigorously that $\alpha_u^+ < 1$ for *all* $\lambda > 0$ (we do know that $\alpha_u^+ > 0$ for all $\lambda > 0$ [46]). We emphasize that estimating α_u^+ is only a problem of *one-body dynamics* however, which is simpler from both a theoretical and a numerical standpoint. A rough numerical study we conducted suggests that $\alpha_u^+ < 1$ also holds for $0 \ll \lambda < 8$, and we think it would be interesting to pursue the numerical aspects further. Moreover, explicit rigorous upper and lower bounds for α_u^+ exist [51, 52, 45]. Asymptotically, they behave like $\frac{2\log(1+\phi)}{\log\lambda}$ for large λ and they can be used to obtain quantitative estimates, such as

$$0.1 < \alpha_u^+ < 0.5$$

for all $12 \leq \lambda \leq 7,000$. We stress the upper bound by 0.5 because the particular case $\alpha_u^+ = 0.5$ is sometimes called diffusive transport and not assigned the "anomalous" label.

3.3 Sketch of proof

Following [125], we map the XY chain to free fermions via the Jordan-Wigner transformation. That is, we introduce the spin raising and lowering operators

$$S^{\pm} = \frac{1}{2}\left(\sigma^1 \pm i\sigma^2\right),$$

and define

$$c_1 = S_1^-, \qquad c_x = \sigma_1^3 \dots \sigma_{x-1}^3 S_x^-. \tag{3.9}$$

These operators satisfy the CAR and allow us to rewrite the Hamiltonian as

$$H_N = \sum_{x=1}^N \sum_{y=1}^N c_x^\dagger (\mathfrak{h}_N)_{x,y} c_y.$$

Here, $\mathfrak{h}_N$ is the operator $\mathfrak{h}$ defined in (3.5), but with a zero boundary condition at site $N+1$. At this stage, H_N can be diagonalized by a standard Bogoliubov transformation. One finds the following formula [96] for the Heisenberg dynamics (3.3) of the fermion operators:

$$c_x(t) = \sum_{y=1}^N \left(e^{-2i\mathfrak{h}_N t}\right)_{x,y} c_y. \tag{3.10}$$

Definition 3.3.1. *We say that* $\mathbf{LR}_{\text{fermi}}(\alpha)$ *holds if there exist positive constants* C, ξ, v *such that for all integers* x, x', N *with* $1 \le x < x' \le N$ *and all times* $t > 0$*, the bound*

$$\|[c_x(t), B]\| + \|[c_x^\dagger(t), B]\| \le C\|B\|e^{-\xi(|x-x'|-vt^\alpha)} \tag{3.11}$$

holds for all observables $B \in \mathcal{O}_{x'}$.

As we will see, (3.10) allows us to prove $\mathbf{LR}_{\text{fermi}}(\alpha)$ by controlling the one-body transport created by $\mathfrak{h}$. This is not surprising, because (3.10) is an expression of the fact that we are now describing free particles.

The problem that arises, though, is that the Jordan-Wigner transformation (3.9) is *highly non-local*, while a Lieb-Robinson bound is of course an *inherently local* statement. The key lemma, which is somewhat surprising at first sight, however, says

Lemma 3.3.2. $\mathbf{LR}_{\text{fermi}}(\alpha)$ *is equivalent to* $\mathbf{LR}(\alpha)$.

The point is that, as originally realized in [96] and adapted here to our purposes, inverting the non-local Jordan-Wigner transformation essentially just requires *summing* up fermionic LR bounds: By an iteration argument, which is based only on $(AB)(t) = A(t)B(t)$ and the usual commutator rules, one can show

$$\|[S_x^-(t), B]\| \le 2\sum_{y=1}^{x} \left(\|[c_y(t), B]\| + \|[c_y^\dagger(t), B]\|\right) \tag{3.12}$$

for all $B \in \mathcal{O}_{x'}$. By taking adjoints and using commutator rules, similar bounds hold for S_x^-, $S_x^- S_x^+$, $S_x^+ S_x^-$ and hence for all elements of the four-dimensional algebra of observables $\mathcal{O}_x$. Assuming that $\mathbf{LR}_{\text{fermi}}(\alpha)$ holds, we now see that $\mathbf{LR}(\alpha)$ follows from (3.12) and the trivial, but important, fact that

$$\sum_{y=1}^{x} e^{-\xi(|y-x'|-vt^\alpha)} \propto e^{-\xi(|x-x'|-vt^\alpha)}.$$

For more details and the argument for the converse statement, see [48]. In conclusion, we found that the price of non-locality was the additional sum over y in (3.12), but we can afford this because *tails of exponentially decaying series still decay exponentially.*

To prove Theorem 2, thanks to Lemma 1, it remains to characterize the values of α for which $\mathbf{LR}_{\text{fermi}}(\alpha)$ holds. We first show that $\alpha > \alpha_u^+$ implies $\mathbf{LR}_{\text{fermi}}(\alpha)$. By (3.10) and the fact that c_y and B commute for $y < x'$, we get

$$\|[c_x(t), B]\| \leq \|B\| \sum_{y=x'}^{N} \left|\langle\delta_x|e^{-2i\mathfrak{h}_N t}|\delta_y\rangle\right| . \tag{3.13}$$

Since spatial translation corresponds to a shift of the (anyway arbitrary) phase offset ω, modulo some technical difficulties, the right-hand side is equal to

$$\sum_{y=x'-x-1}^{N-x-1} \left|\langle\delta_1|e^{-2i\mathfrak{h}_N t}|\delta_y\rangle\right| \tag{3.14}$$

and this expression is already quite similar to the definition of the "outside probability" in (3.6). This explains why we can apply techniques developed in [42, 51, 52, 45] to study the transport exponent α_u^+ to our situation. A rough outline of the by now standard approach reads:

(a) use Dunford's formula

$$\langle\delta_1|e^{-2i\mathfrak{h}_N t}|\delta_y\rangle = -\frac{1}{2\pi i}\int_\Gamma e^{-itz}\langle\delta_1|\frac{1}{-2\mathfrak{h}_N - z}|\delta_y\rangle \mathrm{d}z$$

to express the time-evolution in terms of resolvents (Γ is a simple positively oriented contour around the spectrum of $-2\mathfrak{h}_N$),

(b) bound matrix elements of resolvents in terms of transfer matrix norms, by studying individual solutions,

(c) bound transfer matrix norm by the exponentially decaying right-hand side in $\mathbf{LR}_{\text{fermi}}(\alpha)$, by studying the Fibonacci trace map.

However, the original results of [42, 51, 52, 45] do not translate directly to our situation. Firstly, the operator $\mathfrak{h}$ lives on the half-line, while $\mathfrak{h}_N$ has a zero boundary condition at $N+1$. This is a minor obstruction and can be removed, for an upper bound, by one-rank perturbation theory on the level of resolvents.

The bigger problem is that the summands in (3.14) are *not squared*, as they are in (3.6), which may of course make for a much larger sum. The technical solution we have found to this will not be presented here for the sake of brevity and instead we refer the interested reader to [48].

We now turn to the converse direction in Theorem 2. We prove the logically equivalent statement that $\mathbf{LR}_{\text{fermi}}(\alpha)$ implies $\alpha \geq \alpha_u^+$. Using (3.10) and an appropriate trial state to bound the operator norm (see [48] for details), we obtain the key estimate

$$\|[c_x(t), S_{x'}^+]\| \geq \left|\langle \delta_x | e^{-2i\mathfrak{h}_N t} | \delta_{x'} \rangle\right|$$

(compare with (3.13)). Thus, $\mathbf{LR}_{\text{fermi}}(\alpha)$ implies

$$\left|\langle \delta_x | e^{-2i\mathfrak{h}_N t} | \delta_{x'} \rangle\right| \leq C e^{-\xi(|x-x'|-vt^\alpha)}$$

for all $1 \leq x \leq x' \leq N$ and all $t > 0$. We take the limit $N \to \infty$ to pass to the half-line operator,

$$\left|\langle \delta_x | e^{-2i\mathfrak{h} t} | \delta_{x'} \rangle\right| \leq C e^{-\xi(|x-x'|-vt^\alpha)} \tag{3.15}$$

for all $x, x' \in \mathbb{N}$ and all $t > 0$. Using this on definition (3.6) gives

$$P(t^\beta, t) \leq \frac{C^2}{1-e^{-2\xi}} e^{-2\xi(t^\beta - v(t/2)^\alpha)} \leq \tilde{C} e^{-\xi t^\beta}$$

whenever $\beta > \alpha$. By definitions (3.7), (3.8) we conclude that $\beta \geq \alpha_u^+$, so $\alpha \geq \alpha_u^+$.

3.4 The random dimer model

We explain why our method does not extend to yield an anomalous LR bound with *power-law tails* for the random dimer model [63]. The focus is on ideas here, for a detailed discussion see [48].

Recall the one-body discrete Schrödinger operator $\mathfrak{h}$ from (3.5). In the random dimer model, the potential h_n is a random variable taking either of the two values $\pm\lambda$, each with probability 1/2 say, but these values must always occur in pairs (or dimers). The intuition, due to Anderson's work, that a one-dimensional disordered quantum system should exhibit localization is only almost correct here: There exist critical energies $E_c = \pm\lambda$ for which the transfer matrices across dimers commute and the system shows anomalous transport. As it turns out, the anomalous transport is so fast that $\alpha_u^+ = 1$ and so we cannot hope for an $\mathbf{LR}(\alpha)$ with $\alpha < 1$.

Intuitively, this is because $\alpha_u^+ = 1$ means that the probablity to find the particle within a distance t^β of its initial location after time t, is *not* exponentially small for $\beta < 1$. However, in the random dimer model, this probability is *polynomially* small for some $\beta < 1$. In fact, there are similar transport exponents $\tilde{\beta}^+(p)$, related to time-averaged p-th moments of the position operator, which characterize when this is the case and which were determined explicitly in [102, 103].

With this in mind, one may hope to use our method to find an *anomalous LR bound with power-law tails*, which would be of the general form

$$\|[A(t), B]\| \leq C\|A\|\|B\| \left(\frac{|t|^{\gamma(p)}}{|x - x'|} \right)^p \tag{3.16}$$

for any $p \geq 0$ and some $0 < \gamma(p) < 1$, that is related to $\tilde{\beta}^+(p)$. A problem arises, however, when we want to "pull back" the LR bound through the Jordan-Wigner transformation, as we did to prove Lemma 1. As we explained, the non-locality gives rise to the extra sum in (3.14). While we stressed that the sum was irrelevant in the case of exponential decay, *power-law decay decreases by one order under summation* and it turns out that this restricts $\gamma(p)$ in (3.16) to $\gamma(p) > 1$. Of course, the ordinary LR bound is then again a better estimate and the argument is inconclusive.

3.5 Conclusions

We have sketched the rigorous proof of anomalous Lieb-Robinson bounds (3.4) for isotropic XY chains with a quasi-periodic transverse field, which can be viewed as models for quasi-crystals. To our knowledge, this is the first derivation of anomalous quantum many-body transport.

The characterization of the correct exponent α in the anomalous LR bound (3.4) as the *one-body* transport exponent α_u^+ yields rigorous and quantitative bounds on it and opens the anomalous LR bound up to numerical study.

We also present the concept of an anomalous LR bound with power-law tails (3.16). While our argument is inconclusive for the random dimer model, we understand exactly why it fails. In particular, it would yield power-law LR bounds for models with somewhat smaller values of the transport exponent $\tilde{\beta}^+(p)$, if such models exist.

Chapter 4

ON POLYNOMIAL LIEB-ROBINSON BOUNDS FOR THE XY CHAIN IN A DECAYING RANDOM FIELD

Marius Lemm and Martin Gebert

4.1 Introduction

It is well known that a single quantum particle in one dimension which is subjected to an arbitrarily weak random potential exhibits exponential Anderson localization [7, 116]. In the presence of interactions, one enters the subject of many-body localization (MBL) which has been a hot topic of condensed-matter physics in recent years, see e.g. [15, 16, 65, 77, 101, 139] and references therein. On a heuristic level, MBL is described as *absence of thermalization.* Proposed criteria for this include the validity of an area law for the entanglement entropy and absence of information propagation (e.g. a zero-velocity Lieb-Robinson bound and logarithmic in time growth of the entanglement entropy). For an extensive list of possible criteria, see the review [81]. The very special MBL phase is expected to break down for sufficiently weak randomness, in what is called the *MBL transition* [144, 171].

A possible starting point for understanding MBL is the XY quantum spin chain in an i.i.d. random field. This is an *integrable toy model* which can be mapped to non-interacting fermions in a random environment. Since the fermions are then localized in the usual Anderson sense, it can be shown rigorously that this model enjoys an area law for the entanglement entropy for large classes of states [1, 2, 146] and a zero-velocity Lieb-Robinson bound [31, 96]. A continuum analogue of this toy model, the disordered Tonks-Girardeau gas, was recently shown to display features of MBL for bosons, such as the absence of BEC and superfluidity [155], even at zero temperature.

However, a shortcoming of the toy model (apart from integrability) is that it will never display a transition to a non-MBL phase because the fermions are localized at arbitrarily small disorder strength (which is equivalent to arbitrarily large interaction strength).

In this paper, we propose a variation of the XY chain with disorder which *rigorously displays features suggesting that such a phase transition might occur* as the disorder strength is varied. The model is the isotropic XY chain on the half line with a random and *decaying* external field in the z direction. The Hamiltonian reads

$$H_n^{XY}(\omega) := -\sum_{j=1}^{n-1} \left(\sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y\right) + \lambda \sum_{j=1}^{n} \frac{V_j(\omega)}{j^{1/2}} \sigma_j^z$$

where the V_j are i.i.d. random variables satisfying $\mathbb{E}[V_j] = 0$ and $\mathbb{E}[V_j^2] = 1$. Moreover, $\lambda > 0$ is a parameter describing the disorder strength. Note the decaying envelope $j^{-1/2}$ for the random field. It is "critical" in that the potential is just barely not in $\ell^2(\mathbb{N})$. For other decay rates, the random field is either too weak or too strong to observe a qualitative transition from MBL to non-MBL features (such as transport) when λ is varied.

We now explain in which sense our system exhibits features suggesting a phase transition from transport to localization as the disorder strength $\lambda > 0$ is increased. While our results will be more general and include bounds on the particle number transport as well, the key notion for quantifying many-body transport for this model are new *anomalous polynomial Lieb-Robinson (PLR) bounds.* The traditional Lieb-Robinson (LR) bounds [124, 138] apply to general local Hamiltonians defined on a lattice and establish the existence of a certain "light cone" in spacetime outside of which correlations are exponentially small.

We say PLR(a, b) holds for parameters $0 \leq a \leq 1$ and $b > 0$, if there exists a universal constant $C > 0$ such that for any observables A supported at site 1 and B supported at site $k > 1$, we have the bound

$$\|[\tau_t^n(A), B]\| \leq C\|A\|\|B\| \left(\frac{t^a}{k}\right)^b. \tag{4.1}$$

Here τ_t^N is the Heisenberg time evolution generated by the Hamiltonian H_n^{XY}, see (4.3), and $\|\cdot\|$ is the standard operator norm. Intuitively, PLR(a, b) says that in time t, information (as measured by the commutator of the initially localized observables) propagates at most a distance of order t^a, up to errors decaying like x^{-b} away from the bent "light cone" $t^a = k$ in spacetime. The case $a = 1$ corresponds to ballistic transport.

We now discuss our results in words; the precise statements are given later. For simplicity, in this discussion A is supported at site 1 and B is supported at site $k > 1$.

- When λ is *large enough*, the system is "polynomially localized" in the sense that

$$\mathbb{E}\Big[\sup_{t\in\mathbb{R}} \|[\tau_t^n(A), B]\|\Big] \le C\|A\|\|B\| \left(\frac{1}{k}\right)^{\kappa\lambda^2-5/4} \tag{4.2}$$

  for a coefficient $0 < \kappa \le \frac{5}{16}$ (Theorem 4.3.2). This is a disorder-averaged version of PLR$(0, \kappa\lambda^2 - 5/4)$ and may be understood as a *zero-velocity PLR bound*. It is of course only effective when $\kappa\lambda^2 - 5/4 > 0$.

- When λ is *small enough*, PLR(a, b) cannot hold if a is too small or b is too large (Corollary 4.3.9). In other words, there exist observables A, B for which the bound (4.1) fails and in this sense transport is at least of order t^a. Concretely, in Corollary 4.3.9 we show that for $\lambda < 2$, (4.1) fails with probability one if $0 \le a \le 1$ and $b > 1/2$ satisfy

$$a\left(1 + \frac{1}{2b-1}\right) < 1.$$

  In particular, for any $0 \le a < 1$, there exists $b > 1/2$ large enough such that (4.1) fails with probability one.

Remark 4.1.1. *(i) It follows from [48, Thm. 2.6] and Proposition 4.3.8 that if only exponentially small errors are tolerated in an LR bound, then our model will exhibit ballistic transport for all $\lambda > 0$. This fits with the localization being only polynomial in type, even for large λ.*

(ii) We emphasize that our results do not *exclude that for small λ, an analogue of* (4.2) *holds with the exponent $\kappa\lambda^2 - 5/4$ replaced by a number $b \le 1/2$. If this were true, it would be misleading to speak of a true transition from non-trivial transport to localization and it is for this reason that we do not claim to prove such a transition.*

(iii) For the PLR(a, b) bounds defined by (4.1) *and* (4.2)*, we only consider observables A supported at site* 1*. If A is supported at a site $j > 1$, the decaying factor is* not *replaced by the distance of the supports $|j - k|$ (as would be the case in a direct polynomial generalization of the LR*

bound, compare [47, 48]), but instead by $\min\{j,k\}/\max\{j,k\}$. *The precise statement is in Theorem 4.3.2. The reason why one cannot expect the distance* $|j-k|$ *is that the system is far from being translation-invariant.*

To prove the results, we use the standard method of expressing the XY chain in terms of free fermions via the Jordan-Wigner transformation. The basic idea is to take bounds for the corresponding one-body system [56, 80, 110, 111] and to pull them through the (non-local) Jordan-Wigner transformation by using ideas of Hamza, Sims and Stolz [96].

[96] considered a non-decaying random external field which yields an exponentially localized system, see also [112, 161]. Here we apply the method of [96] to a situation in which errors decay only polynomially. Related papers which study the dependence of parameters in LR bounds and their generalizations on the external field are [47, 48, 50, 105]. The idea of studying polynomial LR bounds was conceived in [47, 48], but there it was only shown that the idea does *not* apply to the random dimer model (a model with anomalous one-body transport).

For large λ, we use the fact that the Kunz-Souillard method utilized in [56] actually yields a polynomial bound on the eigenfunction correlator (4.16). We are grateful to David Damanik for pointing this out to us.

As mentioned before, we also show similar results for particle number transport. For this we adapt the techniques from [1], where such bounds were studied for non-decaying i.i.d. randomness, to our situation with polynomial decay. Similar bounds on particle number transport were also proved in the recent paper [155] on the disordered Tonks-Girardeau gas, a continuum analogue of the disordered XY chain.

Overall, our results follow rather directly by combining the above mentioned methods. Nonetheless, we believe that this alternative toy model provides an opportunity to study a phase transition, in terms of transport properties, from a mathematical and physics perspective and can stimulate further research. In particular, we have also attempted without success to prove analogous results for the entanglement entropy of eigenstates in the spirit of the recent works [1, 2, 66, 146]. However we ran into difficulty bounding the entanglement entropy of eigenstates in the "localization regime" of large λ because of the growth in j of the bound (4.16). We believe that this question constitutes an interesting open problem.

4.2 The model

The XY Chain in a random decaying external field

For every $n \in \mathbb{N} = \{1, 2, 3, \ldots\}$, we consider the Hilbert space

$$\mathcal{H}_n = \bigotimes_{j=1}^{n} \mathbb{C}^2.$$

On $\mathcal{H}_n$, the Hamiltonian of the isotropic XY chain with a random decaying external field is given by

$$H_n^{XY}(\omega) := -\sum_{j=1}^{n-1} \left(\sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y\right) + \lambda \sum_{j=1}^{n} \frac{V_j(\omega)}{j^{1/2}} \sigma_j^z,$$

where $\lambda > 0$ is a coupling constant. The sequence $\left(V_j(\omega)\right)_{j \in \mathbb{N}}$ is a family of iid random variables on a probability space $(\Omega, \Sigma, \mathbb{P})$. We assume that its single-site distribution has zero mean and is absolutely continuous with a bounded density of compact support and $\mathbb{E}[V_j^2] = 1$. In the above,

$$\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

are the *Pauli matrices* and $\sigma_j^{x,y,z}$ is short-handed for

$$\mathbb{1}_1 \otimes \ldots \mathbb{1}_{j-1} \otimes \sigma^{x,y,z} \otimes \mathbb{1}_{j+1} \ldots \otimes \mathbb{1}_n$$

for $1 \leq j \leq n$. In the following we omit the ω-dependence for brevity. For a finite set $J \subset \mathbb{N}$, we define the algebra of observables supported on J by

$$\mathcal{A}_J = \bigotimes_{j \in J} \mathcal{B}(\mathbb{C}^2),$$

where $\mathcal{B}(\mathbb{C}^2)$ is the set of all complex 2×2 matrices. We will often make use of the fact that for $J \subset J'$, there is a natural embedding of $\mathcal{A}_J$ into $\mathcal{A}_{J'}$ by tensoring with the identity on $J' \setminus J$. Also, we set $\mathcal{A}_j \equiv \mathcal{A}_{\{j\}}$.

Finally, the *Heisenberg dynamics* of an observable $A \in \mathcal{A}_J$ under the Hamiltonian H_n^{XY} is defined by

$$\tau_t^n(A) := e^{itH_n^{XY}} A e^{-itH_n^{XY}}. \tag{4.3}$$

The Jordan-Wigner transformation

We use the standard procedure, going back to [125], of mapping the XY chain to free fermions via the Jordan-Wigner transformation.

For the details of the diagonalization procedure, we refer to Section 3.1 in [96]. Here we only recall what we need to establish notation. The first step is to introduce the lowering operator

$$a_j = \frac{1}{2}\left(\sigma_j^x - i\sigma_j^y\right) = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}_j \tag{4.4}$$

and its adjoint the raising operator a_j^* for all $1 \le j \le n$. The Jordan-Wigner transformation maps these to the fermion operators

$$c_1 = a_1, \quad c_j = \sigma_1^z \dots \sigma_{j-1}^z a_j \quad \text{for } 2 \le j \le n. \tag{4.5}$$

The $\{c_j\}$ then satisfy the canonical anticommutation relations (CAR). We have the identity

$$a_j^* a_j = c_j^* c_j. \tag{4.6}$$

In terms of the fermion operators, the Hamiltonian reads,

$$H_n^{XY} = 2\mathcal{C}^* H_n \mathcal{C} - \sum_{j=1}^{n} \tilde{V}_j \tag{4.7}$$

where $\mathcal{C} := (c_1, ..., c_n)^T$ and $\widetilde{V}_j := \frac{\lambda}{j^{1/2}} V_j$. The $n \times n$ matrix H_n is given by

$$H_n = \begin{pmatrix} \widetilde{V}_1 & 1 & & \\ 1 & \ddots & \ddots & \\ & \ddots & \ddots & 1 \\ & & 1 & \widetilde{V}_n \end{pmatrix}, \tag{4.8}$$

Note that H_n can be identified with a discrete Schrödinger operator on the half line, i.e. on $\ell^2(\mathbb{N})$, with the random decaying potential $\{\tilde{V}_j\}$ and zero boundary conditions at site $n+1$. The constant $\sum_{j=1}^{n} \tilde{V}_j$ in (4.7) does not change the Heisenberg dynamics (4.3) and can thus be ignored in the following.

We will often use that the Heisenberg dynamics of the c_j operators is given in the following simple fashion.

Proposition 4.2.1. *[96, Sec. 3] For all $1 \le j, k \le n$, the identity*

$$\tau_t^n(c_j) = \sum_{m=1}^{n} \langle \delta_j, e^{-2itH_n} \delta_m \rangle c_m \tag{4.9}$$

holds and consequently

$$\|[\tau_t^n(a_j), B]\| \leq 2 \sum_{l=1}^{j} \sum_{m=1}^{n} |\langle \delta_l, e^{-2itH_n} \delta_m \rangle| \left(\|[c_m, B]\| + \|[c_m^*, B]\| \right). \tag{4.10}$$

Proof. The first equality follows from diagonalizing the one-particle operator H_n. For details see [96, Eq. (3.15)]. Taking adjoints, the same is also true for c_k^*. Using the Leibniz rule for commutators, i.e.

$$[AB, C] = A[B, C] + [A, C]B \tag{4.11}$$

we obtain the estimate

$$\|[\tau_t^n(c_j^* c_j), B]\| \leq \sum_{m=1}^{n} \langle \delta_j, e^{-2itH_n} \delta_m \rangle \left(\|[c_m, B]\| + \|[c_m^*, B]\| \right). \tag{4.12}$$

The latter inequality also holds for the adjoint $c_j c_j^*$.

To see inequality (4.10), we note that $(\sigma_j^z)^{-1} = \sigma_j^z$ for all $1 \leq j \leq n$ gives

$$a_j = \sigma_{j-1}^z ... \sigma_1^z c_j. \tag{4.13}$$

Thus, an iteration of the Leibniz rule (4.11) implies

$$\begin{aligned} \|[\tau_t^n(a_j), B]\| &= \|[\tau_t^n(\sigma_{j-1}^z ... \sigma_1^z c_j), B]\| \\ &\leq \|[\tau_t^n(c_j), B]\| + \sum_{l=1}^{j-1} \|[\tau_t^n(\sigma_l^z), B]\|. \end{aligned} \tag{4.14}$$

Since $\sigma_l^z = 2c_l^* c_l - \mathrm{id}_{\mathbb{C}^2}$, the identity (4.9) and the bound (4.12) imply

$$\begin{aligned} (4.14) \leq & \sum_{m=1}^{n} |\langle \delta_j, e^{-2itH_n} \delta_m \rangle| \|[c_m, B]\| \\ & + 2 \sum_{l=1}^{j-1} \sum_{m=1}^{n} |\langle \delta_l, e^{-2itH_n} \delta_m \rangle \left(\|[c_m, B]\| + \|[c_m^*, B]\| \right). \end{aligned} \tag{4.15}$$

□

4.3 Polynomial Lieb-Robinson bounds

Localization for large enough λ

We start with recalling an old result by [56] which provides bounds on the eigenfunction correlator of the Anderson model with a random decaying potential.

Lemma 4.3.1. *Let H_n be the operator given in* (4.8)*. Then there exist constants $C, \kappa > 0$ such that for all $n \in \mathbb{N}$ and all $1 \leq j \leq k \leq n$, we have*

$$\mathbb{E}\big[\sup_{|g|\leq 1} |\langle \delta_j, g(H_n)\delta_k\rangle|\big] \leq \frac{C}{\lambda}(jk)^{1/4}\left(\frac{j}{k}\right)^{\kappa\lambda^2}. \tag{4.16}$$

In particular, one can choose $g(x) = e^{-itx}$ in the above. The exponent κ will feature in all of the following bounds and we show later that it satisfies $\kappa \leq \frac{5}{16}$, see Corollary 4.3.11.

Proof. We estimate

$$\mathbb{E}\big[\sup_{|g|\leq 1} |\langle \delta_j, g(H_n)\delta_k\rangle|\big] \leq \mathbb{E}\Big[\sum_{E\in\sigma(H_n)} |\psi_E^n(j)||\psi_E^n(k)|\Big] =: \overline{\rho}^n(j,k,\mathbb{R}) \tag{4.17}$$

where the sequence $\left(\psi_E^n\right)_{E\in\sigma(H_n)}$ denotes the normalized eigenvectors of H_n counted with multipicity. An adaption of [56, Prop. III.1] implies

$$\overline{\rho}^n(j,k,\mathbb{R}) \leq \frac{C}{\lambda^2}(jk)^{1/4}\left(\frac{j}{k}\right)^{\kappa\lambda^2}. \tag{4.18}$$

The latter follows from inequality [56, Eq. III.16] using the bounds [56, Eq. III.14 and eq. III.15] and we remark that in the result [56, Eq. III.4] the 1/2-exponent should be replaced by a 1/4-exponent. □

As a consequence, we obtain a disorder-averaged polynomial Lieb-Robinson bound with $a = 0$ for the spin chain H_n^{XY}.

Theorem 4.3.2. *Let κ be as in Lemma 4.3.1 above. Suppose that $\kappa\lambda^2 > \frac{5}{4}$. Then there exists a constant $C > 0$ such that for all choices of $1 \leq j \leq k \leq n$,*

$$\mathbb{E}\big[\sup_{t\in\mathbb{R}} \|[\tau_t^n(A), B]\|\big] \leq C\|A\|\|B\|(jk)^{5/4}\left(\frac{j}{k}\right)^{\kappa\lambda^2} \tag{4.19}$$

holds for all observables $A \in \mathcal{A}_j$ and $B \in \mathcal{A}_{k,\dots,n}$.

We emphasize that the constant C is also uniform in n.

Proof. Note that $\mathcal{A}_j$ is spanned by the matrices $\{a_j, a_j^*, a_j a_j^*, a_j^* a_j\}$. According to Proposition 4.2.1, we can estimate

$$\|[\tau_t^n(a_j), B]\| \leq 2\sum_{l=1}^{j}\sum_{m=1}^{n} |\langle \delta_l, e^{-2itH_n}\delta_m\rangle| \left(\|[c_m, B]\| + \|[c_m^*, B]\|\right) \tag{4.20}$$

We note that $[c_m, B] = 0$ for all $m < k$. Hence, Lemma 4.3.1 implies

$$\begin{aligned}\mathbb{E}(4.20) \leq & \frac{4C}{\lambda^2}\|B\| \sum_{l=1}^{j} \sum_{m=k}^{n} (lm)^{1/4} \left(\frac{l}{m}\right)^{\kappa\lambda^2} \\ \leq & \frac{4C}{\lambda^2}\|B\| \sum_{l=1}^{j} \sum_{m=k}^{\infty} (lm)^{1/4} \left(\frac{l}{m}\right)^{\kappa\lambda^2} \\ \leq & \frac{C}{\lambda^2}\|B\|(jk)^{5/4} \left(\frac{j}{k}\right)^{\kappa\lambda^2}\end{aligned} \tag{4.21}$$

for some constant $C > 0$ which is finite for $\lambda > \sqrt{\frac{5}{4\kappa}}$. Taking adjoints the same estimate is true for a_j^*. For the products $a_j^* a_j$ and $a_j a_j^*$, we use the Leibniz rule (4.11). □

Remark 4.3.3. *Instead of the distance $|j - k|$ of the supports of the observables, which would appear in a straightforward polynomial generalization of the traditional LR bound as was proposed in [47, 48], the right hand side depends on the quotient j/k. Note that the distance $|j - k|$ is not so natural for our model, which is far from being translation-invariant.*

However, if we consider observables A supported at a fixed *site, say the site* 1*, the bound* (4.19) *reduces to a polynomial Lieb-Robinson bound involving the distance of the supports. Let $A \in \mathcal{A}_1$. Then the bound*

$$\mathbb{E}\Big[\sup_{t\in\mathbb{R}} \|[\tau_t^n(A), B]\|\Big] \leq C\|A\|\|B\| \left(\frac{1}{k}\right)^{\kappa\lambda^2 - 5/4} \tag{4.22}$$

holds uniformly in $n \in \mathbb{N}$ and $B \in \mathcal{A}_{k,\dots,n}$ for any $1 < k \leq n$.

For small t the above is not satisfactory. One can improve the result:

Proposition 4.3.4. *Let κ be as in Lemma 4.3.1. There exists a constant C such that for all choices of $1 \leq j \leq k \leq n$,*

$$\mathbb{E}\left[\|[\tau_t^n(A), B]\|\right] \leq C\|A\|\|B\||t|\left(\frac{1}{k}\right)^{\kappa\lambda^2 - 5/4} \tag{4.23}$$

holds for all observables $A \in \mathcal{A}_1$, $B \in \mathcal{A}_{k,\dots,n}$.

Proof. We follow the proof of [96, Cor. 3.4]. Define

$$f(t) := [\tau_t(A), B]. \tag{4.24}$$

Then, $f(t)$ solves the ODE

$$f'(t) = i[f(t), \tau_t^n(H_1)] - i[[B, \tau_t^n(H_1)], \tau_t^n(A)]. \tag{4.25}$$

where $H_1 := \sigma_1^x\sigma_2^x + \sigma_1^y\sigma_2^y + V_1\sigma_1^z$. Following [136, App. A] we obtain

$$\|f(t)\| \leq \int_0^{|t|} \mathrm{d}s \, \|[\tau_s^n(H_1), B]\|. \tag{4.26}$$

Since H_1 is supported on $\mathcal{A}_1 \otimes \mathcal{A}_2$ we use Theorem 4.3.2 to obtain a time independent bound on the integrand which yields the theorem. □

Lower bounds on transport for small enough λ

In this section we restrict ourselves to pairs of observables for which one of the observables is supported at the site 1.

Definition 4.3.5. *Let $0 \leq a \leq 1$ and $b \geq 0$. We say that H_n^{XY} exhibits the polynomial Lieb-Robinson bound PLR(a, b), if there exists a constant $C > 0$ such that for all $n \in \mathbb{N}$*

$$\|[\tau_t^n(A), B]\| \leq C\|A\|\|B\| \left(\frac{t^a}{k}\right)^b \tag{4.27}$$

holds for all $A \in \mathcal{A}_1$, $B \in \mathcal{A}_{k,\dots,n}$.

Let H be the discrete Schrödinger operator on $\ell^2(\mathbb{N})$ which arises as the inductive limit of the family $(H_n)_{n\in\mathbb{N}}$.

Definition 4.3.6. *We define the p-th moment of the position operator*

$$|X|^p(t) := \sum_{k\in\mathbb{N}} k^p |\langle e^{-itH}\delta_j, \delta_k\rangle|^2 \tag{4.28}$$

and its time-average

$$\langle |X|^p \rangle(T) := \frac{2}{T}\int_0^\infty \mathrm{d}t \, e^{-2t/T} |X|^p(t) \tag{4.29}$$

for all $T > 0$. The upper and lower transport exponents are defined by

$$\beta^-(p) := \liminf_{t\to\infty} \frac{\ln |X|^p(t)}{p \ln t} \quad \text{and} \quad \beta^+(p) := \limsup_{t\to\infty} \frac{\ln |X|^p(t)}{p \ln t} \tag{4.30}$$

and their averaged versions are defined by

$$\langle\beta^-(p)\rangle := \liminf_{T\to\infty} \frac{\ln\langle |X|^p\rangle(T)}{p \ln T} \quad \text{and} \quad \langle\beta^+(p)\rangle := \limsup_{T\to\infty} \frac{\ln\langle |X|^p\rangle(T)}{p \ln T}. \tag{4.31}$$

Theorem 4.3.7. *Assume* PLR(a,b) *holds for some* $0 \leq a \leq 1$ *and* $b > 1/2$. *Then,*

$$\limsup_{\epsilon \to 0} \beta^+(2b-1-\epsilon) \leq a\left(1 + \frac{1}{2b-1}\right). \tag{4.32}$$

Proof. The strong resolvent-convergence of H_n to H (this follows e.g. from the geometric resolvent identity) implies the convergence

$$\lim_{n\to\infty} \langle e^{itH_n}\delta_1, \delta_k\rangle = \langle e^{itH}\delta_1, \delta_k\rangle, \tag{4.33}$$

for any $1 \leq k \leq n$. Hence, Fatou's lemma implies the inequality

$$\begin{aligned}\sum_{k\in\mathbb{N}} k^{2b-1-\epsilon}|\langle e^{-itH}\delta_1, \delta_k\rangle|^2 &= \lim_{M\to\infty} \sum_{1\leq k\leq M} k^{2b-1-\epsilon}|\langle e^{-itH}\delta_1, \delta_k\rangle|^2 \\ &\leq \lim_{M\to\infty} \liminf_{n\to\infty} \sum_{1\leq k\leq M} k^{2b-1-\epsilon}|\langle e^{-itH_n}\delta_1, \delta_k\rangle|^2, \end{aligned} \tag{4.34}$$

where $\epsilon > 0$ is arbitary.

Now, we bound the one-body propagation in terms of the many-body propagation using [48, Lm. 4.1]. It implies that for any $1 \leq k \leq n$

$$|\langle e^{-itH_n}\delta_1, \delta_k\rangle| \leq \|[\tau_t^n(c_1), a_k^*]\|. \tag{4.35}$$

Using this and the assumption that PLR(a,b) holds, we bound

$$(4.34) \leq t^{2ab} \sum_{k\in\mathbb{N}} k^{-1-\epsilon}. \tag{4.36}$$

Since the latter is summable for any $\epsilon > 0$, this implies

$$\beta^+(2b-1-\epsilon) \leq \frac{2ab}{2b-1-\epsilon} \tag{4.37}$$

and therefore (4.32) follows. □

Proposition 4.3.8. *Let* $p > \frac{\lambda}{4}$. *The lower bound*

$$\beta^+(p) \geq 1 - \frac{\lambda}{4p} \tag{4.38}$$

holds $\mathbb{P}$*-almost surely. In the case of* $\lambda < 2$ *one has*

$$\beta^+(p) = 1 \tag{4.39}$$

$\mathbb{P}$*-almost surely.*

Before we give the proof, which is based on results in [80, 110, 111], we discuss the consequences of combining Theorem 4.3.7 and Proposition 4.3.8. What we obtain can be interpreted as lower bounds on transport, as we explained in the introduction, however see also the caveat in Remark 4.1.1(iii).

Corollary 4.3.9. *Let* (a,b) *be a pair of* $0 \le a \le 1$ *and* $b > 1/2$. *If either of the following two conditions applies, then, with probability one,* $\mathrm{PLR}(a,b)$ *cannot hold.*

- $\lambda < 2$ *and* $a\left(1 + \frac{1}{2b-1}\right) < 1$
- $\lambda < 4(2b-1)$ *and* $a\left(1 + \frac{1}{2b-1}\right) < 1 - \frac{\lambda}{4(2b-1)}$.

In particular, if $\lambda < 2$, *then for any fixed* $0 \le a < 1$ *there exists* $b > 1/2$ *large enough such that PLR*(a,b) *cannot hold.*

Remark 4.3.10. *A shortcoming of our results is that we need to assume* $b > 1/2$, *see Remark 4.1.1(iii). This is ultimately a consequence of summing up one-body transport bounds when inverting the Jordan-Wigner transformation (compare Proposition 4.2.1) and is therefore intimately connected to the core of the method.*

We also get a bound on the maximal power of the polynomial decay coefficient κ which was introduced considered in the previous section.

Corollary 4.3.11. *The constant* κ *from Proposition 4.3.1 satisfies* $\kappa \le \frac{5}{16}$.

Proof. Note that κ is independent of λ. Fix $\lambda < 2$ and $p > 0$. By Proposition 4.3.8, $\sup_{t>0} |X|^p(t) = \infty$. Recalling the definition (4.28) of $|X|^p(t)$ and using the estimate in Lemma 4.3.1 then gives $p + 1/4 - \kappa\lambda^2 \ge -1$. Sending $\lambda \to 2$ and $p \to 0$ yields $\kappa \le \frac{5}{16}$. □

It remains to give the

Proof of Prop. 4.3.8. For equation (4.38), we apply the lower bound [80, Thm. 5.1, Eq. (5.3)] to the function $f \in C_c^\infty(\mathbb{R})$ with $f \equiv 1$ on $\sigma(H)$. This provides for any $\varepsilon > 0$ the bound

$$\langle |X| \rangle_j^p(T) \ge C_\omega(p,\varepsilon) T^{p-2\gamma-\varepsilon}, \tag{4.40}$$

$\mathbb{P}$-almost surely, where $\gamma := \inf_{E\in(-2,2)} \frac{\lambda}{8-2E^2}$. This implies

$$\langle \beta^-(p)\rangle \geq 1 - \frac{\lambda}{4p}. \tag{4.41}$$

The chain of inequalities $\langle \beta^-(p)\rangle \leq \langle \beta^+(p)\rangle \leq \beta^+(p)$ gives the result. To see the last inequality, note that $\beta := \beta^+(p) > 0$ implies for any $\epsilon > 0$, $|X|_1^p(t) \leq Ct^{p\beta+\epsilon}$. This readily gives

$$\langle |X|_1^p\rangle(T) = \frac{2}{T}\int_0^\infty \mathrm{d}t\, e^{-2t/T}|X|_1^p(t) \leq CT^{p\beta+\epsilon} \tag{4.42}$$

and the inequality $\langle \beta^+(p)\rangle \leq \beta$.

For equation (4.39), we use [110, Thm 5.1] with $m = p$, where we have to prove its assumption, which is $P_c\delta_1 \neq 0$. Here, P_c is the orthogonal projection onto continuous part of the spectrum. Since $|\lambda| < 2$, the operator H exhibits singular continuous spectrum [111], thus $P_c \neq 0$. Now, $P_c\delta_1 \neq 0$ follows from cyclicity of δ_1, which can be proven by induction because the Hamiltonian acts on the half space $\ell^2(\mathbb{N})$ only. □

4.4 Propagation bounds for the number operator

In this section, we derive bounds on the propagation of the number operator by combining ideas from [1] with the bounds on the one-body dynamics discussed before. We recall that [1] derived such bounds for the case of non-decaying randomness (see also [155] for a continuum analogue).

We define the number operator and the local number operator by

$$\mathcal{N} := \sum_{j=1}^{n} a_j^* a_j \quad \text{and} \quad \mathcal{N}_S := \sum_{j\in S} a_j^* a_j, \tag{4.43}$$

where a_j is given in (4.4) and $S \subset \{1, ..., n\}$. This measures the number of up-spins in S. Let

$$\rho = \bigotimes_{j=1}^{n} \rho_j, \qquad \rho_j := \begin{pmatrix} \eta_j & 0 \\ 0 & 1-\eta_j \end{pmatrix} \tag{4.44}$$

and $0 \leq \eta_j \leq 1$. We denote by $\rho_t := e^{-itH_n}\rho e^{itH_n}$ the time evolution of the state ρ and by $\langle A\rangle_\rho := \mathrm{tr} A\rho$ the expectation of an observable A with respect to the state ρ.

Theorem 4.4.1. *Let $\kappa > 0$ be as in Lemma 4.3.1. There exists a constant $C > 0$ such that for every $n \geq 1$ and $S \subset \{1, \ldots, n\}$,*

$$\mathbb{E}\Big[\sup_{t\geq 0}\langle \mathcal{N}_S\rangle_{\rho_t}\Big] \leq \frac{C}{\lambda}\sum_{j\in S}\sum_{k=1}^{n}\eta_k (jk)^{1/4}\left(\frac{\min\{j,k\}}{\max\{j,k\}}\right)^{\kappa\lambda^2}. \tag{4.45}$$

This follows directly by combining results of [1] with Lemma 4.3.1.

Remark 4.4.2. *To illustrate the above we split $\{1,...,n\} = I \cup J$ with $I := \{1,...,m\}$ and $J := \{m+1,...,n\}$ for $n > m \in \mathbb{N}$. We set $\eta_j = 0$ on I and $\eta_j = 1$ on the complement J. In other words $\rho = |\varphi\rangle\langle\varphi|$ with the vector*

$$|\varphi\rangle = |\downarrow\rangle^{\otimes m} \otimes |\uparrow\rangle^{\otimes(n-m+1)} \tag{4.46}$$

in standard notation. Let $m > l \in \mathbb{N}$ and $S = \{1,...,l\}$. For $\kappa\lambda^2 > 5/4$, the above theorem implies the bound

$$\mathbb{E}\Big[\sup_{t\geq 0}\langle \mathcal{N}_S\rangle_{\rho_t}\Big] \leq C\left(\frac{l}{m}\right)^{\kappa\lambda^2}(lm)^{5/4} \tag{4.47}$$

for a constant $C > 0$ uniform in l, m, n. This is a time-independent bound on the number of up-spins which propagate from J into S and it decays as the distance $m \to \infty$ (when λ is large enough to guarantee $\kappa\lambda^2 > 5/4$).

Proof. The same computation that gives [1, eq. (41)] shows

$$\langle \mathcal{N}_S\rangle_{\rho_t} = \sum_{j\in S}\sum_{k=1}^{n}|\langle \delta_j, e^{2itH_n}\delta_k\rangle|^2\eta_k. \tag{4.48}$$

Using this, Lemma 4.3.1 implies

$$\mathbb{E}\Big[\sup_{t\geq 0}\langle \mathcal{N}_S\rangle_{\rho_t}\Big] \leq \sum_{j\in S}\sum_{k=1}^{n}\eta_k\mathbb{E}\Big[\sup_{t\geq 0}|\langle \delta_j, e^{2itH_n}\delta_k\rangle|^2\Big] \tag{4.49}$$

The assertion now follow from $|\langle \delta_j, e^{2itH_n}\delta_k\rangle|^2 \leq |\langle \delta_j, e^{2itH_n}\delta_k\rangle|$ and Lemma 4.3.1. ☐

Theorem 4.4.3. *If for some $0 \leq a \leq 1 < b$ and all $k, n \in \mathbb{N}$ with $k \leq n$*

$$\langle \mathcal{N}_1\rangle_{\rho_t} \leq \left(\frac{t^a}{k}\right)^b \tag{4.50}$$

holds for all ρ of the form (4.44) and $\eta_j = 0$ for $j < k$. Then, the upper transport exponent satisfies the bound

$$\limsup_{\varepsilon\to 0}\beta^+(b-1-\varepsilon) \leq \frac{ab}{b-1}. \tag{4.51}$$

Again, Proposition 4.3.8 then gives restrictions on the possible values of $0 \leq a \leq 1 < b$ for which (4.50) can hold. Therefore Theorem 4.4.3 may be interpreted as a lower bound on the transport of particles (from sites k and larger to the site 1) if at most error of order x^{-b} with $b > 1$ can ignored, compare Remark 4.1.1(iii).

Proof. Let ρ_k be given as in (4.44) with $\eta_j = \delta_{j,k}$. By (4.48)

$$\langle \mathcal{N}_1 \rangle_{\rho_t^k} = |\langle \delta_1, e^{-itH_n} \delta_k \rangle|^2. \tag{4.52}$$

Hence, the computation in (4.34) and assumption (4.50) imply that for any $p > 0$

$$\begin{aligned} |X|^p(t) &\leq \lim_{M\to\infty} \liminf_{n\to\infty} \sum_{1\leq k\leq M} k^p |\langle e^{-itH_n}\delta_1, \delta_k\rangle|^2 \\ &\leq \sum_{k\in\mathbb{N}} k^p \left(\frac{t^a}{k}\right)^b = t^{ab} \sum_{k\in\mathbb{N}} k^{p-b}. \end{aligned} \tag{4.53}$$

Taking $p = b - 1 - \varepsilon$ for an $\varepsilon > 0$, the last sum is finite and this gives the assertion. $\square$

Chapter 5

MULTI-COMPONENT GINZBURG-LANDAU THEORY: MICROSCOPIC DERIVATION AND EXAMPLES

Rupert L. Frank and Marius Lemm

5.1 Introduction

Since its advent in 1950 [83], Ginzburg–Landau (GL) theory has become ubiquitous in the description of superconductors and superfluids near their critical temperature T_c. GL theory is a phenomenological theory that describes the superconductor on a macroscopic scale. Apart from being a very successful physical theory, it also has a rich mathematical structure which has been extensively studied, see e.g. [40, 71, 87, 152] and references therein. Microscopically, superconductivity arises due to an effective attraction betweeen electrons, causing them to condense into Cooper pairs. In 1957 Bardeen, Cooper and Schrieffer [14], were the first to explain the origin of the attractive interaction in crystalline s-wave superconductors. By integrating out phonon modes, they arrived at their effective "BCS theory", in which one restricts to a certain class of trial states now known as BCS states. In 1959, Gor'kov [85] argued how the microscopic BCS theory with a rank-one interaction gives rise to the macroscopic GL theory near T_c. An alternative argument is due to de Gennes [57].

The first mathematically rigorous proof that Ginzburg–Landau theory arises from BCS theory, on macroscopic length scales and for temperatures close to T_c, was given in [73] under the non-degeneracy assumption that there is only one type of superconductivity present in the system. The derivation there allows for local interactions and external fields and hence applies to superfluid ultracold Fermi gases, a topic of considerable current interest.

In the present paper, we use the same formalism as in [73] and study microscopically derived Ginzburg–Landau theories involving multiple types of superconductivity for systems without external fields.

We first discuss the main result of part I, which forms the basis for the applications in parts II and III. Afterwards, we discuss the physical motivation for studying multi-component GL theories and the extent to which our model applies to realistic systems. The introduction closes with a description of the main results of parts II and III.

Main result of part I

As in [73], we employ a variational formulation of BCS theory [11, 119] with an isotropic electronic dispersion relation. We use previous rigorous results about this theory in the absence of external fields [72, 89, 92, 93]. Particularly important is the result of [89] that the critical temperature T_c can be characterized by the following linear criterion. T_c is the unique value of $T \geq 0$ for which the "effective gap operator"

$$K_T + V(\mathbf{x}) = \frac{-\nabla^2 - \mu}{\tanh\left(\frac{-\nabla^2-\mu}{2T}\right)} + V(\mathbf{x})$$

has zero as its lowest eigenvalue. Here V is the electron-electron interaction potential. Throughout the microscopic derivation of GL theory in [73], it is *assumed that zero is a non-degenerate eigenvalue* of $K_{T_c} + V$. For radially symmetric V, this means that the order parameter is an s-wave, i.e. it is spherically symmetric.

The **main result of part I**, Theorem 5.2.10, is that for systems without external fields the microscopic derivation of GL theory also holds when the eigenvalue is *degenerate* of arbitrary order $n > 1$. (A general argument shows that always $n < \infty$.) The arising GL theory now features precisely n order parameters $\psi_1, \ldots, \psi_n$. It turns out that one can use the same general strategy as in [73].

In fact, one can classify approximate minimizers of the BCS free energy via the GL theory. Given an orthonormal basis $\{a_1, \ldots, a_n\}$ of $\ker(K_{T_c} + V)$, Theorem 5.2.10 (ii) says that, near the critical temperature, the Cooper pair wave function α of a BCS state of almost minimal free energy (i.e. the Cooper pair wave function realized by the physical system) is approximately given by a linear combination of the $\{a_1, \ldots, a_n\}$ of the form

$$\alpha \approx \sqrt{\frac{T_c - T}{T_c}} \sum_{j=1}^{n} \psi_j a_j, \qquad (5.1)$$

where the "amplitudes" $\psi_1, \ldots, \psi_n \in \mathbb{C}$ almost minimize the corresponding GL function.

The results of [73] allow for the presence of weak external fields which vary on the macroscopic scale. A key step is to establish semiclassical estimates under weak regularity assumptions. We emphasize that in our case the system has no external fields and is therefore translation-invariant. This simplifies several technical difficulties present in [73]. In particular, the semiclassical analysis of [73] reduces to an ordinary Taylor expansion. The result of the expansion is stated as Theorem 5.5.3 and we give the simplified proof for the translation-invariant situation. We do this (a) to obtain optimal error bounds and (b) to hopefully make the emergence of GL theory more transparent in our technically simpler situation.

Physical motivation

Background. The degenerate case corresponds to systems which have *multiple order parameters*, i.e. which can host multiple types of superconductivity. Physically, this situation occurs e.g. for *unconventional superconductors*. By definition, these are materials in which an effective attractive interaction of electrons leads to the formation of Cooper pairs, but the effective attraction is not produced by the usual electron-phonon interactions. (Identifying the underlying mechanisms is a major open problem in condensed matter physics.)

Two important classes of unconventional superconductors are the layered cuprates and iron-based compounds, typically designed to have large values of T_c ("high-temperature superconductors"). Many of these materials possess tetragonal lattice symmetry, though the prominent example of YBCO has orthorhombic symmetry. There is strong experimental evidence for the occurrence of d-wave order parameters in these materials, in contrast to the pure s-wave order parameter in conventional superconductors. More precisely, phase-sensitive experiments with Josephson junctions [108, 109, 168, 169, 174] have evidenced the presence of a $d_{x^2-y^2}$-wave order parameter (for tetragonal symmetry) and of mixed $(s+d_{x^2-y^2})$-wave order parameters (for orthorhombic symmetry).

There also exist proposals of d-wave super*fluidity* for molecules in optical lattices [115].

Multi-component Ginzburg–Landau theories. On the theoretical side, one of the most important tools for studying unconventional superconductors are multi-component Ginzburg-Landau theories [8, 24, 104, 120, 150, 162, 170, 172, 175, 176]. Many of these papers study the symmetry properties near the vortex cores in two-component GL theories. A very common example is a GL theory with $(s+d_{x^2-y^2})$-wave order parameters; this case has also been studied mathematically in [61, 107]. The effect of an an anisotropic order parameter on the upper critical field was studied in [118].

Another avenue where two-component GL theories have been successful is in the description of type I.5 superconductors [10, 34, 157]. These are systems in which the magnetic field penetration depth lies in between the coherence lengths of the different order parameters (of course this effect only manifests itself in an external magnetic field).

Microscopically derived GL theories. In many of the papers cited above, the GL theories that are studied are first obtained microscopically by using Gor'kov's formal expansion of Green's functions. The advantage of having a microscopically derived GL theory is that it has some remaining "microscopic content". By this we mean:

1. One can directly associate each macroscopic order parameters with a certain symmetry type of the system's Cooper pair wave function. Therefore, if we can classify the minimizers of the microscopically derived GL theory, we understand exactly which Cooper pair wave functions α can occur in the physical system in configurations of almost minimal free energy.

2. One has explicit formulae for computing the GL coefficients as integrals over microscopic quantities.

The first point is expressed by (5.1) above and is therefore a corollary of Theorem 5.2.10. The second point is represented by formulae (5.21),(5.22) in Theorem 5.2.10.

While the papers cited above provide important insight about the vortex structure in unconventional superconductors, they are restricted in that the GL theories are obtained using the formal Gorkov procedure and that almost exclusively two-component GL theories are studied. Our Theorem 5.2.10 provides a rigorous microscopic derivation of n-component GL theories with n arbitrary starting from a BCS theory with an isotropic electronic dispersion.

Physical assumptions of our model. We discuss the main physical assumptions of our model and the resulting limitations in its applicability to realistic systems.

(a) *Translation-invariance.* We view the degenerate translation-invariant systems as toy models for multi-component superconductivity. We believe that the examples of multi-component GL theories studied in part II are already rich enough to show that the translation-invariant case can be interesting. From a technical perspective, translation invariance yields major technical simplifications. In particular, the semiclassical analysis of [73] reduces to a Taylor expansion.

(b) *BCS theory with a Fermi-Dirac normal state.* There are two assumptions here: First, we start from a BCS theory (meaning a theory in which electrons can form Cooper pairs and which restricts to BCS-type trial states). The question whether such a theory can be used to describe unconventional superconductors is unresolved [120]. Second, we work with a BCS theory for which the normal state is given by the usual Fermi-Dirac distribution. Most realistic unconventional superconductors are strongly interacting systems with a non-Fermi liquid normal state [120, 156].

(c) *Isotropy.* We study a BCS theory in which the electrons live in the continuum and have an isotropic dispersion. Many of the known examples of unconventional superconductors are layered compounds which are effectively two-dimensional. When we say that their order parameter has $d_{x^2-y^2}$-wave symmetry, then this only means that it has a four-lobed shape similar to that of $k_x^2-k_y^2$ for $-\pi < k_x, k_y < \pi$, but its precise dependence on k_x, k_y depends on the symmetry group of the two-dimensional lattice [120]. Order parameters of the form $k_x^2 - k_y^2$ have been studied as a first approximation to unconventional superconductors, see e.g. [150, 172, 175].

For the examples in part II, we consider a spherically symmetric interaction potential, resulting in a fully isotropic BCS theory. Consequently, the d-wave order parameters that we consider are the "usual" ones, known from atomic physics (see section 5.3). By isotropy, all the d-waves (there are two in two dimensions and five in three dimensions) are energetically equal. The examples in part II show that even this isotropic microscopic theory can lead to rather rich coupling phenomena of anisotropic macroscopic order parameters, as we discuss next.

(d) *Spin singlet order parameter.* We restrict to order parameters which are singlets in spin space. This is indeed the case for unconventional superconductors [120], but it excludes systems with p-wave order parameters such as superfluid Helium-3.

Main results of part II

In part II, we compute the n-component GL theories that arises from the BCS theory according to Theorem 5.2.10 for several exemplary cases. For each situation, we make some observations about the minimizers of the GL energy and their symmetries and give a physical interpretation.

Throughout part II, V is assumed to be spherically symmetric, so the BCS theory becomes fully isotropic. The order parameters can then be described by the decomposition into angular momentum sectors (see section 5.3) and we consider the case of pure d-wave and mixed $(s+d)$-wave order parameter. Here and in the following, we write *"GLn"* for "n-component Ginzburg–Landau theory". The dimension D will be either two or three.

(i) Let $D = 3$. Assume the Cooper pair wave function is a linear combination of the five linearly independent d-waves with a given radial part. **Theorem 5.3.1** explicitly computes the microscopically derived GL5 energy and gives a full description of all its minimizers. Surprisingly, the GL5 energy in three dimensions exhibits the emergent symmetry group $O(5)$, see Corollary 5.3.3 (i), which is considerably larger than the original $O(3)$ symmetry group coming from the spherical symmetry and reflection symmetry of V.

(ii) Let $D = 2$. Assume the Cooper pair wave function is a linear combination of the two linearly independent d-waves with a given radial part. **Theorem 5.3.5** explicitly computes the microscopically derived GL2 energy and gives a full description of all its minimizers. We find that the $(d_{x^2-y^2}, d_{xy})$ order parameter must be of the form $(\psi, \pm i\psi)$ with $|\psi|$ minimizing an appropriate GL1. In particular, the minimizers of this GL2 form a double cover of the minimizer of a GL1.

(iii) Let $D = 3$. Assume the Cooper pair wave function is a linear combination of the five linearly independent d-waves with a given radial part *and* the s-wave with another given radial part. **Theorem 5.3.7** explicitly computes the microscopically derived GL6 energy. It also gives a simple characterization of the parameter values for which the pure d-wave minimum is always unstable under s-wave perturbations and of the parameter values for which, vice-versa, the pure s-wave minimum is unstable under d-wave perturbations. As a consequence, we give parameter values for which s- and d-waves must *couple non-trivially* to be energy-minimizing.

We also consider the mixed $(s+d)$-wave case in $D = 2$ dimensions. The result is presented in Remark 5.3.9 (v) for brevity.

Main results of part III

Recall from the discussion of part I above, that the candidate Cooper pair wave functions are the ground states of the effective gap operator $K_{T_c} + V$. A priori, it is not at all clear that the fully isotropic BCS theory can produce ground state sectors of $K_{T_c} + V$ which are not spherically symmetric. In particular, it is not clear that the examples considered in part II actually exist.

In fact, if K_{T_c} is replaced by the Laplacian $-\nabla^2$ we have a Schrödinger operator and under very general conditions on the potential V, the Perron-Frobenius theorem implies that the ground state is in fact *non-degenerate*, see e.g. Theorem 11.8 in [123]. For spherically symmetric V, this means the ground state is also spherically symmetric ("s-wave").

In part III, we remedy this by exhibiting examples of spherically symmetry potentials V such that the ground state sector of $K_{T_c} + V$ can in fact have *arbitrary* angular momentum. These potentials will be of the form

$$V_{\lambda,R}(\mathbf{x}) = -\lambda\delta(|\mathbf{x}| - R)$$

in three dimensions. Here λ and R are positive parameters. The result holds for open intervals of the parameters values, so it is "not un-generic".

5.2 Part I: Microscopic derivation of GL theory in the degenerate case

BCS theory

We consider a gas of fermions in $\mathbb{R}^D$ with $1 \leq D \leq 3$ at temperature $T > 0$ and chemical potential $\mu \in \mathbb{R}$, interacting via the two-body potential $V(\mathbf{x})$. We assume that $V(\mathbf{x}) = V(-\mathbf{x})$ is reflection symmetric. We do not consider external fields, so the system is translation-invariant. A BCS state Γ can then be conveniently represented as a 2×2 matrix-valued Fourier multiplier on $L^2(\mathbb{R}^3) \oplus L^2(\mathbb{R}^3)$ of the form

$$\widehat{\Gamma}(\mathbf{p}) = \begin{pmatrix} \widehat{\gamma}(\mathbf{p}) & \widehat{\alpha}(\mathbf{p}) \\ \overline{\widehat{\alpha}(\mathbf{p})} & 1 - \widehat{\gamma}(\mathbf{p}) \end{pmatrix}, \tag{5.2}$$

for all $\mathbf{p} \in \mathbb{R}^D$. Here, $\widehat{\gamma}(\mathbf{p})$ denotes the Fourier transform of the one particle-density matrix and $\widehat{\alpha}(\mathbf{p})$ the Fourier transform of the Cooper pair wave function. We require $\widehat{\alpha}(\mathbf{p}) = \widehat{\alpha}(-\mathbf{p})$ and $0 \leq \Gamma(\mathbf{p}) \leq 1$ as a matrix, which is equivalent to $0 \leq \widehat{\gamma}(\mathbf{p}) \leq 1$ and $|\widehat{\alpha}(\mathbf{p})|^2 \leq \widehat{\gamma}(\mathbf{p})(1 - \widehat{\gamma}(\mathbf{p}))$. The *BCS free energy per unit volume* reads, in suitable units

$$\mathcal{F}_T^{BCS}(\Gamma) = \int_{\mathbb{R}^D} (\mathbf{p}^2 - \mu)\widehat{\gamma}(\mathbf{p})\,\mathrm{d}\mathbf{p} - TS[\Gamma] + \int_{\mathbb{R}^D} V(\mathbf{x})|\alpha(\mathbf{x})|^2\,\mathrm{d}\mathbf{x}, \tag{5.3}$$

where the *entropy per unit volume* is given by

$$S[\Gamma] = -\int_{\mathbb{R}^D} \mathrm{Tr}_{\mathbb{C}^2}\left[\widehat{\Gamma}(\mathbf{p}) \log \widehat{\Gamma}(\mathbf{p})\right]\,\mathrm{d}\mathbf{p}. \tag{5.4}$$

Remark 5.2.1 (BCS states). *(i) In general [11, 73], $SU(2)$-invariant BCS states are represented as 2×2 block operators*

$$\Gamma = \begin{pmatrix} \gamma & \alpha \\ \overline{\alpha} & 1 - \overline{\gamma} \end{pmatrix}$$

where γ, α are operators on $L^2(\mathbb{R}^D)$ with kernel functions $\gamma(\mathbf{x}, \mathbf{y})$ and $\alpha(\mathbf{x}, \mathbf{y})$ in $L^2(\mathbb{R}^D) \oplus L^2(\mathbb{R}^D)$. Since $0 \leq \Gamma \leq 1$ is Hermitian, $\gamma(\mathbf{x}, \mathbf{y}) = \overline{\gamma(\mathbf{y}, \mathbf{x})}$ and $\alpha(\mathbf{x}, \mathbf{y}) = \alpha(\mathbf{y}, \mathbf{x})$. In the translation-invariant case considered here, these kernel functions are assumed to be of the form $\gamma(\mathbf{x} - \mathbf{y})$ and $\alpha(\mathbf{x} - \mathbf{y})$. Since convolution by γ, α becomes multiplication in Fourier space, we can equivalently describe the BCS state by its Fourier transform $\widehat{\Gamma}$ defined in (5.2) *above. In the translation-invariant case, the symmetries of γ, α turn into the relations $\gamma(\mathbf{x}) = \overline{\gamma(-\mathbf{x})}$ and $\alpha(\mathbf{x}) = \alpha(-\mathbf{x})$*

or equivalently $\widehat{\gamma}(\mathbf{p}) = \overline{\widehat{\gamma}(\mathbf{p})}$ *and* $\widehat{\alpha}(\mathbf{p}) = \widehat{\alpha}(-\mathbf{p})$*. Finally, since we are interested in states with minimal free energy, we may also assume*

$$\widehat{\gamma}(\mathbf{p}) = \widehat{\gamma}(-\mathbf{p}) \tag{5.5}$$

and this was already used on the bottom right element in (5.2)*. To see this, let* $\widehat{\Gamma}$ *be a BCS state not satisfying* (5.5)*, set* $\widehat{\Gamma}_r(\mathbf{p}) := \widehat{\Gamma}(-\mathbf{p})$ *and observe that*

$$\mathcal{F}_T^{BCS}\left(\frac{\Gamma + \Gamma_r}{2}\right) < \mathcal{F}_T^{BCS}(\Gamma)$$

by strict concavity of the entropy and reflection symmetry of all terms in $\mathcal{F}_T^{BCS}$*.*

(ii) Note that $\alpha(\mathbf{x}, \mathbf{y}) = \alpha(\mathbf{y}, \mathbf{x})$ *means that the Cooper pair wave function is symmetric in its arguments. To obtain a fermionic wave function, we would eventually tensor* α *with an antisymmetric spin singlet. Since* α *is reflection-symmetric in the translation-invariant case,* α *must be of even angular momentum if* V *is radial.*

The restriction to symmetric α *is a consequence of assuming* $SU(2)$ *invariance in the heuristic derivation of the BCS free energy [89, 119]. This means the full Cooper pair wave function must be a spin singlet and so its spatial part* α *must be symmetric. Note that this excludes systems, e.g. superfluid Helium-3, which display a p-wave order parameter.*

(iii) For more background on the BCS functional, in particular a heuristic derivation from the many-body quantum Hamiltonian in which one restricts to quasi-free states, assumes $SU(2)$ *invariance and drops the direct and exchange terms, see [119] or the appendix in [89]. Recently, [27] justified the last step for translation-invariant systems by proving that dropping the direct and exchange terms only leads to a renormalization of the chemical potential* μ*, for a class of short-ranged potentials.*

We make the following technical assumption on the interaction potential.

Assumption 5.2.2. *We either have* $V \in L^{p_V}(\mathbb{R}^D)$ *with* $p_V = 1$ *for* $D = 1$*,* $1 < p_V < \infty$ *for* $D = 2$ *and* $p_V = 3/2$ *for* $D = 3$*, or we have*

$$V(\mathbf{x}) = V_{\lambda,R}(|\mathbf{x}|) := -\lambda\delta(|\mathbf{x}| - R), \tag{5.6}$$

when $D = 1, 2, 3$ *and* $\lambda, R > 0$*.*

We note

Proposition 5.2.3. *A potential V satisfying Assumption 5.2.2 is infinitesimally form-bounded with respect to $-\nabla^2$.*

We quote a result of [89], which provides the foundation for studying the variational problem associated with $\mathcal{F}_T^{BCS}$. Define

$$\mathcal{D} := \Big\{\Gamma \text{ as in (5.2)} \,:\, 0 \le \widehat{\Gamma} \le 1,\, \widehat{\gamma} \in L^1(\mathbb{R}^D, (1+\mathbf{p}^2)\,\mathrm{d}\mathbf{p}),\, \alpha \in H^1_{sym}(\mathbb{R}^D)\Big\}$$

with $H^1_{sym}(\mathbb{R}^D) = \big\{\alpha \in H^1(\mathbb{R}^D) \,:\, \alpha(\mathbf{x}) = \alpha(-\mathbf{x})\, a.e.\big\}$.

Proposition 5.2.4 (Prop. 2 in [89])**.** *Under Assumption 5.2.2 on V, the BCS free energy* (5.3) *is bounded below on $\mathcal{D}$ and attains its minimum.*

The physical interpretation rests on the following

Definition 5.2.5 (Superconductivity)**.** *The system described by $\mathcal{F}_T^{BCS}$ is* superconducting *(or* superfluid*, depending on the context) iff any minimizer Γ of $\mathcal{F}_T^{BCS}$ has off-diagonal entry $\alpha \not\equiv 0$.*

It was shown in [89] that the question whether the system is superconducting can be reduced to the following linear criterion, which we will use heavily. (In [89], the results are proved for $D = 3$ and without the restriction to the reflection-symmetric subspace of $L^2(\mathbb{R}^D)$, but it was already observed in [73] that the statement holds as stated here.)

Proposition 5.2.6 (Theorems 1 and 2 in [89])**.** *Define the operator*

$$K_T := \frac{-\nabla^2 - \mu}{\tanh\left(\frac{-\nabla^2-\mu}{2T}\right)} \tag{5.7}$$

as a Fourier multiplier and consider $K_T + V$ in the Hilbert space

$$L^2_{sym}(\mathbb{R}^D) := \{f \in L^2(\mathbb{R}^D) \,:\, f(\mathbf{x}) = f(-\mathbf{x}) \ a.e.\}. \tag{5.8}$$

Then:

(i) the system is superconducting in the sense of Definition 5.2.5 iff $K_T + V$ has at least one negative eigenvalue.

(ii) *there exists a unique critical temperature* $0 \leq T_c < \infty$ *such that*

$$\begin{aligned} K_{T_c} + V &\geq 0, \\ \inf \operatorname{spec}(K_T + V) &< 0, \quad \forall T < T_c. \end{aligned} \tag{5.9}$$

T_c is unique because the quadratic form associated with K_T is strictly monotone in T. In a nutshell, the reason why the operator $K_T + V$ appears, is that it is the Hessian of the map

$$\phi \mapsto \mathcal{F}_T^{BCS}\left(\Gamma_0 + \begin{pmatrix} 0 & \phi \\ \overline{\phi} & 0 \end{pmatrix}\right)$$

at $\phi = 0$ with Γ_0 the normal state of the system, see (5.13), and naturally, the positivity of the Hessian is related to minimality. For the details, we refer to [89]. In the following, we make

Assumption 5.2.7. *V is such that $T_c > 0$.*

By Theorem 3 in [89], $V \leq 0$ and $V \not\equiv 0$ implies $T_c > 0$ in $D = 3$ and this result is stable under addition of a small positive part.

Definition 5.2.8 (Ground-state degeneracy)**.** *We set*

$$n := \dim \ker(K_{T_c} + V). \tag{5.10}$$

Remark 5.2.9. *(i) We always have $n < \infty$. The reason is that, by Assumption 5.2.2 on V, the essential spectrum of $K_T + V$ is contained in $[2T, \infty)$. Therefore, zero is an isolated eigenvalue of $K_{T_c} + V$ of finite multiplicity and so $n < \infty$.*

(ii) A sufficient condition for $n = 1$ is that $\widehat{V} \leq 0$ and $\widehat{V} \not\equiv 0$ [72, 92].

(iii) For Schrödinger operators $-\nabla^2 + V$, the ground state is non-degenerate by the Perron-Frobenius theorem. That is, one always has the analogue of $n = 1$ in that case. One may therefore wonder if $n > 1$ ever holds. In part III, we present a class of radial potentials such that for open intervals of parameter values, we have $n > 1$. In fact, one can tune the parameters such that $\ker(K_{T_c} + V)$ *lies in an* arbitrary *angular momentum sector.*

GL theory

In GL theory, one aims to find "order parameters" that minimize the GL energy. The minimizers then describe the macroscopic relative density of superconducting charge carriers, up to spontaneous symmetry breaking. Microscopically, they describe the center of mass coordinate of the Cooper pair wave function α. In our case, translation-invariance implies that the order parameters are complex-valued constants, which are non-zero iff the system is superconducting.

When $n = 1$ (and the system is translation-invariant), there is a single order parameter $\psi \in \mathbb{C}$ and for $T < T_c$ the GL energy is of the all-familiar "Mexican hat" shape

$$\mathcal{E}^{GL}(\psi) = c|\psi|^4 - d|\psi|^2, \qquad c, d > 0. \tag{5.11}$$

Below, in Theorem 5.2.10, we show that for $n > 1$, the GL energy is of the form

$$\mathcal{E}^{GL}(\mathfrak{a}) = \int f_4(p)|\mathfrak{a}(\mathbf{p})|^4 \mathrm{d}\mathbf{p} - \int f_2(p)|\mathfrak{a}(\mathbf{p})|^2 \mathrm{d}\mathbf{p} \tag{5.12}$$

and $\mathfrak{a}$ varies over the n-dimensional set $\ker(K_{T_c} + V)$. The functions f_4 and f_2 are explicit; they are radial ($p \equiv |\mathbf{p}|$) and positive for $T < T_c$.

Thus, we see that *the Mexican hat shape is characteristic for the translation-invariant case, even in the presence of degeneracies.* However, there exists *nontrivial coupling* (i.e. mixed terms) between the different basis elements of $\ker(K_{T_c} + V)$ in general.

Result

We write Γ_0 for the minimizer of the free energy $\mathcal{F}_T^{BCS}$ as in (5.3) but with $V \equiv 0$. That is, Γ_0 describes a free Fermi gas at temperature T and for this reason we call Γ_0 the "normal state" of the system. From the Euler-Lagrange equation, one easily obtains

$$\widehat{\Gamma}_0(\mathbf{p}) = \begin{pmatrix} \widehat{\gamma}_0(\mathbf{p}) & 0 \\ 0 & 1 - \widehat{\gamma}_0(\mathbf{p}) \end{pmatrix}, \tag{5.13}$$

where

$$\widehat{\gamma}_0(\mathbf{p}) = \frac{1}{1 + \exp((\mathbf{p}^2 - \mu)/T)} \tag{5.14}$$

is the well-known Fermi-Dirac distribution. (Of course, Γ_0 depends on μ and T, but for the following we implicitly assume that it has the same values of μ, T as the free energy under consideration.)

We now state our first main result. It says that an appropriate n-component GL theory arises from BCS theory on the macroscopic scale and for temperatures close to T_c. Recall that $p \equiv |\mathbf{p}|$.

Theorem 5.2.10. *Let V satisfy Assumptions 5.2.2 and 5.2.7 and let $\mu \in \mathbb{R}$, $T < T_c$. Recall that $n = \dim\ker(K_{T_c} + V)$. Then:*

(i) As $T \uparrow T_c$,

$$\begin{aligned} &\min_{\Gamma} \mathcal{F}_T^{BCS}(\Gamma) - \mathcal{F}_T^{BCS}(\Gamma_0) \\ &= \left(\frac{T_c - T}{T_c}\right)^2 \min_{\mathfrak{a} \in \ker(K_{T_c}+V)} \mathcal{E}^{GL}(\mathfrak{a}) + O\left((T_c - T)^3\right), \end{aligned} \tag{5.15}$$

where $\mathcal{E}^{GL}$ is defined by

$$\begin{aligned} \mathcal{E}^{GL}(\mathfrak{a}) =& \frac{1}{T_c} \int_{\mathbb{R}^D} \frac{g_1((p^2-\mu)/T_c)}{(p^2-\mu)/T_c} \left|K_{T_c}(p)\right|^4 \left|\mathfrak{a}(\mathbf{p})\right|^4 \mathrm{d}\mathbf{p} \\ &- \frac{1}{2T_c} \int_{\mathbb{R}^D} \frac{1}{\cosh^2\left(\frac{p^2-\mu}{2T_c}\right)} \left|K_{T_c}(p)\right|^2 \left|\mathfrak{a}(\mathbf{p})\right|^2 \mathrm{d}\mathbf{p}. \end{aligned} \tag{5.16}$$

Here we used the auxiliary functions

$$\begin{aligned} g_0(z) :=& \frac{\tanh(z/2)}{z} \\ g_1(z) :=& -g_0'(z) = z^{-1} g_0(z) - \frac{1}{2} z^{-1} \frac{1}{\cosh^2(z/2)} \\ K_T(p) :=& \frac{p^2-\mu}{\tanh\left(\frac{p^2-\mu}{2T}\right)}. \end{aligned} \tag{5.17}$$

(ii) Moreover, if Γ is an approximate minimizer of $\mathcal{F}_T^{BCS}$ in the sense that

$$\mathcal{F}_T^{BCS}(\Gamma) - \mathcal{F}_T^{BCS}(\Gamma_0) = \left(\frac{T_c - T}{T_c}\right)^2 \left(\min_{\mathfrak{a} \in \ker(K_{T_c}+V)} \mathcal{E}^{GL}(\mathfrak{a}) + \varepsilon\right), \tag{5.18}$$

for some $0 < \varepsilon \le M$, then we can decompose its off-diagonal element $\widehat{\alpha}$ as

$$\widehat{\alpha}(\mathbf{p}) = \sqrt{\frac{T_c - T}{T_c}} \mathfrak{a}_0(\mathbf{p}) + \xi, \tag{5.19}$$

where $\|\xi\|_2 = O_M(T_c - T)$ and $\mathfrak{a}_0 \in \ker(K_{T_c} + V)$ is an approximate minimizer of the GL energy, i.e.

$$\mathcal{E}^{GL}(\mathfrak{a}_0) \le \min \mathcal{E}^{GL} + \varepsilon + O_M(T_c - T).$$

(Here O_M means that the implicit constant depends on M.)

The idea is that near T_c, where superconductivity is weak, the normal state Γ_0 is the prime competitor for the development of a small off-diagonal component $\widehat{\alpha}$ of the BCS minimizer. Theorem 5.2.10 then says that the lowest-order deviation from the normal state is well-described by a GLn whose coefficients are given explicitly as integrals over microscopic quantities.

Remark 5.2.11. *(i) We can equivalently rewrite the GL energy in terms of "order parameters" $\psi_1, \ldots, \psi_n$ as follows. We fix an orthonormal basis $\{a_j\}$ of $\ker(K_{T_c} + V)$ and decompose $\mathfrak{a} \in \ker(K_{T_c} + V)$ as $\mathfrak{a}(\mathbf{p}) = \sum_{j=1}^n \psi_j \widehat{a}_j(\mathbf{p})$. The basis coefficients $\psi_1, \ldots, \psi_n \in \mathbb{C}$ are the n order parameters, each one corresponds to a different "type" of superconductivity $\widehat{a}_j$. The GL energy (5.16) can then be rewritten in the equivalent form*

$$\mathcal{E}^{GL}(\psi_1, \ldots, \psi_n) = \sum_{i,j,k,m} c_{ijkm} \overline{\psi_i \psi_j} \psi_k \psi_m - \sum_{i,j} d_{ij} \overline{\psi_i} \psi_j. \tag{5.20}$$

Here the "GL coefficients" c_{ijkm}, d_{ij} are given by

$$c_{ijkm} = \frac{1}{T_c^2} \int_{\mathbb{R}^D} \frac{g_1((p^2 - \mu)/T_c)}{p^2 - \mu} \left| K_{T_c}(p) \right|^4 \overline{\widehat{a}_i(\mathbf{p}) \widehat{a}_j(\mathbf{p})} \widehat{a}_k(\mathbf{p}) \widehat{a}_m(\mathbf{p}) \, \mathrm{d}\mathbf{p} \tag{5.21}$$

$$d_{ij} = \frac{1}{2T_c} \int_{\mathbb{R}^D} \frac{1}{\cosh^2\left(\frac{p^2 - \mu}{2T_c}\right)} \left| K_{T_c}(p) \right|^2 \overline{\widehat{a}_i(\mathbf{p})} \widehat{a}_j(\mathbf{p}) \, \mathrm{d}\mathbf{p}. \tag{5.22}$$

The minimum in (5.15) turns into the minimum over all $\psi_1, \ldots, \psi_n \in \mathbb{C}$. In part II, we compute the integrals (5.21),(5.22) for special symmetry types and study the resulting minimization problem given by (5.20).

(ii) If one assumes $n = 1$, this result is a corollary of Theorem 1 in [73], which is obtained by restricting it to translation-invariant systems. (When comparing, note that [73] rescale the BCS free energy to macroscopic units.) In this case, the microscopically derived GL theory is simply of the form (5.11).

(iii) Note that the error term in (5.15) is $O(T_c - T)$ higher than the order at which the GL energy enters. Such an error bound is probably optimal because the semiclassical expansion of Lemma 5.5.4 will contribute terms at this order. It improves on the error term that one would obtain from Theorem 1 of [73] in the case $n = 1$.

We note that writing $\min \mathcal{E}^{GL}$ in the above theorem is justified because

Proposition 5.2.12. *The microscopically derived Ginzburg–Landau energy satisfies* $\inf_{\mathbb{C}^n} \mathcal{E}^{GL} > -\infty$. *Moreover, the infimum is attained.*

When $T \geq T_c$, it was proved in [89] that the unique minimizer of $\Gamma \mapsto \mathcal{F}_T^{BCS}(\Gamma)$ is the normal state Γ_0. In other words, the left-hand side in (5.15) vanishes identically for all $T \geq T_c$. Nonetheless, one can still ask if GL theory describes *approximate* minimizers of the BCS free energy similarly to Theorem 5.2.10 (ii) when $T - T_c$ is positive but small. Indeed, *above* T_c approximate minimizers must have *small* GL order parameters (as one would expect):

Proposition 5.2.13. *Suppose* $T > T_c$ *and* Γ *satisfies*

$$\mathcal{F}_T^{BCS}(\Gamma) - \mathcal{F}_T^{BCS}(\Gamma_0) = \varepsilon \left(\frac{T - T_c}{T_c} \right)^2,$$

with $0 < \varepsilon \leq M$. *Let* $\{a_j\}$ *be any choice of basis for* $\ker(K_{T_c} + V)$.

Then, there exist $\psi_1, \ldots, \psi_n \in \mathbb{C}^n$ *and* $\xi \in L^2(\mathbb{R}^D)$ *such that*

$$\widehat{\Gamma}_{12} \equiv \widehat{\alpha} = \sqrt{\frac{T - T_c}{T_c}} \sum_{j=1}^{n} \psi_j \widehat{a}_j + \xi$$

with $\|\xi\|_2 = O_M\left(T - T_c\right)$ *and*

$$\sum_{i=1}^{n} |\psi_i|^2 \leq \frac{\varepsilon}{\lambda_{\min}} + O_M\left(T_c - T\right) \tag{5.23}$$

as $T \to T_c$. *Here* $\lambda_{\min} > 0$ *is a system-dependent parameter.*

5.3 Part II: Examples with d-wave order parameters

Angular momentum sectors

In order to explicitly compute the GL coefficients given by formulae (5.21), (5.22), we make some assumptions on the potential V. First and foremost, we assume that V *is radially symmetric.* We can then decompose $L^2(\mathbb{R}^3)$ into angular momentum sectors. We review here some basic facts about these and establish notation. For the *spherical harmonics*, we use the definition

$$Y_l^m(\vartheta, \varphi) = \sqrt{\frac{(2l+1)}{4\pi} \frac{(l-m)!}{(l+m)!}}\, P_l^m(\cos\vartheta) e^{im\varphi}, \tag{5.24}$$

where P_l^m is the associated Legendre function, which we define with a factor of $(-1)^m$ relative to the Legendre polynomial P_m. While we will use the Y_l^m in the proofs, it will be convenient to state the results in the basis of *real-valued spherical harmonics* defined by

$$Y_{l,m} = \begin{cases} \frac{i}{\sqrt{2}}\left(Y_l^m - (-1)^m Y_l^{-m}\right), & \text{if } m < 0 \\ Y_0^0, & \text{if } m = 0 \\ \frac{1}{\sqrt{2}}\left(Y_l^m + (-1)^m Y_l^{-m}\right), & \text{if } m > 0. \end{cases} \tag{5.25}$$

We let $\mathcal{S}_l = \operatorname{span}\{Y_l^m\}_{m=-l,\dots,l} = \operatorname{span}\{Y_{l,m}\}_{m=-l,\dots,l}$ and define

$$\mathcal{H}_l = L^2(\mathbb{R}_+; r^2 \mathrm{d}r) \otimes \mathcal{S}_l, \qquad (r \equiv |\mathbf{x}|). \tag{5.26}$$

We employ the usual physics terminology

$$\mathcal{H}_0 \equiv \{s\text{-waves}\}, \quad \mathcal{H}_1 \equiv \{p\text{-waves}\}, \quad \mathcal{H}_2 \equiv \{d\text{-waves}\}. \tag{5.27}$$

Note that $\mathcal{H}_0$ is just the set of spherically symmetric functions and $Y_{2,2} \propto \frac{x^2-y^2}{x^2+y^2}$ is the $d_{x^2-y^2}$-wave in this classification. In analogy to Fourier series, we have the orthogonal decomposition [164]

$$L^2(\mathbb{R}^3) = \bigoplus_{l=0}^{\infty} \mathcal{H}_l. \tag{5.28}$$

Recall that $r \equiv |\mathbf{x}|$. The Laplacian in 3-dimensional polar coordinates reads

$$\nabla^2 = \nabla^2_{\text{rad}} + \frac{\nabla^2_{S^2}}{r^2}, \tag{5.29}$$

where $\nabla^2_{\text{rad}} = r^{-2}\partial_r(r^2\partial_r)$ and $\nabla^2_{S^2}$ is the Laplace-Beltrami operator, which acts on spherical harmonics by

$$-\nabla^2_{\mathbb{S}^2} Y_{l,m} = l(l+1) Y_{l,m}. \tag{5.30}$$

Since K_T commutes with the Laplacian and V clearly leaves the decomposition (5.28) invariant, we observe that the eigenstates of $K_T + V$ can be labeled by l (in physics terminology, l is a "good quantum number"). To make contact with unconventional superconductors, we will suppose we are in either of the two cases:

- $\ker(K_{T_c} + V) = \operatorname{span}\{\rho_2\} \otimes \mathcal{S}_2$, *"pure d-wave case"*

- $\ker(K_{T_c}+V) = \mathrm{span}\{\rho_0\}\otimes\mathcal{S}_0 + \mathrm{span}\{\rho_2\}\otimes\mathcal{S}_2$, *"mixed $(s+d)$-wave case".*

Here $\rho_0, \rho_2 \in L^2(\mathbb{R}_+; r^2\mathrm{d}r)$ are radial functions. They are determined as the ground states of an appropriate l-dependent operator acting on radial functions. We assume that these radial ground states are non-degenerate for simplicity. This assumption is satisfied for the examples we give in part III, but may not be satisfied in general.

Results

The pure d-wave case in three dimensions

Theorem 5.3.1 (Pure d-wave case, 3D)**.** *Let $D=3$. Let V be such that Theorem 5.2.10 applies and such that $\ker(K_{T_c}+V) = \mathrm{span}\{\rho_2\}\otimes\mathcal{S}_2$ for some $0\not\equiv\rho_2\in L^2(\mathbb{R}_+; r^2\mathrm{d}r)$. Let $\{a_{2,m}\}_{m=-2,\ldots,2}$ be an orthonormal basis of the kernel such that*

$$\widehat{a}_{2,m}(\mathbf{p}) = \varrho(p) Y_{2,m}(\vartheta,\varphi) \tag{5.31}$$

for an appropriate $\varrho\in L^2(\mathbb{R}_+; p^2\mathrm{d}p)$ (explicitly, ϱ is the Fourier-Bessel transform (5.131) of ϱ). Let ψ_m denote the GL order parameter corresponding to $\widehat{a}_{2,m}$ for $-2\le m\le 2$. Then:

(i) The GL energy that arises from BCS theory as described in Theorem 5.2.10 reads

$$\mathcal{E}^{GL}_{d\text{-wave}}(\psi_{-2},\ldots,\psi_2) = \frac{5c}{14\pi}\left(\left(\sum_{m=-2}^{2}|\psi_m|^2-\tau\right)^2 - \tau^2 + \frac{1}{2}\left|\sum_{m=-2}^{2}\psi_m^2\right|^2\right). \tag{5.32}$$

where $\tau := \frac{7\pi d}{5c}$ and

$$c = \int_0^\infty f_4(p)\mathrm{d}p, \qquad d = \int_0^\infty f_2(p)\mathrm{d}p. \tag{5.33}$$

Here, we introduced the positive and radially symmetric functions

$$\begin{aligned} f_4(p) =& \frac{p^2}{T_c^2}\frac{g_1\left(\frac{p^2-\mu}{T_c}\right)}{p^2-\mu}|K_{T_c}(p)\varrho(p)|^4 \\ f_2(p) =& \frac{p^2}{2T_c}\frac{1}{\cosh^2\left(\frac{p^2-\mu}{2T_c}\right)}|K_{T_c}(p)\varrho(p)|^2. \end{aligned} \tag{5.34}$$

See (5.17) for the definition of g_1 and $K_T(p)$.

(ii) We have $\min \mathcal{E}^{GL}_{d\text{-wave}} = -\frac{5c}{14\pi}\tau^2$*. The set of minimizers is*

$$\mathcal{M}_{d\text{-wave}} = \left\{ (\psi_{-2}, \dots, \psi_2) \in \mathbb{C}^5 : \sum_{m=-2}^{2} |\psi_m|^2 = \tau \text{ and } \sum_{m=-2}^{2} \psi_m^2 = 0 \right\}. \tag{5.35}$$

Remark 5.3.2. *(i) The existence of V such that the assumption we made on* $\ker(K_{T_c} + V)$ *holds for an open interval of parameter values follows from statement (i) of Theorem 5.4.1 by choosing* $l_0 = 2$.

(ii) Observe that the minimization problem in (5.32) *is trivial, i.e. (ii) is immediate.*

(iii) Recall that we normalized the GL order parameters such that they are related to the Cooper pair wave function via (5.19)*. For the special case* (5.35)*, we see that a minimizing vector will have absolute value* $\sqrt{\tau}$*. We can then reduce to the case where a minimizing vector lies on the* unit *sphere by rescaling the order parameters. The advantage of this other normalization is that it allows to interpret the absolute value of the order parameters as* relative *densities of superconducting charge carriers.*

We discuss what symmetry of $\mathcal{E}^{GL}$ one can expect. First of all, GL theory always has the global $U(1)$ gauge symmetry $\psi_j \mapsto e^{i\phi}\psi_j$ (this is due to the presence of the absolute value signs in (5.20)). Second, $SO(3)$ acts on spherical harmonics by pre-composition, i.e. for $g \in SO(3)$ and $\omega \in \mathbb{S}^2$,

$$gY_{l,m}(\omega) := Y_{l,m}(g^{-1}\omega) = \sum_{m'} A^g_{mm'} Y_{l,m'}$$

where $A^g \in O(2l+1)$ is the analogue of the well-known Wigner d-matrix for real spherical harmonics [9]. By changing the angular integration variable in (5.21) and (5.22) from $g\omega$ to ω, it is easy to see that

$$\mathcal{E}^{GL}((A^g)^{-1}\vec{\psi}) = \mathcal{E}^{GL}(\vec{\psi}),$$

where we introduced $\vec{\psi} = (\psi_{-2}, \dots, \psi_2)$. Since $Y_{l,m}$ is reflection-symmetric for even l, we can extend the action to all of $O(3)$ and retain the invariance of $\mathcal{E}^{GL}$. This shows that we can expect $\mathcal{E}^{GL}$ to have symmetry groups $U(1)$ and $O(3)$. However:

Corollary 5.3.3. *In the situation of Theorem 5.3.1:*

(i) For all $\phi \in [0, 2\pi)$, $\mathcal{R} \in O(5)$ *and* $\vec{\psi} \in \mathbb{C}^5$,

$$\mathcal{E}^{GL}(e^{i\phi}\mathcal{R}\vec{\psi}) = \mathcal{E}^{GL}(\vec{\psi}) \tag{5.36}$$

Moreover, $O(5)$ *acts transitively and faithfully on* $\mathcal{M}_{d\text{-}wave}$.

(ii) $\mathcal{M}_{d\text{-}wave}$ *is a 7-dimensional manifold in* $\mathbb{R}^{10}$.

(iii) Any minimizer of $\mathcal{E}^{GL}_{d\text{-}wave}$ *has at least* two *non-zero entries* ψ_j.

Remark 5.3.4. *(i) Surprisingly, the emergent symmetry group* $O(5)$ *is considerably larger than the* $O(3)$*-symmetry discussed above. (Recall also that* A^g *from above is in* $O(5)$*, so that the* $O(3)$*-symmetry is really contained in the* $O(5)$*-symmetry.) The particularly nice form of the* $O(5)$ *action is a consequence of choosing the real-valued spherical harmonics as a basis.*

(ii) We interpret faithfulness of the group action as saying that $\mathcal{M}_{d\text{-}wave}$ *is "truly" invariant under the full* $O(5)$.

(iii) Transitivity means that the set of minimizers $\mathcal{M}_{d\text{-}wave}$ *is a single orbit under the* $O(5)$ *symmetry. In other words, there exists a* unique minimizer modulo symmetry.

(iv) We interpret (iii) as a proof of non-trivial coupling between the real-valued *d-wave channels (it is of course a basis-dependent statement).*

Proof. The invariance under multiplication by $e^{i\phi}$ is trivial. To see the $O(5)$ symmetry, we use real coordinates because they also provide an interesting change in perspective. Writing $\vec{\psi} = \vec{x} + i\vec{y}$ with $\vec{x}, \vec{y} \in \mathbb{R}^5$, the GL energy becomes

$$\mathcal{E}^{GL}(\vec{x} + i\vec{y}) = \frac{5c}{14\pi}\left(\left(\vec{x}^2 + \vec{y}^2 - \tau\right)^2 - \tau^2 + \frac{1}{2}\left|\vec{x}^2 - \vec{y}^2\right|^2 + |\vec{x}\cdot\vec{y}|^2\right). \tag{5.37}$$

This is clearly invariant under the $O(5)$-action $\vec{x} + i\vec{y} \mapsto \mathcal{R}\vec{x} + i\mathcal{R}\vec{y}$. We can rewrite the set of minimizers as

$$\mathcal{M}_{d\text{-wave}} = \left\{(\vec{x}, \vec{y}) \in \mathbb{R}^5 \times \mathbb{R}^5 \,:\, \vec{x}^2 = \vec{y}^2 = \frac{\tau}{2},\, \vec{x}\cdot\vec{y} = 0\right\}. \tag{5.38}$$

Without loss of generality, we may set $\tau/2 = 1$, so that $\mathcal{M}_{d\text{-wave}}$ is just the set of pairs of orthonormal $\mathbb{R}^5$-vectors. To see that the $O(5)$-action is transitive, consider the orbit of $(e_1, e_2) \in \mathcal{M}_{d\text{-wave}}$, namely $\{(\mathcal{R}e_1, \mathcal{R}e_2) : \mathcal{R} \in O(5)\}$. Since any two orthonormal vectors can appear as the first two columns of an orthogonal matrix, we have transitivity. To see that the action is faithful, note that for any two distinct $\mathcal{R}, \tilde{\mathcal{R}} \in O(5)$, there exists e_i such that $\mathcal{R}e_i \neq \tilde{\mathcal{R}}e_i$.

For (ii), we employ the implicit function theorem and observe that the Jacobian associated with the functions $\vec{x}^2, \vec{y}^2, \vec{x} \cdot \vec{y}$ from (5.38) has rank 3. Finally, (iii) is immediate from (5.35). □

The pure d-wave case in two dimensions

Note that the two-dimensional analogue of the space $\mathcal{S}_l$, namely the homogeneous polynomials of order l on $\mathbb{S}^1$, is spanned by $\cos(l\varphi)$ and $\sin(l\varphi)$. Thus assumption (5.39) below is the two-dimensional analogue of the assumption $\ker(K_{T_c} + V) = \operatorname{span}\{\rho_2\} \otimes \mathcal{S}_2$ in Theorem 5.2.10 above.

Theorem 5.3.5 (Pure d-wave case, 2D)**.** *Let $D = 2$. Let V be such that Theorem 5.2.10 applies and such that $\ker(K_{T_c} + V) = \operatorname{span}\{a_{xy}, a_{x^2-y^2}\}$ with*

$$\widehat{a}_{x^2-y^2}(\mathbf{p}) = \varrho(p)\frac{\cos(2\varphi)}{\sqrt{\pi}}, \qquad \widehat{a}_{xy}(\mathbf{p}) = \varrho(p)\frac{\sin(2\varphi)}{\sqrt{\pi}}, \tag{5.39}$$

for an appropriate, normalized $0 \not\equiv \varrho \in L^2(\mathbb{R}_+, p\mathrm{d}p)$. Let $\psi_{x^2-y^2}$ and ψ_{xy} denote the corresponding GL order parameters. Then:

(i) The GL energy that arises from BCS theory as described in Theorem 5.2.10 reads

$$\begin{aligned}&\mathcal{E}^{GL}_{d\text{-wave},2D}(\psi_{x^2-y^2}, \psi_{xy}) \\ &= \frac{c}{2\pi}\left\{\left(|\psi_{x^2-y^2}|^2 + |\psi_{xy}|^2 - \frac{\pi d}{c}\right)^2 - \frac{\pi^2 d^2}{c^2} + \frac{1}{2}\left|\psi_{x^2-y^2}^2 + \psi_{xy}^2\right|^2\right\}\end{aligned} \tag{5.40}$$

where c, d are defined in the same way as in Theorem 5.3.1 with $f_2(p), f_4(p)$ replaced by $f_2(p)/p, f_4(p)/p$.

(ii) We have $\min \mathcal{E}^{GL}_{d\text{-wave},2D} = -\frac{\pi d^2}{2c}$. The set of minimizers is

$$\begin{aligned}&\mathcal{M}_{d\text{-wave},2D} \\ &= \left\{(\psi_{x^2-y^2}, \psi_{xy}) \in \mathbb{C}^2 : |\psi_{x^2-y^2}|^2 + |\psi_{xy}|^2 = \frac{\pi d}{c},\ \psi_{x^2-y^2}^2 + \psi_{xy}^2 = 0\right\} \\ &= \left\{(\psi, \pm i\psi) \in \mathbb{C}^2 : |\psi|^2 = \frac{\pi d}{2c}\right\}\end{aligned} \tag{5.41}$$

Remark 5.3.6. *(i) Statement (i) directly implies the first equality in* (5.41) *and the second equality is elementary. Note that the result can be conveniently stated in terms of the complex-valued spherical harmonics as well.*

(ii) From the second equation in (5.41)*, we see that the minimizers of the GL2 for a pure d-wave superconductor in two dimensions (in the cosine, sine basis) form a double cover of the minimizers of the usual "Mexican-hat" GL1.*

(iii) A similar result holds for any pure angular momentum sector in two dimensions.

The mixed $(s+d)$-wave case

We write $\Re[z]$ for the real part of a complex number z.

Theorem 5.3.7 (Mixed $(s+d)$-wave case, 3D)**.** *Let $D=3$. Let V be such that Theorem 5.2.10 applies and such that* $\ker(K_{T_c}+V)=\operatorname{span}\{\rho_0\}\otimes\mathcal{S}_0+\operatorname{span}\{\varrho_2\}\otimes\mathcal{S}_2$ *for some* $0\not\equiv\rho_0,\rho_2\in L^2(\mathbb{R}_+;r^2\mathrm{d}r)$*. As an orthonormal basis, take $a_{2,m}$ as in Theorem 5.3.1 and a_s with*

$$\widehat{a}_s(\mathbf{p})=\varrho_s(p)\,Y_{0,0}(\vartheta,\varphi). \tag{5.42}$$

Let ψ_m, $(m=-2,\dots,2)$ and ψ_s denote the GL order parameters corresponding to the respective basis functions. Then:

(i) The microscopically derived GL energy reads

$$\begin{aligned}&\mathcal{E}^{GL}_{(s+d)\text{-}wave}(\psi_s,\psi_{-2},\dots,\psi_2)\\&=\mathcal{E}^{GL}_{s\text{-}wave}(\psi_s)+\mathcal{E}^{GL}_{d\text{-}wave}(\psi_{-2},\dots,\psi_2)+\mathcal{E}^{GL}_{coupling}(\psi_s,\psi_{-2},\dots,\psi_2)\end{aligned} \tag{5.43}$$

where $\mathcal{E}^{GL}_{d\text{-}wave}(\psi_{-2},\dots,\psi_2)$ is given by (5.32)*,*

$$\mathcal{E}^{GL}_{s\text{-}wave}(\psi_s)=\frac{c^{(4s)}}{4\pi}\left(\left(|\psi_s|^2-\tau_s\right)^2-\tau_s^2\right), \tag{5.44}$$

with $\tau_s = \frac{2\pi d^{(2s)}}{c^{(4s)}}$, *and*

$$\begin{aligned}
&\mathcal{E}^{GL}_{coupling}(\psi_s, \psi_{-2}, \dots, \psi_2) \\
&= \frac{c^{(2s)}}{2\pi}\left(2|\psi_s|^2 \sum_{m=-2}^{2} |\psi_m|^2 + \Re\left[\overline{\psi_s}^2\left(\sum_{m=-2}^{2}\psi_m^2\right)\right]\right) + \frac{\sqrt{5}c^{(s)}}{7\pi} \\
&\quad\times\left(\Re\left[\overline{\psi_s}\left(2\psi_0|\psi_0|^2 + \sum_{m=\pm1,2}|m|(-1)^{m+1}(2\psi_0|\psi_m|^2 + \overline{\psi_0}\psi_m^2)\right)\right]\right. \\
&\qquad + \sqrt{3}\Re\left[\overline{\psi_s}\sum_{m=\pm1} m\left(2\psi_2|\psi_m|^2 + \overline{\psi_2}\psi_m^2\right)\right] \\
&\qquad \left. + 2\sqrt{3}\Re\left[\overline{\psi_s}\left(\overline{\psi_{-2}}\psi_1\psi_{-1} + 2\psi_{-2}\Re\left[\overline{\psi_1}\psi_{-1}\right]\right)\right]\right).
\end{aligned} \tag{5.45}$$

The coefficients c, d *are given by* (5.33). *Moreover, for* $m = 1, 2, 4$, *we introduced*

$$c^{(ms)} = \int_0^\infty f_4(p) g_s(p)^m \, \mathrm{d}p, \qquad d^{(2s)} = \int_0^\infty f_2(p) g_s(p)^2 \, \mathrm{d}p, \tag{5.46}$$

with f_2, f_4 *as in* (5.34) *and*

$$g_s(p) = \left|\frac{\varrho_s(p)}{\varrho(p)}\right|. \tag{5.47}$$

(ii) The following are equivalent:

- $dc^{(2s)} < \frac{5}{7} cd^{(2s)}$,
- *for all sufficiently small* $\varepsilon > 0$, *and for any minimizer* $(\psi_{-2}, \dots, \psi_2)$ *of* $\mathcal{E}^{GL}_{d\text{-}wave}$, *there exists* ψ_s *with* $|\psi_s| = \varepsilon$ *such that*

$$\mathcal{E}^{GL}_{(s+d)\text{-}wave}(\psi_s, \psi_{-2}, \dots, \psi_2) < \mathcal{E}^{GL}_{d\text{-}wave}(\psi_{-2}, \dots, \psi_2) = \min \mathcal{E}^{GL}_{d\text{-}wave}. \tag{5.48}$$

(iii) The following are equivalent:

- $d^{(2s)} c^{(2s)} \leq dc^{(4s)}$,
- *for all sufficiently small* $\varepsilon > 0$, *and for any minimizer* ψ_s *of* $\mathcal{E}^{GL}_{s\text{-}wave}$, *there exists* $(\psi_{-2}, \dots, \psi_2)$ *with* $|\psi_m| < \varepsilon$ *for* $m = -2, \dots, 2$ *such that*

$$\mathcal{E}^{GL}_{(s+d)\text{-}wave}(\psi_s, \psi_{-2}, \dots, \psi_2) < \mathcal{E}^{GL}_{s\text{-}wave}(\psi_s) = \min \mathcal{E}^{GL}_{s\text{-}wave}. \tag{5.49}$$

We see that $\mathcal{E}^{GL}_{(s\,+\,d)\text{-wave}}$ yields a much richer GL theory than $\mathcal{E}^{GL}_{d\text{-wave}}$. Especially the terms which depend on the relative phases of several GL order parameters make this a rather challenging minimization problem. Accordingly, we no longer have an explicit characterization of the set of minimizers. However, using (ii) and (iii) above, we immediately obtain

Corollary 5.3.8 (Non-trivial coupling of s- and d-waves)**.** *In the situation of Theorem 5.3.7 suppose that* $dc^{(2s)} < \frac{5}{7}cd^{(2s)}$ *and* $d^{(2s)}c^{(2s)} \leq dc^{(4s)}$*. Then any minimizer* $(\psi_s, \psi_{-2}, \ldots, \psi_2)$ *of* $\mathcal{E}^{GL}_{(s\,+\,d)\text{-wave}}$ *must satisfy* $\psi_s \neq 0$ *and* $\psi_m \neq 0$ *for some* $-2 \leq m \leq 2$*.*

Remark 5.3.9. *(i) The existence of* V *such that the assumption required by Theorem 5.3.7 on* $\ker(K_{T_c} + V)$ *holds for appropriate parameter values follows from statement (ii) of Theorem 5.4.1.*

(ii) Using the same method and the two-dimensional analogues of all quantities above, one can also compute the GL3 that arises for a two-dimensional isotropic $(s + d)$*-wave superconductor*

$$
\begin{aligned}
&4\pi\mathcal{E}^{GL}_{(s\,+\,d)\text{-wave},2D}(\psi_s, \psi_{x^2-y^2}, \psi_{xy}) \\
&= 3c|\psi_{x^2-y^2}|^4 + 3c|\psi_{xy}|^4 + 2c^{(4s)}|\psi_s|^4 + 2c\Re[\overline{\psi_{x^2-y^2}}^2\psi_{xy}^2] \\
&\quad + 4c|\psi_{x^2-y^2}|^2|\psi_{xy}|^2 + 4c^{(2s)}\Re[\overline{\psi_s}^2(\psi_{x^2-y^2}^2 + \psi_{xy}^2)] \\
&\quad + 8c^{(2s)}|\psi_s|^2(|\psi_{x^2-y^2}|^2 + |\psi_{xy}|^2) \\
&\quad - 4\pi d\left(|\psi_{x^2-y^2}|^2 + |\psi_{xy}|^2\right) - 4\pi d^{(2s)}|\psi_s|^2
\end{aligned}
\tag{5.50}
$$

Its complexity lies somewhere between the GL theories in Theorems 5.3.5 and 5.3.7. Setting $\psi_{xy} = 0$ *(that is, we forbid the* d_{xy} *channel ad hoc), we obtain the GL2*

$$
\begin{aligned}
&4\pi\mathcal{E}^{GL}_{(s\,+\,d)\text{-wave},2D}(\psi_s, \psi_{x^2-y^2}, 0) \\
&= 3c|\psi_{x^2-y^2}|^4 + 2c^{(4s)}|\psi_s|^4 + 4c^{(2s)}\Re[\overline{\psi_s}^2\psi_{x^2-y^2}^2] \\
&\quad 82c^{(2s)}|\psi_s|^2|\psi_{x^2-y^2}|^2 - 4\pi d|\psi_{x^2-y^2}|^2 - 4\pi d^{(2s)}|\psi_s|^2
\end{aligned}
\tag{5.51}
$$

Compare this with $\mathcal{E}^{GL}_{d\text{-wave},2D}$ *from Theorem 5.3.5. While one cannot complete the square because the coefficients differ in a way that depends on the microscopic details, notice that the only phase-dependent term is of the form*

$$
4c^{(2s)}\Re[\overline{\psi_s}^2\psi_{x^2-y^2}^2]
\tag{5.52}
$$

with $c^{(2s)} > 0$*. It is then clear that for minimizers, the* $d_{x^2-y^2}$*- and* s*-wave order parameters must have a relative phase of* $\pm i$*.*

5.4 Part III: Radial potentials with ground states of arbitrary angular momentum

In this part, $D = 3$ and $\mu > 0$. Recall that

$$K_T(p) = \frac{p^2 - \mu}{\tanh\left(\frac{p^2-\mu}{2T}\right)}, \tag{5.53}$$

and the operator K_T is multiplication by the function $K_T(p)$ in Fourier space. Recall the definition (5.6) of the Dirac delta potentials

$$V_{\lambda,R}(\mathbf{x}) = -\lambda\delta(|\mathbf{x}| - R),$$

for $\lambda, R > 0$.

The following theorem says that, given a non-negative integer l_0, we can choose parameter values for μ, λ, R from appropriate open intervals such that the zero-energy ground state sector of $K_{T_c} + V_{\lambda,R}$ lies entirely within the angular momentum sector $\mathcal{H}_{l_0}$.

Theorem 5.4.1. *(i) Let l_0 be a non-negative integer. For every $R > 0$, there exist an open interval $I \subset \mathbb{R}_+$ and $\lambda_* > 0$ such that for all $\mu \in I$ and all $\lambda \in (0, \lambda_*)$ there exists $T_c > 0$ such that*

$$\inf \operatorname{spec}(K_{T_c} + V_{\lambda,R}) = 0, \tag{5.54}$$

$$\ker(K_{T_c} + V_{\lambda,R}) = \operatorname{span}\{\rho_{l_0}\} \otimes \mathcal{S}_{l_0}, \tag{5.55}$$

$$\inf \operatorname{spec}(K_T + V) < 0, \quad \forall T < T_c. \tag{5.56}$$

Explicitly, the (non-normalized) radial part is

$$\rho_{l_0}(r) = r^{-1/2} \int_0^\infty p \frac{\mathcal{J}_{l_0+\frac{1}{2}}(rp)\mathcal{J}_{l_0+\frac{1}{2}}(Rp)}{K_{T_c}(p)} \mathrm{d}p. \tag{5.57}$$

(ii) For every $R > 0$, there exists $T_* > 0$ such that for all $T_c < T_*$, there exist $\mu, \lambda > 0$ such that

$$\inf \operatorname{spec}(K_{T_c} + V_{\lambda,R}) = 0, \tag{5.58}$$

$$\ker(K_{T_c} + V_{\lambda,R}) = \operatorname{span}\{\rho_0\} \otimes \mathcal{S}_0 + \operatorname{span}\{\rho_2\} \otimes \mathcal{S}_2, \tag{5.59}$$

$$\inf \operatorname{spec}(K_T + V) < 0, \quad \forall T < T_c. \tag{5.60}$$

with ρ_0, ρ_2 as in (5.57).

Remark 5.4.2. *(i) To be completely precise, in (i) there exists T_0 such that the analogue of* (5.54)-(5.56) *holds with T_0 in place of T_c. Then $T_c = T_0$ by definition* (5.9).

(ii) The parameter R can be removed by rescaling μ, λ and T appropriately.

(iii) In statement (i), for given $\mu \in I$, $\lambda \in (0, \lambda_*)$ and $R > 0$, T_c is given as the unique solution to the implicit relation

$$1 = \lambda \int_0^\infty \frac{pR}{K_{T_c}(p)} \mathcal{J}^2_{l_0+1/2}(pR)\mathrm{d}p. \tag{5.61}$$

(iv) The fact that statement (i) holds for open intervals of μ and λ values is to be interpreted as saying that the occurrence of degenerate ground states for $K_{T_c} + V_{\lambda,R}$ is "not un-generic". This may be surprising at first sight, because if one replaces $K_T + V$ by the Schrödinger operator $-\nabla^2 + V$, the Perron-Frobenius Theorem (see e.g. [123]) implies that the ground state is always simple.

(v) The proof critically uses that $K_T(p)$ is small (for small enough T) on the set $\{\mathbf{p} : \mathbf{p}^2 = \mu\}$. Note that this set would be empty for $\mu < 0$.

(vi) It is interesting to compare Theorem 5.4.1 with Theorem 2.2 from [72] which characterizes the critical temperature in the weak-coupling limit $\lambda \to 0$ through an effective Hilbert-Schmidt operator $\mathcal{V}_\mu$ acting only on L^2 of the Fermi sphere. For radial potentials, [72] shows that $\ker(K_{T_c}+V) \subset \mathcal{H}_{l_0}$ *for all sufficiently small λ iff l_0 is the unique minimizer of*

$$l \mapsto \frac{\sqrt{\mu}}{2\pi^2} \int V(\mathbf{x})|j_l(\sqrt{\mu}|\mathbf{x}|)|^2 \mathrm{d}\mathbf{x} \tag{5.62}$$

where $j_l(z) = \sqrt{\frac{\pi}{2z}} J_l(z)$ is the spherical Bessel function of the first kind. While our proof here will be independent of [72], one can take $V = V_{\lambda,R}$ in (5.62) *to see that the key fact needed to prove* $\ker(K_{T_c} + V) \subset \mathcal{H}_{l_0}$ *is that there is a point at which $j_{l_0}^2 > \sup_{l \neq l_0} j_l^2$. This is the content of Theorem 5.8.1.*

We conclude by discussing the conceivable extensions of Theorem 5.4.1. Statement (i) also holds if $K_T + V$ is defined on all of $L^2(\mathbb{R}^3)$ instead of just on $L^2_{\text{symm}}(\mathbb{R}^3)$, so there is nothing special about even functions in (i).

Statement (ii) can not be generalized as much: (a) it will not hold when odd functions are also considered and (b) it does not generalize to arbitrary pairs (l_0, l_0+2) with l_0 even. The reason is that, as demonstrated within the proof of Theorem 5.4.1, for small enough T, (ii) is equivalent to the existence of a point where $\mathcal{J}_{1/2} > \mathcal{J}_{l+1/2}$ for all even $l \geq 1$. The generalizations to more l-values described above require the analogous inequalities for Bessel functions. However, these facts will not hold in the cases above, as becomes plausible when considering Figure 5.1.

5.5 Proofs for part I

The strategy of the proof follows [73].

We introduce the family of BCS states Γ_Δ from which the trial state generating the upper bound will be chosen. The relative entropy identity (5.68) rewrites the difference of BCS free energies as terms involving Γ_Δ.

The *main simplification* of our proof as compared to [73] is then in the "semi-classical" Theorem 5.5.3. While [73] requires elaborate semiclassical analysis for analogous results, the proof in our technically simpler translation-invariant case reduces to an ordinary Taylor expansion.

Afterwards, we discuss how one concludes Theorem 5.2.10 by separately proving an upper and a lower bound. In the lower bound, the degeneracy requires modifying the arguments from [73] slightly.

Relative entropy identity

All integrals are over $\mathbb{R}^D$ unless specified otherwise. We introduce the family of operators

$$\widehat{\Gamma}_\Delta := \frac{1}{1+\exp(\widehat{H}_\Delta/T)}, \qquad \widehat{H}_\Delta := \begin{pmatrix} \mathfrak{h} & \widehat{\Delta} \\ \overline{\widehat{\Delta}} & -\mathfrak{h} \end{pmatrix}. \tag{5.63}$$

Here Δ is an even function on $\mathbb{R}^D$ and we have introduced

$$\mathfrak{h}(p) = p^2 - \mu, \tag{5.64}$$

the energy of a single unpaired electron of momentum $\mathbf{p}$. Note that the choice $\widehat{\Delta} \equiv 0$ in (5.63) indeed yields the normal state Γ_0 defined in (5.13).

Recall that Γ is a BCS state iff $0 \leq \widehat{\Gamma} \leq 1$ and $\widehat{\Gamma}$ is of the form (5.2).

Proposition 5.5.1. Γ_Δ *defined by* (5.63) *is a BCS state and*

$$\widehat{\Gamma}_\Delta(\mathbf{p}) = \begin{pmatrix} \widehat{\gamma}_\Delta(\mathbf{p}) & \widehat{\alpha}_\Delta(\mathbf{p}) \\ \overline{\widehat{\alpha}_\Delta(\mathbf{p})} & 1-\widehat{\gamma}_\Delta(\mathbf{p}) \end{pmatrix}$$

with

$$\widehat{\gamma}_\Delta(\mathbf{p}) = \frac{1}{2}\left(1-(p^2-\mu)\frac{\tanh(E_\Delta(\mathbf{p})/(2T))}{E_\Delta(\mathbf{p})}\right), \tag{5.65}$$

$$\widehat{\alpha}_\Delta(\mathbf{p}) = -\frac{\widehat{\Delta}(\mathbf{p})}{2}\frac{\tanh(E_\Delta(\mathbf{p})/(2T))}{E_\Delta(\mathbf{p})}, \tag{5.66}$$

$$E_\Delta(\mathbf{p}) = \sqrt{\mathfrak{h}(p)^2+|\Delta(\mathbf{p})|^2}. \tag{5.67}$$

Proof. It is obvious from (5.63) that $0 \leq \widehat{\Gamma}_\Delta(\mathbf{p}) \leq 1$. Since $(\widehat{H}_\Delta)^2 = E_\Delta^2 I_2$ and since $\tanh(x)/x$ only depends on x^2, it follows that

$$\begin{aligned}\widehat{\Gamma}_\Delta &= \frac{1}{1+\exp(\widehat{H}_\Delta/T)} = \frac{1}{2}\left(1-\tanh(\widehat{H}_\Delta/(2T))\right)\\ &= \frac{1}{2}\left(1-\frac{\widehat{H}_\Delta}{E_\Delta}\tanh(E_\Delta/(2T))\right),\end{aligned}$$

which yields (5.65) and (5.66). □

We now give an identity which rewrites the difference $\mathcal{F}_T^{BCS}(\Gamma)-\mathcal{F}_T^{BCS}(\Gamma_0)$ in terms of more manageable quantities involving Γ_Δ, one of them is the relative entropy.

Proposition 5.5.2 (Relative Entropy Identity, [73])**.** *Let* Γ *be an admissible BCS state and* $\mathfrak{a} \in H^1_{sym}(\mathbb{R}^D)$. *Set* $\widehat{\Delta} = 2\widehat{V\mathfrak{a}}$. *It holds that*

$$\begin{aligned}&\mathcal{F}_T^{BCS}(\Gamma)-\mathcal{F}_T^{BCS}(\Gamma_0)\\ &= -\frac{T}{2}\mathrm{Tr}\left[\log\left(1+e^{-\widehat{H}_\Delta/T}\right)-\log\left(1+e^{-\widehat{H}_0/T}\right)\right]\\ &\quad+\frac{T}{2}\mathfrak{H}(\Gamma,\Gamma_\Delta)-\int V|\mathfrak{a}|^2\,\mathrm{d}\mathbf{x}+\int V|\alpha-\mathfrak{a}|^2\,\mathrm{d}\mathbf{x}\end{aligned} \tag{5.68}$$

where $\mathfrak{H}(\Gamma,\Gamma_\Delta)$ *is the* relative entropy *defined by*

$$\mathfrak{H}(\Gamma,\Gamma_\Delta) := \mathrm{Tr}\left[\phi(\widehat{\Gamma},\widehat{\Gamma}_\Delta)\right]. \tag{5.69}$$

Here we introduced

$$\phi(x,y) = x(\log(x)-\log(y))+(1-x)(\log(1-x)-\log(1-y)), \quad \forall 0\leq x,y\leq 1.$$

Proof. This is a computation, see [73] or [74]. □

For the sake of comparability with [73], we note that in the translation-invariant case the L^2-trace per unit volume of a locally trace-class operator (which they denote by Tr) is just the integral of its Fourier transform and so

$$\mathrm{Tr}[\Gamma] = \int_{\mathbb{R}^D} \mathrm{Tr}_{\mathbb{C}^2}[\widehat{\Gamma}(\mathbf{p})]\,\mathrm{d}\mathbf{p}.$$

"Semiclassical" expansion

We prove Theorem 5.5.3 by a Taylor expansion, which is sufficient because of the simplifications introduced by the translation-invariance. The analogous results in [73] require many more pages of challenging semiclassical analysis.

The result and the key lemma

Recall the definition of g_1 in (5.17). The following is the main consequence of the Taylor expansion

Theorem 5.5.3. *Let* $\widehat{\Delta} = 2h\widehat{V\mathfrak{a}}$ *for some* $\mathfrak{a} \in \ker(K_{T_c} + V)$. *Define* $h > 0$ *by*

$$h = \sqrt{\frac{T_c - T}{T_c}}. \tag{5.70}$$

Then, as $h \to 0$,

$$\mathcal{F}_T^{BCS}(\Gamma_\Delta) - \mathcal{F}_T^{BCS}(\Gamma_0) = h^4 E_2 + O(h^6), \tag{5.71}$$

where

$$E_2 = \frac{1}{16T_c^2}\int \frac{g_1(\mathfrak{h}(p)/T_c)}{\mathfrak{h}(p)}|t(\mathbf{p})|^4\,\mathrm{d}\mathbf{p} - \frac{1}{8T_c}\int \frac{1}{\cosh^2(\mathfrak{h}(p)/(2T_c))}|t(\mathbf{p})|^2\,\mathrm{d}\mathbf{p} \tag{5.72}$$

with $t = 2\widehat{V\mathfrak{a}}$.

We emphasize that this is the place where the effective gap operator appears in the analysis. The choice $\mathfrak{a} \in \ker(K_{T_c} + V)$ ensures that there are no $O(h^2)$ terms in the expansion (5.71).

The theorem follows from the key

Lemma 5.5.4. *Let* Γ_Δ *be given by* (5.63) *with* $\widehat{\Delta}(p) = ht(p)$ *for a function* t *satisfying*

$$t \in L^q(\mathbb{R}^D) \text{ with } \begin{cases} q = \infty & \text{if } D = 1, \\ 4 < q < \infty & \text{if } D = 2, \\ q = 6 & \text{if } D = 3. \end{cases} \tag{5.73}$$

Then, as $h \to 0$*,*

(i)

$$\begin{aligned} &-\frac{T}{2}\mathrm{Tr}\left[\log\left(1+e^{-\widehat{H}_\Delta/T}\right) - \log\left(1+e^{-\widehat{H}_0/T}\right)\right] \\ &= h^2 E_1 + h^4 E_2 + O(h^6) \end{aligned} \tag{5.74}$$

where E_2 *is defined by* (5.72) *and (see* (5.17) *for* g_0*)*

$$E_1 = -\frac{1}{4T_c}\int g_0(\mathfrak{h}(p)/T_c)|t(\mathbf{p})|^2\,\mathrm{d}\mathbf{p}, \tag{5.75}$$

(ii)

$$\|\alpha_\Delta - \check{\phi}\|_{H^1} = O(h^3) \tag{5.76}$$

with $\phi(\mathbf{p}) = -h\frac{t(p)}{2T_c}g_0(\mathfrak{h}(\mathbf{p})/T_c)$*.*

This may be compared to Theorems 2 and 3 in [73].

To conclude Theorem 5.5.3 from the key lemma, we need a regularity result for the translation-invariant operator.

Proposition 5.5.5. *Let* $a \in H^1(\mathbb{R}^D)$ *satisfy* $(K_{T_c} + V)a = 0$*. Then,* $\widehat{a} \in L^\infty(\mathbb{R}^D)$*. Let* $t := \widehat{Va}$ *and* $\langle p \rangle := (1+p^2)^{1/2}$*. Then,* $\langle p \rangle^{-1} t \in L^2(\mathbb{R}^D)$ *and* t *satisfies* (5.73)*.*

Proof. Recall Assumption 5.2.2 on the potential V. When $V \in L^{p_V}(\mathbb{R}^D)$, then the result follows from Proposition 2 in [73]. For the potentials $V_{\lambda,R}$ in $D = 3$, the regularity properties can be read off directly from the explicit solution of the eigenvalue problem $(K_{T_c} + V_{\lambda,R})a = 0$, see (5.133) in the proof of Lemma 5.7.1 for its Fourier representation. Indeed, since $Y_{l,m}$ and the Bessel function of the first kind $\mathcal{J}_{l+1/2}$ are smooth and bounded with $\mathcal{J}_{l+1/2}(0) = 0$ and since $E < 2T$, we get $\widehat{a} \in L^\infty$. Moreover,

$$t(\mathbf{p}) \propto Y_{l,m}(\vartheta,\varphi)\,\frac{\mathcal{J}_{l+1/2}(pR)}{\sqrt{p}}$$

and since $\mathcal{J}_{l+1/2}$ also decays like $p^{-1/2}$ for large p-values, the regularity properties of t follow. In $D = 1, 2$, one can again solve the eigenvalue problem $(K_{T_c} + V_{\lambda,R})a = 0$ explicitly and obtains the claimed regularity by similar considerations. The details are left to the reader. □

Proof of Theorem 5.5.3. First, note that $t = 2\widehat{V\mathfrak{a}}$ has all the regularity properties needed to apply (i), thanks to Proposition 5.5.5. We invoke the relative entropy identity (5.68) and use Lemma 5.5.4 to find

$$\begin{aligned}&\mathcal{F}_T^{BCS}(\Gamma_\Delta) - \mathcal{F}_T^{BCS}(\Gamma_0)\\&= h^2 E_1 + h^4 E_2 - h^2 \int V|\mathfrak{a}|^2 \mathrm{d}x + \int V|\alpha_\Delta - h\mathfrak{a}|^2 \mathrm{d}x + O(h^6).\end{aligned} \tag{5.77}$$

Observe that

$$g_0(\mathfrak{h}(p)/T_c) = T_c K_{T_c}^{-1}(p). \tag{5.78}$$

By Plancherel and the eigenvalue equation $(K_{T_c} + V)\mathfrak{a} = 0$, (5.77) becomes

$$\mathcal{F}_T^{BCS}(\Gamma_\Delta) - \mathcal{F}_T^{BCS}(\Gamma_0) = h^4 E_2 + \int V|\alpha_\Delta - h\mathfrak{a}|^2 \mathrm{d}\mathbf{x} + O(h^6).$$

Thus, it remains to show

$$\int V(\mathbf{x})|\alpha_\Delta(\mathbf{x}) - h\mathfrak{a}(\mathbf{x})|^2 \, \mathrm{d}\mathbf{x} = O(h^6). \tag{5.79}$$

To see this, recall that V is form-bounded with respect to $-\nabla^2$, so it suffices to prove that $\|\alpha_\Delta - h\mathfrak{a}\|_{H^1} = O(h^3)$. Using the eigenvalue equation and (5.78),

$$\widehat{\mathfrak{a}}(\mathbf{p}) = -K_{T_c}^{-1}(p)\widehat{V\mathfrak{a}}(\mathbf{p}) = -\frac{t(\mathbf{p})}{2T_c} g_0(\mathfrak{h}(p)/T_c)$$

and so (5.79) follows from Lemma 5.5.4 (ii). □

Proof of Lemma 5.5.4

Proof of (i) We have

$$\log\left(1 + e^{-\widehat{H}_\Delta(\mathbf{p})/T}\right) = -\widehat{H}_\Delta(\mathbf{p})/(2T) + \log\cosh(\widehat{H}_\Delta(\mathbf{p})/(2T)).$$

Observe that $\mathrm{Tr}_{\mathbb{C}^2}\left[\widehat{H}_\Delta(\mathbf{p})\right] = 0$, that $x \mapsto \cosh x$ is an even function and that $\widehat{H}_\Delta(\mathbf{p})^2 = E_\Delta(\mathbf{p})^2 I_2$. We find

$$\begin{aligned}\mathrm{Tr}_{\mathbb{C}^2}\left[\log\left(1 + e^{-\widehat{H}_\Delta/T}\right)\right] &= \mathrm{Tr}_{\mathbb{C}^2}\left[\log\cosh(\widehat{H}_\Delta(p)/(2T))\right]\\&= 2\log\cosh(E_\Delta(p)/(2T)).\end{aligned}$$

This and a similar computation for $\Delta = 0$ show that

$$
\begin{aligned}
&-\frac{T}{2}\operatorname{Tr}\left[\log\left(1+e^{-\widehat{H}_\Delta/T}\right)-\log\left(1+e^{-\widehat{H}_0/T}\right)\right]\\
&=-T\int\left(\log\cosh(E_\Delta/(2T))-\log\cosh(\mathfrak{h}/(2T))\right)\,\mathrm{d}\mathbf{p}. \qquad (5.80)
\end{aligned}
$$

We denote the function in (5.80) by

$$
f(h^2):=T(h^2)\left(\log\cosh\left(\frac{E(h^2)}{2T(h^2)}\right)-\log\cosh\left(\frac{E(0)}{2T(h^2)}\right)\right),
$$

where we wrote $E(h^2)$ for E_Δ and $T(h^2)=T_c(1-h^2)$. Note that $E'=|t|^2/(2E)$ and recall the definition (5.17) of g_0 and g_1. By an easy computation

$$
\begin{aligned}
f(0)&=0,\\
f'(0)&=-g_0(\mathfrak{h}/T_c)\frac{|t|^2}{4T_c},\\
\frac{1}{2}f''(0)&=\frac{g_1(\mathfrak{h}/T_c)}{\mathfrak{h}}\frac{|t|^4}{16T_c^2}-\frac{1}{\cosh^2(\mathfrak{h}/(2T_c))}\frac{|t|^2}{8T_c}.
\end{aligned}
$$

With this, we can expand (5.80) as follows

$$
\frac{T}{2}\operatorname{Tr}\left[\log\widehat{\Gamma}_\Delta-\log\widehat{\Gamma}_0\right] \qquad (5.81)
$$

$$
\begin{aligned}
&=-h^2\int g_0(\mathfrak{h}/T_c)\frac{|t|^2}{4T_c}\,\mathrm{d}\mathbf{p}\\
&\quad+h^4\left(\frac{1}{16T_c^2}\int\frac{g_1(\mathfrak{h}/T_c)}{\mathfrak{h}}|t|^4\,\mathrm{d}\mathbf{p}-\frac{1}{8T_c}\int\frac{1}{\cosh^2\left(\frac{\mathfrak{h}}{2T_c}\right)}|t|^2\,\mathrm{d}\mathbf{p}\right)+O(h^6). \qquad (5.82)
\end{aligned}
$$

It remains to check that the $O(h^6)$ term is indeed finite. Using the Lagrange remainder in Taylor's formula, it suffices to show

$$
\int\sup_{0<\delta<h^2}\frac{1}{3!}|f'''(\delta)|\,\mathrm{d}\mathbf{p}<\infty. \qquad (5.83)
$$

We will control this quantity in terms of appropriate integrals over t which are finite by our assumptions on t. We introduce the function

$$
g_2(z):=g_1'(z)+\frac{2}{z}g_1(z)=\frac{1}{2z}\frac{1}{\cosh^2(z/2)}\tanh(z/2). \qquad (5.84)
$$

By a straightforward computation

$$\frac{1}{3!}f'''(\delta) = \frac{1}{8T(\delta)^3}\left[\frac{|t|^6}{12E(\delta)^2}\left(3\frac{g_1(E(\delta)/T(\delta))}{E(\delta)/T(\delta)} - g_2(E(\delta)/T(\delta))\right)\right.$$
$$- \frac{T_c}{2T(\delta)}|t|^4 g_2(E(\delta)/T(\delta))$$
$$\left. + T_c^2|t|^2\left(\frac{1}{\cosh^2\left(\frac{E(\delta)}{2T(\delta)}\right)} - \left(\frac{E(\delta)}{T(\delta)}\right)^2 g_2(E(\delta)/T(\delta))\right)\right].$$

Note that, for h^2 small enough, $T_c/2 \leq T(\delta) \leq 2T_c$ for all $0 < \delta < h^2$. Using this and the fact that $\frac{1}{\cosh^2(z)}$ and $g_2(z)$ are monotone decreasing for $z > 0$, we can estimate

$$\int \sup_{0<\delta<h^2} \frac{1}{3!}|f'''(\delta)|\,\mathrm{d}\mathbf{p}$$
$$\leq C_1 \int |t|^6 \sup_{0<\delta<h^2} E(\delta)^{-2}\left|3\frac{g_1(E(\delta)/T(\delta))}{E(\delta)/T(\delta)} - g_2(E(\delta)/T(\delta))\right| \mathrm{d}\mathbf{p} \tag{5.85}$$
$$+ C_2 \int |t|^4 g_2(\mathfrak{h}/(2T_c))\,\mathrm{d}\mathbf{p} \tag{5.86}$$
$$+ C_3 \int |t|^2\left(\frac{1}{\cosh^2(\mathfrak{h}/(4T_c))} + g_2(\mathfrak{h}/(2T_c)) \sup_{0<\delta<h^2} E(\delta)^2\right) \mathrm{d}\mathbf{p}.$$

Here C_1, C_2, C_3 denote constants which depend on D, T_c and may change from line to line in the following. For definiteness, assume $D = 3$. The arguments for $D = 1, 2$ are similar. Since $g_2(z)$ is a bounded function that decays exponentially for large z, we can use Cauchy-Schwarz and the fact that $\mathfrak{h}(p) \sim C\langle p\rangle^2$ for large p to conclude

$$C_2 \int |t|^4 g_2(\mathfrak{h}/(2T_c))\,\mathrm{d}\mathbf{p} \leq C_2 \int \left(|t|^6 + \langle p\rangle^{-2}|t|^2\right)\,\mathrm{d}\mathbf{p}$$

and the right-hand side is finite by Proposition 5.5.5. Using that $E(\delta)^2 = \mathfrak{h}^2 + \delta|t|^2 \leq \mathfrak{h}^2 + |t|^2$ for small enough h, the same argument applies to the C_3 term in (5.86).

The C_1 term in (5.86) contains a factor $E(\Delta)^{-2}$ which looks troubling because, as $\delta \to 0$, it is of the form $\mathfrak{h}^{-2}$ and thus singular on the sphere $\{\mathbf{p} : \mathbf{p}^2 = \mu\}$ if $\mu > 0$. For the radial integration, this singularity would not be integrable (and we have not even considered the factor $|t|^6$ yet). However, the singularity is canceled by the factor $3g_1(z)/z - g_2(z)$ with $z = E(\delta)/T(\delta)$ in (5.86). To see this, recall the definition (5.17) of g_1 and (5.84) of g_2 and observe that $g_1(z)/z$ and $g_2(z)$ are both even functions. Using the power series representation for

$\frac{1}{\cosh^2}$ and tanh, it is elementary to check that in the expansion of $3g_1(z)/z - g_2(z)$ the coefficients of order z^{-2} and z^0 vanish and so the lowest non-vanishing order is z^2. Therefore, the singularity is removed and since $g_1(z)/z$ and g_2 are bounded, we get

$$\sup_{0<\delta<h^2} E(\delta)^{-2} \left| 3\frac{g_1(E(\delta)/T(\delta))}{E(\delta)/T(\delta)} - g_2(E(\delta)/T(\delta)) \right| \leq C < \infty.$$

Since $\int |t|^6 \,\mathrm{d}\mathbf{p} < \infty$ by our assumption on t, the C_1 term in (5.86) is finite and we have proved (5.83).

Proof of (ii) From (5.66) we have

$$\widehat{\alpha}_\Delta(\mathbf{p}) = -h\frac{t(\mathbf{p})}{2T} g_0(E_\Delta(\mathbf{p})/T).$$

Therefore

$$\|\alpha_\Delta - \check{\phi}\|_{H^1}^2 = h^2 \int \langle p\rangle^2 |t|^2 |f(h^2) - f(0)|^2 \,\mathrm{d}\mathbf{p}, \tag{5.87}$$

where we introduced the function

$$f(h^2) := \frac{g_0(E(h^2)/T(h^2))}{2T(h^2)}. \tag{5.88}$$

Recall that $g_0' = -g_1$. Using this and the fact that for h^2 small enough, $T_c/2 \leq T(\delta) \leq 2T_c$ for all $0 < \delta < h^2$, Taylor's theorem with Lagrange remainder yields

$$\begin{aligned} &|f(h^2) - f(0)| \\ &\leq Ch^2 \sup_{0<\delta<h^2} \left(|g_0(E(\delta)/T(\delta))| + |g_1(E(\delta)/T(\delta))| \left(\frac{|t|^2}{E(\delta)} + E(\delta) \right) \right). \end{aligned}$$

Note that $g_0(z)$ and $g_1(z)/z$ are monotone decreasing and so

$$\begin{aligned} |f(h^2) - f(0)| &\leq Ch^2 \,|g_0(\mathfrak{h}/(2T_c))| + C' \sup_{0<\delta<h^2} \left| \frac{g_1(\mathfrak{h}/(2T_c))}{\mathfrak{h}} \right| \left(|t|^2 + E(\delta)^2 \right) \\ &\leq Ch^2 \left(|g_0(\mathfrak{h}/(2T_c))| + \left| \frac{g_1(\mathfrak{h}/(2T_c))}{\mathfrak{h}} \right| \left(|t|^2 + \mathfrak{h}^2 \right) \right) \\ &\leq Ch^2 \left(|t|^2 \mathfrak{h}^{-3} + \langle \mathfrak{h} \rangle^{-1} \right) \end{aligned}$$

where in the second step we used that $E(\delta) = \mathfrak{h}^2 + \delta|t|^2 \leq \mathfrak{h}^2 + |t|^2$ for small enough h and in the third step we used $g_0(z) \leq C\langle z\rangle^{-1}$ as well as $g_1(z)/z \leq C\langle z\rangle^{-3}$. Assume $D = 3$ for definiteness. We can bound (5.87) as follows

$$h^2 \int \langle p\rangle^2 |t|^2 |f(h^2) - f(0)|^2 \,\mathrm{d}\mathbf{p} \leq Ch^6 \int \left(|t|^6 \langle p\rangle^{-10} + |t|^2 \langle p\rangle^{-2} \right) \,\mathrm{d}\mathbf{p} = Ch^6,$$

where the last equality holds by the assumption on t. This proves (ii). □

Proof of Theorem 5.2.10

We follow the strategy in [73]. That is, we prove theorem Theorem 5.2.10 (i) by separately proving an upper and a lower bound on the left-hand side in (5.15). The upper bound follows by choosing an appropriate trial state Γ_Δ and using the semiclassical expansion of the BCS free energy in the form of Theorem 5.5.3. For the lower bound, we show that the chosen trial states Γ_Δ indeed describe *any* approximate minimizer Γ to lowest order in h (this is precisely statement (ii) in Theorem 5.2.10) and conclude by using the semiclassical expansion once again.

Upper bound

Recall the definition of h in (5.70). In this section we prove

$$\min_{\Gamma} \mathcal{F}_T^{BCS}(\Gamma) - \mathcal{F}_T^{BCS}(\Gamma_0) \leq h^4 \min_{\mathfrak{a}\in\ker(K_{T_c}+V)} \mathcal{E}^{GL}(\mathfrak{a}) + O(h^6), \tag{5.89}$$

where $\mathcal{E}^{GL}$ is given by (5.16).

We get this by using the trial state $\widehat{\Gamma}_\Delta$, defined by (5.63) with the choice

$$\widehat{\Delta} = 2h\widehat{(V\check{\mathfrak{a}})} \tag{5.90}$$

where $\mathfrak{a} \in \ker(K_{T_c}+V)$ minimizes $\mathcal{E}^{GL}$ (recall that minimizers exist by Proposition 5.2.12). Then, (5.89) follows from Theorem 5.5.3 and the fact that evaluating the definition (5.72) of E_2 for the choice

$$t(\mathbf{p}) = \widehat{\Delta}(\mathbf{p})/h = -2K_{T_c}(p)\mathfrak{a}(\mathbf{p})$$

produces the definition (5.16) of $\mathcal{E}^{GL}(\mathfrak{a})$. □

Lower bound: Part A

Following [73], we will prove the lower bound in (5.15) in conjunction with statement (ii) about approximate minimizers. We consider any BCS state Γ satisfying

$$\mathcal{F}_T^{BCS}(\Gamma) - \mathcal{F}_T^{BCS}(\Gamma_0) \leq O(h^4). \tag{5.91}$$

Note that we may restrict to such Γ when minimizing $\mathcal{F}_T^{BCS}$ thanks to the upper bound (5.89) and that (5.91) still includes the approximate minimizers considered in (ii). In **Part A**, we prove Proposition 5.5.6, which says that the off-diagonal element α of such a Γ will be close to a minimizer of $\mathcal{E}^{GL}$. In **Part**

B, we will use this to get $\mathcal{F}_T^{BCS}(\Gamma) - \mathcal{F}_T^{BCS}(\Gamma_\Delta) \geq O(h^6)$ for Δ of the form (5.90) and hence

$$\mathcal{F}_T^{BCS}(\Gamma) - \mathcal{F}_T^{BCS}(\Gamma_0) \geq \mathcal{F}_T^{BCS}(\Gamma_\Delta) - \mathcal{F}_T^{BCS}(\Gamma_0) + O(h^6).$$

Since we know $\mathcal{F}_T^{BCS}(\Gamma_\Delta) - \mathcal{F}_T^{BCS}(\Gamma_0) = h^4\mathcal{E}^{GL}(\psi_1, \ldots, \psi_n) + O(h^6)$ from Theorem 5.5.3, this will imply both the lower bound in (5.15) and statement (ii) about approximate minimizers.

In the remainder of this section, we will prove:

Proposition 5.5.6. *Suppose* Γ *satisfies* (5.91) *and let* P *denote the orthogonal projection onto* $\ker(K_{T_c} + V)$ *and let* $P^\perp = 1 - P$*. Then,* $\|P\alpha\|_2 = O(h)$ *and* $\|P^\perp\alpha\|_2 = O(h^2)$*.*

This implies statement (ii) in Theorem 5.2.10 with $\mathfrak{a}_0 \equiv h^{-1}P\alpha$. The proof of Proposition 5.5.6 will use the following lemma, which bounds the relative entropy $\mathfrak{H}(\Gamma, \Gamma_\Delta)$ from below in terms of a weighted Hilbert-Schmidt norm. The result without the second "bonus" term on the right-hand side first appeared in [90], the improved version is due to [73].

Lemma 5.5.7 (Lemma 1 in [73])**.** *For any* $0 \leq \Gamma \leq 1$ *and* $\Gamma^{(H)} = (1 + \exp(H))^{-1}$*, it holds that*

$$\begin{aligned} \mathfrak{H}(\Gamma, \Gamma^{(H)}) \geq & \operatorname{Tr}\left[\frac{\widehat{H}}{\tanh(\widehat{H}/2)}(\widehat{\Gamma} - \widehat{\Gamma}^{(H)})^2\right] \\ & + \frac{4}{3}\operatorname{Tr}\left[(\widehat{\Gamma}(1-\widehat{\Gamma}) - \widehat{\Gamma}^{(H)}(1-\widehat{\Gamma}^{(H)}))^2\right]. \end{aligned} \tag{5.92}$$

Proof. By the identity (5.7) in [73] and Klein's inequality for 2×2 matrices, (5.92) even holds pointwise in $\mathbf{p}$. $\square$

Here is a quick outline of the proof of Proposition 5.5.6: Following [73], we rewrite $\mathcal{F}_T^{BCS}(\Gamma) - \mathcal{F}_T^{BCS}(\Gamma_0)$ by invoking the relative entropy identity (5.68). Then, we bound the right hand side from below by $\langle \alpha, (K_T + V)\alpha \rangle$, which is therefore negative due to (5.91). Since $K_{T_c} + V \geq 0$ with a spectral gap above zero, this will allow us to conclude that the part of α lying outside of $\ker(K_{T_c} + V)$ must be small, more precisely that $\|\alpha - P\alpha\|_2 = O(h^2)$. To get that $\|P\alpha\|_2$ itself is $O(h)$, we use the second "bonus" term on the right-hand side of Lemma 5.5.7.

Proof of Proposition 5.5.6. Step 1: We first apply the relative entropy identity (5.68) with the choice $\mathfrak{a} = 0$ to get

$$O(h^4) \geq \mathcal{F}_T^{BCS}(\Gamma) - \mathcal{F}_T^{BCS}(\Gamma_0) = \frac{T}{2}\mathfrak{H}(\Gamma, \Gamma_0) + \int V|\alpha|^2 \,\mathrm{d}\mathbf{x}. \tag{5.93}$$

Next, we use Lemma 5.5.7. To evaluate the resulting expression, note that

$$\frac{\widehat{H}_0}{\tanh(\widehat{H}_0/(2T))} = K_T I_{2\times 2},$$
$$\widehat{\Gamma}(1-\widehat{\Gamma}) - \widehat{\Gamma}_0(1-\widehat{\Gamma}_0) = \left(\widehat{\gamma}(1-\widehat{\gamma}) - \widehat{\gamma}_0(1-\widehat{\gamma}_0) - |\widehat{\alpha}|^2\right) I_{2\times 2},$$

are diagonal matrices. We obtain

$$\frac{T}{2}\mathfrak{H}(\Gamma, \Gamma_0) \geq \int \Big(K_T(\cdot)(\widehat{\gamma} - \widehat{\gamma}_0)^2 \,\mathrm{d}\mathbf{p} + K_T(\cdot)|\widehat{\alpha}|^2 + \frac{4T}{3}\left(\widehat{\gamma}(1-\widehat{\gamma}) - \widehat{\gamma}_0(1-\widehat{\gamma}_0) - |\widehat{\alpha}|^2\right)^2 \Big) \,\mathrm{d}\mathbf{p}.$$

We estimate the first term using $K_T(p) \geq 2T$ and find the lower bound

$$\int \left(K_T(\cdot)|\widehat{\alpha}|^2 + 2T(\widehat{\gamma} - \widehat{\gamma}_0)^2 + \frac{4T}{3}\left(\widehat{\gamma}(1-\widehat{\gamma}) - \widehat{\gamma}_0(1-\widehat{\gamma}_0) - |\widehat{\alpha}|^2\right)^2 \right) \mathrm{d}\mathbf{p}.$$

By

$$(x(1-x) - y(1-y))^2 \leq (x-y)^2, \quad \forall 0 \leq x, y \leq 1$$

and the triangle inequality, we get the pointwise estimate

$$\left(2(\widehat{\gamma} - \widehat{\gamma}_0)^2 + \frac{4}{3}\left(\widehat{\gamma}(1-\widehat{\gamma}) - \widehat{\gamma}_0(1-\widehat{\gamma}_0) - |\widehat{\alpha}|^2\right)^2 \right) \geq \frac{4}{5}|\widehat{\alpha}|^4.$$

Going back to (5.93), we have shown that

$$\frac{4T}{5}\|\widehat{\alpha}\|_4^4 + \langle \alpha, (K_T + V)\alpha \rangle \leq O(h^4). \tag{5.94}$$

Step 2: Next, we replace K_T by K_{T_c} in (5.94) to make use of the spectral gap of $K_{T_c} + V$. This is an easy version of what is Step 2 of Part A in [73], which is more involved because it also removes the dependence on the external fields A, W. For us, it suffices to observe that

$$\frac{\mathrm{d}}{\mathrm{d}T} K_T(p) = \frac{1}{2T^2} \frac{\mathfrak{h}(p)^2}{\sinh^2(\mathfrak{h}(p)/(2T))}$$

is uniformly bounded in p for all h small enough such that $T > T_c/2$. By the mean-value theorem, $\|K_T - K_{T_c}\|_\infty \leq O(h^2)$. Using this on (5.94), we find

$$\frac{4T}{5}\|\widehat{\alpha}\|_4^4 + \langle \alpha, (K_{T_c} + V)\alpha \rangle \leq O(h^2)\|\alpha\|_2^2 + O(h^4). \tag{5.95}$$

Let $\kappa > 0$ denote the size of the spectral gap of $K_{T_c} + V$ above energy zero. We write $\alpha = P\alpha + P^\perp\alpha$. Using $(K_{T_c} + V)P\alpha = 0$, we obtain

$$\frac{4T}{5}\|\widehat{\alpha}\|_4^4 + \kappa\|P^\perp\alpha\|_2^2 \leq O(h^2)\|\alpha\|_2^2 + O(h^4). \tag{5.96}$$

For the moment we drop the first term on the left-hand side of (5.96) and use orthogonality to get

$$\|P^\perp\alpha\|_2^2 \leq O(h^2)(\|P\alpha\|_2^2 + \|P^\perp\alpha\|_2^2) + O(h^4)$$

which yields

$$\|P^\perp\alpha\|_2^2 \leq O(h^2)\|P\alpha\|_2^2 + O(h^4). \tag{5.97}$$

Thus, both claims will follow, once we show $\|P\alpha\|_2 = O(h)$.

<u>Step 3:</u> Here the degeneracy requires a slight modification. We now drop the second term on the left-hand side of (5.96) to get

$$\|\widehat{\alpha}\|_4 \leq O(h^{1/2})\|\widehat{\alpha}\|_2^{1/2} + O(h). \tag{5.98}$$

By orthogonality and (5.97),

$$\|\widehat{\alpha}\|_4 \leq O(h^{1/2})\|\widehat{P\alpha}\|_2^{1/2} + O(h), \tag{5.99}$$

On the right-hand side of (5.98) however, the replacement of $\widehat{\alpha}$ by $\widehat{P\alpha}$ requires more work. By the triangle inequality for $\|\cdot\|_4$ and (5.97)

$$\begin{aligned}\|\widehat{\alpha}\|_4 &\geq \|\widehat{P\alpha}\|_4 - \|\widehat{P^\perp\alpha}\|_4 \geq \|\widehat{P\alpha}\|_4 - \|\widehat{P^\perp\alpha}\|_2^{1/2}\|\widehat{P^\perp\alpha}\|_\infty^{1/2}\\ &\geq \|\widehat{P\alpha}\|_4 - O(h^{1/2})\|\widehat{P\alpha}\|_2^{1/2}\|\widehat{P^\perp\alpha}\|_\infty^{1/2}.\end{aligned}$$

We use $\widehat{P^\perp\alpha} = \widehat{\alpha} - \widehat{P\alpha}$ and $|\widehat{\alpha}|^2 \leq \widehat{\gamma}(1-\widehat{\gamma}) \leq 1/4$ pointwise to find $\|\widehat{P^\perp\alpha}\|_\infty \leq \frac{1}{4} + \|\widehat{P\alpha}\|_\infty$. It is slightly more convenient to conclude the argument by choosing an orthonormal basis $\{a_j\}$ for $\ker(K_{T_c} + V)$. This allows us to write

$$P\alpha = h\sum_{j=1}^{n}\psi_j a_j \tag{5.100}$$

By Proposition 5.5.5, $\|\widehat{a_j}\|_\infty \leq C$ for all j and therefore $\|\widehat{P\alpha}\|_\infty \leq O(h)|\psi|_\infty$. We have shown

$$\|\widehat{\alpha}\|_4 \geq \|\widehat{P\alpha}\|_4 - O(h^{1/2})\|\widehat{P\alpha}\|_2^{1/2}(1 + h|\psi|_\infty)^{1/2}.$$

Combining this with (5.99), we obtain

$$\|\widehat{P\alpha}\|_4 \leq O(h^{1/2})\|\widehat{P\alpha}\|_2^{1/2}(1+h|\psi|_\infty)^{1/2} + O(h). \tag{5.101}$$

It remains to bound $\|\widehat{P\alpha}\|_4$ from below in terms of $\|\widehat{P\alpha}\|_2$. Let $R>0$. We split the integration domain into $\{p \leq R\}$ and $\{p > R\}$. Applying Hölder's inequality to the former yields

$$\|\widehat{P\alpha}\|_2^2 \leq CR^{D/2}\|\widehat{P\alpha}\|_4^2 + h^2|\psi|_\infty^2 \sum_{i,j} \int_{\{p>R\}} |\widehat{a}_i||\widehat{a}_j| \,\mathrm{d}\mathbf{p} \tag{5.102}$$

where $C>0$ denotes a constant independent of h, R. Note that for all i,j, Cauchy-Schwarz implies $|\widehat{a}_i||\widehat{a}_j| \in L^1(\mathbb{R}^D)$ and so for $R_0>0$ large enough,

$$\sum_{i,j} \int_{\{p>R_0\}} |\widehat{a}_i||\widehat{a}_j| \,\mathrm{d}\mathbf{p} < \frac{1}{2}.$$

We recall (5.101) to find

$$\|\widehat{P\alpha}\|_2^2 \leq O(h)\|\widehat{P\alpha}\|_2(1+h|\psi|_\infty) + \frac{1}{2}h^2|\psi|_\infty^2 + O(h^2).$$

Since the $\{a_j\}$ in (5.100) are orthonormal, $h|\psi|_\infty \leq \|\widehat{P\alpha}\|_2 \leq \sqrt{n}h|\psi|_\infty$. This implies

$$\left(\frac{1}{2} + O(h)\right)|\psi|_\infty^2 \leq O(1)|\psi|_\infty + O(1). \tag{5.103}$$

Let h be small enough such that the $1/2+O(h)$ term exceeds $1/4$. We conclude that $|\psi|_\infty \leq O(1)$. Since $\|\widehat{P\alpha}\|_2 \leq \sqrt{n}h|\psi|_\infty$, it follows that $\|\widehat{P\alpha}\|_2 \leq O(h)$ as claimed. □

Lower bound: Part B

We use once more the relative entropy identity (5.68). Together with Lemma 5.5.4 (i) and the eigenvalue equation, we get

$$\begin{aligned} &\mathcal{F}_T^{BCS}(\Gamma) - \mathcal{F}_T^{BCS}(\Gamma_0) \\ =&h^4\mathcal{E}^{GL}(P\alpha) + \frac{T}{2}\mathfrak{H}(\Gamma,\Gamma_\Delta) + \int V|\alpha - P\alpha|^2 \,\mathrm{d}\mathbf{x} + O(h^6). \end{aligned} \tag{5.104}$$

We see that to prove the lower bound it remains to show

$$\frac{T}{2}\mathfrak{H}(\Gamma,\Gamma_\Delta) + \int V|\alpha - P\alpha|^2 \,\mathrm{d}\mathbf{x} = \frac{T}{2}\mathfrak{H}(\Gamma,\Gamma_\Delta) + \int V|P^\perp\alpha|^2 \,\mathrm{d}\mathbf{x} \geq O(h^6). \tag{5.105}$$

By Lemma 5.5.7 and the fact that $x \mapsto x/\tanh(x)$ is a monotone function that depends only on x^2, we have

$$\begin{aligned}\frac{T}{2}\mathfrak{H}(\Gamma,\Gamma_\Delta) &\geq \frac{1}{2}\mathrm{Tr}\left[(\widehat{\Gamma}-\widehat{\Gamma}_\Delta)\frac{\widehat{H}_\Delta}{\tanh\left(\widehat{H}_\Delta/(2T)\right)}(\widehat{\Gamma}-\widehat{\Gamma}_\Delta)\right] \\ &= \frac{1}{2}\mathrm{Tr}\left[(\widehat{\Gamma}-\widehat{\Gamma}_\Delta)\frac{E_\Delta}{\tanh\left(E_\Delta/(2T)\right)}(\widehat{\Gamma}-\widehat{\Gamma}_\Delta)\right] \\ &\geq \frac{1}{2}\mathrm{Tr}\left[(\widehat{\Gamma}-\widehat{\Gamma}_\Delta)K_T(\widehat{\Gamma}-\widehat{\Gamma}_\Delta)\right].\end{aligned} \tag{5.106}$$

Since $K_T \geq 0$, we have for every fixed (i.e. h-independent) $0 < \varepsilon < 1$,

$$\begin{aligned}&\frac{1}{2}\mathrm{Tr}\left[(\widehat{\Gamma}-\widehat{\Gamma}_\Delta)K_T(\widehat{\Gamma}-\widehat{\Gamma}_\Delta)\right] \\ &\geq \int K_T|\widehat{\alpha}-\widehat{\alpha}_\Delta|^2\,\mathrm{d}\mathbf{p} \\ &\geq \int K_T|\widehat{P^\perp\alpha}|^2\,\mathrm{d}\mathbf{p} - 2\Re\int K_T\overline{\widehat{P^\perp\alpha}}\left(\widehat{P\alpha}-\widehat{\alpha}_\Delta\right)\mathrm{d}\mathbf{p} \\ &\geq (1-\varepsilon)\int K_T|\widehat{P^\perp\alpha}|^2\,\mathrm{d}\mathbf{p} - C_\varepsilon\int K_T|\widehat{P\alpha}-\widehat{\alpha}_\Delta|^2\,\mathrm{d}\mathbf{p} \\ &\geq (1-\varepsilon)\int K_T|\widehat{P^\perp\alpha}|^2\,\mathrm{d}\mathbf{p} + O(h^6).\end{aligned}$$

In the last step, we used Lemma 5.5.4 (ii) and $K_T(p) \leq C\langle p\rangle^2$ to get

$$\int K_T|\widehat{P\alpha}-\widehat{\alpha}_\Delta|^2\,\mathrm{d}\mathbf{p} = O(h^6). \tag{5.107}$$

Using these estimates on (5.105) and setting $\xi := P^\perp\alpha$, we see that it remains to show that there exists an h-independent choice of $0 < \varepsilon < 1$ such that

$$\langle\xi, ((1-\varepsilon)K_T + V)\xi\rangle \geq O(h^6). \tag{5.108}$$

Recall from step 2 of the proof of Proposition 5.5.6 that $\|K_T - K_{T_c}\|_\infty \leq O(h^2)$. Since also $\|\xi\|_2 = O(h^2)$ by Proposition 5.5.6, we get

$$\langle\xi, ((1-\varepsilon)K_T + V)\xi\rangle = \langle\xi, ((1-\varepsilon)K_{T_c} + V)\xi\rangle + O(h^6).$$

We claim that there exists a constant $c > 0$ such that

$$\langle\xi, (K_{T_c} + V)\xi\rangle \geq c\langle\xi, K_{T_c}\xi\rangle. \tag{5.109}$$

Choosing ε sufficiently small will then give $\langle\xi, (1-\varepsilon)K_{T_c} + V)\xi\rangle \geq 0$. Thus, it remains to prove (5.109). Since V_- is infinitesimally form-bounded with respect to K_{T_c}, we have for any $\delta > 0$

$$(1-\delta)K_{T_c} \leq K_{T_c} - V_- + C_\delta \leq K_{T_c} + V + C_\delta \tag{5.110}$$

or

$$K_{T_c} \leq C_1(K_{T_c}+V)+C_2. \tag{5.111}$$

Now, on $\ker(K_{T_c}+V)^{\perp}$, it also holds that $K_{T_c}+V-\kappa \geq 0$ where $\kappa > 0$ denotes the gap size. Thus, for all $\lambda > 0$,

$$K_{T_c} \leq (C_1+\lambda)(K_{T_c}+V)+C_2-\lambda\kappa, \quad \text{on} \ker(K_{T_c}+V)^{\perp} \tag{5.112}$$

and choosing $\lambda = C_2/\kappa$, we see that (5.109) follows. This proves (i).

Statement (ii) was proved along the way: Any approximate minimizer satisfies (5.91) and hence Proposition 5.5.6 implies that its off-diagonal part can be split into $\alpha = P\alpha + \xi$ with $\|\xi\| = O(h^2)$. Since P is the projection onto $\ker(K_{T_c}+V)$, $P\alpha \in \ker(K_{T_c}+V)$. Moreover, $\mathfrak{a}_0 \equiv h^{-1}P\alpha$ approximately minimizes the GL energy because the proof of the lower bound shows that for all Γ satisfying (5.91) (not just for actual minimizers),

$$\mathcal{F}_T^{BCS}(\Gamma) - \mathcal{F}_T^{BCS}(\Gamma_0) \geq h^4 \mathcal{E}^{GL}(\mathfrak{a}_0) + O(h^6).$$

This finishes the proof of Theorem 5.2.10. □

Proofs of Propositions 5.2.3, 5.2.12 and 5.2.13

Proof of Proposition 5.2.3. For the L^{p_V} potentials, this is a standard argument combining Hölder's inequality and Sobolev's inequality.

Consider the potentials (5.6), i.e. $V(\mathbf{x}) = -\lambda\delta(|\mathbf{x}|-R)$ with $\lambda, R > 0$. Let $f \in H^1(\mathbb{R}^D)$. We first consider the case $D=1$. Then

$$\langle f, Vf\rangle = -\lambda |f(R)|^2.$$

We apply the simplest Sobolev inequality

$$2\sup_{x\in\mathbb{R}} |u(x)| \leq \int_{-\infty}^{\infty} |u'(x)| \mathrm{d}x, \quad \forall u \in W^{1,1}(\mathbb{R}), \tag{5.113}$$

(which follows from the fundamental theorem of calculus) with the choice $u(s) = f(s)^2$. By (5.113) and Cauchy-Schwarz, we get

$$|f(R)|^2 \leq \int_{-\infty}^{\infty} |f(x)f'(x)| \mathrm{d}x \leq \varepsilon \|f'\|_2^2 + \frac{1}{4\varepsilon}\|f\|_2^2$$

for any $\varepsilon > 0$. This proves the claimed infinitesimal form-boundedness of V when $D=1$.

Let now $D = 2, 3$. We have

$$\langle f, Vf \rangle = -\lambda \int_{\mathbb{S}^{D-1}} R^{D-1} |f(R\omega)|^2 \mathrm{d}\sigma(\omega),$$

where $\mathrm{d}\sigma$ is the usual surface measure on $\mathbb{S}^{D-1}$. Observe that the inequality (5.113) implies

$$2 \sup_{s>0} |u(s)| \leq \int_0^\infty |u'(s)| \mathrm{d}s, \quad \forall u \in W_0^{1,1}(\mathbb{R}_+).$$

We use this with the choice $u(s) = s^{D-1} f(s\omega)^2$, pointwise in $\omega \in \mathbb{S}^2$, and find

$$\begin{aligned} &\int_{\mathbb{S}^{D-1}} R^{D-1} |f(R\omega)|^2 \mathrm{d}\sigma(\omega) \\ &\leq \int_{\mathbb{S}^{D-1}} \int_0^\infty \left(\frac{D-1}{2} s^{D-2} |f(s\omega)|^2 + s^{D-1} |f(s\omega) \partial_s f(s\omega)| \right) \mathrm{d}s \mathrm{d}\sigma(\omega). \end{aligned} \tag{5.114}$$

Consider the first term in the parentheses. We split the integration domain into $s > 1$ and $s \leq 1$ and estimate $s^{D-2} < s^{D-1}$ in the first region. By applying Hölder's inequality in the second region, we get

$$\begin{aligned} \int_{\mathbb{S}^{D-1}} \int_0^\infty s^{D-2} |f(s\omega)|^2 \mathrm{d}s \mathrm{d}\sigma(\omega) &< \|f\|_2^2 + \int_{\mathbb{S}^{D-1}} \int_0^1 s^{D-2} |f(s\omega)|^2 \mathrm{d}s \mathrm{d}\sigma(\omega) \\ &\leq \|f\|_2^2 + \left(\int_0^1 s^{D-8/3} \mathrm{d}s \right)^{3/5} \|f\|_5^2 \\ &= \|f\|_2^2 + C \|f\|_5^2 \end{aligned}$$

where C is a finite constant, since $D - 8/3 > -1$. The L^5 norm is infinitesimally form-bounded with respect to $-\nabla^2$ by the usual argument via Sobolev's inequality.

We come to the second term in (5.114) in parentheses. By Cauchy-Schwarz, for every $\varepsilon > 0$, it is bounded by

$$\varepsilon \int_{\mathbb{S}^{D-1}} \int_0^\infty s^{D-1} |\partial_s f(s\omega)|^2 \mathrm{d}s \mathrm{d}\sigma(\omega) + \frac{1}{4\varepsilon} \|f\|_2^2.$$

The first term is the quadratic form corresponding to (the negative of) the radial part of the Laplacian, see (5.29). It differs from the full Laplacian by a multiple of the Laplace-Beltrami operator $-\nabla^2_{\mathbb{S}^{D-1}}$, i.e. a nonnegative operator. This implies infinitesimal form-boundedness when $D = 2, 3$. $\square$

Proof of Proposition 5.2.12. Recall (5.16)

$$\begin{aligned}\mathcal{E}^{GL}(\mathfrak{a}) =&\frac{1}{T_c}\int_{\mathbb{R}^D} \frac{g_1((p^2-\mu)/T_c)}{(p^2-\mu)/T_c} \left|K_{T_c}(p)\right|^4 \left|\mathfrak{a}(\mathbf{p})\right|^4 \mathrm{d}\mathbf{p} \\ &- \frac{1}{2T_c}\int_{\mathbb{R}^D} \frac{1}{\cosh^2\left(\frac{p^2-\mu}{2T_c}\right)} \left|K_{T_c}(p)\right|^2 \left|\mathfrak{a}(\mathbf{p})\right|^2 \mathrm{d}\mathbf{p},\end{aligned}$$

We denote the quartic term by $A(\mathfrak{a})$ and the quadratic term by $-B(\mathfrak{a})$. Note that $A, B > 0$ whenever $\mathfrak{a}$ is not identically zero.

We use the basis representation of the GL energy mentioned in Remark 5.2.11 (i). That is, we fix a basis $\{a_j\}$ of $\ker(K_{T_c}+V)$ and write $\mathfrak{a}(\mathbf{p}) = \sum_{j=1}^n \psi_j \widehat{a}_j(\mathbf{p})$ with $(\psi_1, \ldots, \psi_n) \in \mathbb{C}^n$. Then we write

$$(\psi_1, \ldots, \psi_n) = L\omega, \qquad L \geq 0,\, \omega \in S(\mathbb{C}^n),$$

where $S(\mathbb{C}^n)$ is the unit sphere in $\mathbb{C}^n$. It follows that

$$\begin{aligned}\inf_{(\psi_1,\ldots,\psi_n)\in\mathbb{C}^n} \mathcal{E}^{GL}(\psi_1, \ldots, \psi_n) &= \inf_{\omega\in S(\mathbb{C}^n)} \inf_{L\geq 0} \mathcal{E}^{GL}(L\omega) \\ &= \inf_{\omega\in S(\mathbb{C}^n)} \inf_{L\geq 0} \left(L^4 A(\omega) - L^2 B(\omega)\right) \\ &= \inf_{\omega\in S(\mathbb{C}^n)} \frac{-B(\omega)^2}{4A(\omega)}\end{aligned}$$

and since A, B are continuous functions which never vanish on the compact set $S(\mathbb{C}^n)$, the last infimum is finite and attained. □

Proof of Proposition 5.2.13. The same argument that proves Theorem 5.2.10 (ii) applies for $T > T_c$ and yields the same result with the sign of the $|\mathfrak{a}|^2$ term in the GL energy (5.16) flipped. Consequently, the unique minimizer of the GL energy is $\mathfrak{a} = 0$. To see coercivity of the GL energy around this minimizer, we drop the quartic term and rewrite the the quadratic term as in the proof of Proposition 5.2.12 above. We get

$$\mathcal{E}^{GL}(\psi_1, \ldots, \psi_n) \geq \varepsilon \lambda_{min} \sum_{j=1}^n |\psi_j|^2$$

with

$$\lambda_{min} := \min_{\omega\in S(\mathbb{C}^n)} \frac{1}{2T_c} \int_{\mathbb{R}^D} \frac{1}{\cosh^2\left(\frac{p^2-\mu}{2T_c}\right)} \left|K_{T_c}(p)\right|^2 \left|\sum_{j=1}^n \omega_j \widehat{a}_j(\mathbf{p})\right|^2 \mathrm{d}\mathbf{p}.$$

Note that $\lambda_{min} > 0$, since it is the minimum of a positive, continuous function over a compact set. □

5.6 Proofs for part II

Setting

We use the formulation of GL theory from Remark 5.2.11(i). We compute the GL coefficients c_{ijkm} and d_{ij} given by formulae (5.21) and (5.22). They determine the GL energy $\mathcal{E}^{GL}_{d\text{-wave}} : \mathbb{C}^5 \to \mathbb{R}$ via

$$\mathcal{E}^{GL}\left(\tilde{\psi}_{-2}, \ldots, \tilde{\psi}_2\right) = \sum_{i,j,k,m=-2}^{2} c_{ijkm} \overline{\tilde{\psi}_i \tilde{\psi}_j} \tilde{\psi}_k \tilde{\psi}_m - \sum_{i,j=-2}^{2} d_{ij} \overline{\tilde{\psi}_i} \tilde{\psi}_j$$

It remains to pick a convenient basis to compute (5.21) and (5.22). Since the Fourier transform maps $\mathcal{H}_l$ to itself in a bijective fashion, see e.g. [164], we can choose

$$\widehat{a}_m(\mathbf{p}) = \varrho(p)\, Y_m^2(\vartheta, \varphi), \qquad \mathbf{p} \equiv (p, \vartheta, \varphi), \tag{5.115}$$

for an appropriate radial function ϱ. We will denote the GL order parameter corresponding to $\widehat{a}_m$ (in the sense of (5.1)) by $\tilde{\psi}_m$ with $-2 \le m \le 2$. (Note that we use the *ordinary* spherical harmonics Y_2^m (5.24) as a basis because it is more convenient to do computations, but our final result is phrased in terms the basis of *real* spherical harmonics (5.25).)

With the choice (5.115), equations (5.21),(5.22) for the GL coefficients read

$$c_{ijkm} = \int p^{-2} f_4(p) \overline{Y_2^i(\vartheta, \varphi) Y_2^j(\vartheta, \varphi)} Y_2^k(\vartheta, \varphi) Y_2^m(\vartheta, \varphi)\, \mathrm{d}\mathbf{p} \tag{5.116}$$

$$d_{ij} = -\int p^{-2} f_2(p) \overline{Y_2^i(\vartheta, \varphi)} Y_2^j(\vartheta, \varphi)(p)\, \mathrm{d}\mathbf{p}, \tag{5.117}$$

where $i, j, k, m = -2, \ldots, 2$ and we used the functions f_2, f_4 defined in (5.34). Note that f_2, f_4 are positive (since g_1 defined by (5.17) satisfies $\frac{g_1(z)}{z} > 0$) and radially symmetric.

Proof of Theorem 5.3.1

While the radial integrals in (5.116),(5.117) depend on the details of the microscopic potential V through ϱ, the integration over the angular variables can be performed explicitly. Since the spherical harmonics form an orthonormal family with respect to surface measure on $\mathbb{S}^2$, we immediately get

$$d_{ij} = d\delta_{ij}$$

where $d > 0$ is the result of the radial integration in (5.117), i.e.

$$d = \int_0^\infty f_2(p)\, \mathrm{d}p \tag{5.118}$$

i	j	k	m	$c_{ijkm} \cdot 28\pi$
2	2	2	2	$10c$
2	1	2	1	$5c$
1	1	1	1	$10c$
0	2	0	2	$5c$
1	1	0	2	0
0	1	0	1	$5c$
-1	2	-1	2	$5c$
0	1	-1	2	0
0	0	0	0	$15c$
1	-1	1	-1	$10c$
2	-2	2	-2	$10c$
0	0	2	-2	$5c$
0	0	1	-1	$-5c$
1	-1	2	-2	$-5c$

Table 5.1: Non-trivial equivalence classes of Ginzburg–Landau coefficients in the pure d-wave case. c is defined as the result of the radial integration (5.119). Notice that the case $i+j=0$ behaves rather differently. This is due to the fact that the "pair permutation" and "pair sign-flip" symmetries fall together in this case. We keep the factor 5 to ensure better comparability with Table 5.2 later on.

and this is the second relation claimed in (5.33).

Next, we consider (5.116). Firstly, note that c_{ijkm} is always proportional to the result of the radial integration in (5.116), i.e.

$$c = \int_0^\infty f_4(p)\,\mathrm{d}p \tag{5.119}$$

and this is the first relation claimed in (5.33).

It remains to compute the angular part of the integral in (5.116). We express the product of two spherical harmonics of angular momentum $l=2$ as a linear combination of spherical harmonics of angular momentum ranging from $l=0$ to $l=4$. The general relation involves the well-tabulated Clebsch-Gordan coefficients, which we denote by $\langle l_1, l_2; m_1, m_2 | L; M\rangle$, and can be found in textbooks on quantum mechanics (see e.g. [38] p. 1046):

$$Y_{l_1}^{m_1}(\vartheta,\varphi)Y_{l_2}^{m_2}(\vartheta,\varphi) = \sum_{L=|l_1-l_2|}^{l_1+l_2} \sqrt{\frac{(2l_1+1)(2l_2+1)}{4\pi(2L+1)}} \langle l_1,l_2;0,0|L;0\rangle \times \langle l_1,l_2;m_1,m_2|L;m_1+m_2\rangle Y_L^{m_1+m_2}(\vartheta,\varphi). \tag{5.120}$$

Physically, this corresponds to expressing a pair of particles, uncorrelated in the angular variable, in terms of a wave function for the composite system. Since the total angular momentum of the composite system is not determined uniquely by the product wavefunction on the left-hand side, the sum over L appears on the right. However, the total z-component of the angular momentum is determined to be m_1+m_2. This "selection rule" will greatly restrict which c_{ijkm} may be non-zero.

Now, we can use the orthonormality of the spherical harmonics to compute the angular integrals and find

$$c_{ijkm} = \sum_{L=0,2,4} \frac{25c}{4\pi(2L+1)} \langle 2,2;0,0|L;0\rangle^2 \langle 2,2;i,j|L;i+j\rangle \times \langle 2,2;k,m|L;k+m\rangle \delta_{i+j,k+m}, \tag{5.121}$$

where we used that the Clebsch-Gordan coefficients are real-valued and that $\langle l_1,l_2;0,0|L;0\rangle = 0$ unless L is even [38]. Note that the selection rule from above yielded the necessary relation $i+j=k+m$ for $c_{ijkm} \neq 0$.

There are further symmetries: Considering the original expression (5.116), we that $c_{ijkm} = c_{jikm} = c_{ijmk}$. Since (5.121) shows $c_{ijkm} \in \mathbb{R}$, (5.116) also implies that $c_{ijkm} = c_{kmij}$. We subsume these relations as "pair permutation" symmetry. Physically, they correspond to the exchange of Cooper pairs. Moreover, as can be seen from reference tables for Clebsch-Gordan coefficients, we have $c_{ijkm} = c_{(-i)(-j)km}$, to which we will refer as "pair sign-flip" symmetry. Physically, it is a consequence of the invariance of our system under reflection in the xy-plane.

It thus suffices to look up (5.121) in a reference table for Clebsch-Gordan coefficients once for each member of a "pair permutation"and "pair sign-flip" equivalence class, ignoring those tuples (i,j,k,m) which do not satisfy the selection rule $i+j=k+m$. The result is presented in Table 5.1. By counting the number of elements of each equivalence class, we find

$$\begin{aligned}&\mathcal{E}^{GL}_{d\text{-wave}}\left(\tilde{\psi}_{-2},\dots,\tilde{\psi}_2\right)\\&=\frac{5c}{14\pi}\Bigg(\left(\sum_{m=-2}^{2}|\tilde{\psi}_m|^2-\tau\right)^2-\tau^2+\frac{1}{2}|\tilde{\psi}_0|^4+2\sum_{m=1,2}|\tilde{\psi}_m|^2|\tilde{\psi}_{-m}|^2\\&\quad-2\Re\left(\overline{\tilde{\psi}_0}^2\tilde{\psi}_1\tilde{\psi}_{-1}\right)+2\Re\left(\overline{\tilde{\psi}_0}^2\tilde{\psi}_2\tilde{\psi}_{-2}\right)-4\Re\left(\overline{\tilde{\psi}_1\tilde{\psi}_{-1}}\tilde{\psi}_2\tilde{\psi}_{-2}\right)\Bigg),\end{aligned}$$

where $\tau=\frac{7\pi d}{5c}$. Notice that this expression contains a second complete square:

$$\begin{aligned}&\mathcal{E}^{GL}_{d\text{-wave}}\left(\tilde{\psi}_{-2},\dots,\tilde{\psi}_2\right)\\&=\frac{5c}{14\pi}\left(\left(\sum_{m=-2}^{2}|\tilde{\psi}_m|^2-\tau\right)^2-\tau^2+\frac{1}{2}\left|\tilde{\psi}_0^2-2\tilde{\psi}_1\tilde{\psi}_{-1}+2\tilde{\psi}_2\tilde{\psi}_{-2}\right|^2\right)\end{aligned}\tag{5.122}$$

To conclude Theorem 5.3.1, it remains to make the basis change to the real-valued spherical harmonics, i.e. to invert (5.25). On the level of the GL order parameters, this yields the $SU(5)$ transformation

$$\begin{aligned}\tilde{\psi}_0=\psi_0,\qquad\tilde{\psi}_{-1}&=\frac{-\psi_1+i\psi_{-1}}{\sqrt{2}},\qquad\tilde{\psi}_1=\frac{\psi_1+i\psi_{-1}}{\sqrt{2}},\\\tilde{\psi}_{-2}&=\frac{\psi_2-i\psi_{-2}}{\sqrt{2}},\qquad\tilde{\psi}_2=\frac{\psi_2+i\psi_{-2}}{\sqrt{2}}.\end{aligned}\tag{5.123}$$

Proof of Theorem 5.3.5

The situation is as in three dimensions, only simpler. The d_{ij} GL coefficients are again diagonal by orthogonality and they come with a factor d defined in the same way as in Theorem 5.3.1 but with $f_2(p)$ replaced $f_2(p)/p$ since $D=2$ (of course the definition of ϱ has changed as well). For the c_{ijkm} coefficients, instead of considering Clebsch-Gordan coefficients, it suffices to compute

$$\frac{c}{\pi^2}\int_0^{2\pi}\cos(2\varphi)^k\sin(2\varphi)^{4-k}\mathrm{d}\varphi\tag{5.124}$$

for all $0\leq k\leq 4$. Here, the GL coefficient c is defined in the same way as in Theorem 5.3.1. We omit the details.

Proof of Theorem 5.3.7

We compute $\mathcal{E}^{GL}_{(s+d)\text{-wave}}$ by using the formulae (5.21) and (5.22) for the GL coefficients as in the previous section. We already computed most of the GL coefficients, namely all the ones that couple d-waves to d-waves.

i	j	k	m	$c_{ijkm} \cdot 28\pi$
s	2	0	2	$-2\sqrt{5}c^{(1s)}$
s	2	s	2	$7c^{(2s)}$
s	2	1	1	$\sqrt{30}c^{(1s)}$
s	1	0	1	$\sqrt{5}c^{(1s)}$
s	1	s	1	$7c^{(2s)}$
s	1	-1	2	$-\sqrt{30}c^{(1s)}$
s	0	0	0	$2\sqrt{5}c^{(1s)}$
s	s	0	0	$7c^{(2s)}$
s	0	s	0	$7c^{(2s)}$
s	s	s	0	0
s	s	s	s	$7c^{(4s)}$
s	0	2	-2	$-2\sqrt{5}c^{(1s)}$
s	s	2	-2	$7c^{(2s)}$
s	0	1	-1	$-\sqrt{5}c^{(1s)}$
s	s	1	-1	$-7c^{(2s)}$

Table 5.2: Equivalence classes of new Ginzburg–Landau coefficients in the mixed $(s+d)$-wave case. $c^{(1s)}, c^{(2s)}, c^{(4s)}$ are defined in (5.46).

By orthonormality of the spherical harmonics, d_{ij} is still diagonal. For $i, j \neq s$, d is as in (5.118). Notice however that d depends on ϱ through f_2. When $i = j = s$, we have to replace ϱ by ϱ_s, which is conveniently described as multiplication by $g_s = \left|\frac{\varrho_s}{\varrho}\right|$. We conclude that

$$d_{ij} = \begin{cases} d^{(2s)} & \text{if } i = j = s, \\ d\delta_{ij} & \text{otherwise.} \end{cases}$$

with $d^{(2s)}$ as defined in (5.46).

We turn to the quartic GL coefficients c_{ijkm}. Note that the "pair permutation" and "pair sign-flip" symmetries described in the proof of Theorem 5.3.1 still hold. In addition to the results listed in Table 5.1, we now have equivalence classes of c_{ijkm} where some indices are equal to s. Since the corresponding $\widehat{a}_s$ carry zero momentum in the z-direction, the selection rule dictates that c_{ijkm} can only be non-zero if the s replaces a 0-index.

We thus consider all equivalence classes of GL coefficients that can be obtained by replacing a 0 in Table 5.1 by s. We compute their values again via (5.120) (some follow immediately from the fact that $Y_0^0 = 1/\sqrt{4\pi}$). The results are presented in Table 5.2.

Just as for d_{ij}, the $c^{(1s)}, c^{(2s)}, c^{(4s)}$ are the result of a radial integration where for each index equal to s, f_4 is multiplied by a factor g_s. This yields the expressions (5.46) for $c^{(1s)}, c^{(2s)}, c^{(4s)}$. Note that according to Table 5.2, $c_{sss0} = 0$ and thus it is not necessary to define $c^{(3s)}$.

Armed with Table 5.2, it remains to count the number of GL coefficients in each equivalence class. After some algebra, we obtain

$$\begin{aligned}&\mathcal{E}^{GL}_{(s\,+\,d)\text{-wave}}\left(\tilde{\psi}_s, \tilde{\psi}_{-2}, \dots, \tilde{\psi}_2\right)\\ =&\mathcal{E}^{GL}_{d\text{-wave}}(\tilde{\psi}_{-2}, \dots, \tilde{\psi}_2) + \mathcal{E}^{GL}_{s\text{-wave}}(\tilde{\psi}_s) + \mathcal{E}^{GL}_{\text{coupling}}(\tilde{\psi}_s, \tilde{\psi}_{-2}, \dots, \tilde{\psi}_2).\end{aligned} \tag{5.125}$$

where

$$\begin{aligned}&\mathcal{E}^{GL}_{\text{coupling}}(\tilde{\psi}_s, \tilde{\psi}_{-2}, \dots, \tilde{\psi}_2)\\ =&\frac{\sqrt{5}c^{(1s)}}{7\pi}\Bigg(2\Re\left[\overline{\tilde{\psi}_s}\tilde{\psi}_0\left(\sum_{m=0,\pm1}|\tilde{\psi}_m|^2 - 2\sum_{m=\pm2}|\tilde{\psi}_m|^2\right)\right]\\ &\qquad\qquad - 2\sum_{m=1,2} m\Re\left[\overline{\tilde{\psi}_s\tilde{\psi}_0}\tilde{\psi}_m\tilde{\psi}_{-m}\right]\\ &\qquad\qquad + \sqrt{6}\sum_{\sigma=\pm1}\left(\Re\left[\overline{\tilde{\psi}_\sigma}^2\tilde{\psi}_s\tilde{\psi}_{2\sigma}\right] - 2\Re\left[\overline{\tilde{\psi}_s\tilde{\psi}_\sigma}\tilde{\psi}_{-\sigma}\tilde{\psi}_{2\sigma}\right]\right)\Bigg)\\ &+ \frac{c^{(2s)}}{2\pi}\left(2|\tilde{\psi}_s|^2\sum_{m=-2}^{2}|\tilde{\psi}_m|^2 + \Re\left[\overline{\tilde{\psi}_s}^2\left(\tilde{\psi}_0^2 - 2\tilde{\psi}_1\tilde{\psi}_{-1} + 2\tilde{\psi}_2\tilde{\psi}_{-2}\right)\right]\right)\end{aligned}$$

where $\mathcal{E}^{GL}_{d\text{-wave}}(\tilde{\psi}_{-2}, \dots, \tilde{\psi}_2)$ is given by (5.122) and

$$\mathcal{E}^{GL}_{s\text{-wave}}(\tilde{\psi}_s) = \frac{c^{(4s)}}{4\pi}\left(\left(|\tilde{\psi}_s|^2 - \tau_s\right)^2 - \tau_s^2\right)$$

with $\tau_s = \frac{2\pi d^{(2s)}}{c^{(4s)}}$. Statement (i) in Theorem 5.3.1, which gives the expression for $\mathcal{E}^{GL}_{(s\,+\,d)\text{-wave}}$, now follows by transforming into the basis of real spherical harmonics via (5.123).

To prove (ii), we use the GL energy expressed in the basis of real spherical harmonics. Let $\varepsilon > 0$ and take $(\psi_{-2}, \dots, \psi_2) \in \mathcal{M}_{d\text{-wave}}$, the set of minimizers of $\mathcal{E}_{d\text{-wave}}$ described by (5.35). Set $\psi_s = \varepsilon\omega$ with $|\omega| = 1$ and note that

$$\begin{aligned}\mathcal{E}^{GL}_{(s\,+\,d)\text{-wave}}(\psi_s, \psi_{-2}, \dots, \psi_2) =& \inf \mathcal{E}^{GL}_{d\text{-wave}} + \varepsilon\Re[\overline{\omega}z]\\ &+ \varepsilon^2\left(\frac{\tau c^{(2s)}}{\pi} - \frac{\tau_s c^{(4s)}}{2\pi}\right) + \frac{c^{4s}}{4\pi}\varepsilon^4.\end{aligned}$$

for some $z \in \mathbb{C}$, which is independent of ε and w. Consider first the case that $(\psi_{-2}, \ldots, \psi_2) \in \mathcal{M}_{d\text{-wave}}$ is such that $z \neq 0$. Then, we can choose ω such that $Re[\overline{\omega} z] < 0$ and we obtain (5.48) for sufficiently small ε. Thus, suppose that $z = 0$, which is e.g. the case for $(0, \tau/\sqrt{2}, 0, i\tau/\sqrt{2}, 0) \in \mathcal{M}_{d\text{-wave}}$. It is then clear that (5.48) holds iff $\frac{\tau c^{(2s)}}{\pi} < \frac{\tau_s c^{(4s)}}{2\pi}$, or equivalently $dc^{(2s)} < \frac{5}{7} cd^{(2s)}$. This proves (ii).

For statement (iii), let ψ_s be a minimizer of $\mathcal{E}^{GL}_{s\text{-wave}}$, i.e. $|\psi_s|^2 = \tau_s$. Now let $\varepsilon > 0$ and let $(\psi_{-2}, \ldots, \psi_2)$ have entries of the form $\psi_m = \varepsilon \psi'_m$ with $|\psi'_m| < 1$. We have

$$
\begin{aligned}
&\mathcal{E}^{GL}_{(s+d)\text{-wave}}(\psi_s, \psi_{-2}, \ldots, \psi_2) \\
&= \min \mathcal{E}^{GL}_{s\text{-wave}} + \varepsilon^2 \left(\left(-d + \frac{c^{(2s)} \tau_s}{\pi} \right) \sum_m |\psi'_m|^2 + \frac{c^{(2s)}}{2\pi} \Re \left[\overline{\psi_s^2} \sum_{m=-2}^{2} (\psi'_m)^2 \right] \right) \\
&\quad + O(\varepsilon^3)
\end{aligned}
$$

as $\varepsilon \to 0$. The real part is clearly minimal when we choose $\operatorname{Arg}(\psi'_m) = \operatorname{Arg}(\psi_s) + \pi/2$ for all m with $\psi'_m \neq 0$. This choice yields

$$
\begin{aligned}
&\mathcal{E}^{GL}_{(s+d)\text{-wave}}(\psi_s, \psi_{-2}, \ldots, \psi_2) \\
&= \min \mathcal{E}^{GL}_{s\text{-wave}} + \varepsilon^2 \sum_m |\psi'_m|^2 \left(-d + \frac{c^{(2s)} \tau_s}{\pi} \right) + O(\varepsilon^3).
\end{aligned}
$$

When the term in parentheses is strictly negative, which is equivalent to $d^{(2s)} c^{(2s)} < dc^{(4s)}$, we see that $\mathcal{E}^{GL}_{(s+d)\text{-wave}} < \min \mathcal{E}^{GL}_{s\text{-wave}}$ for sufficiently small ε. Vice-versa, when the term in parentheses is strictly positive, $\mathcal{E}^{GL}_{(s+d)\text{-wave}} > \min \mathcal{E}^{GL}_{s\text{-wave}}$ for all small $\varepsilon > 0$.

To conclude statement (iii), it remains to consider the case $d^{(2s)} c^{(2s)} = dc^{(4s)}$, when the $O(\varepsilon^2)$-term vanishes. The leading correction is now given by the $O(\varepsilon^3)$-term and by choosing $\psi_m = 0$ for $m \neq 0$, we find

$$
\mathcal{E}^{GL}_{(s+d)\text{-wave}}(\psi_s, 0, 0, \psi_0, 0, 0) = \min \mathcal{E}^{GL}_{s\text{-wave}} + \varepsilon^3 \frac{2\sqrt{5} c^{(s)}}{7\pi} |\psi'_0|^2 \Re[\overline{\psi_s} \psi'_0] + O(\varepsilon^4).
$$

Letting $\operatorname{Arg}(\psi'_0) = \operatorname{Arg}(\psi_s) + \pi$ shows that $\mathcal{E}^{GL}_{(s+d)\text{-wave}}(\psi_s, 0, 0, \psi_0, 0, 0) < \min \mathcal{E}^{GL}_{s\text{-wave}}$ in this case as well. This proves statement (iv). $\square$

5.7 Proofs for part III

The proof of Theorem 5.4.1 is based on three steps.

- In Lemma 5.7.1, we solve the eigenvalue problem for $K_T + V_{\lambda,R}$ explicitly in each angular momentum sector $\mathcal{H}_l$. The key result is the "eigenvalue condition" (5.128) which gives a formula for the eigenvalue (or energy) E in terms of the other parameters l, μ, T and λ. We will see that one can solve this for λ and one obtains an integral formula which is *monotone* in E. Therefore, instead of showing that E is minimal for $l = l_0$, one can equivalently show that λ is minimal for $l = l_0$.

- In Lemma 5.7.2, we show how, by adapting the parameters μ, T of the "weight function" $p/K_T(p)$, one can conclude that $\int_0^\infty \frac{p}{K_T(p)} f(p)\mathrm{d}k$ is positive, if one assumes that f is strictly positive on an interval.

- By Theorem 5.8.1, for any half-integer Bessel function of the first kind $\mathcal{J}_{l_0+1/2}$, there exists an open interval around its first maximum on which it is strictly larger than (the absolute value of) all other half-integer Bessel functions.

The idea is then to use the eigenvalue condition (5.128) to rephrase the question whether some state in $\mathcal{H}_{l_0}$ has lower energy than all states in $\mathcal{H}_l$ as the more tangible question whether the quantity

$$\int_0^\infty \left(\mathcal{J}_{l_0+1/2}^2(p) - \mathcal{J}_{l+1/2}^2(p)\right) \frac{p}{K_T(p)} \mathrm{d}p$$

is positive. By Theorem 5.8.1 there is an interval of p-values on which the integrand is positive and by Lemma 5.7.2 there are intervals of μ- and T-values such that the entire integral is positive.

Solving the eigenvalue problem

For any radial V, we can block diagonalize $K_T + V$ by using the orthogonal decomposition of $L^2(\mathbb{R}^3)$ into angular momentum sectors (5.28), namely $L^2(\mathbb{R}^3) = \bigoplus_{l=0}^\infty \mathcal{H}_l$ with $\mathcal{H}_l$ defined in (5.26). It is well-known [164] that the Fourier transform leaves each $\mathcal{H}_l$ invariant. Consequently, if we have $\alpha \in H^1(\mathbb{R}^3)$ satisfying the eigenvalue equation

$$(K_T + V)\,\alpha = E\alpha, \tag{5.126}$$

then we can decompose it as $\alpha = \sum_l \alpha_l$ with $\alpha_l \in \mathcal{H}_l$ mutually orthogonal. Taking the Fourier transform of (5.126) and using the fact that $V\alpha_l \in \mathcal{H}_l$ since V is radial, we get from orthogonality

$$K_T(p)\widehat{\alpha}_l(\mathbf{p}) + \widehat{V\alpha_l}(\mathbf{p}) = E\widehat{\alpha}_l(\mathbf{p}),$$

for every $l \geq 0$ and a.e. $\mathbf{p} \in \mathbb{R}^3$. Thus, we can study each component α_l separately. When $V_{\lambda,R}$ is the specific radial potential (5.6), we can say even more.

Lemma 5.7.1. *Let $V_{\lambda,R}$ be as in* (5.6) *and let l be a non-negative integer. We write $\mathcal{J}_{l+\frac{1}{2}}$ for the Bessel function of the first kind of order $l+1/2$. Let $E < 2T$ if $\mu \geq 0$ and $E < \frac{|\mu|}{\tanh(|\mu|/(2T))}$ if $\mu < 0$. Then*

$$\ker\left(K_T + V_{\lambda,R} - E\right) \cap \mathcal{H}_l \neq \emptyset \tag{5.127}$$

is equivalent to the "eigenvalue condition"

$$1 = \lambda \int_0^\infty \frac{pR}{K_T(p) - E} \mathcal{J}^2_{l+\frac{1}{2}}(pR) \mathrm{d}p. \tag{5.128}$$

Moreover, if (5.127) *holds, then* $\ker\left(K_T + V_{\lambda,R} - E\right) = \operatorname{span}\{\rho_l\} \otimes \mathcal{S}_l$ *with*

$$\rho_l(r) = r^{-1/2} \int_0^\infty p \frac{\mathcal{J}_{l+\frac{1}{2}}(rp)\mathcal{J}_{l+\frac{1}{2}}(Rp)}{K_T(p) - E} \mathrm{d}p. \tag{5.129}$$

Since $|\mathcal{J}_{l+\frac{1}{2}}(p)| \leq Cp^{-1/2}$, the numerator in (5.128) and (5.129) poses no threat for convergence of the integral.

Proof. By the definition of $\mathcal{H}_l$, we have

$$\alpha_l(\mathbf{x}) = \sum_{m=-l}^{l} \alpha_{l,m}(r) Y_l^m(\vartheta, \varphi), \qquad \mathbf{x} \equiv (r, \vartheta, \varphi).$$

We suppose α_l satisfies $\left(K_T + V_{\lambda,R}\right)\alpha_l = E\alpha_l$. Recall that the Fourier transform not only leaves each $\mathcal{H}_l$ invariant, it also reduces to the Fourier-Bessel transform $\mathcal{F}_l$ on it [164]. That is, a function of the form $f(\mathbf{x}) = g(r)Y_l^m(\vartheta, \varphi)$ has Fourier transform given by

$$\widehat{f}(\mathbf{p}) = i^{-l} \left(\mathcal{F}_l g\right)(p)\, Y_l^m(\vartheta, \varphi), \qquad \mathbf{p} \equiv (p, \vartheta, \varphi), \tag{5.130}$$

where the Fourier-Bessel transform reads

$$\mathcal{F}_l g(p) = \int_0^\infty s^{3/2} p^{-1/2} \mathcal{J}_{l+\frac{1}{2}}(sp) g(s) \mathrm{d}s. \tag{5.131}$$

We apply the Fourier transform to the eigenvalue equation. By (5.130) and orthogonality of the spherical harmonics,

$$(K_T(p) - E)\mathcal{F}_l \alpha_{l,m}(p) + \mathcal{F}_l(V_{\lambda,R}\alpha_{l,m})(p) = 0$$

for all m and a.e. $\mathbf{p} \in \mathbb{R}^3$. The assumption on E is such that $K_T(p) - E > 0$ and therefore

$$\mathcal{F}_l \alpha_{l,m}(p) = -\frac{\mathcal{F}_l(V_{\lambda,R}\alpha_{l,m})(p)}{K_T(p) - E}. \tag{5.132}$$

So far we only used that the potential is radial. Since $V_{\lambda,R} = -\lambda\delta(|\cdot| - R)$,

$$\begin{aligned} -\mathcal{F}_l(V_{\lambda,R}\alpha_{l,m})(p) &= -\alpha_{l,m}(R)(\mathcal{F}_l V_{\lambda,R})(p) \\ &= \lambda\alpha_{l,m}(R)R^{3/2}p^{-1/2}\mathcal{J}_{l+\frac{1}{2}}(Rp). \end{aligned}$$

Plugging this back into (5.132), we find the following explicit expression for the solution to the eigenvalue problem:

$$\mathcal{F}_l \alpha_{l,m}(p) = \lambda\alpha_{l,m}(R)R^{3/2}p^{-1/2}\frac{\mathcal{J}_{l+\frac{1}{2}}(Rp)}{K_T(p) - E} \tag{5.133}$$

Now we apply $\mathcal{F}_l^{-1}$ which, by unitarity of the Fourier transform, has the operator kernel $r^{-1/2}k^{3/2}\mathcal{J}_{l+\frac{1}{2}}(rk)$ when evaluated at $r > 0$. For all $r > 0$, we have

$$\alpha_{l,m}(r) = \alpha_{l,m}(R)\lambda R^{3/2}r^{-1/2}\int_0^\infty p\frac{\mathcal{J}_{l+\frac{1}{2}}(rp)\mathcal{J}_{l+\frac{1}{2}}(Rp)}{K_T(p) - E}\mathrm{d}p$$

Note that we may assume that for some m, $\alpha_{l,m}(R) \neq 0$, since otherwise $\alpha_l \equiv 0$. Evaluating the above expression for that particular m at $r = R$ gives (5.128). We write $\alpha_{l,m}(R) = c_{l,m}\lambda^{-1}R^{-3/2}$ and absorb $c_{l,m}$ into the angular part $\mathcal{S}_l$ to get (5.129). Clearly the argument works in reverse, proving the claimed equivalence. □

Choosing μ and T

From now on, let $\mu > 0$. The following lemma concerns the quantity

$$\int_0^\infty \frac{p}{K_T(p)}f(p)\mathrm{d}p.$$

Suppose we know that $f > \varepsilon$ on some interval I, while f may be negative outside of I. Our goal in this section is to choose the right values of μ and T such that the above integral is then also positive.

The basic idea is to view $p/K_T(p)$ as a weight function which is centered at the point $p = \sqrt{\mu}$, where it takes a value proportional to T^{-1}. By making T small enough, we can ensure that the neighborhood of the point $p = \sqrt{\mu}$ dominates in the above integral. By choosing $\sqrt{\mu} \in I$ and T sufficiently small, the integral will pick up mostly points where f is positive and will therefore yield a positive value itself. This is spelled out in the following lemma.

We will eventually apply this lemma with $f = \mathcal{J}_{l_0+1/2}^2 - \mathcal{J}_{l+1/2}^2$ and positivity of the above integral will translate via (5.128) to the statement that the angular momentum sector $\mathcal{H}_{l_0}$ has lower energy than $\mathcal{H}_l$.

Lemma 5.7.2. *Let $f : \mathbb{R}_+ \to \mathbb{R}$ be a continuous function satisfying $|f(p)| \leq C_f(1+p^2)^{-1/2}$ for some $C_f > 0$. Suppose there exists $\varepsilon > 0$ and an interval (a,b) such that $f > \varepsilon$ on (a,b). Then,*

(i) for every $\delta > 0$ small enough, there exists $T_* > 0$ and an interval I such that for every $\mu \in I$ and $T \in (0, T_*)$,

$$\int_0^\infty \frac{p}{K_T(p)} f(p) \mathrm{d}p > 0. \tag{5.134}$$

(ii) letting $\delta := \frac{b^2-a^2}{4}$, one can choose

$$I := (a^2+\delta, b^2-\delta), \qquad T_* := \frac{\delta}{2} \exp\left(-\frac{2C_f\left(\sqrt{1+2b^2}+\frac{1}{2b}\right)}{\varepsilon\delta}\right). \tag{5.135}$$

Proof. Let $\mu \in (a^2+\delta, b^2-\delta)$. Since $\frac{p}{K_T(p)} > 0$ and $|\tanh| \leq 1$, we can estimate

$$\int_0^\infty \frac{pf(p)}{K_T(p)} \mathrm{d}p \geq -C_f \int_{[0,a)\cup(b,\infty)} \frac{p}{(1+p^2)^{1/2}|p^2-\mu|} \mathrm{d}p + \varepsilon \int_a^b \frac{p}{K_T(p)} \mathrm{d}p. \tag{5.136}$$

In the first integral, we estimate pointwise

$$|p^2-\mu|^{-1} \leq \delta^{-1}(\chi_{\{p\leq 2b\}} + 2p^{-2}\chi_{\{p>2b\}})$$

with χ_A denoting the characteristic function of a set A. This gives

$$-C_f \int_{[0,a)\cup(b,\infty)} \frac{p}{(1+p^2)^{1/2}|p^2-\mu|} \mathrm{d}p \geq -C_f\delta^{-1}\left(\sqrt{1+2b^2}+\frac{1}{2b}\right) \tag{5.137}$$

In the second integral, we change variables and use $\mu \in (a^2+\delta, b^2-\delta)$ with $\tanh(u)/u > 0$ to get

$$\int_a^b \frac{p}{K_T(p)} \mathrm{d}p = \frac{1}{2}\int_{\frac{a^2-\mu}{2T}}^{\frac{b^2-\mu}{2T}} \frac{\tanh(u)}{u} \mathrm{d}u > \int_{-\frac{\delta}{2T}}^{\frac{\delta}{2T}} \frac{\tanh(u)}{u} \mathrm{d}u > \log\left(\frac{\delta}{2T}\right),$$

where in the last step we also used that $\tanh x \geq 1/2$ for $x \geq 1$. Combining everything, we get

$$\int_0^\infty \frac{pf(p)}{K_T(p)} \mathrm{d}p \geq -C_f\delta^{-1}\left(\sqrt{1+2b^2}+\frac{1}{2b}\right) + \varepsilon \log\left(\frac{\delta}{2T}\right). \tag{5.138}$$

The claim follows from some algebra. □

Proof of Theorem 5.4.1

Proof of (i). By rescaling the parameters μ, λ and T, we may assume that $R = 1$. We fix a non-negative integer l_0 and invoke Theorem 5.8.1 to get $\varepsilon > 0$ and an interval (a, b) on which $\mathcal{J}^2_{l_0+1/2} - \mathcal{J}^2_{l+1/2} > \varepsilon$ for all $l \neq l_0$. Then we apply Lemma 5.7.2 to

$$f := \mathcal{J}^2_{l_0+1/2} - \mathcal{J}^2_{l+1/2},$$

which satisfies

$$|f(p)| \leq 2^{1/2}(1 + p^2)^{-1/2}. \tag{5.139}$$

and so $C_f = 2^{1/2}$ in Lemma 5.7.2. To prove (5.139), ones uses statement (ii) in Lemma 5.8.5 to get $\mathcal{J}^2_\nu(p) \leq M^2_\nu(p) \leq \frac{1}{p}$ for all ν. Together with $|\mathcal{J}_\nu| \leq 1$ from (9.1.60) in [4], this implies $|f(p)| \leq \min\{1, p^{-1}\}$ and hence (5.139).

Note that T_* and I defined in Lemma 5.7.2 (ii) work for all $l \neq l_0$, because they depend on f only through (a, b), which is uniform in f by Theorem 5.8.1, and through $C_f = 2^{3/2}$. Hence, Lemma 5.7.2 provides $T_* > 0$ and an interval I such that for all $\mu \in I$, all $T < T_*$ and all $l \neq l_0$ we have

$$\int_0^\infty \frac{p}{K_T(p)} \left(\mathcal{J}^2_{l_0+1/2}(p) - \mathcal{J}^2_{l+1/2}(p)\right) \mathrm{d}p > 0 \tag{5.140}$$

For every non-negative integer l, we define the function

$$\lambda_l(T, \mu) := \left(\int_0^\infty \frac{p}{K_T(p)} \mathcal{J}^2_{l+1/2}(p) \mathrm{d}p\right)^{-1} \tag{5.141}$$

which is chosen such that λ satisfies the eigenvalue condition (5.128) with $E = 0$. We write

$$E_l(T, \mu, \lambda) := \inf \operatorname{spec} (K_T + V_{\lambda,1}) \big|_{\mathcal{H}_l}.$$

With these definitions, Lemma 5.7.1 says

$$E_l(T, \mu, \lambda_l(T, \mu)) = 0 \tag{5.142}$$

At the heart of our proof is the following monotonicity argument. For all $\mu \in I$, all $T < T_*$ and all $l \neq l_0$, we have

$$0 = E_l(T, \mu, \lambda_l(T, \mu)) < E_l(T, \mu, \lambda_{l_0}(T, \mu)), \tag{5.143}$$

where the inequality holds by the variational principle applied to the operator $(K_T + V_{\lambda,1})\big|_{\mathcal{H}_l}$ and the observation that (5.140) is equivalent to $\lambda_{l_0}(T, \mu) <$

$\lambda_l(T,\mu)$. (The inequality is strict because $\langle\alpha, V_{\lambda,1}\alpha\rangle = -\lambda\alpha(R)^2$ is either strictly monotone decreasing in λ or identically zero and in the latter case the energy has to be at least $2T$.)

This would already prove (5.54) and (5.55) under the condition that one fixes $T < T_*$ and determines λ through (5.140). We find it physically more appealing to fix λ small enough and determine T instead. To this end, we observe that $T \mapsto \lambda_{l_0}(T,\mu)$ is monotone increasing, because $T \mapsto K_T(p)$ is monotone increasing for every $p > 0$. Therefore, for every $\mu \in I$, we have the monotone increasing inverse function

$$\begin{aligned}(0, \lambda_{l_0}(T_*,\mu)) &\to (0, T_*)\\ \lambda &\mapsto T(\lambda,\mu)\end{aligned}$$

satisfying $\lambda_{l_0}(T(\lambda,\mu),\mu) = \lambda$. To remove the μ-dependence from the maximal value for λ, we set

$$\lambda_* := \min_{\mu\in\bar{I}} \lambda(T_*,\mu) \tag{5.144}$$

and note that $\lambda_* > 0$ since the integral in (5.141) is continuous in μ by dominated convergence. For $\lambda < \lambda_*$, (5.142) and (5.143) become

$$E_{l_0}(T(\lambda,\mu),\mu,\lambda) = 0, \qquad E_l(T(\lambda,\mu),\mu,\lambda) > 0, \quad \forall l \neq l_0.$$

This proves that for all $\mu \in I$ and all $\lambda < \lambda_*$, there exists $T_0 < T_*$ (namely $T_0 := T(\lambda,\mu)$) such that (5.54) holds (modulo restoring the R parameter). Moreover, (5.55) is a direct consequence of the explicit characterization of $\ker(K_{T_c} + V)$ in Lemma 5.7.1. Finally, (5.56) follows via the variational principle from the observation that $T \mapsto K_T(p)$ is strictly increasing for all $p > 0$ and so $T \mapsto E_{l_0}(T,\mu,\lambda)$ is strictly increasing as well, as long as it stays below $2T$. □

Proof of (ii). Consider the function

$$\delta_T : \mu \mapsto \int_0^\infty \frac{p}{K_T(p)} \left(\mathcal{J}_{1/2}^2(p) - \mathcal{J}_{5/2}^2(p)\right) \mathrm{d}p.$$

<u>Claim:</u> *There exists $T_{**} > 0$ such that for all $0 < T < T_{**}$ there exists $\mu_T > 0$ such that $\delta_T(\mu_T) = 0$. Moreover, $\sqrt{\mu_T} \to z_{1/2}$ as $T \to 0$, where $z_{1/2} = \min\{z > 0 : \mathcal{J}_{1/2}^2(z) = \mathcal{J}_{5/2}^2(z)\}$.*

The claim follows essentially from the intermediate value theorem. Before we give the details, we explain how one may conclude statement (ii) from the claim. Let $0 < T < T_{**}$. By definition (5.141), $\delta_T(\mu_T) = 0$ implies $\lambda_0(T, \mu_T) = \lambda_2(T, \mu_T)$. By Lemma 5.7.1 and using the notation (5.142),

$$E_0(T, \mu_T, \lambda_0(T, \mu_T)) = E_2(T, \mu_T, \lambda_0(T, \mu_T)) = 0. \tag{5.145}$$

This implies $\subset$ in (5.59) according to Lemma 5.7.1. Equation (5.60) follows by the same monotonicity argument as in the proof of statement (i) above.

In order to prove (5.58) with the choices $\mu \equiv \mu_T$ and $\lambda \equiv \lambda_0(T, \mu_T)$ and the remaining $\supset$ in (5.59), we shall show that there exists $T_* \in (0, T_{**}]$ such that for all $0 < T < T_*$,

$$E_l(T, \mu_T, \lambda_0(T, \mu_T)) > 0, \quad \forall l \geq 4, l \text{ is even}. \tag{5.146}$$

By Theorem 5.8.1 (ii) (with $l_0 = 1$) and Lemma 5.8.6, there exists an open interval containing $z_{1/2}$ such that

$$\mathcal{J}_{5/2}^2 - \sup_{\substack{l \geq 4 \\ l \text{ even}}} \mathcal{J}_{l+1/2}^2 > \varepsilon' \quad \text{on this interval.}$$

As in part (i), Lemma 5.7.2 provides $T_{**} > 0$ and an interval I' containing $z_{1/2}^2$ such that for all $\mu \in I'$, all $T < T_{**}$ and all even $l \geq 4$ we have

$$\int_0^\infty \frac{p}{K_T(p)} \left(\mathcal{J}_{5/2}^2(p) - \mathcal{J}_{l+1/2}^2(p) \right) \mathrm{d}p > 0\,. \tag{5.147}$$

Since the second part of the claim gives $\mu_T \to z_{1/2}^2$ as $T \to 0$, we may assume, after decreasing T_{**} to T_* if necessary, that $\mu_T \in I'$ for all $0 < T < T_*$. Therefore (5.147) implies that $\lambda_0(T, \mu_T) = \lambda_2(T, \mu_T) < \lambda_l(T, \mu_T)$ for all $T < T_*$ and all even $l \geq 4$. By the same variational argument as in (5.143), this implies (5.146).

We now prove the claim. The reader may find it helpful to consider Figure 5.1. Since $\mu \mapsto K_T(p)$ is continuous for every p, $\mu \mapsto \delta_T$ is also continuous by dominated convergence. Let x_l ($l = 0, 2$) denote the first maximum of $\mathcal{J}_{l+1/2}$. It is well-known that $x_0 < x_2$ [145] and that $\mathcal{J}_{1/2}^2(x_0) > \mathcal{J}_{5/2}^2(x_0)$ and $\mathcal{J}_{5/2}^2(x_2) > \mathcal{J}_{1/2}^2(x_2)$ (which is also a very special case of our Theorem 5.8.1 (i)). By continuity these inequalities hold also in neighborhoods of x_0 and x_2. Therefore Lemma 5.7.2 provides open intervals $I_l \subset \mathbb{R}_+$ ($l = 0, 2$), containing x_l, and a $T_{**} > 0$ such that for all $T < T_{**}$, we have $\delta_T > 0$ on I_0 and $\delta_T < 0$ on I_2. By the intermediate value theorem, for any $T < T_{**}$ there is a $\mu_T \in [\sup I_0, \inf I_2]$ with $\delta_T(\mu_T) = 0$. This proves the first part of the claim.

We are left with showing that $\sqrt{\mu_T} \to z_{1/2}$ as $T \to 0$. Since $\mu_T \in [\sup I_0, \inf I_2]$ is bounded, it has a limit point as $T \to 0$. We argue by contradiction and assume that there is a limit point $\tilde{z}$ different from $z_{1/2}$. By Lemma 5.8.6, $z_{1/2}$ is also the position of the first critical point of $\mathcal{J}_{l+3/2}$. By the interlacing properties of the zeros of Bessel functions and their derivatives, see e.g. [145], $z_{1/2} \in (x_0, x_2)$ and there is no other point $z \in (x_0, x_2)$ at which $\mathcal{J}_{1/2}^2(z) = \mathcal{J}_{5/2}^2(z)$. Therefore $\mathcal{J}_{1/2}^2 - \mathcal{J}_{5/2}^2$ is either strictly positive or strictly negative at $\tilde{z}$ and, by continuity, also in an open interval containing $\tilde{z}$. Lemma 5.7.2 provides an open interval $\tilde{I}$ containing $\tilde{z}^2$ and a $\tilde{T} > 0$ such that $\delta_T(\mu)$ is either strictly positive or strictly negative for all $T < \tilde{T}$ and $\mu \in \tilde{I}$. Since $\tilde{z}$ is a limit point of $\sqrt{\mu_T}$, there is a sequence $T_m \to 0$ with $\mu_{T_m} \to \tilde{z}^2$. In particular, $\mu_{T_m} \in \tilde{I}$ and $T_m < \tilde{T}$ for all sufficiently large m. Thus, $\delta_{T_m}(\mu_{T_m})$ is either strictly positive or strictly negative for all sufficiently large m. This, however, contradicts the construction of μ_T, according to which $\delta_T(\mu_T) = 0$ for all $T < T_{**}$. Thus, we have shown that $\sqrt{\mu_T} \to z_{1/2}$. □

5.8 Properties of Bessel functions

While one might expect the following fact about Bessel functions to be known, it appears to be new:

At its first maximum, a half-integer Bessel function is strictly larger than (the absolute value of) all other half-integer Bessel functions.

The precise statement is in Theorem 5.8.1 (i) below. It extends to families of Bessel functions $\{\mathcal{J}_{\nu+k}\}_{k\in\mathbb{Z}_+}$ with $\nu \in [0,1]$, in particular to the family of integer Bessel functions. We acknowledge a helpful discussion on mathoverflow.net [135] that led to Lemma 5.8.5.

Let l_0 be a non-negative integer. We recall that the Bessel function $\mathcal{J}_{l_0+1/2}$ (of the first kind, of order $l_0 + 1/2$) vanishes at the origin and then increases to its first maximum, whose location we denote as usual by $j'_{l_0+1/2,1}$. The following theorem says that at $j'_{l_0+1/2,1}$, $\mathcal{J}_{l_0+1/2}^2$ is strictly larger than any other $\mathcal{J}_{l+1/2}^2$ with l a non-negative integer different from l_0.

Theorem 5.8.1. *Let $\mathbb{Z}_+$ denote the set of non-negative integers and let $l_0 \in \mathbb{Z}_+$. Recall that $j'_{l_0+1/2,1}$ denotes the position of the first maximum of $\mathcal{J}_{l_0+1/2}$.*

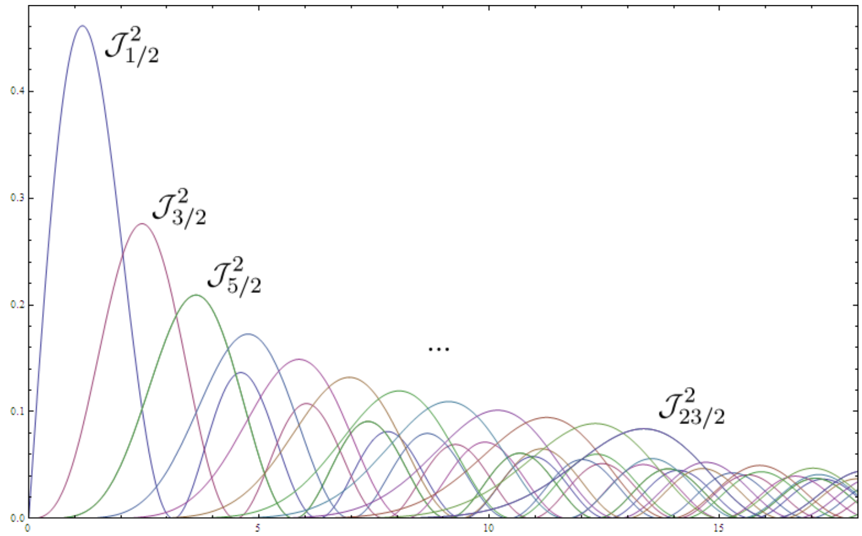

Figure 5.1: A plot of the squared Bessel functions $\mathcal{J}^2_{1/2}, \mathcal{J}^2_{3/2}, \mathcal{J}^2_{5/2}, \dots, \mathcal{J}^2_{23/2}$. Observe that in an open interval around its maximum, each function is the largest one among all the shown ones (in particular it is the largest among all the $\mathcal{J}^2_{l+1/2}$ according to Lemma 5.8.3).

(i) There exist $\varepsilon > 0$ *and an open interval* I *containing* $j'_{l_0+1/2,1}$ *such that*

$$\mathcal{J}^2_{l_0+1/2} - \sup_{l \in \mathbb{Z}_+ \setminus \{l_0\}} \mathcal{J}^2_{l+1/2} > \varepsilon \quad \text{on } I. \tag{5.148}$$

(ii) If $l_0 \geq 1$*, then* $\mathcal{J}_{l_0-1/2}(j'_{l_0+1/2,1}) = \mathcal{J}_{l_0+3/2}(j'_{l_0+1/2,1})$ *and there exist* $\varepsilon' > 0$ *and an open interval* I' *containing* $j'_{l_0+1/2,1}$ *such that*

$$\min\{\mathcal{J}^2_{l_0-1/2}, \mathcal{J}^2_{l_0+3/2}\} - \sup_{\substack{l \geq l_0+3 \\ l-l_0 \text{ odd}}} \mathcal{J}^2_{l+1/2} > \varepsilon' \quad \text{on } I'. \tag{5.149}$$

Remark 5.8.2. *Statement (i) is the key result and implies Theorem 5.4.1 (i). Statement (ii) is used to prove Theorem 5.4.1 (ii).*

The proof of (i) in Theorem 5.8.1 is split into three Lemmata, each treating one of the following three regimes of l:

$$\begin{aligned} \mathcal{L}_{>} &:= \{l \in \mathbb{Z}_+ \ : \ l > l_0\}, \\ \mathcal{L}_{\lesssim} &:= \left\{l \in \mathbb{Z}_+ \ : \ l < l_0,\ j_{l+1/2,1} \geq j'_{l_0+1/2,1}\right\}, \\ \mathcal{L}_{\ll} &:= \left\{l \in \mathbb{Z}_+ \ : \ l < l_0,\ j_{l+1/2,1} < j'_{l_0+1/2,1}\right\}. \end{aligned}$$

Here, as usual, $j_{l+1/2,1}$ denotes the first positive zero of $\mathcal{J}_{l+1/2}$. The most cumbersome regime is $\mathcal{L}_{\ll}$. The proof there is based on a combination of some hands-on elementary estimates and bounds on the zeros of Bessel functions and their derivatives, which we could not find in the usual reference books [4],[173]. The first regime $\mathcal{L}_>$ is the easiest

Lemma 5.8.3. *There exist $\varepsilon_1 > 0$ and an open interval I_1 containing $j'_{l_0+1/2,1}$ such that*

$$\mathcal{J}^2_{l_0+1/2} - \sup_{l>l_0} \mathcal{J}^2_{l+1/2} \geq \varepsilon_1 \quad \text{on } I_1 \tag{5.150}$$

Proof. According to [117], the function

$$\nu \mapsto \max_y |\mathcal{J}_\nu(y)|$$

is strictly decreasing. Therefore

$$\varepsilon_1 := \frac{1}{2}\left(\mathcal{J}^2_{l_0+1/2}(j'_{l_0+1/2,1}) - \max_y \mathcal{J}^2_{l_0+3/2}(y)\right)$$

is strictly positive. By continuity, there exists an open interval I_1 containing $j'_{l_0+1/2,1}$ such that for all $x \in I_1$,

$$|\mathcal{J}^2_{l_0+1/2}(j'_{l_0+1/2,1}) - \mathcal{J}^2_{l_0+1/2}(x)| < \varepsilon_1.$$

For $x \in I_1$, we have

$$\begin{aligned} \mathcal{J}^2_{l_0+1/2}(x) - \sup_{l>l_0} \mathcal{J}^2_{l+1/2}(x) &> -\varepsilon_1 + \mathcal{J}^2_{l_0+1/2}(j'_{l_0+1/2,1}) - \sup_{l>l_0} \max_y \mathcal{J}^2_{l+1/2}(y) \\ &\geq -\varepsilon_1 + \mathcal{J}^2_{l_0+1/2}(j'_{l_0+1/2,1}) - \max_y \mathcal{J}^2_{l_0+3/2}(y) \\ &= \varepsilon_1. \end{aligned}$$

□

Lemma 5.8.4. *There exist $\varepsilon_2 > 0$ and an open interval I_2 containing $j'_{l_0+1/2,1}$ such that*

$$\mathcal{J}^2_{l_0+1/2} - \sup_{l\in\mathcal{L}_{\lesssim}} \mathcal{J}^2_{l+1/2} \geq \varepsilon_2 \quad \text{on } I_2.$$

Proof. Since the supremum of finitely many continuous functions is itself continuous, it suffices to prove $\mathcal{J}^2_{l_0+1/2}(j'_{l_0+1/2,1}) > \mathcal{J}^2_{l+1/2}(j'_{l_0+1/2,1})$ for every $l \in \mathcal{L}_{\lesssim}$. We define the sequence $\{a_l\}_{l\in\mathcal{L}_{\lesssim}}$ by

$$\mathcal{J}_{l+1/2}(j'_{l_0+1/2,1}) = a_l \mathcal{J}_{l_0+1/2}(j'_{l_0+1/2,1}). \tag{5.151}$$

With this definition, the recurrence relation for Bessel functions from (9.1.27) in [4] appears in the form of a second-order difference equation

$$a_{l-1} = 2\frac{l+1/2}{x_0} a_l - a_{l+1} \tag{5.152}$$

with initial conditions $a_{l_0} = 1$ and $a_{l_0-1} = (l_0 + 1/2)/j'_{l_0+1/2,1}$. It is well-known that the latter quantity is strictly less than one, see eq. (3) on p. 486 of [173]. Moreover, $a_l \geq 0$ for all $l \in \mathcal{L}_{\lesssim}$, because $j_{l+1/2,1} \geq j'_{l_0+1/2,1}$ and all Bessel functions are positive before they first become zero. An easy induction lets us conclude from (5.152) that $a_l < a_{l+1} < 1$ for all $l \in \mathcal{L}_{\lesssim}$. In particular, $a_l \leq a_{l_0-1} = (l_0 + 1/2)/j'_{l_0+1/2,1} < 1$. Recalling the definition (5.151) of a_l, this proves the claim. □

We finally come to the regime $\mathcal{L}_{\ll}$. As a tool, we will use the "modulus" function defined by

$$M_\nu := \sqrt{\mathcal{J}_\nu^2 + \mathcal{Y}_\nu^2},$$

where $\mathcal{Y}_\nu$ is the Bessel function of the second kind. The first two statements of the following Lemma are known facts about the modulus function. Statement (iii) is the key result to derive (iv).

Lemma 5.8.5. *(i) The map $\nu \mapsto M_\nu(x)$ is strictly increasing for all $x > 0$.*

(ii) For all $x > \nu$,

$$M_\nu^2(x) < \frac{2}{\pi} \frac{1}{\sqrt{x^2 - \nu^2}}.$$

(iii) If $l_0 \geq 11$, there exists $l_1 < l_0$ such that we have both,

(iii.a) $\mathcal{J}^2_{l_0+1/2}(j'_{l_0+1/2,1}) > M^2_{l_1+1/2}(j'_{l_0+1/2,1})$

(iii.b) $j_{l_1+1/2,1} > j'_{l_0+1/2,1}$

(iv) There exist $\varepsilon_3 > 0$ and an open interval I_3 containing $j'_{l_0+1/2,1}$ such that

$$\mathcal{J}^2_{l_0+1/2} - \sup_{l \in \mathcal{L}_{\ll}} \mathcal{J}^2_{l+1/2} \geq \varepsilon_3 \quad \text{on } I_3.$$

The intuition why such l_1 as in (iii) should exist is based on a heuristic argument of which we learned through [135], involving asymptotic formulae for the relevant expression. To turn this into a rigorous proof, we need to replace the asymptotics by bounds that hold for all l_0 (or at least for all $l_0 \geq 11$). [78] contains results which are sufficient for our purposes when combined with a number of elementary estimates.

Proof. Statement (i) is a direct consequence of Nicholson' formula, see p. 444 in [173], and the fact that $K_0 > 0$. Statement (ii) is formula (1) on p. 447 of [173].

We come to statement (iii). For convenience, we write $m = l + 1/2$, so in particular $m_0 = l_0 + 1/2$. We also abbreviate $x_0 = j'_{l_0+1/2,1}$. The basic idea (inspired by asymptotics) is to choose

$$m_1 = m_0 - c m_0^{1/3}$$

with c small enough to have (iii.a) hold but large enough to have (iii.b) hold. By (i), (iii.a) is implied by

$$\frac{2}{\pi} \frac{1}{\sqrt{x_0^2 - m_1^2}} < \mathcal{J}_{m_0}^2(x_0). \tag{5.153}$$

By [78], we have the lower bound

$$x_0 > m_0 \exp\left(2^{-1/3} a_1' m_0^{-2/3} - 1.06 m_0^{-4/3}\right) \tag{5.154}$$

for all $m_0 \geq 11.5$. Here, a_1' is the absolute value of the first zero of the derivative of the Airy function, with a numerical value of about 1.018793. From $m_0 \geq 11.5$, we can conclude that the argument of the exponential in (5.154) is greater than $0.6 m_0^{-2/3}$. Thus, by the elementary estimate $e^y \geq 1 + y$, (5.154) implies the more manageable lower bound

$$x_0 > m_0 + 0.6 m_0^{1/3}$$

Setting $m_1 = m_0 - c m_0^{1/3}$ with c to be determined and using the above bound on x_0, as well as $m_0 \geq 11.5$, we see that (5.153) is implied by

$$\frac{2}{\pi} \frac{1}{\sqrt{1.26 + 2c - 0.19c^2}} < \left(m_0^{1/3} \max_x |\mathcal{J}_{m_0}(x)|\right)^2 \tag{5.155}$$

According to [117], $\nu \mapsto \nu^{1/3} \max_x |\mathcal{J}_\nu(x)|$ is an increasing function and so we can estimate the right-hand side in (5.155) from below by $\nu^{2/3} \max_x \mathcal{J}_\nu(x)^2$ for any $1/2 \leq \nu \leq m_0$. Unfortunately, the numerical value one obtains for the "worst case" $\nu = 1/2$ is not good enough to also get (iii.b). Instead, we assume that $c \leq 1$ and use $m_0 \geq 11.5$ to get $m_0 - c m_0^{-1/3} \geq 8.5$ and so

$$\left(m_0^{1/3} \max_x |\mathcal{J}_{m_0}(x)|\right)^2 > \left((8.5)^{1/3} \max_x |\mathcal{J}_{8.5}(x)|\right)^2 > 0.42$$

where the last inequality can be read off from a plot, for example. Therefore, (5.155) holds if we can find $c \leq 1$ that satisfies

$$\frac{2}{\pi} \frac{1}{\sqrt{1.26 + 2c - 0.19c^2}} < 0.42 \tag{5.156}$$

and it is easily seen that this holds for $c \in [0.5, 1]$.

Now, we want to ensure that c is also small enough to have (iii.b) hold, i.e. $j_{m_1} > x_0$. To this end, we invoke two more facts:

- the upper bound

$$x_0 < m_0 + 0.89 m_0^{1/3}. \tag{5.157}$$

  This is a consequence of the bound

$$x_0 < m_0 \exp\left(2^{-1/3} a_1' m_0^{-2/3}\right)$$

  from [78], where again $a_1' \approx 1.018793$, by noting that $m_0 \geq 11.5$ implies that the argument of the exponential, call it y, satisfies $y < 1.59$. On $[0, 1.59]$, we can estimate $\exp(y) < 1 + 1.09y$, as one can verify e.g. by plotting and this yields (5.157).

- the lower bound

$$j_{m_1} > m_1 + 1.85 m_1^{1/3} \tag{5.158}$$

  which we obtained from the optimal lower bound proved in [149] by rounding down. This is better than the bound one can derive from a corresponding result of [78] as we did above.

From (5.157) and (5.158), we see that $j_{m_1} > x_0$ will follow from

$$(m_0 - c m_0^{1/3}) + 1.85 (m_0 - c m_0^{1/3})^{1/3} > m_0 + 0.89 m_0^{1/3}, \tag{5.159}$$

Since $c \leq 1$ and $m_0 \geq 11.5$, we have $1 - c m_0^{-2/3} > 0.8$ and so (5.159) is implied by

$$c < (0.8)^3 * 1.85 - 0.89 = 0.827.$$

So any choice of $c \in [0.5, 0.8]$ will ensure that (iii.a) and (iii.b) hold.

We prove statement (iv). By continuity, it suffices to prove $\mathcal{J}_{l_0+1/2}^2(x_0) > \mathcal{J}_l^2(x_0)$ for all $l \in \mathcal{L}_{\ll}$ (which we recall means $l < l_0$ with $j_{l+1/2} \leq x_0$). Assume first that $l_0 \geq 11$. Choosing l_1 as in statement (iii), (iii.a) states

$$\mathcal{J}_{l_0+1/2}^2(x_0) > M_{l_1+1/2}^2(x_0) \tag{5.160}$$

and (iii.b) implies that $l_1 \in \mathcal{L}_{\lesssim}$. By the monotonicity of $\nu \mapsto j_\nu$, it holds that $l \in \mathcal{L}_{\ll}$ implies $l < l_1$. Thus, the definition of M_ν and statement (i) imply

$$\mathcal{J}_{l+1/2}^2 \leq M_{l+1/2}^2 \leq M_{l_1+1/2}^2. \tag{5.161}$$

Together with (5.160), this implies (iv) for $l_0 \geq 11$. Since for $l_0 = 0, 1$ there are no $l \ll l_0$, we may assume $l_0 \geq 2$. For $2 \leq l_0 \leq 10$, one can then check by hand that (5.160) holds with the choice $l_1 = l_0 - 2$. Since $l_0 - 1 \in \mathcal{L}_{\lesssim}$, we get that $l \in \mathcal{L}_{\ll}$ implies $l \leq l_1$ and so (5.161) applies for all such l. $\square$

Lemma 5.8.6. *For any positive integer l,*

$$\min\{z > 0 : \mathcal{J}^2_{l-1/2}(z) = \mathcal{J}^2_{l+3/2}(z)\} = j'_{l+1/2,1} \tag{5.162}$$

and $\mathcal{J}_{l-1/2}, \mathcal{J}_{l+1/2}, \mathcal{J}_{l+3/2}$ are positive on $(0, j'_{l+1/2,1}]$.

Proof. We recall the recurrence relation from (9.1.27) in [4], which says that for all $\nu, z > 0$,

$$\mathcal{J}_{\nu-1}(z) - \mathcal{J}_{\nu+1}(z) = 2\mathcal{J}'_\nu(z).$$

Applying this with $\nu = l + 1/2$, $z = j'_{l+1/2,1}$ we obtain $\mathcal{J}_{l-1/2}(j'_{l+1/2,1}) = \mathcal{J}_{l+3/2}(j'_{l+1/2,1})$ and hence $\leq$ in (5.162). Notice that by the interlacing properties of zeros and extrema of Bessel functions, see e.g. [145], $j'_{l+1/2,1}$ is to the left of the first positive zeros of $\mathcal{J}_{l-1/2}, \mathcal{J}_{l+1/2}, \mathcal{J}_{l+3/2}$. Since Bessel functions are positive before they reach their first positive zero, we conclude that $\mathcal{J}_{l-1/2}, \mathcal{J}_{l+1/2}, \mathcal{J}_{l+3/2}$ are positive on $(0, j'_{l+1/2,1}]$. In particular, $\mathcal{J}_{l-1/2}, \mathcal{J}_{l+3/2}$ are positive at the left side of (5.162), call it z_l, and so we can take square roots to get $\mathcal{J}_{l-1/2}(z_l) = \mathcal{J}_{l+3/2}(z_l)$. By the recurrence relation from above, $\mathcal{J}'_{l+3/2}(z_l) = 0$ implying $z_l \geq j'_{l+1/2,1}$, as claimed. □

It remains to give the

Proof of Theorem 5.8.1. Statement (i) is a direct consequence of Lemmata 5.8.3 to 5.8.5.

For statement (ii) we first observe that for any positive integer l,

$$\mathcal{J}^2_{l-1/2} > \mathcal{J}^2_{l+3/2}, \quad \text{on } (0, j'_{l+1/2,1}). \tag{5.163}$$

In fact, by standard asymptotics, this inequality holds near zero and, according to Lemma 5.8.6, $j'_{l+1/2,1}$ is the first point of intersection of $\mathcal{J}^2_{l-1/2}$ and $\mathcal{J}^2_{l+3/2}$. Therefore the inequality holds on all of $(0, j'_{l+1/2,1})$, as claimed.

We now use the fact that $j'_{l+1/2,1}$ is increasing in l [145]. Choose I' to be an open interval containing $j'_{l_0+1/2,1}$ whose closure is contained in $(0, j'_{l_0+5/2,1})$. Then by (5.163) (with $l = l_0 + 2$) and continuity there is an $\epsilon' > 0$ such that

$$\mathcal{J}^2_{l_0+3/2} \geq \mathcal{J}^2_{l_0+7/2} + \epsilon' \quad \text{on } I'.$$

Applying (5.163) successively with $l = l_0 + 4, l_0 + 6, \ldots$, we conclude that

$$\mathcal{J}^2_{l_0+3/2} \geq \sup_{\substack{l \geq l_0+3 \\ l-l_0 \text{ odd}}} \mathcal{J}^2_{l+1/2} + \epsilon' \quad \text{on } I',$$

which is one part of the claim. Finally, we want to prove the same inequality with $\mathcal{J}^2_{l_0-1/2}$ on the left side (with possibly smaller ϵ' and I'). Clearly, (5.163) implies that this is true on $I' \cap (0, j'_{l_0+1/2,1}]$. Now use continuity to find $\delta > 0$ such that $\mathcal{J}^2_{l_0-1/2} \geq \mathcal{J}^2_{l_0+3/2} - \epsilon'/2$ on $[j'_{l_0+1/2,1}, j'_{l_0+1/2,1} + \delta]$. Thus,

$$\mathcal{J}^2_{l_0-1/2} \geq \mathcal{J}^2_{l_0+7/2} + \epsilon'' \quad \text{on } I''$$

with $\epsilon'' = \epsilon'/2$ and $I'' = I' \cap (0, j'_{l_0+1/2,1} + \delta)$. As before, (5.163) now implies the inequality in part (ii). This completes the proof. $\square$

Chapter 6

CONDENSATION OF FERMION PAIRS IN A DOMAIN

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6.1 Introduction

We consider a gas of fermions at zero temperature in $d = 1, 2, 3$ dimensions and at chemical potential $\mu < 0$. The particles are confined to an open and bounded domain $\Omega \subseteq \mathbb{R}^d$ with Dirichlet (i.e. zero) boundary conditions. They interact via a microscopic local two-body potential V which admits a two-body bound state. Additionally, the particles are subjected to a weak external field W, which varies on a macroscopic length scale.

At low particle density, this leads to tightly bound fermion pairs. The pairs will approximately look like bosons to one another and, since we are at zero temperature, they will form a Bose-Einstein condensate (BEC). It was understood in the 1980s [119] [141] that BCS theory, initially used to describe Cooper pair formation in superconductors on much larger (but still microscopic) length scales [14], also applies in this situation. Moreover, the macroscopic variations of the condensate density are given in terms of the nonlinear Gross-Pitaevskii (GP) theory [60][148][151]. An effective GP theory was recently derived mathematically starting from the microscopic BCS theory, see [28][94] for the stationary case and [91] for the dynamical case. This is in the spirit of Gorkov's paper [85] on how Ginzburg-Landau theory arises from BCS theory for superconductors *at positive temperature*. The latter problem has been intensely studied mathematically in recent years [73][75][74][76][95].

The papers mentioned above all work under the assumption that the system has no boundary (either by working on the torus or on the whole space). In the present paper, we start from low-density BCS theory with Dirichlet boundary conditions and we show that the effective macroscopic GP theory *also has Dirichlet boundary conditions.*

Our result is new even in the linear setting. The formal statement and its comparatively short proof can be found in Appendix 6.12 and we hope that this part may serve to illustrate the ideas. In a nutshell, in the linear case we consider the two-body Schrödinger operator

$$H_h := \frac{h^2}{2}(-\Delta_{\Omega,x} + W(x) - \Delta_{\Omega,y} + W(y)) + V\left(\frac{x-y}{h}\right),$$

acting on $L^2(\Omega\times\Omega)$, where $-\Delta_\Omega$ is the Dirichlet Laplacian. H_h describes the energy of a fermion pair confined to Ω. While the center of mass variable $\frac{x+y}{2}$ and the relative variable $x-y$ *do not decouple due to the boundary conditions*, we show that, up to first subleading order as $h\to 0$, the ground state energy of H_h can be computed in a decoupled manner. Namely, one can separately minimize (a) in the relative variable without boundary conditions and (b) in the center of mass variable with Dirichlet boundary conditions and combine the results to obtain the leading and subleading terms in the asymptotics for the ground state energy of H_h as $h\downarrow 0$. For the details, we refer to Theorem 6.12.1.

At positive temperature, de Gennes [58] predicted that BCS theory with Dirichlet boundary conditions should instead lead to a Ginzburg-Landau theory with *Neumann boundary conditions*. We believe that the discrepancy with our result here is due to the fact that we study the system in the low density limit.

BCS theory with a boundary

Let $\Omega\subset\mathbb{R}^d$, $d=1,2,3$, be open; further assumptions on Ω are described below. In the BCS model, one considers so-called *BCS states* (also called "quasi-free" states), which are fully described by an operator

$$\Gamma = \begin{pmatrix} \gamma & \alpha \\ \overline{\alpha} & 1-\overline{\gamma} \end{pmatrix}, \qquad 0\le\Gamma\le 1 \tag{6.1}$$

acting on $L^2(\Omega)\oplus L^2(\Omega)$. Physically, γ is the one-body density matrix and α is the fermion pairing function, see also Remark 5.2.1 (ii). The condition $0\le\Gamma\le 1$ implies that $0\le\gamma\le 1$, $\overline{\alpha}=\alpha^*$ and $0\le\alpha\overline{\alpha}\le\gamma-\gamma^2$. (The last inequality can be proved by observing that $\gamma-\gamma^2-\alpha\overline{\alpha}$ is the top left entry of the non-negative block operator $\Gamma(1-\Gamma)$ and must therefore be a non-negative operator as well.)

We let $h>0$ denote the ratio between the microscopic and macroscopic length scales; it will be a small parameter in our study. The energy of unpaired electrons at chemical potential $\mu<0$ is described by the one-body Hamiltonian

$$\mathfrak{h} = -h^2\Delta_\Omega + h^2 W - \mu, \qquad W:\Omega\to\mathbb{R}.$$

Here, $-\Delta_\Omega$ is the Dirichlet Laplacian on Ω. By definition, it is the self-adjoint operator corresponding to the quadratic form

$$\int_\Omega |\nabla f(x)|^2 \mathrm{d}x, \qquad f \in H_0^1(\Omega).$$

The *BCS energy* of a BCS state Γ is given by

$$\mathcal{E}_\mu^{BCS}(\Gamma) = \mathrm{Tr}\,[\mathfrak{h}\gamma] + \iint_{\Omega^2} V\left(\frac{x-y}{h}\right) |\alpha(x,y)|^2 \mathrm{d}x\mathrm{d}y. \tag{6.2}$$

Here and in what follows, we denote by $\gamma(x,y)$ and $\alpha(x,y)$ the integral kernels of the operators γ and α. (The fact that γ and α are indeed integral operators is guaranteed by Definition 6.1.5 of admissible BCS states.)

Remark 6.1.1. *(i) The formulation of the BCS model that we use is due to [11][119]. A heuristic derivation from the quantum many-body Hamiltonian can be found in the appendix to [89].*

(ii) The matrix elements of a BCS state Γ have the following physical significance. If we write $\langle\cdot\rangle$ for the expectation value of an observable in the system state, then $\gamma(x,y) = \langle a_x^\dagger a_y\rangle$ is the one-particle density matrix and $\alpha(x,y) = \langle a_x a_y\rangle$ is the fermion pairing function. (Here $a_x^\dagger, a_x$ denote the fermion creation and annihilation operators.)

(iii) We ignore spin variables. Implicitly, the pairing function $\alpha(x,y)$ (which is symmetric since $\alpha^* = \overline{\alpha}$) is to be tensored with a spin singlet*, yielding an antisymmetric two-body wave function, as is required for fermions.*

(iv) For simplicity, we do not include an external magnetic field in the model. There is no apparent obstruction to applying the methods with a sufficiently regular and weak external magnetic field as in [73][74][94].

Throughout, we make

Assumption 6.1.2 (Regularity of V and W)**.** *$V : \mathbb{R}^d \to \mathbb{R}$ is a locally integrable function that is infinitesimally form-bounded with respect to $-\Delta$ (the ordinary Laplacian) and V is reflection-symmetric, i.e. $V(x) = V(-x)$. Moreover, $-\Delta + V$ admits a ground state of negative energy $-E_b$.*

We also assume that $W \in L^{p_W}(\Omega)$ with $2 \le p_W \le \infty$ if $d=1$, $2 < p_W \le \infty$ if $d=2$ and $3 \le p_W \le \infty$ if $d=3$.

Remark 6.1.3. *(i) The assumption that $-\Delta + V$ admits a ground state is critical for the fermion pairs to condense. Without it, the pairs would prefer to drift far apart to be energy-minimizing. (Strictly speaking, each fermion pair is described by the operator $-2\Delta + 2V$ and has the ground state energy $-2E_b$. We have made the factor two disappear for notational convenience; observe also the lack of a symmetrization factor $1/2$ in front of the V term in (6.2).)*

(ii) The integrability assumption on W is such that $W\psi \in L^2(\Omega)$ for every $\psi \in H_0^1(\Omega)$ and the numerical value of p_W is derived from the critical Sobolev exponent.

Note that the assumption implies that W is infinitesimally form-bounded with respect to $-\delta$. However, the assumption is stronger than infinitesimal form-boundedness and the two places where we use this additional strength are (a) for the semiclassical expansion (Lemma 6.3.2) and (b) for Davies' approximation result (Lemma 6.7.2).

Assumption 6.1.4 (Regularity of Ω)**.** *The open set $\Omega \subseteq \mathbb{R}^d$ is a bounded Lipschitz domain.*

We recall that a set Ω is a Lipschitz domain if its boundary can be locally represented as the graph of a Lipschitz continuous function. The formal definition is given in Appendix 6.11.

Definition 6.1.5 (Admissible states)**.** *We say that a BCS state Γ of the form* (6.1) *is* admissible, *if* $\mathrm{Tr}[\gamma^{1/2}(1-\Delta_\Omega)\gamma^{1/2}] < \infty$*. Here $\gamma^{1/2}$ denotes the square root in the sense of operators.*

An admissible state Γ has the integral kernel $\alpha \in H_0^1(\Omega^2)$ thanks to the operator inequality $\alpha\overline{\alpha} \leq \gamma$ and $\alpha^* = \overline{\alpha}$ (we skip the proof, see the last step in the proof of Proposition 6.4.2 for a closely related argument). We note

Proposition 6.1.6. *$\mathcal{E}_\mu^{BCS}$ is bounded from below on the set of admissible states Γ.*

In principle, this is a standard argument based on the operator inequality $\alpha\overline{\alpha} \leq \gamma$ and our assumption that V is infinitesimally form-bounded with respect to $-\Delta$. However, a little care has to be taken regarding the boundary conditions;

we leave the proof to the interested reader because the required ideas appear throughout the paper.

In this paper, we shall study the minimization problem

$$E_\mu^{BCS} := \inf_{\Gamma \text{ admissible}} \mathcal{E}_\mu^{BCS}(\Gamma). \tag{6.3}$$

Note that $E_\mu^{BCS} > -\infty$ by Proposition 6.1.6. We are especially interested in the occurrence of $E_\mu^{BCS} < 0$ and in that case we say that the system exhibits *fermion pairing.*

Here is the reasoning behind this definition: We will consider chemical potentials $\mu = -E_b + Dh^2$ with $D \in \mathbb{R}$ so that $\mathfrak{h} \geq 0$ for h small enough, see Proposition 6.5.3. Then $E_\mu^{BCS} < 0$ implies that any minimizer Γ must satisfy $\alpha \neq 0$, i.e. it must have a non-trival fermion pairing function α.

Main results. We now discuss our main results in words, they are stated precisely in Section 6.1 below.

By the monotonicity of $\mu \mapsto E_\mu^{BCS}$ for every fixed $h > 0$, there exists a unique critical chemical potential $\mu_c(h)$ such that we have fermion pairing iff $\mu > \mu_c(h)$. The first natural question is then whether one can compute $\mu_c(h)$. In our **first main result**, **Theorem 6.1.7**, we show that

$$\mu_c(h) = -E_b + h^2 D_c + O(h^{2+\nu}), \quad \text{as } h \downarrow 0.$$

That is, to lowest order in h, $\mu_c(h)$ is just one half of the binding energy of a fermion pair. The subleading correction term $D_c \in \mathbb{R}$ is the ground state energy of an explicit Dirichlet eigenvalue problem on Ω (the linearization of the GP theory below).

Physically, the choice of $\mu \approx \mu_c(h)$ corresponds to small density; this is explained after Proposition 6.1.11. We expect that for μ above and close to $\mu_c(h)$, the fermion pairs look like bosons to each other and (since we are at zero temperature) the pairs will form a Bose-Einstein condensate, which will then be describable by a Gross-Pitaevskii (GP) theory.

Accordingly, in our **second main result**, **Theorem 6.1.10**, we derive an effective, macroscopic GP theory of fermion pairs from the BCS model for all $\mu = -E_b + Dh^2$ with $D \in \mathbb{R}$. The resulting GP theory *also has Dirichlet boundary conditions.*

Theorems 6.1.7 and 6.1.10 show that the boundary conditions make a significant difference on the (macroscopic!) GP scale, a physically non-trivial fact. The results hold for the rather general class of bounded Lipschitz domains.

Related works. The BCS model that we consider has received considerable interest in recent years in mathematical physics. Most closely related to our paper are the derivations of effective GP theories for periodic boundary conditions in [94] and for a system in $\mathbb{R}^3$ at fixed particle number [28]. The dynamical analogue of this derivation was performed in [91]. The related, and technically more challenging, case of BCS theory close to the critical temperature for pair formation has also been considered: In [72][89], the critical temperature was described by a linear criterion. The analogue of Theorem 6.1.7 for the upper and lower critical temperatures was the content of [74]. In [75, 76] and especially [73] effective macroscopic Ginzburg-Landau theories have been derived.

We emphasize that all of these papers assume that the system has no boundary (either by working on the torus or on the whole space) and the same holds true for the resulting effective GP or GL theories. (We also mention that the derivation in [28] depends on $\|W\|_{L^\infty(\mathbb{R}^d)} < \infty$ and so one cannot obtain the Dirichlet boundary conditions as the limiting case of a sufficiently deep potential well from [28].)

Our main contribution is thus to show the *non-trivial effect of boundary conditions on the effective macroscopic GP theory*. As we mentioned in the introduction, this is in some contrast to de Gennes' arguments [58] at positive temperature and positive density.

Main result 1: The critical chemical potential

Considering definitions (6.2) and (6.3) of the BCS energy, we see that the non-positive function $\mu \mapsto E_\mu^{BCS}$ is monotone decreasing (and concave). This allows us to define the critical chemical potential $\mu_c(h)$ as the unique number (potentially infinity) such that

$$\mu_c(h) := \inf \left\{ \mu < 0 \ : \ E_\mu^{BCS} < 0 \right\} \tag{6.4}$$

If $\mu_c(h)$ is finite, then the monotonicity and continuity of the function $\mu \mapsto E_\mu^{BCS}$ allows us to write $\left\{ \mu \ : \ E_\mu^{BCS} < 0 \right\} = (\mu_c(h), \infty)$. The definition (6.4) is analogous to the definition of the upper and lower critical temperature in

[74], but the explicit dependence of the BCS energy on μ simplifies matters here.

Our first main result gives an asymptotic expansion of $\mu_c(h)$ in h up to second order, where the subleading term D_c is given as an appropriate Dirichlet eigenvalue, namely

$$D_c := \inf \operatorname{spec}_{L^2(\Omega)} \left(-\frac{1}{4}\Delta_\Omega + W \right) \tag{6.5}$$

The result is the analogue of the main result in [74] for the critical temperature.

Theorem 6.1.7 (Main result 1)**.** *We have*

$$\mu_c(h) = -E_b + D_c h^2 + O(h^{2+\nu}), \quad \text{as } h \downarrow 0$$

The exponent of the error term is $\nu := \min\{d/2, c_\Omega - \delta\}$ where $\delta > 0$ is arbitrarily small and $c_\Omega \in (0,1]$ depends only on Ω, see Remark 6.1.8 (iii) below.

Remark 6.1.8. *(i) It follows from the definition of D_c that the Dirichlet boundary conditions have a non-trivial effect on the value of $\mu_c(h)$.*

(ii) The critical value D_c is uniquely determined by $E_D^{GP} = 0$ for $D \leq D_c$ and $E_D^{GP} < 0$ for $D > D_c$, where E_D^{GP} is defined in (6.7) *and* (6.8) *below. For the proof, see Lemma 2.5 in [74].*

(iii) The constant c_Ω in the definition of ν is the constant such that the Hardy inequality (6.65) *holds on Ω. Under additional assumptions on Ω, quantitative information on c_Ω is known: If Ω is convex or if $\partial\Omega$ is given as the graph of a C^2 function, then $c_\Omega = 1$ which is optimal [30][132][134] and if $\Omega \subset \mathbb{R}^2$ is simply connected, then we can take $c_\Omega = 1/2$ [6].*

(iv) The asymptotic expansion of $\mu_c(h)$ to this order is the same as the expansion of the ground state energy of the two-body Schrödinger operator *H_h, see Theorem 6.12.1. Intuitively, this is due to the fact that at $\mu_c(h)$ fermion pairing just onsets, so the order parameter is small and the non-linear terms become negligible.*

Main result 2: Effective GP theory

Definition 6.1.9. *(i) We write α_* for the unique positive and L^2-normalized ground state of $-\Delta+V$. By definition, it satisfies $(-\Delta+V)\alpha_* = -E_b\alpha_*$.*

We let

$$g_{BCS} := (2\pi)^{-d} \int_{\mathbb{R}^d} (p^2 + E_b)|\widehat{\alpha}_*(p)|^4 \mathrm{d}p. \tag{6.6}$$

(ii) For any $D \in \mathbb{R}$ and $\psi \in H^1(\mathbb{R}^d)$, we define the Gross-Pitaevskii (GP) energy functional by

$$\mathcal{E}_D^{GP}(\psi) := \int_{\mathbb{R}^d} \left(\frac{1}{4}|\nabla\psi(X)|^2 + (W(X) - D)|\psi(X)|^2 + g_{BCS}|\psi(X)|^4 \right) \mathrm{d}X. \tag{6.7}$$

Here and in the following, we extend $W : \Omega \to \mathbb{R}$ by zero to obtain a function on $\mathbb{R}^d$ to compute the integral.

(iii) Given a domain $U \subset \mathbb{R}^d$, we will consider its Dirichlet GP energy, defined as

$$E_{U,D}^{GP} := \inf_{\psi \in H_0^1(U)} \mathcal{E}_D^{GP}(\psi). \tag{6.8}$$

Here and in the following, we extend $\psi \in H_0^1(U)$ by zero to obtain a function in $H^1(\mathbb{R}^d)$.

We now state our second main result. It says that the GP theory $\mathcal{E}_D^{GP}$ arises from $\mathcal{E}_{-E_b+Dh^2}^{BCS}$ as the scale parameter h goes to zero.

Theorem 6.1.10 (Main result 2)**.** *Let $\mu = -E_b + Dh^2$ with $D \in \mathbb{R}$.*

(i) As $h \downarrow 0$, we have

$$E_\mu^{BCS} = h^{4-d} E_{\Omega,D}^{GP} + O(h^{4-d+\nu}), \tag{6.9}$$

where ν is as in Theorem 6.1.7.

(ii) Let Ω be convex. Suppose that Γ is a BCS state such that

$$\mathcal{E}_\mu^{BCS}(\Gamma) \leq E_\mu^{BCS} + \varepsilon h^{4-d}$$

for some small $\varepsilon > 0$. Then, its upper right entry α in the sense of (6.1) *can be decomposed as*

$$\alpha(x,y) = h^{1-d}\psi\left(\frac{x+y}{2}\right)\alpha_*\left(\frac{x-y}{h}\right) + \xi\left(\frac{x+y}{2}, x-y\right) \tag{6.10}$$

with $\psi \in H_0^1(\Omega)$ satisfying $\mathcal{E}_D^{GP}(\psi) \leq E_{\Omega,D}^{GP} + \varepsilon + O(h^\nu)$ and $\xi \in H_0^1(\Omega \times \mathbb{R}^d)$ such that

$$\|\xi\|_{L^2(\Omega\times\mathbb{R}^d)}^2 + h^2\|\nabla\xi\|_{L^2(\Omega\times\mathbb{R}^d)}^2 \leq O(h^{4-d}). \tag{6.11}$$

The interpretation of Theorem 6.1.10 (ii) is that *GP theory describes the center-of-mass part* of the fermion pairing function of any *approximate minimizer* of the BCS energy. To see this, observe first that ξ is an error term in (6.10), because for the first term in (6.10) the norm in (6.11) is of order h^{2-d}. Therefore, to leading order in h, the fermion pairing function of any approximate BCS minimizer is of the form $\psi\left(\frac{x+y}{2}\right)\alpha_*\left(\frac{x-y}{h}\right)$. Here α_* describes the pair binding on the microscopic scale h. By contrast, ψ describes the center-of-mass of the pairs on a macroscopic scale and it must be an approximate minimizer of the GP energy.

If Ω is not convex, one can still get a weaker version of Theorem 6.1.10 (ii) in which ψ and the Dirichlet energy live on a slightly enlarged domain, see Theorem 6.2.1 (LB).

We close the presentation by explaining why the choice of $\mu = -E_b + Dh^2$ corresponds to a low density limit.

Proposition 6.1.11 (Convergence of the one-body density)**.** *Let Γ be a BCS state satisfying the inequality $\mathcal{E}^{BCS}_{-E_b+Dh^2}(\Gamma) \leq E^{BCS}_{-E_b+Dh^2} + o(h^{4-d})$ (e.g. Γ is an approximate minimizer as in Theorem 6.1.10 (ii)) and let ρ_γ denote its one-body density (i.e. $\rho_\gamma(x) = \gamma(x,x)$ if γ is continuous). Then we have*

$$h^{d-2}\rho_\gamma \rightharpoonup |\psi_*|^2, \qquad \text{in } L^{p'_W}(\Omega) \tag{6.12}$$

where ψ_* is a minimizer of E^{GP}_D. p'_W is the Hölder dual exponent of p_W.

We mention that minimizers of E^{GP}_D exist and are unique up to a complex phase by Proposition 6.2.5 (though they may be identically zero).

The proof of Proposition 6.1.11 is in Appendix 6.9. It is a classical argument which is based on Theorem 6.1.10 and the fact that the one-body density ρ_γ and the external field W are "dual variables" [84][129].

Note that we can test (6.12) against the indicator function 1_Ω to obtain the expected particle number

$$N := \int_\Omega \rho_\gamma \mathrm{d}x = h^{2-d}\int_\Omega |\psi_*|^2 \mathrm{d}x + o(h^{2-d}),$$

compare (1.14) in [94]. The expected particle density in microscopic units is given by

$$h^d N = h^2 \|\psi_*\|^2_{L^2(\Omega)} + o(h^2) \to 0.$$

We see that our scaling limit indeed corresponds to low density. (We point out that the physical model is somewhat pathological in $d = 1$ because even N will go to zero as $h \to 0$. Since N is only the *expected* particle number, the model still makes sense in principle, but it is of course debatable that statistical mechanics still applies in this case.)

Outline of the paper

The proof of the main results is based on two distinct key results.

- In **key result 1** (Theorem 6.2.1), we bound the BCS energy over Ω in terms of GP energies on a slightly smaller domain than Ω (upper bound) and on a slightly larger domain than Ω (lower bound). If Ω is convex, the lower bound simplifies to the GP energy on Ω itself. The general strategy here is as in [73][91][94], though some technical difficulties arise from the Dirichlet boundary conditions, see (i) and (ii) below. This part only requires Ω to have finite Lebesgue measure.

- In **key result 2** (Theorem 6.2.2), we show that the GP energy is *continuous under approximations of the domain* Ω, if Ω is a bounded Lipschitz domain. The idea is to use Hardy inequalities to control the boundary decay of GP minimizers using the fact that these lie in the operator domain of the Dirichlet Laplacian. This approach is due to Davies [54][55] who treated the linear case of Dirichlet eigenvalues. (Davies does not treat continuity under exterior approximations because a Hardy inequality is not sufficient for this to hold, see the example in Remark 6.2.4)

We point out that key result 1 concerns the many-body system. Key result 2, by contrast, is a continuity result for a certain class of nonlinear functionals on $\mathbb{R}^d$ and is based on ideas from spectral theory and geometry.

In **Section 6.2**, we present the two key results in detail and derive the two main results from them.

In **Section 6.3**, we present the semiclassical expansion (Lemma 6.3.2). This is an important tool in the proof of all parts of Theorem 6.2.1 (key result 1). The version here is very close to the one in [28], though we generalize it somewhat as described in (iii) below.

In **Section 6.4**, we prove the upper bound part of Theorem 6.2.1. We construct a trial state following [28][91], with an appropriate cutoff to ensure that it satisfies the Dirichlet boundary conditions. The semiclassical expansion then yields an upper bound by a GP energy in a slightly smaller region than Ω. One finishes the proof by applying the continuity of the GP energy under domain approximations (key result 2).

In **Sections 6.5-6.6**, we prove the lower bound part of Theorem 6.2.1. The overall strategy is as in [28][73]: One first proves an a priori decomposition result yielding (6.10) for the off diagonal entry α of any approximate BCS minimizer Γ (with H^1 control on the involved functions). This is Theorem 6.5.1 and it shows that the GP order parameter is naturally associated with the center of mass variable $\frac{x+y}{2}$ (living on the macroscopic scale). Then, one can use the semiclassical expansion on the main part of α to finish the proof.

While the overall strategy is as in [28][73], there are some significant difficulties due to the boundary conditions:

(i) The boundary conditions prevent the variables in the center of mass frame from decoupling as usual. This poses a problem, because the GP energy/order parameter should only depend on the center of mass variable. The solution we have found to this is to *forget the boundary conditions in the relative coordinate altogether*. (Note that this gives a lower bound, since Dirichlet energies decrease under an increase of the underlying function spaces.) In this way, we *decouple the variables* in the center of mass frame. Moreover, one has not lost much, thanks to the exponential decay of the Schrödinger eigenfunction α_* governing the relative coordinate via (6.10). This idea is most clearly seen in Appendix 6.12.

(ii) The center of mass variable $\frac{x+y}{2}$ naturally takes values in the set

$$\tilde{\Omega} := \frac{\Omega + \Omega}{2}.$$

After some steps in the lower bound, we are led to a GP energy on $\tilde{\Omega}$. Note that when Ω is convex, $\tilde{\Omega} = \Omega$ and so one is essentially done at this stage. If Ω is not convex, however, some additional work is required. The idea is to use the exponential decay of α_* again, the details are in Section 6.6.

(iii) We observe that the arguments from [28] can be extended to dimensions $d = 1, 2$ and to external potentials which satisfy $W \in L^{p_W}(\Omega)$. We do not see, however, that the arguments can be extended to the case $W = \infty$ on a set of positive measure (i.e. the Dirichlet boundary conditions).

In **Section 6.7**, we prove key result 2, Theorem 6.2.2. The crucial input are Davies' ideas [54][55] of deriving continuity of the Dirichlet energy under domain approximations from the Hardy inequality, see Lemma 6.7.2. Along the way, we need Theorem 6.7.3 which says that the Hardy inequality holds along a suitable sequence of exterior approximations Ω_ℓ to Ω, with uniform dependence of the Hardy constants on ℓ, and may be of independent interest.

Theorem 6.7.3 is proved in Appendix 6.11 by extending Necas' proof [140] of the Hardy inequality on any bounded Lipschitz domain. The appendix also contains the proofs of some technical results used in the main text, as well as a presentation of the *linear version of our main results*, the asymptotics of the ground state energy of the two-body Schrödinger operator H_h mentioned in the introduction (see Appendix 6.12).

Notation. We write $C, C', \ldots$ for positive, finite constants whose value may change from line to line. We typically do not track their dependence on parameters which are assumed to be fixed throughout, such as the dimension d and the potentials V and W. The dependence on D will be explicit only where relevant.

We will suppress the parameter dependence on μ and D in the following. That is, we will write $\mathcal{E}_\mu^{BCS} \equiv \mathcal{E}^{BCS}, \mathcal{E}_D^{GP} \equiv \mathcal{E}^{GP}$, etc.

Finally, we will abuse notation and identify a function $\psi \in H_0^1(U)$ on some domain $U \subset \mathbb{R}^d$ with the function on $\mathbb{R}^d$ that is obtained by extending ψ by zero. We note that this extension lies in $H^1(\mathbb{R}^d)$

6.2 The two key results

Key result 1: Bounds on the BCS energy

We bound the BCS energy on Ω in terms of GP energies on interior approximations of Ω for an upper bound ("UB") and on exterior approximations of Ω for a lower bound ("LB").

Let $\Omega \subset \mathbb{R}^d$ be an open set of finite Lebesgue measure. For $\ell > 0$, define the interior and exterior approximations of Ω

$$\Omega_\ell^- := \{X \in \Omega \ : \ \mathrm{dist}(X, \Omega^c) > \ell\}, \tag{6.13}$$

$$\Omega_\ell^+ := \left\{X \in \mathbb{R}^d \ : \ \mathrm{dist}(X, \Omega) < \ell\right\}, \tag{6.14}$$

and define $\Omega_0^\pm := \Omega$.

Theorem 6.2.1 (Key result 1)**.** *Let $\ell(h) := h\log(h^{-q})$ with $q > 0$ sufficiently large but fixed. Let $\mu = -E_b + Dh^2$ for some fixed $D \in \mathbb{R}$. Then:*

(UB) For every function $\psi \in H_0^1(\Omega_{\ell(h)}^-)$, there exists an admissible BCS state Γ_ψ such that

$$\mathcal{E}^{BCS}(\Gamma_\psi) = h^{4-d}\mathcal{E}^{GP}(\psi) + O(h^{5-d})(\|\psi\|_{H^1(\mathbb{R}^d)}^2 + \|\psi\|_{H^1(\mathbb{R}^d)}^4). \tag{6.15}$$

The implicit constant depends continuously on D.

(LB) Let Γ be an admissible BCS state satisfying $\mathcal{E}^{BCS}(\Gamma) \leq C_\Gamma h^{4-d}$. Then, there exists $\psi \in H_0^1(\Omega_{\ell(h)}^+)$ such that

$$\mathcal{E}^{BCS}(\Gamma) \geq h^{4-d}\mathcal{E}^{GP}(\psi) + O(h^{4-d+\nu'}), \tag{6.16}$$

where $\nu' = \min\{d/2, 1\}$. Moreover, there exists $\xi \in H_0^1(\tilde{\Omega} \times \mathbb{R}^d)$, $\tilde{\Omega} := \frac{\Omega + \Omega}{2}$, such that α can be decomposed as in (6.10) *and we have the bounds*

$$\begin{aligned} &\|\nabla\psi\|_{L^2(\Omega_{\ell(h)}^+)} \leq C\|\psi\|_{L^2(\Omega_{\ell(h)}^+)} \leq O(1), \\ &\|\xi\|_{L^2(\tilde{\Omega}\times\mathbb{R}^d)}^2 + h^2\|\nabla\xi\|_{L^2(\tilde{\Omega}\times\mathbb{R}^d)}^2 \leq O(h^{4-d})(\|\psi\|_{L^2(\tilde{\Omega})}^2 + C_\Gamma) \end{aligned} \tag{6.17}$$

The implicit constants depend continuously on D.

(LBC) If Ω is convex, then one can take $\ell(h) = 0$ everywhere in (LB). In particular, there exists $\psi \in H_0^1(\Omega)$ such that

$$\mathcal{E}^{BCS}(\Gamma) \geq h^{4-d}\mathcal{E}^{GP}(\psi) + O(h^{4-d+\nu'}). \tag{6.18}$$

Key result 2: Continuity of the GP energy under domain approximations

The following theorem says that, on any bounded Lipschitz domain Ω, we have continuity of the GP energy under domain approximations. The continuity is derived from the Hardy inequality (6.65) in an approach due to Davies [54][55], see also [68]. The details are in Section 6.7.

We recall Definition 6.1.9 of the GP energies and the conventions made therein.

Theorem 6.2.2. *Assume that Ω is a bounded Lipschitz domain. For $\ell > 0$, define $\Omega_\ell^\pm$ as before in Theorem 6.2.1. Then, there exists a constant $c_\Omega \in (0,1]$ such that*

$$|E^{GP}_{\Omega_\ell^\pm} - E^{GP}_\Omega| \leq O(\ell^{c_\Omega}). \tag{6.19}$$

Moreover, the statement holds irrespectively of the value of the parameters g_{BCS} and D in (6.8). *In particular it holds for $g_{BCS} = D = 0$ and then it shows that*

$$|D_c^\pm(\ell) - D_c| \leq O(\ell^{c_\Omega}), \qquad D_c^\pm(\ell) := \inf \operatorname{spec}_{L^2(\Omega)} \left(-\frac{1}{4}\Delta_{\Omega_\ell^\pm} + W \right). \tag{6.20}$$

Here $D_c \equiv D_c^\pm(0)$ is defined in (6.5).

Remark 6.2.3. *The constant c_Ω is the same as in Theorem 6.1.7; see Remark 6.1.8 (iii) for quantitative results on c_Ω if more information on Ω is known.*

We close with a cautionary example, which shows that a two-sided continuity result such as (6.19) cannot be valid without additional assumptions on the regularity of the boundary $\partial\Omega$.

Remark 6.2.4 (Exterior approximation is delicate)**.** *Consider the slit domain $\Omega = [-1,1]^2 \setminus ((-1,0] \times \{0\})$. The slit will disappear for any exterior approximation Ω_ℓ^+ ($\ell > 0$) and this will lead to an order one decrease of the GP energy. Therefore, the GP energy on Ω is* not continuous under exterior approximation. *(However, it is continuous under interior approximation: As discussed in Section 6.7, this follows from the validity of the Hardy inequality* (6.65) *on Ω, and since $\Omega \subset \mathbb{R}^2$ is simply connected, it satisfies the Hardy inequality with $c_\Omega = 1/2$ [6].)*

On GP minimizers

We collect some standard results about GP minimizers for later use. We recall Definition 6.1.9 of the GP energy.

Proposition 6.2.5. *(i) For any $\psi \in H^1(\mathbb{R}^d)$, we have the coercivity inequality*

$$\mathcal{E}^{GP}(\psi) \geq C_1 \|\psi\|^2_{H_0^1(\mathbb{R}^d)} - (C_2 + D)^2, \tag{6.21}$$

where the constants $C_1, C_2 > 0$ are independent of D.

(ii) *Let $U \subset \mathbb{R}^d$ be an open set of finite Lebesgue measure. Then $E_U^{GP} > -\infty$. Moreover, there exists a minimizer for E_U^{GP} and it is unique up to multiplication by a complex phase. Minimizing sequences are precompact in $H_0^1(U)$.*

(iii) *There exists $C > 0$, independent of U and D, such that the minimizer ψ_* corresponding to E_U^{GP} satisfies*

$$\|\Delta_U \psi_*\|_{L^2(U)} \leq C(1 + |D|)(\|\psi_*\|_{H_0^1(U)} + \|\psi_*\|_{H_0^1(U)}^3). \tag{6.22}$$

For completeness, the standard proof of these results is included in Appendix 6.8.

Derivation of the main results from the key results

In this section, we assume that the two key results (Theorems 6.2.1 and 6.2.2) hold.

Proof of main result 1, Theorem 6.1.7

Upper bound. Let $\mu = -E_b + Dh^2$ with $D = D_c + C_0 h^\nu$ for some constant $C_0 > 0$ to be determined. We will show that for large enough $C_0 > 0$, there exists an admissible BCS state Γ such that

$$\mathcal{E}^{BCS}(\Gamma) < 0. \tag{6.23}$$

By Definition (6.4) (and the comment following it), this implies the claimed upper bound $\mu_c(h) \leq -E_b + D_c h^2 + C_0 h^{2+\nu}$.

We let $\ell \equiv \ell(h) = h \log(h^{-q})$ with $q > 0$ large enough and we recall definitions (6.13) and (6.20) of Ω_ℓ^- and $D_c^-(\ell)$. Following [74] p.209, we choose $\psi = \theta \psi_\ell$, where $\theta > 0$ and $\psi_\ell \in H_0^1(\Omega_\ell^-)$ is the eigenfunction

$$(-\Delta_{\Omega_\ell^-} + W)\psi_\ell = D_c^-(\ell)\psi_\ell.$$

Optimizing over θ yields

$$\mathcal{E}^{GP}(\psi) = -C(D - D_c^-(\ell))^2, \qquad \theta = C'\sqrt{D - D_c^-(\ell)}. \tag{6.24}$$

Hence, any relevant norm of $\psi = \theta\psi_\ell$ is proportional to $\sqrt{D - D_c^-(\ell)}$. Since $\psi \in H_0^1(\Omega_{\ell(h)}^-)$, we can apply Theorem 6.2.1 (UB) to get an admissible BCS state Γ_ψ such that

$$\begin{aligned} h^{d-4}\mathcal{E}^{BCS}(\Gamma_\psi) =& \mathcal{E}^{GP}(\psi) + O(h^\nu)(\|\psi\|^2_{H^1(\mathbb{R}^d)} + \|\psi\|^4_{H^1(\mathbb{R}^d)}) \\ =& - C(D - D_c^-(\ell))^2 + O(h^\nu)(\theta^2\|\psi_\ell\|^2_{H^1(\mathbb{R}^d)} + \theta^4\|\psi_\ell\|^4_{H^1(\mathbb{R}^d)}). \end{aligned}$$

We have the a priori bound $\|\psi_\ell\|_{H^1(\mathbb{R}^d)} \leq O(1)$. Indeed, the infinitesimal-form boundedness of W with respect to $-\Delta_{\Omega_\ell^-}$ implies

$$\|\psi_\ell\|_{H^1(\mathbb{R}^d)} - C \leq D_c^-(\ell) \leq D_c^-(\ell_0),$$

where $\ell_0 > 0$ is fixed. In the second step, we used the fact that Dirichlet energies increase when the underlying domain decreases.

By our choice of D and the last part of Theorem 6.2.2, there exists $C_1 > 0$ such that

$$D = D_c + C_0 h^\nu \geq D_c^-(\ell) + (C_0 - C_1)h^\nu$$

and so, for $C_0 > C_1$,

$$h^{d-4}\mathcal{E}^{BCS}(\Gamma_\psi) \leq -C(C_0 - C_1)^2 h^{2\nu} + O(h^{2\nu})(C_0 - C_1).$$

We recall that the implicit constant depends on D in a continuous way. Let C_2 denote the maximum absolute value that this constant takes on the interval $[D_c - 1, D_c + 1]$. We choose $C_0 = 2C_2/C + C_1$. Then, for all small enough $h > 0$, $D = D_c + C_0 h^\nu \in [D_c - 1, D_c + 1]$ and consequently

$$h^{d-4}\mathcal{E}^{BCS}(\Gamma_\psi) \leq h^{2\nu}(C_0 - C_1)(-C(C_0 - C_1) + C_2) < 0.$$

This proves (6.23) and hence the claimed upper bound on $\mu_c(h)$. □

Lower bound (convex case). Let $\mu = -E_b + Dh^2$ and $D = D_c - C_0 h^\nu$ with C_0 to be determined. Let Γ be a BCS state satisfying $\mathcal{E}^{BCS}(\Gamma) \leq 0$. We will show that $\Gamma \equiv 0$ and this will prove the claim $\mu_c(h) \geq -E_b + h^2 D_c - C_0 h^{2+\nu}$.

Assumption 6.1.2 on W implies that it is infinitesimally form-bounded with respect to $-\Delta_\Omega$ on $H_0^1(\Omega)$ and from this one derives that $\mathfrak{h} \geq 0$ for sufficiently small h, see Proposition 6.5.3. Therefore, the zero state is the unique minimizer of the first term $\mathrm{Tr}[\mathfrak{h}\gamma]$ in $\mathcal{E}^{BCS}$ and it suffices to show that $\alpha \equiv 0$ to get $\Gamma = 0$.

We apply Theorem 6.2.1 (LBC) with $C_\Gamma = 0$ and obtain $\psi \in H_0^1(\Omega)$ such that

$$0 \geq h^{d-4}\mathcal{E}^{BCS}(\Gamma) \geq \mathcal{E}^{GP}(\psi) + O(h^\nu)\|\psi\|^2_{H_0^1(\Omega)}.$$

We drop the (non-negative) quartic term in $\mathcal{E}^{GP}$ for a lower bound and use the definition of D_c to get

$$\mathcal{E}^{GP}(\psi) \geq (D_c - D)\|\psi\|^2_{L^2(\Omega)}$$

The analogue of the first relation in (6.17) in the convex case is $\|\psi\|^2_{H^1_0(\Omega)} \leq C\|\psi\|^2_{L^2(\Omega)}$. It gives

$$0 \geq (C(D_c - D) + O(h^\nu))\|\psi\|^2_{H^1_0(\Omega)}. \tag{6.25}$$

Recall that the implicit constant depends on D in a continuous way and let C_2 denote its maximum value on the interval $[D_c - 1, D_c + 1]$. Taking $D = D_c - C_0 h^\nu$ with $C_0 = 2C_2/C$, we get from (6.25) that $\psi \equiv 0$ for small enough $h > 0$.

Since $C_\Gamma = 0$, the analogue of the second bound in (6.17) in the convex case yields $\xi \equiv 0$ and so $\alpha \equiv 0$ as claimed.

Lower bound (non convex case). We write $\ell \equiv \ell(h)$ throughout. We apply Theorem 6.2.1 (LB) and argue as in the convex case to find

$$0 \geq h^{d-4}\mathcal{E}^{BCS}(\Gamma) \geq (D_c^+(\ell) - D + O(h^\nu))\|\psi\|^2_{L^2(\Omega)}.$$

Now, the last part of Theorem 6.2.2 gives $D_c^+(\ell) - D + O(h^\nu) = D_c - D + O(h^\nu)$. This can be made positive by choosing C_0 large enough in the same way as above. We conclude that $\psi = 0$ and so $\xi = 0$ by (6.17) and $C_\Gamma = 0$ (since we assume $\mathcal{E}^{BCS}(\Gamma) \leq 0$). This completes the proof of Theorem 6.1.7. □

Proof of main result 2, Theorem 6.1.10

We let $\mu = -E_b + Dh^2$ with $D \in \mathbb{R}$ fixed and we let $\ell(h) = h\log(h^{-q})$, with $q \geq 1$ large but fixed.

Upper bound. By Proposition 6.2.5, the minimization problem $E^{GP}_{\Omega^-_{\ell(h)}}$ has a unique minimizer, call it $\psi_- \in H^1_0(\Omega^-_{\ell(h)})$. We apply Theorem 6.2.1 (UB) with $\psi = \psi_-$ to obtain an admissible BCS state Γ_{ψ_-} such that

$$\begin{aligned} E^{BCS} \leq \mathcal{E}^{BCS}(\Gamma_{\psi_-}) =& h^{4-d}\mathcal{E}^{GP}(\psi_-) + O(h^{5-d})(\|\psi_-\|^2_{H^1(\mathbb{R}^d)} + \|\psi_-\|^4_{H^1(\mathbb{R}^d)}) \\ \leq& h^{4-d}E^{GP}_{\Omega^-_{\ell(h)}} + O(h^{5-d})(1 + E^{GP}_{\Omega^-_{\ell(h)}})^2. \end{aligned}$$

In the second step, we used the fact that ψ_- is a minimizer and the coercivity (6.21).

Now we apply Theorem 6.2.2. Since $\ell(h) = O(h^{1-\delta})$ for every $\delta > 0$, we get

$$E^{BCS} \leq h^{4-d} E_{\Omega}^{GP} + O(h^{4-d+\nu}),$$

where ν is as in Theorem 6.1.7.

Lower bound. Thanks to the upper bound right above, for any minimizer Γ of the BCS energy, we have

$$\mathcal{E}^{BCS}(\Gamma) \leq h^{4-d}(E_{\Omega}^{GP} + \varepsilon)$$

for all $\varepsilon > 0$. In particular, $\mathcal{E}^{BCS}(\Gamma) \leq C_\Gamma h^{4-d}$ and so Γ satisfies the assumption in Theorem 6.2.1 (LB) and (LBC).

If Ω is convex, the claim follows directly from Theorem 6.2.1 (LBC).

If Ω is a non convex bounded Lipschitz domain, Theorem 6.2.1 (LB) yields $\psi \in H_0^1(\Omega_{\ell(h)}^+)$ such that

$$\mathcal{E}^{BCS}(\Gamma) \geq h^{4-d}\mathcal{E}^{GP}(\psi) + O(h^{4-d+\nu'}) \geq h^{4-d} E_{\Omega_{\ell(h)}^+}^{GP} + O(h^{4-d+\nu'}).$$

The lower bound now follows from Theorem 6.2.2. This finishes the proof of Theorem 6.1.10. □

6.3 Semiclassical expansion

We state an important tool for the proof of Theorem 6.2.1, the semiclassical expansion. The version here is essentially the one from [28].

Though not strictly necessary for the result, it will be convenient for us to assume the following decay condition

Definition 6.3.1. *We say that a function $\mathfrak{a} \in L^2(\mathbb{R}^d)$ decays exponentially in the L^2 sense with the rate ρ, if*

$$\int_{\mathbb{R}^d} e^{2\rho|s|} |\mathfrak{a}(s)|^2 \mathrm{d}s < \infty. \tag{6.26}$$

Recall that α_* denotes the unique ground state of $-\Delta + V$. It is well known that weak assumptions on the potential V imply the exponential decay of α_* in an L^2 sense. The fact that infinitesimal form-boundedness of V is sufficient is essentially contained in [160] but was known to the experts even earlier. That is, there exists $\rho_* > 0$ such that

$$\int_{\mathbb{R}^d} e^{2\rho_*|s|}|\alpha_*(s)|^2 \mathrm{d}s < \infty. \tag{6.27}$$

In particular, we can apply the following lemma with $\mathfrak{a} = \alpha_*$ later on.

Lemma 6.3.2 (Semiclassics)**.** *For $\psi, \mathfrak{a} \in H^1(\mathbb{R}^d)$, we set*

$$\mathfrak{a}_\psi(x,y) := h^{-d}\psi\left(\frac{x+y}{2}\right)\mathfrak{a}\left(\frac{x-y}{h}\right), \quad x,y \in \mathbb{R}^d. \tag{6.28}$$

Suppose that $\mathfrak{a}(x) = \mathfrak{a}(-x)$ and that $\mathfrak{a}$ decays exponentially in the L^2 sense of Definition 6.3.1.

Then:

(i)

$$\begin{aligned} &\mathrm{Tr}[(-h^2\delta - \mu)\mathfrak{a}_\psi\overline{\mathfrak{a}_\psi}] + \iint_{\mathbb{R}^d\times\mathbb{R}^d} V\left(\frac{x-y}{h}\right)|\mathfrak{a}_\psi(x,y)|^2 \mathrm{d}x\mathrm{d}y \\ =&h^{-d}\|\psi\|^2_{L^2(\mathbb{R}^d)}\langle \mathfrak{a}\,|{-\Delta} + E_b + V|\,\mathfrak{a}\rangle \\ &+ \|\mathfrak{a}\|^2_{L^2(\mathbb{R}^d)}\left(\frac{h^{2-d}}{4}\|\nabla\psi\|^2_{L^2(\mathbb{R}^d)} + h^{-d}(-E_b - \mu)\|\psi\|^2_{L^2(\mathbb{R}^d)}\right). \end{aligned}$$

(ii) There exists a constant $C > 0$ such that

$$\begin{aligned} &\left|\mathrm{Tr}[W\mathfrak{a}_\psi\overline{\mathfrak{a}_\psi}] - h^{-d}\|\mathfrak{a}\|^2_{L^2(\mathbb{R}^d)}\int_{\mathbb{R}^d} W(X)|\psi(X)|^2\mathrm{d}X\right| \\ \leq&Ch^{1-d}\|\mathfrak{a}\|^2_{L^2(\mathbb{R}^d)}\|W\|_{L^{p_W}(\Omega)}\|\psi\|^2_{H^1(\mathbb{R}^d)}. \end{aligned}$$

(iii) Let

$$\begin{aligned} g_{BCS}(\mathfrak{a}) : &= (2\pi)^{-d}\int_{\mathbb{R}^d}(p^2 + E_b)|\hat{\mathfrak{a}}(p)|^4\mathrm{d}p, \\ g_0(\mathfrak{a}) : &= (2\pi)^{-d}\int_{\mathbb{R}^d}|\hat{\mathfrak{a}}(p)|^4\mathrm{d}p \end{aligned} \tag{6.29}$$

Then, as $h \downarrow 0$,

$$\begin{aligned} &\mathrm{Tr}[(-h^2\delta + E_b + h^2W)\mathfrak{a}_\psi\overline{\mathfrak{a}_\psi}\mathfrak{a}_\psi\overline{\mathfrak{a}_\psi}] \\ =&h^{-d}g_{BCS}(\mathfrak{a})\|\psi\|^4_{L^4(\mathbb{R}^d)} + O(h^{1-d})\|\psi\|^4_{H^1(\mathbb{R}^d)}, \end{aligned}$$

and

$$\mathrm{Tr}[\mathfrak{a}_\psi\overline{\mathfrak{a}_\psi}\mathfrak{a}_\psi\overline{\mathfrak{a}_\psi}] = h^{-d}g_0(\mathfrak{a})\|\psi\|^4_{L^4(\mathbb{R}^d)} + O(h^{1-d})\|\psi\|^4_{H^1(\mathbb{R}^d)}.$$

Lemma 6.3.2 was proved in in [28] for $d = 3$, $\mathfrak{a} = h\alpha_*$, $W \in L^\infty(\mathbb{R}^3)$ and at fixed particle number. We sketch the proof in Appendix 6.10 to show that it generalizes to the present version.

Remark 6.3.3. *To see that $g_{BCS}(\mathfrak{a}), g_0(\mathfrak{a}) < \infty$, observe that the decay assumption* (6.26) *implies $\mathfrak{a} \in L^1(\mathbb{R}^d) \cap H^1(\mathbb{R}^d)$ and so $\widehat{\mathfrak{a}}$ is bounded.*

6.4 Proof of Theorem 6.2.1 (UB)

The idea of the proof is to construct an appropriate trial state and then to use the semiclassical expansion from Lemma 6.3.2.

The trial state

The trial state Γ_ψ is defined as in [28], following an idea of [91], see (6.31) below. However, we multiply α_* by an appropriate cutoff function χ, in order to satisfy the Dirichlet boundary conditions in the relative variable.

Definition 6.4.1 (Trial state)**.** *Let $\chi \in C_c^\infty(\mathbb{R}^d)$ be a symmetric cutoff function, i.e. $\chi(r) = \chi(-r)$, $0 \le \chi \le 1$ and $\chi \equiv 1$ on B_1 and* $\operatorname{supp}\chi \subset B_{3/2}$*. Let $\ell(h) = h\phi(h)$ with $\lim_{h\to 0} \phi(h) = \infty$ and define*

$$\mathfrak{a}(r) := \chi\left(\frac{r}{\phi(h)}\right) h\alpha_*(r). \tag{6.30}$$

For any $\psi \in H^1(\mathbb{R}^d)$, we define $\mathfrak{a}_\psi$ by (6.28) *and*

$$\gamma_\psi := \mathfrak{a}_\psi \overline{\mathfrak{a}_\psi} + (1 + h^{1/2})\mathfrak{a}_\psi \overline{\mathfrak{a}_\psi} \mathfrak{a}_\psi \overline{\mathfrak{a}_\psi}, \qquad \Gamma_\psi := \begin{pmatrix} \gamma_\psi & \mathfrak{a}_\psi \\ \overline{\mathfrak{a}_\psi} & 1 - \overline{\gamma_\psi} \end{pmatrix}. \tag{6.31}$$

Proposition 6.4.2. *Let $\psi \in H_0^1(\Omega^-_{\ell(h)})$. For all sufficiently small h, Γ_ψ is an admissible BCS state.*

Proof. $0 \le \Gamma_\psi \le 1$ holds by a short computation, see [28]. We show that $\mathfrak{a}_\psi \in H_0^1(\Omega^2)$. First, we observe that $\operatorname{supp}\mathfrak{a}_\psi \subseteq \Omega^2$. To see this, we note that $\operatorname{supp}\psi \subseteq \Omega^-_{\ell(h)}$ and $\operatorname{supp}\mathfrak{a} \subseteq \operatorname{supp}\chi(\cdot/\phi(h)) \subseteq B_{3\phi(h)/2}$ and therefore

$$\operatorname{supp}\mathfrak{a}_\psi \subseteq \left\{(x,y) \in \mathbb{R}^d \times \mathbb{R}^d \ : \ \frac{x+y}{2} \in \Omega^-_{\ell(h)},\ \frac{x-y}{2} \in B_{3\ell(h)/4}\right\},$$

where we also used $h\phi(h) = \ell(h)$. By construction, $\operatorname{dist}(\frac{x+y}{2}, \Omega^c) \ge \ell(h)$ and by expressing

$$(x,y) = \left(\frac{x+y}{2} + \frac{x-y}{2}, \frac{x+y}{2} - \frac{x-y}{2}\right),$$

we obtain that, indeed, $\operatorname{supp}\mathfrak{a}_\psi \subseteq \Omega^2$.

It remains to show that, after extending ψ and $\mathfrak{a}$ by zero to $\mathbb{R}^d$, we have $\mathfrak{a}_\psi \in H^1(\mathbb{R}^d \times \mathbb{R}^d)$. By using $\mathfrak{a}(r) = \mathfrak{a}(-r)$ to symmetrize the derivatives and changing to center-of-mass coordinates (6.40), we indeed get an upper bound on $\|\mathfrak{a}_\psi\|_{H^1(\mathbb{R}^d\times\mathbb{R}^d)}$ in terms of the (finite) quantities $\|\psi\|_{H^1(\mathbb{R}^d)}$ and $\|\mathfrak{a}\|_{H^1(\mathbb{R}^d)}$. We leave the details to the reader, as similar computations appear several times in the lower bound, see e.g. the proof of Lemma 6.5.2.

This proves $\mathfrak{a}_\psi \in H^1_0(\Omega^2)$. To see that γ_ψ satisfies Definition 6.1.5, we note that $\gamma_\psi \leq 3\mathfrak{a}_\psi\overline{\mathfrak{a}_\psi}$ since $\overline{\mathfrak{a}_\psi}\mathfrak{a}_\psi \leq \overline{\gamma_\psi} \leq 1$. We can then bound

$$\begin{aligned}\sqrt{1-\Delta_\Omega}\gamma_\psi\sqrt{1-\Delta_\Omega} \leq& 3\sqrt{1-\Delta_\Omega}\mathfrak{a}_\psi\overline{\mathfrak{a}_\psi}\sqrt{1-\Delta_\Omega}\\ =&3\sqrt{1-\Delta_\Omega}\mathfrak{a}_\psi\left(\sqrt{1-\Delta_\Omega}\mathfrak{a}_\psi\right)^*\end{aligned}$$

by a product of two Hilbert Schmidt operators and therefore it is trace class.

□

Controlling the effect of the cutoff

When we apply the semiclassical expansion in Lemma 6.3.2, we want to remove the effect of the cutoff, i.e. we want to replace $\mathfrak{a}$ by α_*, up to higher order corrections. We will get this from the estimates in Proposition 6.4.3 below, which follow essentially from the exponential decay (6.27) of α_*.

We recall definition (6.29) of $g_{BCS}(\mathfrak{a})$ and $g_0(\mathfrak{a})$.

Proposition 6.4.3. *We have*

$$\|\mathfrak{a}\|^2_{L^2(\mathbb{R}^d)} = h^2\left(1 + O(e^{-2\rho_*\phi(h)})\right), \tag{6.32}$$

$$g_{BCS}(\mathfrak{a}) = h^4\left(g_{BCS} + O(e^{-\rho_*\phi(h)/2})\right), \tag{6.33}$$

$$g_0(\mathfrak{a}) = h^4\left(g_0(\alpha_*) + O(e^{-\rho_*\phi(h)/2})\right), \tag{6.34}$$

$$\langle\mathfrak{a}\,|-\Delta + E_b + V|\,\mathfrak{a}\rangle = h^2 O(e^{-2\rho_*\phi(h)}). \tag{6.35}$$

Proof. For (6.32), we observe

$$\begin{aligned}\|h\alpha_*\|^2_{L^2(\mathbb{R}^d)} - \|\mathfrak{a}\|^2_{L^2(\mathbb{R}^d)} =& h^2\int_{\mathbb{R}^d}|\alpha_*(r)|^2\left(1-\chi\left(\frac{r}{\phi(h)}\right)^2\right)\mathrm{d}r\\ \leq& h^2\int_{B^c_{\phi(h)}}|\alpha_*(r)|^2\mathrm{d}r \leq Ch^2e^{-2\rho_*\phi(h)}.\end{aligned}$$

In the last step, we used the fact that α_* satisfies the decay assumption (6.27). This proves (6.32) since $\|\alpha_*\|_{L^2(\mathbb{R}^d)} = 1$.

To get (6.33), we first write

$$|h\widehat{\alpha}_*|^4 - |\hat{\mathfrak{a}}|^4 = \left(|h\widehat{\alpha}_*|^2 + |\hat{\mathfrak{a}}|^2\right)\left(|h\widehat{\alpha}_*| + |\hat{\mathfrak{a}}|\right)\left(|h\widehat{\alpha}_*| - |\hat{\mathfrak{a}}|\right). \tag{6.36}$$

The smallness comes from the last term. Indeed, the decay assumption (6.27) gives

$$\begin{aligned}\sup_{p\in\mathbb{R}^d} \left||h\widehat{\alpha}_*(p)| - |\hat{\mathfrak{a}}(p)|\right| &\le \sup_{p\in\mathbb{R}^d} |h\widehat{\alpha}_*(p) - \hat{\mathfrak{a}}(p)| \le \|h\alpha_* - \mathfrak{a}\|_{L^1(\mathbb{R}^d)} \\ \le & h\int_{B^c_{\phi(h)}} |\alpha_*(r)|\mathrm{d}r = h\int_{B^c_{\phi(h)}} |\alpha_*(r)|e^{\rho_* r}e^{-\rho_* r}\mathrm{d}r \le Che^{-\rho_*\phi(h)/2}.\end{aligned}$$

Note also that (6.27) implies $\|\widehat{\alpha}_*\|_{L^\infty(\mathbb{R}^d)} \le (2\pi)^{-d/2}\|\alpha_*\|_{L^1(\mathbb{R}^d)} \le C$ and consequently $\|\widehat{\mathfrak{a}}\|_{L^\infty(\mathbb{R}^d)} \le Ch$. Applying these estimates to (6.36), we get

$$|h\widehat{\alpha}_*|^4 - |\hat{\mathfrak{a}}|^4 \le Ch^2 e^{-\rho_*\phi(h)/2}\left(|h\widehat{\alpha}_*|^2 + |\hat{\mathfrak{a}}|^2\right).$$

Recall the definition (6.29) and observe that $g_{BCS}(\alpha_*) = g_{BCS}$ from (6.6). Hence,

$$\begin{aligned}|g_{BCS}(\mathfrak{a}) - h^4 g_{BCS}| \le & Ch^2 e^{-\rho_*\phi(h)/2}\int_{\mathbb{R}^d}(p^2 + E_b)\left(|h\widehat{\alpha}_*|^2 + |\hat{\mathfrak{a}}|^2\right)\mathrm{d}p \\ \le & Ch^2 e^{-\rho_*\phi(h)/2}\left(h^2\|\alpha_*\|^2_{H^1(\mathbb{R}^d)} + \|\mathfrak{a}\|^2_{H^1(\mathbb{R}^d)}\right).\end{aligned}$$

To conclude the claim (6.33), it remains to see that $\|\mathfrak{a}\|^2_{H^1(\mathbb{R}^d)} \le Ch^2$ as $h \downarrow 0$. For the L^2 part of the H^1 norm this follows from $\chi^2 \le 1$. For the derivative term, we denote $\chi_h \equiv \chi(\cdot/\phi(h))$ and use the Leibniz rule to get

$$\|\nabla\mathfrak{a}\|^2_{L^2(\mathbb{R}^d)} \le 2h^2\left(\|\chi_h\nabla\alpha_*\|^2_{L^2(\mathbb{R}^d)} + \|\alpha_*\nabla\chi_h\|^2_{L^2(\mathbb{R}^d)}\right).$$

For the first term, we use $\chi^2 \le 1$ to get

$$\|\chi_h\nabla\alpha_*\|^2_{L^2(\mathbb{R}^d)} \le \|\chi_h\nabla\alpha_*\|^2_{L^2(\mathbb{R}^d)} \le C.$$

The second term is in fact much smaller:

$$\|\alpha_*\nabla\chi_h\|^2_{L^2(\mathbb{R}^d)} \le Ce^{-2\rho_*\phi(h)}. \tag{6.37}$$

Indeed, by Hölder's inequality and (6.27) we have

$$\begin{aligned}\|\alpha_*\nabla\chi_h\|^2_{L^2(\mathbb{R}^d)} = & \|\alpha_*\nabla\chi_h\|^2_{L^2(B_{2\phi(h)}\setminus B_{\phi(h)})} \le e^{-2\rho_*\phi(h)}\|\nabla\chi_h\|^2_{L^\infty(\mathbb{R}^d)} \\ = & e^{-2\rho_*\phi(h)}\phi(h)^{-2}\|\nabla\chi\|^2_{L^\infty(\mathbb{R}^d)} \le Ce^{-2\rho_*\phi(h)}.\end{aligned}$$

In the last step we used $\phi(h) \to \infty$ as $h \to 0$. This proves (6.37) and completes the proof of (6.33). The argument for (6.34) is even simpler.

Finally, we come to (6.35). Since $(-\Delta + E_b + V)\alpha_* = 0$,

$$\langle \mathfrak{a} \,|{-\Delta} + E_b + V|\, \mathfrak{a}\rangle = h\langle \mathfrak{a}\,|[-\Delta, \chi_h]|\, \alpha_*\rangle = h^2 \|\alpha_* \nabla \chi_h\|^2_{L^2(\mathbb{R}^d)}.$$

Therefore, (6.35) follows from (6.37) and Proposition 6.4.3 is proved. □

Conclusion

Given a function $\psi \in H_0^1(\Omega^-_{\ell(h)})$, we define Γ_ψ as in Proposition 6.4.2. We have

$$\begin{aligned}\mathcal{E}^{BCS}(\Gamma_\psi) =& \mathrm{Tr}[\mathfrak{h}\mathfrak{a}_\psi \overline{\mathfrak{a}_\psi}] + \iint_{\mathbb{R}^d\times\mathbb{R}^d} V\left(\frac{x-y}{h}\right) |\mathfrak{a}_\psi(x,y)|^2 \mathrm{d}x\mathrm{d}y \\ &+ (1+h^{1/2})\mathrm{Tr}[\mathfrak{h}\mathfrak{a}_\psi \overline{\mathfrak{a}_\psi}\mathfrak{a}_\psi \overline{\mathfrak{a}_\psi}].\end{aligned}$$

We apply the semiclassical expansion in Lemma 6.3.2 (note that the assumptions are satisfied by $\mathfrak{a}$, since it is as regular as α_* and of compact support). We find, using $D = h^{-2}(\mu + E_b)$,

$$\begin{aligned}&\mathcal{E}^{BCS}(\Gamma_\psi) \\ =&h^{-d}\|\psi\|^2_{L^2(\mathbb{R}^d)} \langle \mathfrak{a} \,|{-\Delta} + E_b + V|\, \mathfrak{a}\rangle \\ &+ \|\mathfrak{a}\|^2_{L^2(\mathbb{R}^d)} \left(\frac{h^{2-d}}{4}\|\nabla\psi\|^2_{L^2(\mathbb{R}^d)} - h^{2-d}D\|\psi\|^2_{L^2(\mathbb{R}^d)}\right) \\ &+ h^{2-d}\|\mathfrak{a}\|^2_{L^2(\mathbb{R}^d)} \int_{\mathbb{R}^d} W(X)|\psi(X)|^2 \mathrm{d}X + h^{-d} g_{BCS}(\mathfrak{a}) \|\psi\|^4_{L^4(\mathbb{R}^d)} \\ &+ O(h^{5-d})(\|\psi\|^2_{H^1(\mathbb{R}^d)} + \|\psi\|^4_{H^1(\mathbb{R}^d)})\end{aligned}$$

The main term in this expression is h^{4-d} times the GP energy defined in (6.8), up to errors which are controlled by Proposition 6.4.3 and the choice $\phi(h) = \log(h^{-q})$ with q sufficiently large compared to $1/\rho_*$. We find

$$\mathcal{E}^{BCS}(\Gamma_\psi) = \mathcal{E}^{GP}(\psi) + (O(h^{5-d}) - Ch^{6-d}D)(\|\psi\|^2_{H^1(\mathbb{R}^d)} + \|\psi\|^4_{H^1(\mathbb{R}^d)}).$$

Note that the constant in front of the error term is an affine function of D; in particular it is continuous in D. This proves Theorem 6.2.1 (UB). □

6.5 Proof of Theorem 6.2.1 (LB): Decomposition

We prove Theorem 6.2.1 (LB) and (LBC) together. (The situation will drastically simplify for convex Ω in due course.)

In this first part of the proof, we consider any BCS state Γ satisfying $\mathcal{E}^{BCS}(\Gamma) \leq C_\Gamma h^{4-d}$ and we show that its off-diagonal element α can be decomposed as in (6.10), with good a priori H^1 control on all the functions involved. Recall that

$$\tilde{\Omega} := \frac{\Omega + \Omega}{2}.$$

Theorem 6.5.1 (Decomposition and a priori bounds)**.** *Suppose that* $\mu = -E_b + Dh^2$ *for some* $D \in \mathbb{R}$ *and that* Γ *is an admissible BCS state satisfying* $\mathcal{E}^{BCS}(\Gamma) \leq C_\Gamma h^{4-d}$. *Then, there exist* $\psi \in H_0^1(\tilde{\Omega})$ *and* $\xi \in H_0^1(\tilde{\Omega} \times \mathbb{R}^d)$ *such that* α*, the upper right entry of* Γ*, can be decomposed as in* (6.10)*. Moreover, we have the bounds*

$$\begin{aligned} &\|\nabla\psi\|_{L^2(\tilde{\Omega})} \leq C\|\psi\|_{L^2(\tilde{\Omega})} \leq O(1), \\ &\|\xi\|^2_{L^2(\tilde{\Omega}\times\mathbb{R}^d)} + h^2\|\nabla\xi\|^2_{L^2(\tilde{\Omega}\times\mathbb{R}^d)} \leq O(h^{4-d})(\|\psi\|^2_{L^2(\tilde{\Omega})} + C_\Gamma). \end{aligned} \tag{6.38}$$

The implicit constants depend continuously on D*.*

The key input to the proof is the spectral gap of the operator $-\Delta + V$ above its ground state energy $-E_b$.

Center of mass coordinates

Define the set

$$\mathcal{D} := \left\{(X, r) \in \tilde{\Omega} \times \mathbb{R}^d \ : \ X + \frac{r}{2}, X - \frac{r}{2} \in \Omega\right\}.$$

Lemma 6.5.2. *Suppose that* $\mu = -E_b + Dh^2$*. Let* Γ *be an admissible BCS state. Set* $\tilde{\alpha}(X, r) := \alpha(X + r/2, X - r/2)$ *so that* $\tilde{\alpha} \in H_0^1(\mathcal{D})$*. Then, for sufficiently small* $h > 0$*, we have*

$$\begin{aligned} \mathcal{E}^{BCS}(\Gamma) \geq \iint_{\mathcal{D}} \overline{\tilde{\alpha}(X,r)} \Bigg(&-\frac{h^2}{4}\Delta_X - h^2\Delta_r + h^2 W(X + r/2) - \mu \\ &+ V(r/h)\Bigg)\tilde{\alpha}(X,r)\mathrm{d}r\mathrm{d}X + \frac{E_b}{2}\mathrm{Tr}[\alpha\overline{\alpha}\alpha\overline{\alpha}]. \end{aligned}$$

We separate the following statement from the proof for later use. The constant 1/2 is not sharp, but it is sufficient for the purpose of proving a priori bounds.

Proposition 6.5.3. *For* h *small enough,* $\mathfrak{h} \geq E_b/2 > 0$.

Proof. By Assumption 6.1.2 W is infinitesimally form-bounded with respect to $-\Delta_\Omega$. Hence, $|W| \leq -\frac{1}{2}\delta + C$ and $\mathfrak{h} \geq -\frac{h^2}{2}\delta - \mu - h^2 C$ hold in the sense of quadratic forms. Since $\mu = -E_b + Dh^2$, this implies that $\mathfrak{h} \geq \frac{E_b}{2}$ for small enough $h > 0$. □

We come to the

Proof of Lemma 6.5.2. The key input is that for any BCS state, we have the operator inequality $\alpha\overline{\alpha} + \gamma^2 \leq \gamma$. For small enough h, we have $\mathfrak{h} \geq 0$ by Proposition 6.5.3. Hence, we can apply $\alpha\overline{\alpha} + \gamma^2 \leq \gamma$ to the term $\mathrm{Tr}[\mathfrak{h}\gamma] = \mathrm{Tr}[\mathfrak{h}^{1/2}\gamma\mathfrak{h}^{1/2}]$ in the BCS energy to get

$$\mathcal{E}^{BCS}(\Gamma) \geq \mathrm{Tr}[\mathfrak{h}\alpha\overline{\alpha}] + \iint_{\Omega^2} V\left(\frac{x-y}{h}\right)|\alpha(x,y)|^2 \mathrm{d}x\mathrm{d}y + \mathrm{Tr}[\mathfrak{h}\gamma^2]. \tag{6.39}$$

We estimate the last term further. By Proposition 6.5.3, $\alpha\overline{\alpha} \leq \gamma$ and the fact that $A \mapsto \mathrm{Tr}[A^2]$ is operator monotone, we have

$$\mathrm{Tr}[\mathfrak{h}\gamma^2] \geq \frac{E_b}{2}\mathrm{Tr}[\gamma^2] \geq \frac{E_b}{2}\mathrm{Tr}[\alpha\overline{\alpha}\alpha\overline{\alpha}].$$

We now rewrite the first two terms in (6.39) in center of mass coordinates. Using $\alpha(x,y) = \alpha(y,x)$ (Γ is Hermitian), we can write out the first term as

$$\mathrm{Tr}[\mathfrak{h}\alpha\overline{\alpha}] = \iint_{\Omega^2} \overline{\alpha(x,y)}\left(-h^2\Delta_x + h^2 W(x) - \mu + V\left(\frac{x-y}{h}\right)\right)\alpha(x,y)\mathrm{d}x\mathrm{d}y$$

$$= \iint_{\Omega^2} \overline{\alpha(x,y)}\left(-\frac{h^2}{2}\Delta_x - \frac{h^2}{2}\Delta_y + h^2 W(x) - \mu + V\left(\frac{x-y}{h}\right)\right)\alpha(x,y)\mathrm{d}x\mathrm{d}y.$$

Now we change to center-of-mass coordinates

$$X = \frac{x+y}{2}, \qquad r = x-y, \qquad \tilde{\alpha}(X,r) := \alpha(X + r/2, X - r/2). \tag{6.40}$$

Since the Jacobian is equal to one and $\Delta_x + \Delta_y = \frac{1}{2}\Delta_X + 2\Delta_r$, Lemma 6.5.2 follows. □

Definition of the order parameter ψ

An important idea is that from now on we isometrically embed $H_0^1(\mathcal{D}) \subset H_0^1(\tilde{\Omega} \times \mathbb{R}^d)$ by extending functions by zero. Note that all local norms are left invariant by the extension, in particular $\|\tilde{\alpha}\|_{L^2(\mathcal{D})} = \|\tilde{\alpha}\|_{L^2(\tilde{\Omega}\times\mathbb{R}^d)}$.

We define the order parameter ψ and establish some of its basic properties. For a fixed $X \in \tilde{\Omega}$, we define the fiber

$$\mathcal{D}_X := \left\{ r \in \mathbb{R}^d \ : \ (X, r) \in \mathcal{D} \right\} = \left\{ r \in \mathbb{R}^d \ : \ X + \frac{r}{2}, X - \frac{r}{2} \in \Omega \right\}.$$

Proposition 6.5.4. *For $\tilde{\alpha} \in H_0^1(\mathcal{D}) \subset H_0^1(\tilde{\Omega} \times \mathbb{R}^d)$, define*

$$\psi(X) := h^{-1} \int_{\mathcal{D}_X} \alpha_*(r/h) \tilde{\alpha}(X, r) \mathrm{d}r, \qquad \text{for all } X \in \tilde{\Omega}, \quad (6.41)$$

$$\tilde{\alpha}_\psi(X, r) := h^{1-d} \psi(X) \alpha_*(r/h), \qquad \text{for a.e. } X \in \tilde{\Omega},\ r \in \mathbb{R}^d, \quad (6.42)$$

$$\xi(X, r) := \tilde{\alpha}(X, r) - \tilde{\alpha}_\psi(X, r), \qquad \text{for a.e. } X \in \tilde{\Omega},\ r \in \mathbb{R}^d. \quad (6.43)$$

Then:

(i) $\psi \in H_0^1(\tilde{\Omega})$ *and* $\xi \in H_0^1(\tilde{\Omega} \times \mathbb{R}^d)$.

(ii) We have the norm identities

$$\begin{aligned} \|\tilde{\alpha}\|_{L^2(\mathcal{D})}^2 &= h^{2-d} \|\psi\|_{L^2(\tilde{\Omega})}^2 + \|\xi\|_{L^2(\tilde{\Omega} \times \mathbb{R}^d)}^2, \\ \|\nabla_X \tilde{\alpha}\|_{L^2(\mathcal{D})}^2 &= h^{2-d} \|\nabla \psi\|_{L^2(\tilde{\Omega})}^2 + \|\nabla_X \xi\|_{L^2(\tilde{\Omega} \times \mathbb{R}^d)}^2. \end{aligned} \quad (6.44)$$

Proof. From the definition of the weak derivative, we get that $\psi \in H_0^1(\tilde{\Omega})$ with

$$\nabla \psi(X) = h^{-1} \int_{\mathcal{D}_X} \alpha_*(r/h) \nabla_X \tilde{\alpha}(X, r) \mathrm{d}r. \quad (6.45)$$

Since $\alpha_* \in H^1(\mathbb{R}^d)$ and $H_0^1(\tilde{\Omega} \times \mathbb{R}^d)$ is a vector space, we also get $\xi \in H_0^1(\tilde{\Omega} \times \mathbb{R}^d)$. This proves claim (i). For claim (ii), we observe the orthogonality relation

$$\int_{\mathbb{R}^d} \alpha_*(r/h) \xi(X, r) \mathrm{d}r = 0, \quad (6.46)$$

which holds for a.e. $X \in \tilde{\Omega}$. Thus, by expanding the square that one gets from (6.43) and using $\|\alpha_*(\cdot/h)\|_{L^2(\mathbb{R}^d)}^2 = h^d$,

$$\|\tilde{\alpha}\|_{L^2(\mathcal{D})}^2 = \|\tilde{\alpha}\|_{L^2(\tilde{\Omega} \times \mathbb{R}^d)}^2 = h^{2-d} \|\psi\|_{L^2(\tilde{\Omega})}^2 + \|\xi\|_{L^2(\tilde{\Omega} \times \mathbb{R}^d)}^2.$$

This is the first identity in (6.44). The second one follows by an analogous argument using (6.45). ∎

Bound on the W term

Lemma 6.5.5. *Let* $\tilde{\alpha} \in H_0^1(\mathcal{D}) \subset H_0^1(\tilde{\Omega} \times \mathbb{R}^d)$ *and let* $\tilde{\alpha}_\psi$ *and* ξ *be as in Proposition 6.5.4. For every* $\varepsilon > 0$*, there exists* $C_\varepsilon > 0$ *such that*

$$\int_{\tilde{\Omega}} \int_{\mathbb{R}^d} |W(X + r/2)||\tilde{\alpha}_\psi(X, r)|^2 \mathrm{d}r\mathrm{d}X \leq h^{4-d} \left(\varepsilon \|\nabla\psi\|^2_{L^2(\tilde{\Omega})} + C_\varepsilon \|\psi\|^2_{L^2(\tilde{\Omega})}\right)$$
$$\int_{\tilde{\Omega}} \int_{\mathbb{R}^d} |W(X + r/2)||\xi(X, r)|^2 \mathrm{d}r\mathrm{d}X \leq h^2 \left(\varepsilon \|\nabla\xi\|^2_{L^2(\tilde{\Omega}\times\mathbb{R}^d)} + C_\varepsilon \|\xi\|^2_{L^2(\tilde{\Omega}\times\mathbb{R}^d)}\right).$$

holds for sufficiently small h.

Proof. Recall that $\tilde{\alpha} = \tilde{\alpha}_\psi + \xi$, see (6.43). In the following, we freely identify functions with their extensions by zero to all of $\mathbb{R}^d$, respectively to all of $\mathbb{R}^d \times \mathbb{R}^d$. By the semiclassical expansion in Lemma 6.3.2(ii),

$$\begin{aligned}
&\int_{\tilde{\Omega}} \int_{\mathbb{R}^d} |W(X + r/2)||\tilde{\alpha}_\psi(X, r)|^2 \mathrm{d}r\mathrm{d}X \\
\leq &h^{2-d} \int_{\mathbb{R}^d} |W(X)||\psi(X)|^2 \mathrm{d}X + Ch^{3-d} \|W\|_{L^{p_W}(\mathbb{R}^d)} \|\psi\|^2_{H^1(\mathbb{R}^d)} \\
= &h^{2-d} \int_{\Omega} |W(X)||\psi(X)|^2 \mathrm{d}X + Ch^{3-d} \|W\|_{L^{p_W}(\Omega)} \|\psi\|^2_{H_0^1(\tilde{\Omega})}.
\end{aligned}$$

In the second step, we used our knowledge of where the functions are actually supported. Recall that W is infinitesimally form-bounded with respect to $-\delta$. Hence, for every $\varepsilon > 0$, there exists $C_\varepsilon > 0$ such that

$$\int_{\Omega} |W(X)||\psi(X)|^2 \mathrm{d}X \leq \varepsilon \|\nabla\psi\|^2_{L^2(\Omega)} + C_\varepsilon \|\psi\|^2_{L^2(\Omega)}$$

This proves the first claimed bound.

By Hölder's inequality (on the space $\tilde{\Omega} \times \mathbb{R}^d$ with Lebesgue measure) and the Sobolev interpolation inequality (on $\mathbb{R}^d \times \mathbb{R}^d$), we get that for every $\varepsilon > 0$, there exists $C_\varepsilon > 0$ such that

$$\begin{aligned}
&\int_{\tilde{\Omega}} \int_{\mathbb{R}^d} |W(X + r/2)||\xi(X, r)|^2 \mathrm{d}r\mathrm{d}X \\
\leq &2^{d/2} |\tilde{\Omega}|^{1/2} \|W\|_{L^2(\Omega)} \|\xi\|^2_{L^4(\tilde{\Omega}\times\mathbb{R}^d)} \\
= &2^{d/2} |\tilde{\Omega}|^{1/2} \|W\|_{L^2(\Omega)} \|\xi\|^2_{L^4(\mathbb{R}^d\times\mathbb{R}^d)} \\
\leq &2^{d/2} |\tilde{\Omega}|^{1/2} \|W\|_{L^2(\Omega)} \left(\varepsilon \|\nabla\xi\|^2_{L^2(\tilde{\Omega}\times\mathbb{R}^d)} + C_\varepsilon \|\xi\|^2_{L^2(\tilde{\Omega}\times\mathbb{R}^d)}\right).
\end{aligned}$$

Since $p_W \geq 2$ in all dimensions, this finishes the proof of Lemma 6.5.5. □

Proof of Theorem 6.5.1

The auxiliary results proved so far combine to give the following H^1 type lower bound on $\mathcal{E}^{BCS}$. From it, the a priori bounds stated in Theorem 6.5.1 will readily follow.

Lemma 6.5.6. *Assume that $\mu = -E_b + Dh^2$. Let $\tilde{\alpha} \in H_0^1(\mathcal{D}) \subset H_0^1(\tilde{\Omega} \times \mathbb{R}^d)$ be decomposed as $\tilde{\alpha} = \tilde{\alpha}_\psi + \xi$ as in Proposition 6.5.4. Then, there exist constants $c_1, c_2 > 0$ such that*

$$\begin{aligned}\mathcal{E}^{BCS}(\Gamma) \geq & c_1 h^2 \left(h^{2-d} \|\nabla \psi\|^2_{L^2(\tilde{\Omega})} + \|\nabla \xi\|^2_{L^2(\tilde{\Omega}\times\mathbb{R}^d)} \right) + c_1 \|\xi\|^2_{L^2(\tilde{\Omega}\times\mathbb{R}^d)} \\ & - (\mu + E_b + c_2 h^2) \|\tilde{\alpha}\|^2_{L^2(\tilde{\Omega}\times\mathbb{R}^d)} + \frac{E_b}{2} \mathrm{Tr}[\alpha\overline{\alpha}\alpha\overline{\alpha}].\end{aligned}$$

holds for all sufficiently small h.

Proof. Given the bounds from Lemma 6.5.5 on the W term, one can follow the proof of Lemma 3 in [28]. The key ingredient is the spectral gap of the operator $-\Delta + V$ above its ground state (and the standard fact that the gap can be used to obtain H^1 control on the error term). □

Proof of Theorem 6.5.1. Let $\mu = -E_b + Dh^2$ and let Γ be a BCS state satisfying $\mathcal{E}^{BCS}(\Gamma) \leq C_\Gamma h^{4-d}$. By Lemma 6.5.6 and $\mu = -E_b + Dh^2$, we have

$$\begin{aligned}h^2(c_2 + D)\|\tilde{\alpha}\|^2_{L^2(\tilde{\Omega}\times\mathbb{R}^d)} + C_\Gamma h^{4-d} \geq & h^2 \left(h^{2-d} \|\nabla \psi\|^2_{L^2(\tilde{\Omega})} + \|\nabla \xi\|^2_{L^2(\tilde{\Omega}\times\mathbb{R}^d)} \right) \\ & + \|\xi\|^2_{L^2(\tilde{\Omega}\times\mathbb{R}^d)} + \mathrm{Tr}[\alpha\overline{\alpha}\alpha\overline{\alpha}]\end{aligned} \tag{6.47}$$

We will eventually use all the terms in this equation. We write $c_2 + D = O(1)$. All the following implicit constants are obtained from this one in a continuous way and will therefore be continuous in D.

We begin by concluding from (6.47) that

$$\|\xi\|^2_{L^2(\tilde{\Omega}\times\mathbb{R}^d)} \leq h^2(c_2 + D)\|\tilde{\alpha}\|^2_{L^2(\tilde{\Omega}\times\mathbb{R}^d)} + C_\Gamma h^{4-d}. \tag{6.48}$$

From the first identity in (6.44), we therefore get

$$\|\alpha\|^2_{L^2(\Omega^2)} \leq h^{2-d}\|\psi\|^2_{L^2(\tilde{\Omega})} + O(h^2)\|\alpha\|^2_{L^2(\Omega^2)} + C_\Gamma h^{4-d}$$

and so, for all sufficiently small h,

$$\|\alpha\|^2_{L^2(\Omega^2)} \leq C h^{2-d}\|\psi\|^2_{L^2(\tilde{\Omega})} + C_\Gamma h^{4-d}. \tag{6.49}$$

Applying (6.49) to (6.47) and dropping some non-negative terms, we conclude

$$\|\nabla\psi\|^2_{L^2(\tilde{\Omega})} \leq C(\|\psi\|^2_{L^2(\tilde{\Omega})} + C_\Gamma), \tag{6.50}$$

$$\|\xi\|^2_{L^2(\tilde{\Omega}\times\mathbb{R}^d)} + h^2\|\nabla\xi\|^2_{L^2(\tilde{\Omega}\times\mathbb{R}^d)} \leq O(h^{4-d})\left(\|\psi\|^2_{L^2(\tilde{\Omega})} + C_\Gamma\right). \tag{6.51}$$

Thus, to prove (6.38), it remains to show

Lemma 6.5.7. *$\|\psi\|_{L^2(\tilde{\Omega})} = O(1)$.*

Remark 6.5.8. *At this stage, [28] prove Lemma 6.5.7 (in three dimensions) by using $\|\psi\|^2_{L^2} \leq h\|\alpha\|^2_{L^2} = h\mathrm{Tr}[\alpha\overline{\alpha}] \leq h\mathrm{Tr}[\gamma]$ and the fact that they work at fixed particle number $\mathrm{Tr}[\gamma] = N/h$. Since we do not have this assumption, we use the semiclassical expansion of the quartic term $\mathrm{Tr}[\alpha\overline{\alpha}\alpha\overline{\alpha}]$ similarly as in [73]. Here, as in the proof of Lemma 6.6.1 and in [28], one uses that in the Schatten norm estimate $\|\xi\|_{\mathfrak{S}^4} \leq \|\xi\|_{\mathfrak{S}^2}$, the right hand side is still of higher order in h for dimensions $d \leq 3$.*

Proof of Lemma 6.5.7. We retain only the trace on the right-hand side of (6.47),

$$Ch^2\|\alpha\|^2_{L^2(\Omega^2)} + C_\Gamma h^{4-d} = Ch^2\|\tilde{\alpha}\|^2_{L^2(\tilde{\Omega}\times\mathbb{R}^d)} + C_\Gamma h^{4-d} \geq \mathrm{Tr}[\alpha\overline{\alpha}\alpha\overline{\alpha}]. \tag{6.52}$$

For the following argument, we extend all the relevant kernels to functions on $\mathbb{R}^d \times \mathbb{R}^d$. In this way, we can identify $\mathrm{Tr}[\alpha\overline{\alpha}\alpha\overline{\alpha}] \equiv \|\alpha\|^4_{\mathfrak{S}^4}$, where $\|\cdot\|_{\mathfrak{S}^p}$ denotes the Schatten trace norm of an operator on $L^2(\mathbb{R}^d)$. Equation (6.43) may be rewritten as

$$\begin{aligned} \alpha = \alpha_\psi + \tilde{\xi}, \qquad \alpha_\psi(x,y) &= h^{1-d}\psi\left(\frac{x+y}{2}\right)\alpha_*\left(\frac{x-y}{h}\right), \\ \tilde{\xi}(x,y) &= \xi\left(\frac{x+y}{2}, x-y\right). \end{aligned} \tag{6.53}$$

Here and in the following, the kernel functions $\alpha_\psi, \tilde{\xi}$ are understood to be functions on $\mathbb{R}^d \times \mathbb{R}^d$ (obtained by extension by zero). The Schatten norms satisfy the triangle inequality and are monotone decreasing in p. Also, the $\|\cdot\|_{\mathfrak{S}^2}$ norm of any operator agrees with the $\|\cdot\|_{L^2(\mathbb{R}^d\times\mathbb{R}^d)}$ norm of its kernel. From these facts, we obtain

$$\begin{aligned} \|\alpha\|_{\mathfrak{S}^4} &\geq \|\alpha_\psi\|_{\mathfrak{S}^4} - \|\tilde{\xi}\|_{\mathfrak{S}^4} \geq \|\alpha_\psi\|_{\mathfrak{S}^4} - \|\tilde{\xi}\|_{\mathfrak{S}^2} = \|\alpha_\psi\|_{\mathfrak{S}^4} - \|\tilde{\xi}\|_{L^2(\mathbb{R}^d\times\mathbb{R}^d)} \\ &= \|\alpha_\psi\|_{\mathfrak{S}^4} - \|\xi\|_{L^2(\tilde{\Omega}\times\mathbb{R}^d)} \geq \|\alpha_\psi\|_{\mathfrak{S}^4} + O(h)\|\alpha\|_{L^2(\Omega^2)} + O(h^{2-d/2}). \end{aligned}$$

In the last step, we used (6.48). From this, (6.52) and (6.49), we get

$$\begin{aligned}\|\alpha_\psi\|_{\mathfrak{S}^4}^4 &\le C\left(\|\alpha\|_{\mathfrak{S}^4}^4 + h^4\|\alpha\|_{L^2(\Omega^2)}^4 + O(h^{8-2d})\right)\\ &\le C\left(h^2\|\alpha\|_{L^2(\Omega^2)}^2 + h^4\|\alpha\|_{L^2(\Omega^2)}^4 + O(h^{4-d})\right)\\ &\le C\left(h^{4-d}\|\psi\|_{L^2(\tilde\Omega)}^2 + h^{8-2d}\|\psi\|_{L^2(\tilde\Omega)}^4 + O(h^{4-d})\right).\end{aligned} \tag{6.54}$$

Along the way, we used $8-2d > 4-d$ for $d = 1,2,3$. After extension by zero, $\psi \in H^1(\mathbb{R}^d)$ and we apply Lemma 6.3.2 (iv) to get

$$\|\alpha_\psi\|_{\mathfrak{S}^4}^4 = h^{4-d} g_0(\alpha_*)\|\psi\|_{L^4(\tilde\Omega)}^4 + O(h^{5-d})\|\psi\|_{H_0^1(\tilde\Omega)}^4.$$

Then, by (6.50) and Hölder's inequality, $\|\alpha_\psi\|_{\mathfrak{S}^4}^4 \ge Ch^{4-d}\|\psi\|_{L^2(\tilde\Omega)}^4$. Combining this estimate with (6.54) and using $8-2d > 4-d$, we get

$$\|\psi\|_{L^2(\tilde\Omega)}^4 \le C\|\psi\|_{L^2(\tilde\Omega)}^2 + O(1)$$

This proves $\|\psi\|_{L^2(\tilde\Omega)} \le O(1)$ and hence Lemma 6.5.7 and Theorem 6.5.1. □

6.6 Proof of Theorem 6.2.1 (LB): Semiclassics

From a priori bounds to GP theory

We begin by deriving a lower bound in terms of GP energy on $\tilde\Omega$, by assuming a decomposition with a priori bounds as in Theorem 6.5.1 and applying the semiclassical expansion from Lemma 6.3.2.

Accordingly, in this section, ψ and ξ are general functions, not necessarily the ones defined previously in Proposition 6.2.5 (they will be the same for convex domains).

Lemma 6.6.1. *Let $\mu = -E_b + Dh^2$ and define $\nu' := \min\{d/2, 1\}$. Let Γ be a BCS state such that α can be decomposed as in (6.10) for some $\psi \in H_0^1(\tilde\Omega)$ and $\xi \in H_0^1(\tilde\Omega \times \mathbb{R}^d)$. Moreover, suppose that $\|\psi\|_{H_0^1(\tilde\Omega)} \le O(1)$ and ξ satisfies the bound in (6.38). Then, wee have*

$$\mathcal{E}^{BCS}(\Gamma) \ge h^{4-d}\mathcal{E}^{GP}(\psi) + O(h^{4-d+\nu'})\|\psi\|_{H_0^1(\tilde\Omega)}^2. \tag{6.55}$$

The implicit constant depends continuously on D.

Proof of Lemma 6.6.1

It will be convenient to define the auxiliary energy functional

$$\begin{aligned}\mathcal{E}_{LB}(\alpha) :=&\mathrm{Tr}[(-h^2\Delta_\Omega + h^2W - \mu)\alpha\overline{\alpha}]\\ &+ \iint_{\Omega\times\Omega} V\left(\frac{x-y}{h}\right)|\alpha(x,y)|^2 \mathrm{d}x\mathrm{d}y + \mathrm{Tr}[\mathfrak{h}\alpha\overline{\alpha}\alpha\overline{\alpha}].\end{aligned}$$

We first note that this auxiliary functional provides a lower bound to the BCS energy. The basic idea is to replace γ by expressions in α using $\alpha\overline{\alpha} \leq \gamma$ as in the proof of Lemma 6.5.2. However some additional difficulty is present here because the last term in $\mathcal{E}_{LB}(\alpha)$ still features $\mathfrak{h}$ and so we need the stronger operator inequality (6.56) below.

Proposition 6.6.2. *For sufficiently small h, we have $\mathcal{E}^{BCS}(\Gamma) \geq \mathcal{E}_{LB}(\alpha)$, where α denotes the off-diagonal element of the BCS state Γ.*

Proof of Proposition. The claim will follow from the operator inequality

$$\gamma \geq \alpha\overline{\alpha} + \alpha\overline{\alpha}\alpha\overline{\alpha}. \tag{6.56}$$

To prove (6.56), we start by observing that $1 - \overline{\gamma} \leq (1 + \overline{\gamma})^{-1}$ by the spectral theorem. Consequently

$$0 \leq \Gamma = \begin{pmatrix} \gamma & \alpha \\ \overline{\alpha} & 1-\overline{\gamma} \end{pmatrix} \leq \begin{pmatrix} \gamma & \alpha \\ \overline{\alpha} & (1+\overline{\gamma})^{-1} \end{pmatrix}.$$

The Schur complement formula implies

$$\gamma \geq \alpha(1 + \overline{\gamma})\overline{\alpha}.$$

Using $\overline{\gamma} \geq \overline{\alpha}\alpha$, we find

$$\gamma \geq \alpha(1 + \overline{\gamma})\overline{\alpha} \geq \alpha\overline{\alpha} + \alpha\overline{\alpha}\alpha\overline{\alpha}$$

which proves (6.56). To conclude, let h be sufficiently small such that $\mathfrak{h} \geq 0$, see Proposition 6.5.3. Then (6.56) yields

$$\mathrm{Tr}[\mathfrak{h}\gamma] \geq \mathrm{Tr}[\mathfrak{h}\alpha\overline{\alpha}[+\mathrm{Tr}[\mathfrak{h}\alpha\overline{\alpha}\alpha\overline{\alpha}]$$

and this proves Proposition 6.6.2. □

The following key lemma says that we can apply the semiclassical expansion to the auxiliary energy functional with the desired result.

Lemma 6.6.3. *Under the assumptions of Lemma 6.6.1, we use the splitting $\alpha = \alpha_\psi + \tilde{\xi}$ from (6.53). Then*

$$\mathcal{E}_{LB}(\alpha) \geq \mathcal{E}_{LB}(\alpha_\psi) + O(h^{4-d+\nu'})\|\psi\|^2_{H^1_0(\tilde{\Omega})}.$$

The implicit constant depends continuously on D.

Before we prove this lemma, we note that it directly implies Lemma 6.6.1. Indeed, it gives

$$\mathcal{E}^{BCS}(\Gamma) \geq \mathcal{E}_{LB}(\alpha) \geq \mathcal{E}_{LB}(\alpha_\psi) + O(h^{4-d+\nu'})\|\psi\|^2_{H^1_0(\tilde{\Omega})}.$$

All the terms in $\mathcal{E}_{LB}(\alpha_\psi)$ were computed in the semiclassical expansion in Lemma 6.3.2. On the result of the expansion, we use the eigenvalue equation $(-\delta + V + E_b)\alpha_* = 0$ and recall $g_{BCS}(\alpha_*) = g_{BCS}$ from (6.6). This yields $\mathcal{E}^{GP}(\psi)$ plus the appropriate error terms. These are of the claimed size because $\|\psi\|_{H^1(\mathbb{R}^d)} \leq O(1)$ by Theorem 6.5.1 and $\mu = -E_b + Dh^2$ by assumption. Moreover, they depend on the previously derived error terms in explicit continuous ways and are therefore also continuous in D.

It remains to give the

Proof of Lemma 6.6.3. We treat the terms in $\mathcal{E}_{LB}$ in four separate parts. First, by changing to center-of-mass coordinates (6.40), compare the proof of Lemma 3 in [28],

$$\begin{aligned}
&\mathrm{Tr}[(-h^2\Delta_\Omega + E_b)\alpha\overline{\alpha}] + \iint_{\mathbb{R}^d\times\mathbb{R}^d} V\left(\frac{x-y}{h}\right)|\alpha(x,y)|^2 \mathrm{d}x\mathrm{d}y \\
\geq &\mathrm{Tr}[(-h^2\Delta_\Omega + E_b)\alpha_\psi\overline{\alpha_\psi}] + \iint_{\mathbb{R}^d\times\mathbb{R}^d} V\left(\frac{x-y}{h}\right)|\alpha_\psi(x,y)|^2 \mathrm{d}x\mathrm{d}y.
\end{aligned} \tag{6.57}$$

Second, from $\mu = -E_b + Dh^2$, (6.49) and (6.38), we get

$$-(\mu + E_b)\mathrm{Tr}[\alpha\overline{\alpha}] \geq -(\mu + E_b)\mathrm{Tr}[\alpha_\psi\overline{\alpha_\psi}] + O(h^{6-d})\|\psi\|^2_{L^2(\tilde{\Omega})}. \tag{6.58}$$

Next, by Cauchy-Schwarz, Lemma 6.5.5 and (6.38):

$$\begin{aligned}
\mathrm{Tr}[W\alpha\overline{\alpha}] \geq &\mathrm{Tr}[W\alpha_\psi\overline{\alpha_\psi}] - C\left(\|\xi\|^2_{L^2(\tilde{\Omega}\times\mathbb{R}^d)} + h^2\|\nabla\xi\|^2_{L^2(\tilde{\Omega}\times\mathbb{R}^d)}\right) \\
&- C\left(\|\xi\|^2_{L^2(\tilde{\Omega}\times\mathbb{R}^d)} + h^2\|\nabla\xi\|^2_{L^2(\tilde{\Omega}\times\mathbb{R}^d)}\right)^{1/2} h^{1-\frac{d}{2}}\|\psi\|_{H^1_0(\tilde{\Omega})} \\
\geq &\mathrm{Tr}[W\alpha_\psi\overline{\alpha_\psi}] + O(h^{3-d}).
\end{aligned}$$

Using $\mathfrak{h} = -h^2\Delta_\Omega + h^2 W - \mu$, the claim will then follow from

$$\mathrm{Tr}[\mathfrak{h}\alpha\overline{\alpha}\alpha\overline{\alpha}] \geq \mathrm{Tr}[\mathfrak{h}\alpha_\psi\overline{\alpha_\psi}\alpha_\psi\overline{\alpha_\psi}] + O(h^{4-d+\nu'}). \tag{6.59}$$

This can be obtained by expanding the quartic and using the a priori bounds (6.38), see the proof of (7.12) in [28]. Modifications are only needed for the W

term, which we control via form-boundedness (instead of using $\|W\|_{L^\infty}$). Consider e.g. the term $\mathrm{Tr}[W\alpha_\psi\overline{\alpha}\alpha\overline{\tilde{\xi}}]$. By cyclicity of the trace, Hölder's inequality for Schatten norms and form-boundedness,

$$\begin{aligned}\mathrm{Tr}[W\alpha_\psi\overline{\alpha}\alpha\overline{\tilde{\xi}}] \leq&\|\alpha\|_{\mathfrak{S}^6}^2\|\sqrt{|W|}\alpha_\psi\|_{\mathfrak{S}^6}\|\sqrt{|W|}\mathrm{sgn}(W)\tilde{\xi}\|_{\mathfrak{S}^2}\\ =&\|\alpha\|_{\mathfrak{S}^6}^2\|\overline{\alpha_\psi}|W|\alpha_\psi\|_{\mathfrak{S}^3}^{1/2}\|\overline{\tilde{\xi}}|W|\tilde{\xi}\|_{\mathfrak{S}^1}^{1/2}\\ \leq&C\|\alpha\|_{\mathfrak{S}^6}^2\left(\|\nabla\alpha_\psi\|_{\mathfrak{S}^6}+\|\alpha_\psi\|_{\mathfrak{S}^6}\right)\left(\|\nabla\tilde{\xi}\|_{\mathfrak{S}^2}+\|\tilde{\xi}\|_{\mathfrak{S}^2}\right).\end{aligned}\tag{6.60}$$

In the last step, we used the fact that form-boundedness of W implies the operator inequality $|W|\leq C(1-\Delta)$. The resulting expression is up to constants the first term on the right hand side in (7.16) of [28] and is estimated there for $d=3$. The bounds directly generalize to all $d=1,2,3$ and we briefly sketch the conclusion of the argument in that general case.

First, one uses $\alpha=\alpha_\psi+\xi$, the triangle inequality for the $\mathfrak{S}^6$-norm and the fact that $\|\cdot\|_{\mathfrak{S}^6}\leq\|\cdot\|_{\mathfrak{S}^2}$ to get

$$\|\alpha\|_{\mathfrak{S}^6}^2\leq C\left(\|\alpha_\psi\|_{\mathfrak{S}^6}^2+\|\xi\|_{\mathfrak{S}^2}^2\right).$$

Now one can bound all the terms by generalizing the estimates in Lemma 1 of [28] to all $d=1,2,3$ and by the a priori bounds from Theorem 6.5.1 (recall that the Hilbert-Schmidt norm is equal to the $L^2\times L^2$ norm of the kernel). This gives

$$\begin{aligned}\|\alpha_\psi\|_{\mathfrak{S}^2}\leq O(h^{1-d/2}),\qquad \|\alpha_\psi\|_{\mathfrak{S}^6}\leq O(h^{1-d/6}),\\ \|\tilde{\xi}\|_{\mathfrak{S}^2}\leq O(h^{2-d/2}),\qquad \|\nabla\tilde{\xi}\|_{\mathfrak{S}^2}\leq O(h^{1-d/2}),\\ \|\nabla\alpha_\psi\|_{\mathfrak{S}^6}\leq C\left(\|\nabla_X\alpha_\psi\|_{\mathfrak{S}^6}+\|\nabla_r\alpha_\psi\|_{\mathfrak{S}^6}\right)\leq O(h^{-d/6})\end{aligned}$$

and we conclude that

$$h^2\mathrm{Tr}[W\alpha_\psi\overline{\alpha}\alpha\overline{\tilde{\xi}}]\leq O(h^{5-d}).$$

The same idea applies to all the other W dependent terms in the expansion of the quartic and we obtain (6.59). This proves Lemma 6.6.3 and consequently Lemma 6.6.1. □

Proof of Theorem 6.2.1 (LBC)

Let Ω be convex and let Γ be an approximate BCS minimizer, i.e. $\mathcal{E}^{BCS}(\Gamma)\leq C_\Gamma h^{4-d}$. We apply Theorem 6.5.1 and then Lemma 6.6.1. Since $\Omega=\tilde{\Omega}$ by convexity, this finishes the proof. □

Proof of Theorem 6.2.1 (LB)

Let Ω be a non-convex bounded Lipschitz domain. The order parameter ψ defined in Proposition 6.5.4 now lives on $\tilde{\Omega} = \frac{\Omega+\Omega}{2}$, which may be a much larger set than Ω.

Decay of the order parameter

We first show that ψ in fact *decays exponentially* away from Ω. This follows easily from its definition (6.41) and the exponential decay of α_*, see (6.27).

Proposition 6.6.4. *There exists a constant $C_0 > 0$ such that for every $\ell > 0$ and almost every $X \in \tilde{\Omega}$ with $\operatorname{dist}(X, \Omega) \geq \ell$, we have*

$$|\psi(X)| \leq C_0 h^{d/2-1} e^{-\rho_* \frac{2\ell}{h}} \|\tilde{\alpha}(X, \cdot)\|_{L^2(\mathcal{D}_X)} \tag{6.61}$$

$$|\nabla\psi(X)| \leq C_0 h^{d/2-1} e^{-\rho_* \frac{2\ell}{h}} \|\nabla_X \tilde{\alpha}(X, \cdot)\|_{L^2(\mathcal{D}_X)}. \tag{6.62}$$

Proof. Let $\ell > 0$ and $X \in \tilde{\Omega}$ with $\operatorname{dist}(X, \Omega) \geq \ell$. The key observation is that the triangle inequality implies

$$\mathcal{D}_X \subseteq \left\{ r \in \mathbb{R}^d \ : \ |r| > 2\ell \right\},$$

where $\mathcal{D}_X$ was defined in Proposition 6.5.4. Therefore, by Cauchy-Schwarz and (6.27)

$$\begin{aligned} |\psi(X)| &\leq h^{-1} \int_{\mathcal{D}_X} |\alpha_*(r/h)||\tilde{\alpha}(X, r)| \mathrm{d}r \\ &= h^{-1} \int_{\mathcal{D}_X} e^{-\rho_* \frac{r}{h}} e^{\rho_* \frac{r}{h}} |\alpha_*(r/h)||\tilde{\alpha}(X, r)| \mathrm{d}r \\ &\leq C_0 h^{d/2-1} e^{-\rho_* \frac{2\ell}{h}} \|\tilde{\alpha}(X, \cdot)\|_{L^2(\mathcal{D}_X)}. \end{aligned}$$

This proves (6.61). Starting from (6.45), the same argument gives (6.62). $\square$

Conclusion by a cutoff argument

With Proposition 6.6.4 at our hand, we just have to cut off part of ψ that lives sufficiently far away from Ω. We first apply Theorem 6.5.1 to get the decomposition and the a priori bounds stated there. Then, we define

$$\begin{aligned} \psi_1(X) &:= \eta_{\frac{\ell(h)}{4}, \Omega^+_{\ell(h)}}(X) \psi(X), \\ \xi_1(X, r) &:= \xi(X, r) + (\psi(X) - \psi_1(X)) \alpha_*(r/h). \end{aligned}$$

Here Ω_ℓ^+ was defined in (6.14), the cutoff function $\eta_{\ell,U}$ was defined in (6.66) and $\ell(h) = h\log(h^{-q})$. Note that we also have (6.10) with ψ, ξ replaced by ψ_1, ξ_1.

Note that $\psi_1 \in H_0^1(\Omega_{\ell(h)}^+)$. Hence, the claim will follow from Lemma 6.6.1 applied with the choices $\psi = \psi_1$, $\xi = \xi_1$. It remains to show that its assumptions are satisfied, namely that $\|\psi_1\|_{H_0^1(\Omega_{\ell(h)}^+)} \leq O(1)$ and ξ_1 satisfies (6.38).

For this part, we denote $\eta \equiv \eta_{\frac{c_0\ell(h)}{4},\Omega_{\ell(h)}^+}$ and $\ell \equiv \ell(h)$ for short. We first prove that $\|\psi_1\|_{H_0^1(\Omega_\ell^+)} \leq O(1)$. Using $\eta \leq 1$ and Cauchy-Schwarz, we get

$$\|\psi_1\|_{H_0^1(\Omega_\ell^+)}^2 \leq 2\|\psi\|_{H_0^1(\Omega_\ell^+)}^2 + 2\int_{\Omega_\ell^+(h)} |\nabla\eta|^2|\psi|^2 \mathrm{d}X = O(1) + 2\int_{\Omega_\ell^+} |\nabla\eta|^2|\psi|^2 \mathrm{d}X. \tag{6.63}$$

The term with $|\nabla\eta|$ may look troubling since we can only control $|\nabla\eta| \leq \ell^{-2}$ on $\operatorname{supp}\nabla\eta$. The key insight is that this potential blow up in h is sufficiently dampened on $\operatorname{supp}\nabla\eta$ by the exponential decay of $|\psi|$ established by Proposition 6.6.4. Namely, we will prove

Lemma 6.6.5. $\operatorname{supp}\nabla\eta(p) \subset (\Omega_{\ell/2}^+)^c$

We postpone the proof of this geometrical lemma for now. Assuming it holds, it is straightforward to use the decay estimates from Proposition 6.6.4 to conclude from (6.63) that $\|\psi_1\|_{H_0^1(\Omega_\ell^+)} \leq O(1)$, by choosing q large enough (with respect to $1/\rho_*$).

Next, we show that ξ_1 satisfies (6.38). From Theorem 6.5.1, we already know that ξ satisfies (6.38). When integrating the other term in the definition of ξ_1, we change to center of mass coordinates and write $\psi - \psi_1 = \psi(1-\eta)$. Since $\nabla(1-\eta)$ and $\nabla\eta$ are supported on the same set, one can use the argument from above again on the center of mass integration (i.e. a combination of Lemma 6.6.5 and Proposition 6.6.4). We leave the details to the reader.

To finish the proof of Theorem 6.2.1 (LB), it remains to give the

Proof of Lemma 6.6.5. Let $p \in \mathbb{R}^d$ be a point such that $\nabla\eta(p) \neq 0$. Then, by definition (6.66) of η,

$$\operatorname{dist}(p, (\Omega_\ell^+)^c) < \ell/2.$$

Let $q_\ell \in (\Omega_\ell^+)^c$ be a point such that $\mathrm{dist}(p,(\Omega_\ell^+)^c) = |p - q_\ell|$ and let $q \in \overline{\Omega}$ be a point such that $\mathrm{dist}(p,\Omega) = |p - q|$ (such points exists by a compactness argument). By definition (6.14) of Ω_ℓ^+ and the triangle inequality,

$$\ell \leq \mathrm{dist}(\Omega,(\Omega_\ell^+)^c) \leq |q - q_\ell| \leq |q - p| + |p - q_\ell| < |q - p| + \ell/2.$$

Therefore, $\mathrm{dist}(p,\Omega) = |q - p| > \ell/2$ and so $p \in (\Omega_{\ell/2}^+)^c$. Since p was an arbitrary point with $\nabla\eta(p) \neq 0$ and $(\Omega_{\ell/2}^+)^c$ is closed, Lemma 6.6.5 is proved. □

6.7 Proof of the continuity of the GP energy (Theorem 6.2.2)

Davies' use of Hardy inequalities

This section serves as a preparation to prove the second key result Theorem 6.2.2.

The central idea that we discuss here is Lemma 6.7.2. It is based on the insight of Davies [54][55] that continuity of the Dirichlet energy under interior approximations of a domain U follows from good control on the boundary decay of functions that lie in the operator domain of Δ_U (the decay is better than that of functions that merely lie in the *form domain* of $-\Delta_U$). The key assumption is that the domain U satisfies a Hardy inequality (6.65).

Importantly, *GP minimizers corresponding to* E_U^{GP} *are in* $\mathrm{dom}(\Delta_U)$ *thanks to the Euler Lagrange equation*; this was proved in Proposition 6.2.5.

As its input, the lemma requires the validity of the

Definition 6.7.1 (Hardy inequality)**.** *Let* $U \subseteq \mathbb{R}^d$ *and denote*

$$d_U(x) := \mathrm{dist}(x, U^c). \tag{6.64}$$

We say that U *satisfies a Hardy inequality, if there exist* $c_U \in (0,1]$ *and* $\lambda \in \mathbb{R}$ *such that*

$$\int_U d_U(x)^{-2}|\varphi(x)|^2 \mathrm{d}x \leq \frac{4}{c_U^2}\|\nabla\varphi\|_{L^2(U)}^2 + \lambda\|\varphi\|_{L^2(U)}^2, \qquad \forall \varphi \in C_c^\infty(U). \tag{6.65}$$

We shall refer to c_U *and* λ *as the "Hardy constants".*

We can now state

Lemma 6.7.2. *For any $0 < \ell < 1$, we define the function $\eta_{\ell,U} : \mathbb{R}^d \to [0,\infty)$ by*

$$\eta_{\ell,U}(x) := \begin{cases} 0, & \text{if } 0 \le d_U(x) \le \ell \\ \frac{d_U(x)-\ell}{\ell}, & \text{if } \ell \le d_U(x) \le 2\ell \\ 1, & \text{otherwise.} \end{cases} \tag{6.66}$$

Suppose that U satisfies the Hardy inequality (6.65) for some $c_U \in (0,1]$ and some $\lambda \in \mathbb{R}$. Then, there exists a constant $c > 0$ depending only on c_U and λ such that

$$\mathcal{E}^{GP}(\eta_{\ell,U}\varphi) - \mathcal{E}^{GP}(\varphi) \le c\ell^{c_U} \left(\|\varphi\|_{H_0^1(U)} \|\Delta_U \varphi\|_{L^2(U)} + \|\varphi\|^2_{H_0^1(U)} \right)$$

holds for all $\varphi \in \mathrm{dom}(\Delta_U)$. Moreover, the same bound holds for the quantity $\|\eta_{\ell,U}\varphi\|^2_{H_0^1(U)} - \|\varphi\|^2_{H_0^1(U)}$.

We remark that $\eta_{\ell,U}$ is a Lipschitz continuous function with a Lipschitz constant that is independent of U (this is because d_U has the Lipschitz constant one for all U).

Proof. We write $\eta \equiv \eta_{\ell,U}$. First, we note that the nonlinear term drops out because $|\eta\varphi|^4 - |\varphi|^4 = (\eta^4 - 1)|\varphi|^4 \le 0$ thanks to $0 \le \eta \le 1$. For the gradient term, we note that the Hardy inequality (6.65) is the main assumption in [54][55]. Thus, by Lemma 11 in [55], there exists a $c > 0$ (depending only on the Hardy constants c_U and λ) such that

$$\int_U (|\nabla(\eta\varphi)|^2 - |\nabla\varphi|^2)\mathrm{d}x \le c\ell^{c_U} \|\Delta_U\varphi\|_{L^2(U)} \|\nabla\varphi\|_{L^2(U)}, \quad \forall \varphi \in \mathrm{dom}(-\Delta_U).$$

Since $\eta \le 1$, this already implies the last sentence in Lemma 6.7.2. Using Cauchy-Schwarz, Assumption 6.1.2 on W and Theorem 4 in [55], we get

$$\begin{aligned} &\int_U (W+D)(\eta^2-1)|\varphi|^2\mathrm{d}x \le \int_U (|W|+|D|)(1-\eta^2)|\varphi|^2\mathrm{d}x \\ \le &\left(\|W\varphi\|_{L^2(\Omega)} + |D|\|\varphi\|_{L^2(\Omega)}\right) \left(\int_{U\cap\{d_U \le 2\ell\}} |\varphi|^2 \mathrm{d}x \right)^{1/2} \\ \le &c\left(\|W\|_{L^{p_W}(\Omega)} + |D|\right) \|\varphi\|_{H_0^1(U)} \ell^{1+c_U/2} \left(\|\Delta_U\varphi\|_{L^2(U)} \|\nabla\varphi\|_{L^2(U)} \right)^{1/2} \end{aligned}$$

for another constant c depending only on c_U and λ. We estimate the last term via $2\sqrt{ab} \le a + b$. Then we use that $\ell^{1+c_U/2} \le \ell^{c_U}$ holds for all $c_U \in (0,1]$ and $0 < \ell < 1$. This proves Lemma 6.7.2. □

With Lemma 6.7.2 at our disposal, we need conditions on U such that it satisfies the Hardy inequality (6.65).

It is a classical result of Necas [140] that any bounded Lipschitz domain Ω satisfies a Hardy inequality for some $c_\Omega \in (0,1]$ and some $\lambda \in \mathbb{R}$. Hence, we can apply Lemma 6.7.2 with $U = \Omega$ and this is already sufficient to obtain continuity of the GP energy under *interior* approximation, i.e. Theorem 6.2.2 with Ω_ℓ^-. The details of this argument are given in the next subsection.

To summarize, we see that therefore Necas' result is already sufficient to derive

(i) the upper bounds in the two main results, Theorems 6.1.7 and 6.1.10.

(ii) the complete Theorem 6.1.10 for bounded and *convex* domains Ω. Indeed, Theorem 6.2.1 (LBC) gives the lower bound and the upper bound holds because any convex domains satisfies a Hardy inequality [132][134]. (In fact, the Hardy constants can be taken as $c = 1$ and $\lambda = 0$.)

To prove the lower bounds in the main results for non-convex domains, we need continuity of the GP energy under *exterior* approximation. This relies on the following new theorem which is is an extension of Necas' argument [140]. The proof is deferred to Appendix 6.11.

Theorem 6.7.3. *Let Ω be a bounded Lipschitz domain. There exist $c_\Omega \in (0,1]$, $\lambda \in \mathbb{R}$ and $\ell_0 > 0$, as well as a sequence of exterior approximations $\{\Omega_\ell\}_{0<\ell<\ell_0}$ such that the Hardy inequality* (6.65) *holds with $U = \Omega_\ell$ for all $\ell < \ell_0$.*

Moreover, the sequence of approximations $\{\Omega_\ell\}_\ell$ satisfies the following properties.

(i) There exists a constant $c_0 > 1$ such that $\Omega_\ell^+ \subset \Omega_\ell \subset \Omega_{c_0\ell}^+$.

(ii) There exists a constant $a > 0$ such that

$$\left\{q \in \mathbb{R}^d \ : \ \operatorname{dist}(q, (\Omega_\ell)^c) > a\ell\right\} \subset \Omega. \tag{6.67}$$

We emphasize that the Lipschitz character of Ω is important for the sequence of approximations $\{\Omega_\ell\}_\ell$ to exist. Concretely, properties (i) and (ii) cannot both hold for exterior approximations of the slit domain example presented in Remark 6.2.4 (while there do exist approximations that all satisfy the Hardy inequality with the ℓ-independent constant $c_\Omega = 1/2$).

Proof of Theorem 6.2.2

We begin by observing that $\Omega_\ell^- \subset \Omega \subset \Omega_\ell^+$ trivially gives

$$E^{GP}_{\Omega_\ell^+} \leq E^{GP}_{\Omega} \leq E^{GP}_{\Omega_\ell^-}.$$

Theorem 6.2.2 says that the reverse bounds hold as well, up to the claimed error terms. The basic idea is to take a minimizer on the larger domain and to cut it off near the boundary, where the energy cost of the cutoff is controlled by Lemma 6.7.2.

Interior approximation

The situation is easier for interior approximation, since then we consider GP minimizers and the Hardy inequality on the fixed domain Ω. We want to apply Lemma 6.7.2 and we gather prerequisites.

First, by Proposition 6.2.5, there exists a unique non-negative minimizer corresponding to E^{GP}_Ω, call it ψ, and it satisfies

$$\|\Delta_U \psi\|_{L^2(U)} \leq C(1+|D|)(\|\psi\|_{H_0^1(U)} + \|\psi\|^3_{H_0^1(U)}) \tag{6.68}$$

Second, since Ω is a bounded Lipschitz domain, there exists $c_\Omega \in (0,1]$ and $\lambda \in \mathbb{R}$ such that the Hardy inequality (6.65) holds on $U = \Omega$ [140]. Now we apply Lemma 6.7.2 with the domain $U = \Omega$ and the cutoff function $\eta_{2\ell,\Omega}$. We get

$$\begin{aligned}&\mathcal{E}^{GP}(\eta_{2\ell,\Omega}\psi) \leq \mathcal{E}^{GP}(\psi) + O(\ell^{2/c_\Omega})(\|\psi\|_{H_0^1(\Omega)}\|\Delta_\Omega\psi\|_{L^2(\Omega)} + \|\psi\|^2_{H_0^1(\Omega)})\\ \leq&\mathcal{E}^{GP}(\psi) + O(\ell^{2/c_\Omega})\end{aligned}$$

In the second step, we used (6.68) and the fact that all norms of ψ are independent of ℓ. The definitions of $\eta_{2\ell,\Omega}$ and Ω_ℓ^- are such that $\operatorname{supp} \eta_{2\ell,\Omega} \subset \Omega_\ell^-$. Since $\eta_{2\ell,\Omega}$ is Lipschitz continuous, this implies $\eta_{2\ell,\Omega}\psi \in H_0^1(\Omega_\ell^-)$ and therefore

$$\mathcal{E}^{GP}(\eta_{2\ell,\Omega}\psi) \geq E^{GP}_{\Omega_\ell^-}. \tag{6.69}$$

This proves the claimed continuity under interior approximation.

Exterior approximation

The idea is similar as before, but additional ℓ dependencies complicate the argument somewhat. We let $\{\Omega_\ell\}_{0<\ell<\ell_0}$ be the sequence of exterior approximations given by Theorem 6.7.3. That is, $\Omega_\ell^+ \subset \Omega_\ell$ and the Hardy inequality

(6.65) holds on all $U = \Omega_\ell$ with Hardy constants that are uniformly bounded in ℓ.

By Proposition 6.2.5, there exists a unique non-negative minimizer corresponding to $E^{GP}_{\Omega_\ell}$, call it ψ_ℓ, and it satisfies the analogue of (6.68) with a C that is independent of ℓ.

Recall definition (6.66) of the cutoff function $\eta_{a\ell,\Omega_\ell}$. Here we choose $a > 0$ such that property (ii) in Theorem 6.7.3 holds which is equivalent to

$$\operatorname{supp} \eta_{a\ell,\Omega_\ell} \subset \Omega. \tag{6.70}$$

Now we apply Lemma 6.7.2. We note that the constant c appearing in it depends only on the Hardy constants (and these are uniformly bounded in ℓ). Therefore, using the analogue of (6.68), we get

$$\mathcal{E}^{GP}(\eta_{a\ell,\Omega_\ell}\psi_\ell) \leq \mathcal{E}^{GP}(\psi_\ell) + O(\ell^{2/c})O(\|\psi_\ell\|^2_{H^1_0(\Omega_\ell)} + \|\psi_\ell\|^4_{H^1_0(\Omega_\ell)}). \tag{6.71}$$

Regarding the error term, we note

Lemma 6.7.4. $\|\psi_\ell\|_{H^1_0(\Omega_\ell)} \leq O(1)$.

Proof of Lemma 6.7.4. We use that the GP energy can only increase under a decrease of the underlying domain to get

$$\mathcal{E}^{GP}(\psi_\ell) = E^{GP}_{\Omega_\ell} \leq E^{GP}_{\Omega} \tag{6.72}$$

The claim now follows from the coercivity (6.21), since the constants C_1, C_2, D there do not depend on the underlying domain and hence not on ℓ. □

By (6.70) and the fact that $\eta_{a\ell,\Omega_\ell}$ is a Lipschitz function, we get $\eta_{a\ell,\Omega_\ell}\psi_\ell \in H^1_0(\Omega)$. Returning to (6.71), we can conclude the proof as in (6.69), which yields Theorem 6.2.2. □

6.8 On GP minimizers

We prove Proposition 6.2.5.

Proof of (i). The coercivity (6.21) is a straightforward consequence of the form-boundedness of W and the elementary bound

$$|\psi|^4 - (C + D)|\psi|^2 \geq -(C_2 + D)^2.$$

The constants C_1, C_2 only depend on W.

Proof of (ii). Let $\{\psi_n\}$ be a minimizing sequence corresponding to E_U^{GP}. By the coercivity (6.21), the sequence is bounded in $H_0^1(U)$ and hence weakly $H_0^1(U)$-precompact. Let $\psi_* \in H_0^1(U)$ denote one of its weak limit points. By Rellich's theorem, $\psi_n \to \psi_*$ in $L^2(U)$. Hence,

$$\begin{aligned}
&\left|\int_U W(|\psi_n|^2 - |\psi_*|^2)\mathrm{d}x\right| \\
\leq &\left(\|W\psi_n\|_{L^2(U)} + \|W\psi_*\|_{L^2(U)}\right) \||\psi_n| - |\psi_*|\|_{L^p(U)} \\
\leq &C\|W\|_{L^{p_W}(U)}(\|\nabla\psi_n\|_{H_0^1(U)} + \|\nabla\psi_*\|_{H_0^1(U)})\|\psi_n - \psi_*\|_{L^2(U)} \to 0.
\end{aligned}$$

The last estimate holds by Assumption 6.1.2 on W. The same argument gives the continuity of the D term in $\mathcal{E}^{GP}$.

Let $\# \in \{n, *\}$. We write $\mathcal{E}^{GP}(\psi_\#) = A_\# + B_\#$, where $A_\# = \|\nabla\psi_\#\|^2_{L^2(U)}$ and $B_\#$ contains the remaining terms. Then, the above shows that $B_n \to B_*$. Moreover, by weak convergence is $H_0^1(U)$, $\liminf A_n \geq A_*$, so $E_U^{GP} = \lim(A_n + B_n) \geq A_* + B_*$. Since $A_* + B_* \geq E_U^{GP}$ by definition of E_U^{GP}, we conclude that ψ_* is a minimizer and that $A_n \to A_*$. Thus, $\|\psi_n\|_{H_0^1(U)} \to \|\psi_*\|_{H_0^1(U)}$ and therefore $\psi_n \to \psi_*$ strongly in $H_0^1(U)$.

To prove the uniqueness statement we first note that $\|\nabla|\psi|\|_{L^2(U)} \leq \|\nabla\psi\|_{L^2(U)}$. Moreover, since $\rho \mapsto \|\nabla\sqrt{\rho}\|^2_{L^2(U)}$ is convex and $\rho \mapsto \|\rho\|^2_{L^2(U)}$ is strictly convex, we see that $\mathcal{E}^{GP}(\psi)$ is a strictly convex functional of $|\psi|^2$, and therefore has a unique minimizer.

Proof for (iii). We compute the Euler Lagrange equation for the GP energy and find

$$-\frac{1}{4}\Delta_U\psi_* + (W - D)\psi_* + 2g_{BCS}|\psi_*|^2\psi_* = 0.$$

This equation holds in the dual of $H_0^1(U)$, that is, when tested against $H_0^1(U)$ functions. By our Assumption 6.1.2 on W and Sobolev's inequality, $\Delta_U\psi_*$ is in fact an $L^2(U)$ function and we have the bound

$$\begin{aligned}
\|\Delta_U\psi_*\|_{L^2(U)} =&\|4(W - D)\psi_* + 8g_{BCS}|\psi_*|^2\psi_*\|_{L^2(U)} \\
\leq &C(1 + |D|)(\|\psi_*\|_{H_0^1(U)} + \|\psi_*\|^3_{H_0^1(U)}).
\end{aligned}$$

This finishes the proof of Proposition 6.2.5. □

6.9 Convergence of the one-body density

Proof of Proposition 6.1.11. We fix a real valued $w \in L^{p_W}(\Omega)$ and $t \in \mathbb{R}$ and define $W_t := W + tw$. We denote the BCS/GP energies which are defined with

W_t by $\mathcal{E}_t^{BCS}, E_t^{BCS}, \mathcal{E}_t^{GP}$, etc. On the one hand, our assumption on Γ gives

$$E^{BCS} - E_t^{BCS} \geq \mathcal{E}^{BCS}(\Gamma) - \mathcal{E}_t^{BCS}(\Gamma) + o(h^{4-d}) = th^2 \mathrm{Tr}[\gamma w] + o(h^{4-d}).$$

On the other hand, Theorem 6.1.10 yields

$$E^{BCS} - E_t^{BCS} = h^{4-d}(E^{GP} - E_t^{GP}) + O(h^{4-d+\nu})$$

where the implicit constant depends on w. We denote the unique non-negative minimizer of $\mathcal{E}_t^{GP}$ by ψ_t (see Proposition 6.2.5). Multiplying through by h^{d-4} and taking $h \to 0$, we find

$$\limsup_{h\to 0} th^{d-2}\mathrm{Tr}[\gamma w] \leq E^{GP} - E_t^{GP} \leq \mathcal{E}^{GP}(\psi_t) - \mathcal{E}_t^{GP}(\psi_t) = t\int_\Omega w|\psi_t|^2 \mathrm{d}x. \tag{6.73}$$

We claim that $\psi_t \to \psi_*$ in $H_0^1(\Omega)$. This will imply the main claim (6.12). To see this, one divides (6.73) by t, distinguishing the cases $t > 0$ and $t < 0$, and sends $t \to 0$. Then one uses Rellich's theorem to get $|\psi_t|^2 \to |\psi_0|^2$ in $L^{p_W'}(\Omega)$.

Hence, it remains to prove that $\psi_t \to \psi_*$ in $H_0^1(\Omega)$. This is a simple compactness argument. We denote $\eta_t := \psi_t - \psi_*$. The coercivity (6.21) and the triangle inequality imply that $\|\eta_t\|_{H_0^1(\Omega)}$ remains bounded as $t \to 0$. We have

$$\begin{aligned} 0 \leq & \mathcal{E}^{GP}(\psi_t) - \mathcal{E}^{GP}(\psi_*) = \mathcal{E}_t^{GP}(\psi_t) - \mathcal{E}_t^{GP}(\psi_*) - t\int_\Omega w(2\Re(\eta_t)\psi_* + |\eta_t|^2)\mathrm{d}x \\ \leq & -t\int_\Omega w(2\Re(\eta_t)\psi_* + |\eta_t|^2)\mathrm{d}x \end{aligned}$$

The right hand side vanishes as $t \to 0$, since $\|\eta_t\|_{H_0^1(\Omega)}$ remains bounded as $t \to 0$. Therefore, ψ_t is a sequence of approximate minimizers of $\mathcal{E}^{GP}$. Proposition 6.2.5 (ii) then implies that $\psi_t \to \psi_*$ in $H_0^1(\Omega)$. □

6.10 On the semiclassical expansion

We sketch the proof of Lemma 6.3.2, especially where it departs from similar results in [28]. All norms and all integrals are taken over $\mathbb{R}^d$, unless noted otherwise.

Proof of Lemma 6.3.2. Proof of (i). This follows directly from changing to the center-of-mass coordinates (6.40), compare the proof of Lemma 6.5.2.

Proof of (ii). We write out the trace with operator kernels, change to center-of-mass coordinates (6.40) and apply the fundamental theorem of calculus to get

$$\mathrm{Tr}[W\mathfrak{a}_\psi\overline{\mathfrak{a}_\psi}] = h^{-d}\iint W(X)|\mathfrak{a}(r)|^2\left|\psi\left(X-\frac{hr}{2}\right)\right|^2 \mathrm{d}X\mathrm{d}r$$
$$= h^{-d}\int W(X)|\psi(X)|^2\mathrm{d}X - h^{-d}\eta$$

with

$$\eta = \mathrm{Re}\iint W(X)|\mathfrak{a}(r)|^2\left(\int_0^1 \overline{\psi\left(X-\frac{shr}{2}\right)}hr\cdot\nabla\psi\left(X-\frac{shr}{2}\right)\mathrm{d}s\right)\mathrm{d}X\mathrm{d}r. \tag{6.74}$$

By Hölder's and Sobolev's inequalities, $|\eta| \leq h\|W\|_{L^{p_W}(\Omega)}\|\sqrt{|\cdot|}\mathfrak{a}\|_{L^2}^2\|\psi\|_{H^1}^2$. This is $O(h)$, since $\|\sqrt{|\cdot|}\mathfrak{a}\|_{L^2}^2 < \infty$ by our assumptions on $\mathfrak{a}$.

Proof of (iii). The argument in Lemma 1 in [28] generalizes because the critical Sobolev exponent is always greater or equal to six in $d = 1, 2, 3$ and so all the error terms can be bounded in terms of $\|\psi\|_{H^1(\mathbb{R}^d)}$. We mention that the idea of the proof is to write the trace in terms of operator kernels and to change to the four-body center-of-mass coordinates

$$X = \frac{x_1+x_2+x_3+x_4}{4}, \qquad r_k = x_{k+1}-x_k, \quad k = 1,2,3.$$

Then, one rescales the relative coordinates r_k by h (since they appear as $\mathfrak{a}(r_k/h)$) and expands in h.

When proving the first equation in (iii), the W term requires a different argument. Namely, as in the proof of (6.59), one uses Hölder's inequality for Schatten norms and form-boundedness of W with respect to $-\Delta$ to get

$$|\mathrm{Tr}[W\alpha_\psi\overline{\alpha_\psi}\alpha_\psi\overline{\alpha_\psi}]| \leq C\left(\|\nabla\alpha_\psi\|_{\mathfrak{S}^4}^2 + \|\alpha_\psi\|_{\mathfrak{S}^4}^2\right)\|\nabla\alpha_\psi\|_{\mathfrak{S}^4}^2.$$

Afterwards, one multiplies by h^2 and uses the bounds from Corollary 1 in [28]. This gives the first equation in (iii). For the second equation in (iii), one replaces $\|V\mathfrak{a}\|_{L^1}$ in the estimate of the error term A_2 in [28] by $\|\mathfrak{a}\|_{L^1}$, which is also finite. □

6.11 On Lipschitz domains and Hardy inequalities

We first present the construction of a suitable sequence of exterior approximations to a bounded Lipschitz domain. Then, we prove that this sequence satisfies Hardy inequalities with uniformly bounded Hardy constants (Theorem 6.7.3).

The proof of Theorem 6.7.3 is an extension of Necas' argument [140] for a fixed Lipschitz domain and draws on known results on the geometry of the sequence of the exterior approximations [32][131]. (We remark that we could alternatively work with the naive enlargements Ω_ℓ^+ (6.77), but this would require writing down a non trivial amount of elementary geometry estimates.)

Definitions

We begin by recalling

Definition 6.11.1 (Lipschitz domain)**.** *A bounded domain $\Omega \subseteq \mathbb{R}^d$ is a Lipschitz domain, if its boundary $\partial\Omega$ can be covered by finitely many bounded and open coordinate cylinders $\mathcal{C}_1, \ldots, \mathcal{C}_K \subset \mathbb{R}^d$ such that for all $1 \le k \le K$, there exist $R_k, \beta_k > 0$ and a Cartesian coordinate system such that*

$$\begin{aligned} \partial\Omega \cap \mathcal{C}_k =& \{(\mathbf{x}, f_k(\mathbf{x})) \in B_{R_k} \times \mathbb{R}\}, \\ \Omega \cap \mathcal{C}_k =& \left\{(\mathbf{x}, y) \in B_{R_k} \times \mathbb{R} \ : \ -\beta_k < y < f_k(\mathbf{x})\right\}, \\ \Omega^c \cap \mathcal{C}_k =& \left\{(\mathbf{x}, y) \in B_{R_k} \times \mathbb{R} \ : \ f_k(\mathbf{x}) < y < \beta_k\right\}. \end{aligned}$$

where $f_k : B_{R_k} \to \mathbb{R}$ is a uniformly Lipschitz continuous function on $B_{R_k} \subset \mathbb{R}^{d-1}$, the ball of radius R_k centered at the origin.

The exterior approximations Ω_ℓ are obtained by extending Ω in the direction of a smooth transversal vector field, which any Lipschitz domain is known to host.

By Rademacher's theorem, the Lipschitz continuous function f_k is differentiable almost everywhere. Hence, for every $1 \le k \le K$ and almost every $\mathbf{x} \in B_{R_k}$, we can define the outward normal vector field (to $\partial\Omega$) in the coordinate cylinder $\mathcal{C}_k$ by

$$n(\mathbf{x}) := \frac{(\nabla f_k(\mathbf{x}), -1)}{\sqrt{1 + |\nabla f_k(\mathbf{x})|^2}}. \tag{6.75}$$

Proposition 6.11.2 (Normal and transversal vector fields)**.** *Let Ω be a bounded Lipschitz domain in the sense of Definition 6.11.1. Then, Ω hosts a smooth vector field $v : \mathbb{R}^d \to \mathbb{R}^d$ which is "transversal", i.e. there exists $\kappa \in (0,1)$ such that for all $1 \le k \le K$,*

$$v(\mathbf{x}, f_k(\mathbf{x})) \cdot n(\mathbf{x}) \ge \kappa, \qquad |v(\mathbf{x}, f_k(\mathbf{x}))| = 1, \tag{6.76}$$

for almost every $\mathbf{x} \in B_{R_k}$.

The basic idea for Proposition 6.11.2 is that in each coordinate cylinder $\mathcal{C}_k$ from Definition 6.11.1, one takes the constant vector field e_d, i.e. the y direction, and then one smoothly interpolates between different $\mathcal{C}_k$ via a partition of unity. For the details, see e.g. pages 597-599 in [131] (and note that the surfaces measure, called σ there, and the Lebesgue measure on B_{R_k} are mutually absolutely continuous).

We are now ready to give

Definition 6.11.3 (Exterior approximations)**.** *Let Ω be a bounded Lipschitz domain and let v be the transversal vector field from Proposition 6.11.2. For every $\ell > 0$, define its enlargement by*

$$\hat{\Omega}_\ell := \{p + \ell v(p) \ : \ p \in \Omega\} . \tag{6.77}$$

Bounds on $\hat{\Omega}_\ell$

Each set $\hat{\Omega}_\ell$ has many nice properties if ℓ is small enough, see Proposition 4.19 in [131] (though this is stated for the case $\ell < 0$, analogous results hold for $\ell > 0$, as is also mentioned there). In particular, $\hat{\Omega}_\ell$ is also a bounded Lipschitz domain and there exist coordinate cylinders in which both $\partial\Omega$ and $\partial\hat{\Omega}_\ell$ are represented as the graphs of Lipschitz continuous functions, with Lipschitz constants that are uniformly bounded in ℓ. Moreover:

Proposition 6.11.4. *There exists a constant $c_0 > 0$, such that for all $\ell > 0$ small enough,*

$$\Omega^+_{c_0\ell} \subset \hat{\Omega}_\ell \subset \Omega^+_\ell . \tag{6.78}$$

This lemma will give property (i) in Theorem 6.7.3, up to reparametrizing $\Omega_\ell := \hat{\Omega}_{\ell/c_0}$.

Proof. The second containment follows directly from Proposition 4.15 in [131].

For the first containment, we invoke Proposition 4.19 in [131]. It gives $\overline{\Omega} \subset \hat{\Omega}_\ell$ and consequently

$$\mathrm{dist}(\Omega, \hat{\Omega}^c_\ell) = \mathrm{dist}(\partial\Omega, \hat{\partial}\Omega_\ell). \tag{6.79}$$

We will show that $\mathrm{dist}(\partial\Omega, \partial\hat{\Omega}_\ell) \geq c_0\ell$. By Proposition 4.19 (i) in [131],

$$\partial\hat{\Omega}_\ell = \{p + \ell v(p) \ : \ p \in \partial\Omega\} . \tag{6.80}$$

Hence, by a compactness argument, there exist $p, p' \in \partial\Omega$ such that

$$\mathrm{dist}(\partial\Omega, \partial\hat{\Omega}_\ell) = |p' - (p + \ell v(p))| = |V(p', 0) - V(p, \ell)|,$$

where we introduced the map

$$\begin{aligned} V : \partial\Omega \times (-\ell_0, \ell_0) &\to \mathbb{R}^d \\ (p, s) &\mapsto p + sv(p). \end{aligned} \tag{6.81}$$

By (4.67) in [131], V is bi-Lipschitz if $\ell_0 > 0$ is small enough. In particular, there exists $c_0 > 0$ such that

$$|V(p', 0) - V(p, \ell)| \geq c_0 |(p', 0) - (p, \ell)| \geq c_0 \ell.$$

This proves $\mathrm{dist}(\partial\Omega, \partial\hat{\Omega}_\ell) \geq c_0 \ell$. The claim then follows from (6.79) and definition (6.14) of Ω_ℓ^+. □

Proof of Theorem 6.7.3

We apply Necas' proof [140] to all Ω_ℓ simultaneously (with ℓ sufficiently small) and observe that all the relevant constants can be bounded uniformly in ℓ.

By Proposition 4.19 (ii) in [131], for $\ell_0 > 0$ small enough, there exist coordinate cylinders $\mathcal{C}_1, \ldots, \mathcal{C}_K$ that (a) cover $\partial\Omega_\ell$ for all $0 \leq \ell < \ell_0$ and (b) characterize them as the graph of Lipschitz functions $f_{k,\ell}$ in the e_d direction, as described in Definition 6.11.1. Moreover, the Lipschitz constants of $f_{k,\ell}$ are uniformly bounded in ℓ.

Let $\mathcal{C}_0 \subset \Omega$ be an open set such that $\mathrm{dist}(\mathcal{C}_0, \Omega^c) > 0$ and such that $\Omega \subset \bigcup_{k=0}^K \mathcal{C}_k$. Let $\phi_0, \ldots, \phi_K : \mathbb{R}^d \to \mathbb{R}^d$ be a smooth partition of unity subordinate to this covering, i.e.

$$\mathrm{supp}\, \phi_k \subset \mathcal{C}_k, \qquad \sum_{k=0}^K \phi_k = 1 \text{ on } \bigcup_{k=0}^K \mathcal{C}_k.$$

The key observation is that, locally, the distance $d_\ell := \mathrm{dist}(\cdot, \partial\Omega_\ell)$ is comparable to $f_{k,\ell} - y$ up to constants which depend on the Lipschitz constant of $f_{k,\ell}$ and are thus uniformly bounded in ℓ. Concretely, we have

Lemma 6.11.5. *There exist constants $a > 0$ and $0 < b \leq 1$ such that for all $1 \leq k \leq K$ and all $0 \leq \ell < \ell_0$, we have*

$$\min\{a, b|f_{k,l}(\mathbf{x}) - y|\} \leq d_\ell(\mathbf{x}, y) \leq |f_{k,\ell}(\mathbf{x}) - y| \tag{6.82}$$

for all $(\mathbf{x}, y) \in \mathrm{supp}\phi_k$.

Proof. Fix $1 \leq k \leq K$. The second inequality is trivial because $(\mathbf{x}, f_{k,\ell}(\mathbf{x})) \in \partial\Omega_\ell$ implies

$$d_\ell(\mathbf{x}, y) \leq |(\mathbf{x}, y) - (\mathbf{x}, f_{k,\ell}(\mathbf{x}))| = |f_{k,\ell}(\mathbf{x}) - y|.$$

For the proof of the first inequality in (6.82), we define

$$a := \min_{k=0,\dots,K} \operatorname{dist}(\operatorname{supp}\phi_k, \partial\mathcal{C}_k^c) > 0.$$

Since $\partial\Omega_\ell$ is compact, $d_\ell(\mathbf{x}, y)$ is achieved at some point $p_0 \in \partial\Omega_\ell$. In case $p_0 \notin \mathcal{C}_k$, we can bound

$$d_\ell(\mathbf{x}, y) = |p_0 - (\mathbf{x}, y)| \geq a,$$

and in case $p_0 \in \mathcal{C}_k$ we can write it as $p_0 = (\mathbf{x}_0, f_{k,\ell}(\mathbf{x}_0))$ and proceed as follows. Recall that every $f_{k,\ell}$ is Lipschitz continuous with a Lipschitz constant that is uniformly bounded in ℓ; call the bound L. Hence, for every $\tau \in (0, 1)$,

$$\begin{aligned} d_\ell(\mathbf{x}, y)^2 =& (\mathbf{x} - \mathbf{x}_0)^2 + (y - f_{k,\ell}(\mathbf{x}_0))^2 \\ \geq& (\mathbf{x} - \mathbf{x}_0)^2 + (1 - \tau^{-1})(f_{k,\ell}(\mathbf{x}) - f_{k,\ell}(\mathbf{x}_0))^2 + (1 - \tau)(y - f_{k,\ell}(\mathbf{x}_0))^2 \\ \geq& (1 - L(\tau^{-1} - 1))(\mathbf{x} - \mathbf{x}_0)^2 + (1 - \tau)(y - f_{k,\ell}(\mathbf{x}))^2. \end{aligned}$$

Now one chooses $\tau \in (0, 1)$ so that $1 - L(\tau^{-1} - 1) = 0$. This yields the first inequality in Lemma 6.11.5 with an appropriate $b > 0$. We have thus proved Lemma 6.11.5. □

We resume the proof of Theorem 6.7.3. Take any $\varphi \in C_c^\infty(\Omega_\ell)$ and use the partition of unity to write the left hand side of the Hardy inequality (6.65) as

$$\begin{aligned} \int_{\Omega_\ell} |\varphi(x)|^2 d_\ell(x)^{-2} \mathrm{d}x =& \sum_{k=0}^{K} \int_{\mathcal{C}_k \cap \Omega_\ell} \phi_k(x) |\varphi(x)|^2 d_\ell(x)^{-2} \mathrm{d}x \\ \leq& C\|\varphi\|_{L^2}^2 + \sum_{k=1}^{K} \int_{\mathcal{C}_k \cap \Omega_{\ell_0}} \phi_k(x) |\varphi(x)|^2 d_\ell(x)^{-2} \mathrm{d}x. \end{aligned}$$

where $C = \operatorname{dist}(\mathcal{C}_0, \Omega^c)^{-2} < \infty$. We emphasize that we used $\Omega_\ell \subset \Omega_{\ell_0}$ in the last integral. Now, we write each integral over $\mathcal{C}_k$ in boundary coordinates and apply Lemma 6.11.5. Importantly, the resulting expression is independent of ℓ (it only depends on ℓ_0). Hence, one can conclude the proof, exactly as in [140], by Fubini and the one-dimensional Hardy inequality [88]. This proves the first part of Theorem 6.7.3.

It remains to show properties (i) and (ii) in Theorem 6.7.3. (i) holds by Proposition 6.11.4. For (ii), we take any $q \in \mathbb{R}^d$ such that $\mathrm{dist}(q, \Omega_\ell^c) \geq a\ell$. In particular, $q \in \Omega_\ell$. Hence, if ℓ is small enough, there exists $p \in \Omega$ such that

$$q = p + \ell v(p).$$

Recall that the vector field $v : \mathbb{R}^d \to \mathbb{R}^d$ is differentiable. We introduce the finite and ℓ independent constants

$$C_0 := \|v\|_{L^\infty(\overline{\Omega_{\ell_0}})}, \qquad C_1 := \|\nabla v\|_{L^\infty(\overline{\Omega_{\ell_0}})}.$$

Using the characterization (6.80) and $q \in \Omega_\ell$, we have

$$\begin{aligned} a\ell \leq & \mathrm{dist}(q, \Omega_\ell^c) = \min_{p' \in \partial\Omega} |p + \ell v(p) - p' - \ell v(p')| \\ \leq & (1 + C_1\ell) \min_{p' \in \partial\Omega} |p - p'| = (1 + C_1\ell)\mathrm{dist}(p, \Omega^c). \end{aligned}$$

We can choose ℓ small enough so that $C_1\ell \leq 1$. We get

$$\begin{aligned} \mathrm{dist}(q, \Omega^c) = & \inf_{p' \in \Omega^c} |p + \ell v(p) - p'| \geq \inf_{p' \in \Omega^c} |p - p'| - C_0\ell \\ = & \mathrm{dist}(p, \Omega^c) - C_0\ell \geq \ell(a/2 - C_0). \end{aligned}$$

By choosing $a > 0$ large enough, we get that $q \in \Omega$ as claimed. This finishes the proof of Theorem 6.7.3. □

6.12 The linear case: Ground state energy of a two-body operator

In this section, we discuss a linear version of our main result. It gives an asymptotic expansion of the ground state energy of the two-body operator (6.83), describing a fermion pair which is confined to Ω

While in principle the center of mass and relative coordinate are coupled due to the boundary conditions, the result shows that they contribute to the ground state energy of H_h on different scales in h (and therefore in a decoupled manner).

Theorem 6.12.1. *Let $\Omega \subset \mathbb{R}^d$ be a bounded Lipschitz domain. Given functions $V : \mathbb{R}^d \to \mathbb{R}$ and $W : \Omega \to \mathbb{R}$ satisfying Assumption 6.1.2, we define the two-body operator*

$$H_h := \frac{h^2}{2}(-\Delta_{\Omega,x} + W(x) - \Delta_{\Omega,y} + W(y)) + V\left(\frac{x-y}{h}\right) \tag{6.83}$$

with form domain $H_0^1(\Omega\times\Omega)$*. Then, as* $h\downarrow 0$*,*

$$\inf\operatorname{spec}_{L^2(\Omega\times\Omega)} H_h = -E_b + h^2 D_c + O(h^{2+\nu}), \tag{6.84}$$

where $\nu>0$ *is as in Theorem 6.1.10 (i) and*

$$-E_b = \inf\operatorname{spec}_{L^2(\mathbb{R}^d)}(-\Delta+V), \qquad D_c = \inf\operatorname{spec}_{L^2(\Omega)}\left(-\frac{1}{4}\Delta_\Omega + W\right).$$

This could be proved by following the line of argumentation in the main text and ignoring the nonlinear terms throughout. However, the proof of the lower bound is considerably simpler in the linear case. To not obscure the key ideas, we give the proof in the special case when $W\equiv 0$ and Ω is convex.

It is instructive to think of the even more special case when Ω is an interval, say $\Omega=[0,1]$. This case is depicted in Figure 6.1 and the proof is sketched in the caption.

Proof. We denote the ground state energy of $-\frac{1}{4}\Delta_{\Omega_\ell^-}$ by $D_c^-(\ell)$ (compare (6.20)), where Ω_ℓ^- is defined in (6.13).

Upper bound. We construct a trial state with the following functions: α_*, the ground state satisfying $(-\Delta+V)\alpha_* = -E_b\alpha_*$, χ a cutoff function as described in Definition 6.4.1, and $\psi_{\ell(h)}$, the normalized ground state of $-\Delta_{\Omega^-_{\ell(h)}}$ for $\ell(h)=h\log(h^{-q})$ and $q>0$ large but fixed. In center of mass variables, $X=\frac{x+y}{2}$, $r=x-y$, the trial state then reads

$$\psi_{\ell(h)}(X)\chi\left(\frac{r}{\ell(h)}\right)h^{1-d}\alpha_*\left(\frac{r}{h}\right). \tag{6.85}$$

We apply H_h to this and use the fact that $-\frac{1}{2}\Delta_x - \frac{1}{2}\Delta_y = -\frac{1}{4}\Delta_X - \Delta_r$. The exponential decay of α_* controls the localization error introduced by χ as in the proof of Proposition 6.4.3. Therefore the energy of the trial state is $-E_b + h^2 D_c^-(\ell(h)) + O(h^{2+\nu})$. The second (linear) part of Theorem 6.2.2 with $W\equiv 0$ says that $D_c^-(\ell(h))\le D_c + O(h^\nu)$. Hence the upper bound in (6.84) is proved.

Lower bound. The key idea is to drop the Dirichlet boundary condition in the relative variable. The center of mass coordinates are originally defined on the domain

$$\mathcal{D} := \left\{(X,r)\in\Omega\times\mathbb{R}^d \;:\; X+\frac{r}{2}, X-\frac{r}{2}\in\Omega\right\}.$$

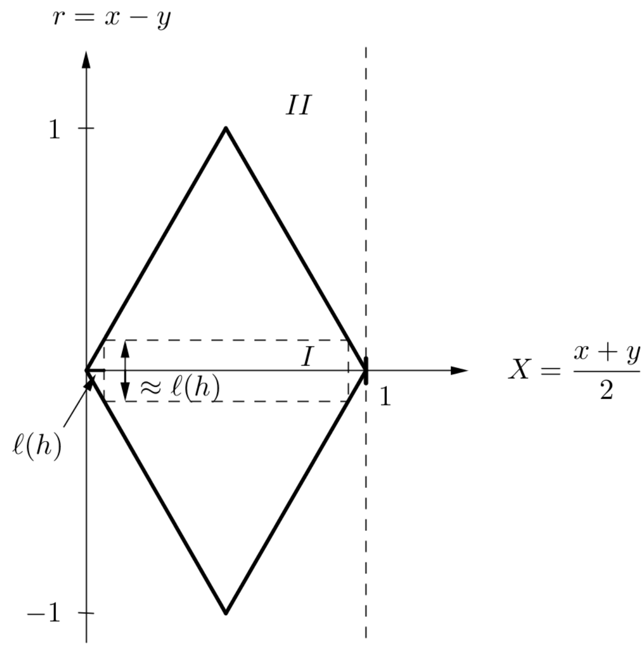

Figure 6.1: When $\Omega = [0,1]$, the region $\Omega \times \Omega$ has a diamond shape when depicted in the center of mass coordinates (X, r). To prove the upper bound in Theorem 6.12.1, one uses a trial state, see (6.85), which is supported on the small dashed rectangular region I, where $\ell(h) = h \log(h^{-q})$ with $q > 0$ large but fixed. When $\Omega = [0,1]$, the Dirichlet eigenfunctions are explicit sine functions and so one does not need to invoke Theorem 6.2.2 to get the upper bound. For the lower bound, one drops the Dirichlet condition in the relative variable, i.e. one extends the problem from the diamond to the strip $II = [0,1] \times \mathbb{R}$. This decouples the X and r variables and directly yields the lower bound.

(Here we use the convexity of Ω.) Observe that $\mathcal{D} \subset \Omega \times \mathbb{R}^d$. On the space $L^2(\Omega \times \mathbb{R}^d)$, we define a new operator

$$\tilde{H}_h = -\frac{h^2}{4}\Delta_{\Omega,X} - h^2\Delta_r + V(r/h),$$

with form domain $H_0^1(\Omega \times \mathbb{R}^d)$. By domain monotonicity we have $\tilde{H}_h \leq H_h$ in the sense of quadratic forms, and therefore

$$\inf \operatorname{spec}_{L^2(\Omega\times\mathbb{R}^d)} \tilde{H}_h \leq \inf \operatorname{spec}_{L^2(\Omega\times\Omega)} H_h. \tag{6.86}$$

Now $\inf \operatorname{spec}_{L^2(\Omega\times\mathbb{R}^d)} \tilde{H}_h$ can be computed exactly since the X and r variables are decoupled and so the corresponding operators commute. The ground state is just

$$\psi_0(X) h^{1-d} \alpha_* \left(\frac{r}{h}\right)$$

where ψ_0 is the normalized ground state of $-\frac{1}{4}\Delta_\Omega$. The energy of this state is precisely equal to $-E_b + h^2 D_c$. By (6.86), the lower bound follows. $\square$

Chapter 7

ON THE ENTROPY OF FERMIONIC REDUCED DENSITY MATRICES

Marius Lemm

7.1 Introduction

The entropy of the k-body reduced density matrix of a quantum state measures the entanglement of k particles with the rest of the system. The antisymmetry of a *fermionic* quantum state has a marked effect on these entropies. For example, there is no fermionic state for which these entropies all vanish and in this sense, a many-fermion system will *always display non-trivial entanglement.*

This is in stark contrast to the bosonic case. Indeed, there are bosonic states, namely product wave functions, for which the entropy of all reduced density matrices vanishes and such states are completely unentangled from this viewpoint.

One commonly considers *Slater determinants* to be the minimally entangled fermionic states, since they arise from the most natural antisymmetrization procedure. Therefore, one often measures the entanglement of a fermionic state relative to Slater determinants, e.g., in the definition of *Slater rank* [5, 64, 147]. A similar idea appears in quantum chemistry, where one separates the indirect electrostatic energy into an "exchange part" and a "correlation part". The correlation part vanishes for Slater determinants, i.e., they are considered to be *uncorrelated modulo antisymmetrization/exchange.*

The intuition that Slater determinants are the minimally entangled fermionic states was recently turned into the following mathematical conjecture by Carlen, Lieb and Reuvers (CLR) [33]. Their conjecture says that the *minimal entropy of a fermionic two-body reduced density matrix is achieved for Slater determinants.* (The value of the minimal entropy is then $\log \binom{N}{2}$ in their convention.) While analogous conjectures can be made for the k-particle density matrices for other values of k, the case $k = 2$ is the most important one for applications to many-body theory. The statement is known when $k = 1$; it was proved by Coleman [39] in 1963.

The conjecture of CLR is part of an effort to better understand the kinds of two-body reduced density matrices that can arise from fermionic pure states. This effort is partly motivated by the N-representability problem in many-body theory.

For further background and results concerning other entanglement measures in many-fermion systems, we refer to [5, 12, 33, 37]. We mention in particular the result of CLR [33] that convex combinations of Slater determinants uniquely minimize the entanglement of formation [19, 20] among fermionic mixed states.

In the present paper, we apply techniques from *quantum information theory*, most notably the monotonicity of the quantum relative entropy under the partial trace, to study the problem posed by CLR. Our *first main result* gives general facts about the entropy of the k-body reduced density matrix of any permutation-invariant pure state as a function of k: It is concave for all $1 \leq k \leq N$ and it is non-decreasing for $1 \leq k \leq \frac{N-1}{2}$ (**Theorem 7.2.4**). Combining the monotonicity with Coleman's theorem, we obtain the lower bound $\log N$ on the entropy of fermionic k-body reduced density matrices for all $k \geq 2$ ([33] proved this for the $k = 2$ case). See Remark 7.2.5 (ii).

In our *second main result*, we show that the relative entropy approach also yields a dimension-dependent bound on the entropy of the two body reduced density matrix (**Theorem 7.2.6**). The bound implies the asymptotic form of the CLR conjecture when the dimension of the underlying Hilbert space is not too large. The proof is inspired by recent work on approximate quantum cloning in collaboration with Mark M. Wilde [121]. (We mention that a similar bound can be obtained from Yang's bound on the largest eigenvalue of the two body reduced density matrix.)

7.2 Setup and results

Basic definitions and facts

We work on the finite-dimensional Hilbert space $(\mathbb{C}^d)^{\otimes N}$, where $1 \leq N \leq d$ are integer-valued parameters. The antisymmetric subspace is given by

$$\mathcal{H}_N := \Lambda^N \mathbb{C}^d, \qquad d_N := \dim \mathcal{H}_N = \binom{d}{N}.$$

By definition, an N-fermion quantum state ρ_N is a density matrix (a non-negative matrix of trace one) that is supported in $\mathcal{H}_N$. We can associate to each ρ_N the family of its k-body reduced density matrices

$$\gamma_k := \mathrm{Tr}_{k+1,\dots,N}[\rho_N].$$

Here $\mathrm{Tr}_{k+1,\dots,N}[\cdot]$ denotes the partial trace over the last $N-k$ variables when we decompose $(\mathbb{C}^d)^{\otimes N} = (\mathbb{C}^d)^{\otimes k} \otimes (\mathbb{C}^d)^{\otimes (N-k)}$. We use the convention that the partial trace is trace-preserving, i.e. $\mathrm{Tr}[\gamma_k] = 1$.

The quantity of interest is the *entropy of the k-body reduced density matrix*

$$S(\gamma_k) := -\mathrm{Tr}[\gamma_k \log \gamma_k], \qquad 1 \leq k \leq N.$$

We view this as the entanglement entropy associated to the decomposition $(\mathbb{C}^d)^{\otimes N} = (\mathbb{C}^d)^{\otimes k} \otimes (\mathbb{C}^d)^{\otimes (N-k)}$; it gives a measure on the entanglement between k of the particles with the remaining $N-k$ ones.

As mentioned in the introduction, we are interested in *lower bounds* on $S(\gamma_k)$, in particular $S(\gamma_2)$, when ρ_N varies over the set of fermionic density matrices. By linearity of the partial trace and concavity of the entropy, we may restrict our considerations to the extreme points of this set, the *pure states*. By definition, a fermionic pure state is a projector

$$|\Psi_N\rangle\langle\Psi_N|, \qquad \Psi_N \in \mathcal{H}_N.$$

In the following, we restrict to the case $\rho_N = |\Psi_N\rangle\langle\Psi_N|$.

A basic fact that will be important for us is that the entanglement entropy of a fermionic pure state is symmetric under reflection at $N/2$, i.e.,

$$S(\gamma_k) = S(\gamma_{N-k}), \qquad \forall\, 1 \leq k \leq N-1. \tag{7.1}$$

The conjecture of Carlen, Lieb and Reuvers

Thanks to Coleman's work [39], we have a good understanding of the case $k = 1$.

Theorem 7.2.1 (Coleman's theorem). *Let $\rho_N = |\Psi_N\rangle\langle\Psi_N|$ for some $\Psi_N \in \mathcal{H}_N$. Then $S(\gamma_1)$ is minimal for Slater determinants, i.e.,*

$$S(\gamma_1) \geq \log N.$$

Remark 7.2.2. *An elementary computation shows that if* $|\Psi_N\rangle = |\phi_1 \wedge \ldots \wedge \phi_N\rangle$ *is a Slater determinant, then* $S(\gamma_k) = \log\binom{N}{k}$ *for any* $1 \le k \le N$*. A detailed proof of this fact can be found e.g. in Appendix E of [121].*

In [33], Carlen, Lieb and Reuvers make the following two conjectures which would give analogues of Coleman's theorem for $k = 2$. The second statement is an asymptotic (and therefore weaker) version of the first one.

Conjecture 7.2.3 (CLR)**.** *Let* $\rho_N = |\Psi_N\rangle\langle\Psi_N|$ *for some* $\Psi_N \in \mathcal{H}_N$*. Then*

$$S(\gamma_2) \ge \log\binom{N}{2}, \tag{7.2}$$

$$\text{or at least} \qquad S(\gamma_2) \ge 2\log N + O(1), \qquad \text{as } N \to \infty. \tag{7.3}$$

In their paper, CLR derive a strengthened subadditivity inequality for the quantum entropy, cf. Theorem 5.1 in [33]. Applied to the problem at hand, they obtain

$$S(\gamma_2) \ge \log N + O(1), \qquad \text{as } N \to \infty. \tag{7.4}$$

Alternatively, as is mentioned in [33], one can use Yang's bound on the largest eigenvalue of γ_2 to find

$$S(\gamma_2) \ge -\|\gamma_2\|_\infty \ge \log(N-1) + \log\left(\frac{d}{d-N+1}\right) \ge \log(N-1). \tag{7.5}$$

Both bounds, (7.4) and (7.5) are off by a factor of two from the conjectured bound (7.3). We investigate the problem using entropy inequalities and as corollaries we obtain bounds which asymptotically behave similarly to (7.4) and (7.5). Establishing the conjectured bound (7.3) remains an interesting open problem.

Main results

Our *first main result* gives general properties of the function $k \mapsto S(\gamma_k)$. It allows us to improve the CLR result (7.4) to (7.8) below. For simplicity, we define

$$S_k := S(\gamma_k).$$

Theorem 7.2.4. *Let* $\rho_N = |\Psi_N\rangle\langle\Psi_N|$ *for some* $\Psi_N \in \mathcal{H}_N$*. The map* $k \mapsto S_k$ *has the following properties.*

(i) ***Monotonicity.*** *For every* $1 \leq k \leq \frac{N}{2} - 1$,

$$S_k \leq S_{k+1}. \tag{7.6}$$

(ii) ***Concavity.*** *For every* $2 \leq k \leq N - 1$,

$$S_k \geq \frac{S_{k+1} + S_{k-1}}{2}. \tag{7.7}$$

Together with the symmetry property $S_k = S_{N-k}$, this theorem provides restrictions on what graphs can be exhibited by $k \mapsto S(\gamma_k)$.

Remark 7.2.5. *(i) Theorem 7.2.4 generalizes verbatim to* bosonic *reduced density matrices. (The proof only uses general inequalities and the symmetry property* $S_k = S_{N-k}$*, which holds for any permutation-invariant pure state.)*

(ii) From the monotonicity (7.6) *and Coleman's theorem, we get*

$$S(\gamma_2) \geq S(\gamma_1) \geq \log N, \tag{7.8}$$

which is to be compared with (7.4) *of [33].*

(iii) In fact, we obtain $S(\gamma_k) \geq \log N$ *for all* $1 \leq k \leq N$*. This shows that, for fermionic pure states, all possible decompositions of the particles into two groups are entangled.*

We now consider the asymptotic version of the CLR conjecture (7.3). It claims that the lower bound (7.8) can be improved to $2 \log N + O(1)$. Our *second main result* implies this as a corollary, provided the dimension $d \geq N$ is not too far from N.

Theorem 7.2.6. *Let* $\rho_N = |\Psi_N\rangle\langle\Psi_N|$ *for some* $\Psi_N \in \mathcal{H}_N$*. Then*

$$S(\gamma_2) \geq S(\gamma_1) + \log\left(\frac{N-1}{d-N+2}\right). \tag{7.9}$$

From Coleman's theorem, we conclude

Corollary 7.2.7. *As* $N \to \infty$*, we have*

$$S(\gamma_2) \geq 2 \log N - \log(d - N + 2) + o(1).$$

In particular, if $d - N = O(1)$ *as* $N \to \infty$*, then* (7.3) *holds.*

Let us explain the role of the dimension d. It does not enter in Conjecture 7.2.3, meaning that the result should be true for all dimensions $d \geq N$ (in particular for infinite-dimensional separable Hilbert spaces). Since our bound (7.9) depends on d, we can only obtain a version of the conjecture for certain values of d.

Note that Conjecture 7.2.3 holds trivially when $d = N$, which is the minimal value of d. (Indeed, in that case $\dim \mathcal{H}_N = 1$ and the only available antisymmetric state $|\Psi_N\rangle$ is necessarily a Slater determinant.) Therefore, it is not too surprising that the number $d - N$ enters in the bound (7.9). The same holds true for the bound (7.5) derived from Yang's theorem.

We close the presentation with two remarks concerning a possible extension of Theorem 7.2.6.

Remark 7.2.8. *(i) In view of Remark 7.2.2, it is natural to generalize Conjecture 7.2.3 to any fixed $k > 2$ by* conjecturing *that $S(\gamma_k) \geq \log \binom{N}{k}$, or at least that*

$$S(\gamma_k) \geq k \log N + O(1), \tag{7.10}$$

as $N \to \infty$. The proof of Theorem 7.2.6 generalizes to this case and yields, together with Coleman's theorem,

$$S(\gamma_k) \geq k \log N - (k-1)\log(d - N + k) + o(1), \tag{7.11}$$

as $N \to \infty$. That is, the generalized conjecture (7.10) *holds for any fixed $k \geq 2$ when $d - N = O(1)$ as $N \to \infty$.*

(ii) It is of course unsatisfactory that the dimension d enters in the bounds (7.9) *and* (7.11)*. For instance, the bounds become worse if one takes a fixed state $|\Psi_N\rangle$ and embeds it in a Hilbert space of increasing dimension d. This particular issue can be remedied however: Given a fixed state $|\Psi_N\rangle$, one can restrict from the outset to the Hilbert space $\Lambda^N \mathbb{C}^{d_\Psi}$ where $d_\Psi \leq d$ is the dimension of the support of γ_1. Then,* (7.9) *also holds with d replaced by d_Ψ. While this allows us to replace the completely arbitrary parameter d with one that actually depends on the state, it does not yield a better bound than* (7.9)*. The reason is that d_Ψ could be very large due to the presence of many small eigenvalues that do not affect $S(\gamma_1)$ very much.*

7.3 Proofs

We now give the proofs of Theorems 7.2.4 and 7.2.6. As mentioned in the introduction, they are mostly based on the symmetry property $S(\gamma_k) = S(\gamma_{N-k})$ and the monotonicity of the quantum relative entropy under the partial trace, which we recall now.

The quantum relative entropy

Definition 7.3.1. *Given two quantum states ρ and σ, their quantum relative entropy is defined by*

$$D(\rho\|\sigma) := \begin{cases} \mathrm{Tr}[\rho(\log\rho - \log\sigma)], & \text{if } \ker\sigma \subset \ker\rho, \\ \infty, & \text{otherwise.} \end{cases}$$

The key property of the quantum relative entropy that we will use is that it decreases under application of the partial trace. Namely, if ρ_{AB}, σ_{AB} are quantum states on a Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$, then

$$D(\rho_{AB}\|\sigma_{AB}) \geq D(\mathrm{Tr}_B[\rho_{AB}]\|\mathrm{Tr}_B[\sigma_{AB}]). \tag{7.12}$$

Proof of Theorem 7.2.4

We begin with the concavity estimate (7.7), since it is slightly easier. Let $2 \leq k \leq N-1$. By (7.12), we have

$$\begin{aligned} &D(\gamma_{k+1}\|\gamma_1 \otimes \gamma_k) - D(\gamma_k\|\gamma_1 \otimes \gamma_{k-1}) \\ =&D(\gamma_{k+1}\|\gamma_1 \otimes \gamma_k) - D(\mathrm{Tr}_{k+1}[\gamma_{k+1}]\|\mathrm{Tr}_{k+1}[\gamma_1 \otimes \gamma_k]) \geq 0. \end{aligned} \tag{7.13}$$

Using that $\log(X_A \otimes Y_B) = \log X_A \otimes I_B + I_A \otimes \log Y_B$ and the definition of the partial trace, we can express the left-hand side in terms of S_{k-1}, S_k and S_{k+1} as follows.

$$\begin{aligned} D(\gamma_{k+1}\|\gamma_1 \otimes \gamma_k) =& \mathrm{Tr}[\gamma_{k+1}\log\gamma_{k+1}] - \mathrm{Tr}[\gamma_{k+1}(\log\gamma_1 \otimes I_{(\mathbb{C}^d)^{\otimes k}} + I_{\mathbb{C}^d} \otimes \log\gamma_k)] \\ =& - S_{k+1} - \mathrm{Tr}[\gamma_1\log\gamma_1] - \mathrm{Tr}[\gamma_k\log\gamma_k] \\ =& - S_{k+1} + S_1 + S_k. \end{aligned}$$

Applying this identity to (7.13), we get $-S_{k+1}+S_1+S_k-(-S_k+S_1+S_{k-1}) \geq 0$ and this is equivalent to (7.7).

Next we prove the monotonicity (7.6). Let $1 \leq k \leq \frac{N-1}{2}$, so that $N-2k-1 \geq 0$. By (7.12), we have

$$\begin{aligned} &D(\gamma_{N-k}\|\gamma_1 \otimes \gamma_{N-k-1}) - D(\gamma_{k+1}\|\gamma_1 \otimes \gamma_k) \\ =&D(\gamma_{N-k}\|\gamma_1 \otimes \gamma_{N-k-1}) - D(\mathrm{Tr}_{k+2,\ldots,N-k}[\gamma_{N-k}]\|\mathrm{Tr}_{k+2,\ldots,N-k}[\gamma_1 \otimes \gamma_{N-k-1}]) \\ \geq&0. \end{aligned}$$

Here we used the convention that $\mathrm{Tr}_{k+2,\ldots,N-k}[X] = X$ if $N-2k-1 = 0$. Using $S_k = S_{N-k}$, we find

$$D(\gamma_{N-k}\|\gamma_1 \otimes \gamma_{N-k-1}) = -S_{N-k} + S_1 + S_{N-k-1} = -S_k + S_1 + S_{k+1}.$$

Therefore, we have $-S_k + S_1 + S_{k+1} - (-S_{k+1} + S_1 + S_k) \geq 0$ which is equivalent to $S_{k+1} \geq S_k$, i.e., (7.6). This concludes the proof of Theorem 7.2.4. $\square$

Proof of Theorem 7.2.6

On $(\mathbb{C}^d)^{\otimes k}$, we introduce the projector P_k onto the subspace

$$\mathcal{H}_k := \Lambda^k \mathbb{C}^d \subset (\mathbb{C}^d)^{\otimes k}, \qquad d_k := \dim \mathcal{H}_k = \binom{d}{k}.$$

We denote $\pi_k := d_k^{-1} P_k$. Note that $\mathrm{Tr}[\pi_k] = 1$, i.e., π_k is a density matrix (called the maximally mixed state on $\mathcal{H}_k$).

We write $S_k = S(\gamma_k)$. Theorem 7.2.6 will be implied by the following two lemmas.

Lemma 7.3.2. *For every* $1 \leq k \leq N$*,*

$$S_k = -D(\gamma_k\|\pi_k) + \log d_k. \tag{7.14}$$

Lemma 7.3.3. *For every* $1 \leq l < m \leq N-1$*, we have* $\mathrm{Tr}_{l+1,\ldots,m}[\pi_m] = \pi_{m-l}$.

We assume that these lemmas holds for now and give the

Proof of Theorem 7.2.6. Thanks to the symmetry $S_k = S_{N-k}$, we have

$$S_2 = S_1 + S_2 - S_1 = S_1 + S_{N-2} - S_{N-1}$$

Using Lemmas 7.3.2 and 7.3.3, we get

$$\begin{aligned} S_2 =&S_1 + \log\left(\frac{d_{N-2}}{d_{N-1}}\right) + D(\gamma_{N-1}\|\pi_{N-1}) - D(\gamma_{N-2}\|\pi_{N-2}) \\ =&S_1 + \log\left(\frac{d_{N-2}}{d_{N-1}}\right) + D(\gamma_{N-1}\|\pi_{N-1}) - D(\mathrm{Tr}_{N-1}[\gamma_{N-1}]\|\mathrm{Tr}_{N-1}[\pi_{N-1}]). \end{aligned} \tag{7.15}$$

By the monotonicity of the relative entropy (7.12), we get

$$S_2 \geq S_1 + \log\left(\frac{d_{N-2}}{d_{N-1}}\right) = S_1 + \log\left(\frac{\binom{d}{N-2}}{\binom{d}{N-1}}\right) = S_1 + \log\left(\frac{N-1}{d-N+2}\right).$$

This proves the claim (7.9). □

It remains to give the proofs of Lemmas 7.3.2 and 7.3.3.

Proof of Lemma 7.3.2. The key observation is that γ_k is a matrix taking $\mathcal{H}_k$ to itself, meaning that

$$\gamma_k = \gamma_k P_k = P_k \gamma_k, \tag{7.16}$$

for every $1 \leq k \leq N$. This follows from

$$|\Psi_N\rangle\langle\Psi_N| = |\Psi_N\rangle\langle\Psi_N| \left(P_k \otimes I_{(\mathbb{C}^d)^{\otimes(N-k)}}\right) = \left(P_k \otimes I_{(\mathbb{C}^d)^{\otimes(N-k)}}\right) |\Psi_N\rangle\langle\Psi_N|$$

and properties of the partial trace. Indeed, we have

$$\begin{aligned}\gamma_k =& \mathrm{Tr}_{k+1,\ldots,N-k}[|\Psi_N\rangle\langle\Psi_N|] = \mathrm{Tr}_{k+1,\ldots,N-k}\left[|\Psi_N\rangle\langle\Psi_N| \left(P_k \otimes I_{(\mathbb{C}^d)^{\otimes(N-k)}}\right)\right] \\ =& \mathrm{Tr}_{k+1,\ldots,N-k}[|\Psi_N\rangle\langle\Psi_N|]P_k = \gamma_k P_k.\end{aligned}$$

This proves the first equality in (7.16); the second one is proved analogously.

Now we use (7.16) to find

$$\begin{aligned}S_k =& -\mathrm{Tr}[\gamma_k \log \gamma_k] = -\mathrm{Tr}[\gamma_k \log(\gamma_k d_k d_k^{-1})] \\ =& -\mathrm{Tr}[\gamma_k \log \gamma_k] - \mathrm{Tr}[\gamma_k P_k \log(d_k)] + \mathrm{Tr}[\gamma_k] \log d_k \\ =& -\mathrm{Tr}[\gamma_k \log \gamma_k] + \mathrm{Tr}[\gamma_k \log(d_k^{-1} P_k)] + \log d_k \\ =& -D(\gamma_k \| \pi_k) + \log d_k.\end{aligned}$$

In the second-to-last step, we used the fact that $\mathrm{Tr}[\gamma_k] = 1$, as well as

$$-P_k \log(d_k) = P_k \log(d_k^{-1}) = P_k \log(d_k^{-1} P_k) P_k.$$

This proves Lemma 7.3.2. □

Proof of Lemma 7.3.3. This is Lemma 12 in [121]. First, observe that

$$\mathrm{Tr}_{l+1,\ldots,m}[\pi_m]$$

maps $\mathcal{H}_l$ to itself by (7.16). Moreover, it commutes with all unitaries U_l on $\mathcal{H}_l$. Indeed, by standard properties of the partial trace and the fact that π_m commutes with all unitaries on $\mathcal{H}_m$,

$$\begin{aligned} U_l \mathrm{Tr}_{l+1,\dots,m}[\pi_m] =& \mathrm{Tr}_{l+1,\dots,m}[(U_l \otimes I_{(\mathbb{C}^d)^{m-l}})\pi_m] = \mathrm{Tr}_{l+1,\dots,m}[\pi_m(U_l \otimes I_{(\mathbb{C}^d)^{m-l}})] \\ =& \mathrm{Tr}_{l+1,\dots,m}[\pi_m]U_l. \end{aligned}$$

Since it commutes with all unitaries, $\mathrm{Tr}_{l+1,\dots,m}[\pi_m] = CI_{\mathcal{H}_l}$ for some constant C. This constant is determined by $\mathrm{Tr}[\mathrm{Tr}_{l+1,\dots,m}[\pi_m]] = 1$ to be $C = d_l^{-1}$. This proves Lemma 7.3.3 and therefore finishes the proof of Theorem 7.2.6. □

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