

GAUGE FIELDS IN THE FUNCTIONAL SCHRODINGER REPRESENTATION

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ABSTRACT

We explore gauge fields in the functional Schrödinger representation. We first consider perturbatively solving quantum electrodynamics using known free field wave functionals. Failures of ordinary perturbative techniques force us to develop techniques to solve nontrivial functional differential equations. These techniques can also be used for Yang-Mills as we also demonstrate. We regularize QED in a new fashion using functional directional derivatives. This may also be generalized to Yang-Mills. We carry out mass renormalization in QED using wave functionals since no one has explicitly done it before. We briefly look at magnetic flux tubes in the Abelian Higgs model to illustrate renormalization in a variational calculation. We also perform a variational calculation using wave functionals in Yang-Mills to see if quantum fluctuations can produce electric flux tubes.

Table of Contents

Acknowledgements	i
Abstract	ii
Chapter 1 Introduction	1
Chapter 2 Free Fields	4
Chapter 3 Quantum Electrodynamics with Wave Functionals	10
A. The Temporal Gauge	10
B. Perturbed Wave Functionals	12
C. Regularization and Renormalization	24
Chapter 4 The Abelian Higgs Model	29
A. The Temporal Gauge and a Choice of Coordinates	29
B. Trial Wave Functionals and Magnetic Flux Tubes	33
Chapter 5 Yang-Mills	35
A. Temporal Gauge	35
B. The Vacuum Wave Functional to First Order	37
C. Regularization	46
D. Do Fluctuations Produce Electric Flux Tubes?	48

Chapter 6	Conclusion	56
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References		58
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Chapter 1 Introduction

The Schrödinger representation for field theory is a natural extension of nonrelativistic quantum mechanics familiar from atomic physics. As is usual, we start with a Hamiltonian. We canonically quantize by postulating commutation relations between coordinates and their conjugate momenta. We represent either the coordinates or their conjugate momenta as derivatives. The Schrödinger equation then becomes a differential equation and we search for eigenfunctions of this operator. These eigenfunctions represent possible states of the system. For field theory in the Schrödinger representation, we must substitute the word functional for function. By functional, we mean "you give me a function and I give a number." The Schrödinger equation then becomes a functional differential equation and we seek eigenfunctionals as solutions. The transition from function to functional is, of course, nontrivial.

We are faced today with nonlinear field theories where perturbative techniques fail. These techniques have not been easily extended to do nonperturbative problems. The search for nonperturbative techniques has led to lattices where much progress has been made. While the lattice is successful numerically, the numerical results have not provided sufficient insight to really understand deeply the fundamental properties of non-Abelian gauge theories. Lattices have also presented some new questions such as what is the nature of fermion doubling on the lattice. Is it only a lattice artifact or is it a property of all regulated field theories?

Since we haven't been able to adequately understand non-Abelian theories analytically with the known techniques and representations, we are justified in developing new ones and redeveloping old ones. The possible value of developing the Schrödinger functional representation goes beyond non-Abelian field

theories, however. Recently, more interest in wave functionals has developed from the work of Hawking and Hartle [1] on the wave function of the universe and by others in formulating quantum field theory on curved spacetimes [2]. One value of the Schrödinger representation is that it facilitates the writing down of the quantized theories. Some of the techniques we develop will carry over to other field theories.

The Schrödinger representation requires us to solve functional differential equations to obtain the stationary states. These functional differential equations involve functional derivatives and are, therefore, different from ordinary functional differential equations which only involve time-delayed ordinary derivatives. We present here a new technique to solve perturbatively those functional equations arising in gauge theories.

Since this representation has been ignored until recently we must also "catch up" with other formalisms and develop techniques to regularize and renormalize. We apply this representation to a nonperturbative problem using a variational calculation to illustrate its value.

Chapter 2 reviews the formalism of the Schrödinger representation for free fields. We can exactly solve these functional differential equations so we use these known wavefunctionals to perturbatively solve quantum electrodynamics in Chapter 3. In Chapter 3, we also illustrate the technique we have developed to solve functional differential equations for interacting fields. We regularize in a new fashion using directional functional derivatives and carry out renormalization (since this hasn't been done before for gauge fields in this representation [3].) In Chapter 4, we briefly explore the Abelian Higgs model and use the Schrödinger representation to show how to do a nonperturbative variational calculation involving magnetic flux tubes. This example also serves to show how

renormalization should be carried out in a variational calculation using wave functionals [4]. In Chapter 5, we examine Yang-Mills and solve the functional differential equation to first order for the vacuum state. We then suggest how to regularize and finish with a variational calculation to see how quantum fluctuations may produce an electric flux tube.

Chapter 2 Free Fields

We begin by reviewing the formalism of the Schrödinger representation for free fields. In this case we have exact solutions. The free fields, of course, provide a basis from which we may perturbatively explore interactive field theories. The free fields also offer the simplest environment in which to see the difference between fermionic and bosonic wave functionals.

As an example of a bosonic theory, let us consider free photons in the temporal gauge.

In the temporal gauge we set $A_0 = 0$. The Hamiltonian for free photons in this gauge is

$$\mathbf{H} = \frac{1}{2} \int \vec{E} \cdot \vec{E} + \vec{B} \cdot \vec{B} d^3x \quad (2.1)$$

where

$$E_i(\vec{x}) = -\dot{A}_i(\vec{x}) \quad \text{and} \quad \vec{B}(\vec{x}) = \vec{\nabla} \times \vec{A}(\vec{x}). \quad (2.2)$$

Canonical quantization gives the equal time commutator

$$[E_i(\vec{x}), A_j(\vec{y})] = i \delta_{ij} \delta(\vec{x} - \vec{y}). \quad (2.3)$$

Working in the Schrödinger representation where $\vec{A}(\vec{x})$ is diagonal means that we may set

$$E_i(\vec{x}) = i \frac{\delta}{\delta A_i(\vec{x})}. \quad (2.4)$$

The Schrödinger equation now becomes the functional differential equation

$$\frac{1}{2} \int d^3x \left[-\frac{\delta}{\delta \vec{A}(\vec{x})} \cdot \frac{\delta}{\delta \vec{A}(\vec{x})} + \vec{B}(\vec{x}) \cdot \vec{B}(\vec{x}) \right] \Psi_n[A] = E_n \Psi_n[A] \quad (2.5)$$

where the eigenfunctions are now eigenfunctionals.

In the temporal gauge there is no Hamiltonian equation of motion for Gauss's Law. Gauss's Law must be added as a constraint on the wave functionals. The wave functionals, $\Psi_n[A]$, must also satisfy

$$(\vec{\nabla} \cdot \vec{E}) \Psi_n[A] = 0 \quad \text{or} \quad \vec{\nabla} \cdot \frac{\delta}{\delta \vec{A}(\vec{x})} \Psi_n[A] = 0 \quad (2.6)$$

which means that the eigenfunctionals cannot depend on the longitudinal component of the vector potentials, $\vec{A}(\vec{x})$.

The vacuum state wave functional, $\Psi_0[A]$, is the lowest energy solution of equation (2.5). It is given by

$$\Psi_0[A] = \exp\left(-\frac{1}{(2\pi)^2} \int \frac{(\vec{\nabla} \times \vec{A}(\vec{x})) \cdot (\vec{\nabla} \times \vec{A}(\vec{y}))}{|\vec{x} - \vec{y}|^2} d^3x d^3y\right). \quad (2.7)$$

This less familiar wave functional becomes transparent when we switch to the momentum representation defined by

$$\vec{A}(\vec{x}) = \frac{1}{(2\pi)^{\frac{3}{2}}} \int \vec{a}(\vec{k}) e^{i\vec{k} \cdot \vec{x}} d^3k \quad \text{and} \quad \frac{\delta}{\delta \vec{A}(\vec{x})} = \frac{1}{(2\pi)^{\frac{3}{2}}} \int \frac{\delta}{\delta \vec{a}(\vec{k})} e^{-i\vec{k} \cdot \vec{x}} d^3k \quad (2.8)$$

where $\Psi_0[A]$ becomes

$$\Psi_0[A] = \exp\left(-\frac{1}{2} \int \frac{(\vec{k} \times \vec{a}(\vec{k})) \cdot (\vec{k} \times \vec{a}(-\vec{k}))}{|\vec{k}|} d^3k\right) \quad (2.9)$$

which is the familiar product of harmonic oscillator ground state wave functions.

The remaining eigenfunctionals of eq. (2.5) may be generated by applying the operator

$$\frac{1}{\sqrt{2|\vec{k}|}} \varepsilon(\vec{k}, \lambda) \cdot \left[-\frac{\delta}{\delta \vec{a}(\vec{k})} + |\vec{k}| \alpha(-\vec{k}) \right] \quad (2.10)$$

to $\Psi_0[A]$. Here, $\varepsilon(\vec{k}, \lambda)$, $\lambda=1,2$ are the polarization vectors orthogonal to \vec{k} . Equation (2.10) is, of course, just the functional form of the raising operator.

Expectation values are now functional integrals. For example, the vacuum expectation value of the gauge invariant operator T is given by

$$\begin{aligned} \frac{\langle 0|T|0\rangle}{\langle 0|0\rangle} &= \int \langle 0|A'\rangle \langle A'|T|A\rangle \langle A|0\rangle DA' DA / \int \langle 0|A\rangle \langle A|0\rangle DA \\ &= \int \Psi_{\mathcal{G}}^*[A] T(A) \Psi_0[A] DA / \int \Psi_{\mathcal{G}}^*[A] \Psi_0[A] DA \end{aligned} \quad (2.11)$$

where T is represented in terms of A so that its matrix, $\langle A'|T|A\rangle$, is diagonal. In the integral we are integrating over the transverse and longitudinal components of the vector potential. Since the eigenfunctionals satisfy the Gauss's Law constraint, they will not depend on the longitudinal component. This means that the eigenfunctionals, $\Psi_n[A]$, will not be normalizable. Expectation values of gauge invariant operators will be meaningful, however, since neither integrands in $\langle 0|T|0\rangle$ nor $\langle 0|0\rangle$ depend on the longitudinal component. We can cancel the "gauge" volume $\int DA_L$ appearing in $\langle 0|T|0\rangle$ with the one in $\langle 0|0\rangle$. Alternatively, we may integrate only over gauge inequivalent configurations by inserting a $\delta(A_L)$ functional in the measure.

Now let us consider fermion wavefunctionals [5]. The Hamiltonian for free Dirac fermions is

$$H = \int d^3x \psi^\dagger(\vec{x}) (-i\alpha \cdot \nabla + \beta m) \psi(\vec{x}). \quad (2.12)$$

Each component of the spinor $\psi(\vec{x})$ will be represented as a Grassmann function [6]. This means that

$$\{\psi_a(\vec{x}), \psi_b(\vec{y})\} = 0 \quad \text{and} \quad \left\{ \frac{\delta}{\delta\psi_a(\vec{x})}, \psi_b(\vec{y}) \right\} = \delta_{ab} \delta(\vec{x}-\vec{y}) . \quad (2.13)$$

Since $i\psi_a^\dagger(\vec{x})$ is conjugate to $\psi_a(\vec{x})$, canonical quantization implies that

$$\{\psi_a^\dagger(\vec{x}), \psi_b(\vec{y})\} = \delta_{ab} \delta(\vec{x}-\vec{y}) \quad (2.14)$$

so we may represent $\psi_a^\dagger(\vec{x})$ as $\frac{\delta}{\delta\psi_a(\vec{x})}$. In the momentum representation defined by

$$\psi(\vec{x}) = \sum_{r=1}^4 \int \frac{d^3k}{(2\pi)^{\frac{3}{2}}} \left(\frac{m}{E_k} \right)^{\frac{1}{2}} b(\vec{k}, r) \omega(\vec{k}, r) e^{i\vec{k} \cdot \vec{x}} \quad (2.15)$$

the Hamiltonian becomes

$$\begin{aligned} H &= \sum_{r=1}^4 \int d^3k \, \varepsilon_r \, \omega_k \, b^\dagger(\vec{k}, r) b(\vec{k}, r) \\ &= \sum_{r=1}^4 \int d^3k \, -\varepsilon_r \, \omega_k \, b(\vec{k}, r) \frac{\delta}{\delta b(\vec{k}, r)} \end{aligned} \quad (2.16)$$

where $\omega_k = E_k = \sqrt{|\vec{k}|^2 + m^2}$, $\varepsilon_r = 1$ for $r=1, 2$, and $\varepsilon_r = -1$ for $r=3, 4$.

Since the reader is probably familiar with the conventions set by Bjorken and Drell [7] we list the correspondence between our convention (left-hand side below) and the convention of BJD (right-hand side).

$$b(\vec{k}, 1) = b(\vec{k}, +)$$

$$b(\vec{k}, 2) = b(\vec{k}, -)$$

$$b(\vec{k}, 3) = d^\dagger(-\vec{k}, -)$$

$$b(\vec{k}, 4) = d^\dagger(-\vec{k}, +)$$

For the spinors,

$$w(\vec{k},1) = u(\vec{k},+)$$

$$w(\vec{k},2) = u(\vec{k},-)$$

$$w(\vec{k},3) = v(-\vec{k},-)$$

$$w(\vec{k},4) = v(-\vec{k},+).$$

The ground state is where all the negative energy states are filled and all of the positive energy states are empty. To determine the ground state wave functional, let us recall the wave functions for a single fermion mode. For a single mode there are two states, $|0\rangle$ and $|1\rangle$, corresponding to the mode being unoccupied or occupied. The wave functions $\langle b(\vec{k},r)|0\rangle$ and $\langle b(\vec{k},r)|1\rangle$ are given by

$$\langle b(\vec{k},r)|0\rangle = b(\vec{k},r) \quad \text{and} \quad \langle b(\vec{k},r)|1\rangle = 1. \quad (2.17)$$

To construct the ground state wave functional, Ω_0 , for the Hamiltonian eq. (2.16), we fill negative energy states and leave positive energy states empty. Thus

$$\Omega_0 = \prod_{r=1}^2 \prod_{\vec{k}} b(\vec{k},r). \quad (2.18)$$

For Grassmann functions, $\psi_a(\vec{x})$, the product $\prod_{\vec{x}} \psi_a(\vec{x}) = \delta[\psi_a(\vec{x})]$, is the δ -functional. This can be easily seen from the formal integration rules for Grassmann functions [6]

$$\int d\psi_a(\vec{x}) = 0 \quad \text{and} \quad \int \psi_b(\vec{x}) d\psi_a(\vec{y}) = \delta_{ab} \delta(\vec{x}-\vec{y}). \quad (2.19)$$

Therefore, the ground state wave functional is a δ -functional, $\Omega_0 = \delta[\psi_+]$, where

ψ_+ is the positive energy part of ψ . Excited state wave functionals may be created by filling the desired modes.

Chapter 3. Quantum Electrodynamics with Wave Functionals

A. The Temporal Gauge

Now that we have a complete wave functional description of free photons and electrons we may now represent quantum electrodynamics (QED) in the temporal gauge in the same way. The Hamiltonian is

$$\begin{aligned} \mathbf{H} = \frac{1}{2} \int d^3x & \left(-\frac{\delta}{\delta \vec{A}(\vec{x})} \cdot \frac{\delta}{\delta \vec{A}(\vec{x})} + \vec{B}(\vec{x}) \cdot \vec{B}(\vec{x}) \right) + \int d^3x \frac{\delta}{\delta \psi(\vec{x})} (-i\vec{\alpha} \cdot \vec{\nabla} + \beta m) \psi(\vec{x}) \\ & - e \int d^3x \frac{\delta}{\delta \psi(\vec{x})} (\vec{\alpha} \cdot \vec{A}(\vec{x})) \psi(\vec{x}). \end{aligned} \quad (3.1)$$

The eigenfunctionals, $\Psi[A, \psi]$, satisfy $\mathbf{H}\Psi[A, \psi] = E\Psi[A, \psi]$. They also must satisfy the Gauss's Law constraint

$$(\vec{\nabla} \cdot \vec{E} - e\rho)\Psi[A, \psi] = 0$$

or

$$\left(i\vec{\nabla} \cdot \frac{\delta}{\delta \vec{A}(\vec{x})} - e \frac{\delta}{\delta \psi_\alpha(\vec{x})} \psi_\alpha(\vec{x}) \right) \Psi[A, \psi] = 0. \quad (3.2)$$

We will develop a perturbative expansion in e to solve $\mathbf{H}\Psi = E\Psi$ using the standard Rayleigh-Schrödinger time-independent perturbation theory. Namely, we write eq.(3.1) as $\mathbf{H}_f + e\mathbf{H}_I$ where \mathbf{H}_I is the third term. \mathbf{H}_f describes free photons and electrons so we know the eigenfunctionals, $\Psi_N^{(0)}$, that satisfy $\mathbf{H}_f \Psi_N^{(0)} = E_N^{(0)} \Psi_N^{(0)}$. We expand $\Psi_N[A, \psi]$ and the energy eigenvalue, E_N , in a power series in e ,

$$\Psi_N = \Psi_N^{(0)} + e \Psi_N^{(1)} + \dots$$

$$E_N = E_N^{(0)} + e E_N^{(1)} + e^2 E_N^{(2)} + \dots \quad (3.3)$$

and place this expansion in $\mathbf{H}\Psi_N = E_N\Psi_N$. Equating both sides of this equation order by order in e we obtain as usual

$$\Psi_N^{(1)}[A, \psi] = \sum_{M \neq N} \frac{\langle \Psi_M^{(0)} | \mathbf{H}_1 | \Psi_N^{(0)} \rangle}{E_N^{(0)} - E_M^{(0)}} \Psi_M^{(0)}[A, \psi] \quad (3.4)$$

$$E_N^{(1)} = \langle \Psi_N^{(0)} | \mathbf{H}_1 | \Psi_N^{(0)} \rangle \quad , \quad E_N^{(2)} = \sum_{M \neq N} \frac{|\langle \Psi_M^{(0)} | \mathbf{H}_1 | \Psi_N^{(0)} \rangle|^2}{E_N^{(0)} - E_M^{(0)}} \quad (3.5)$$

Two problems arise. The first is that eq. (3.4) fails to give the correct form for the perturbed wave functional in the temporal gauge. Eq. (3.5) fails even after the correct perturbed wave functionals are found. Secondly, we must face the additional problem of point particle field theory which is renormalization.

Eq. (3.4) fails because of the Gauss's Law constraint we must impose on the wave functionals in the temporal gauge. The perturbed wave functionals generated by eq. (3.4) do not obey the Gauss's Law constraint to first order. We could circumvent this problem by switching to the Coulomb gauge. In the Coulomb gauge we have no extra constraints on the wave functionals, so eq. (3.4) yields the correct answer. It is instructive, however, to stick to the temporal gauge. To obtain the correct perturbed wave functionals we will instead solve the functional Schrödinger equation directly. The technique we will use will also work for perturbed wave functionals for Yang-Mills. For Yang-Mills we prefer to work in the temporal gauge because of the simplicity of the Hamiltonian in this gauge. The Yang-Mills Coulomb gauge Hamiltonian contains functional determinants which are harder to handle. Also, as is well known, these determinants are actually zero making the Coulomb gauge ambiguous. The determinants present no real problem in perturbation theory but we are

interested in non-perturbative variational calculations where we must deal with them. This makes the temporal gauge far more attractive.

Physically interesting quantities are expectation values of gauge invariant operators. Since we will find that some of these diverge we will have to renormalize. As far as we know, no one has perturbatively carried out renormalization using wave functionals. We will do mass renormalization to lowest order here. If for some reason we were to find that we could not make everything finite by rescaling, then we would have to scrap the Schrödinger representation. But this appears not to be the case.

To renormalize we usually regularize first. We will regularize in a new fashion, one which we can generalize to Yang-Mills. Then we can renormalize by introducing counter terms to the Hamiltonian and suitably modifying the wave functionals. Alternatively, we may calculate the effective potential and use this for renormalization. The effective potential method will be useful for variational calculations so we will briefly discuss it here.

B. Perturbed Wave Functionals

To begin, let us consider a state, $\Psi_{\vec{q}}$, containing one free electron of momentum \vec{q} with spin up. To lowest order this state is given by

$$\Psi_{\vec{q}}^{(0)}[a, b] = \eta \Psi_{\vec{q}}^{(0)} \Omega_{\vec{q}}^{(0)} \quad (3.6)$$

where the normalization $\eta = \prod_{\vec{p}} \left(\frac{|\vec{p}|}{\pi} \right)^{\frac{1}{4}}$ and

$$\Psi_{\vec{q}}^{(0)} = \exp\left(-\frac{1}{2} \int \frac{(\vec{k} \times \vec{a}(\vec{k})) \cdot (\vec{k} \times \vec{a}(-\vec{k}))}{|\vec{k}|} d^3k\right) \quad (3.7)$$

and

$$\Omega_{\vec{q}}^{(0)} = \prod_{r=1}^2 \prod_{\vec{p}} b(\vec{p}, \tau) \quad \text{except } (\vec{p}=\vec{q}, \tau=1) \quad (3.8)$$

We will calculate the lowest-order correction to the energy of the state. The correction to the energy to first order in e will involve the matrix element of the interaction part of the Hamiltonian, H_I , in the state given by eq. (3.6) above. Since eq. (3.6) is gaussian in $\vec{a}(\vec{k})$ and H_I contains a single factor of $\vec{a}(\vec{k})$, the matrix element will be zero. Thus the lowest-order correction will be of order e^2 . To calculate this we will need the wave functional to first order in e .

It is easier to solve the functional Schrödinger equation in the momentum representation give by eqs. (2.8) and (2.15). Let us write H as $H_\gamma + H_e + eH_I$ where

$$H_\gamma = \frac{1}{2} \int \frac{\delta}{\delta \vec{a}(\vec{k})} \cdot \frac{\delta}{\delta \vec{a}(-\vec{k})} + (\vec{k} \times \vec{a}(\vec{k})) \cdot (\vec{k} \times \vec{a}(-\vec{k})) d^3k \quad (3.9)$$

$$H_e = \sum_{r=1}^4 \int d^3k -\varepsilon_r \omega_k b(\vec{k}, \tau) \frac{\delta}{\delta b(\vec{k}, \tau)} \quad (3.10)$$

$$H_I = - \sum_{r, r'=1}^4 \int \frac{d^3k d^3p}{(2\pi)^{\frac{3}{2}}} \left(\frac{m^2}{E_{\vec{p}+\vec{k}} E_{\vec{p}}} \right)^{\frac{1}{2}} w^\dagger(\vec{p}+\vec{k}, \tau') \alpha \cdot \vec{a}(\vec{k}) w(\vec{p}, \tau) \frac{\delta}{\delta b(\vec{p}+\vec{k}, \tau')} b(\vec{p}, \tau) \quad (3.11)$$

The Gauss's Law operator, $\mathbf{G} = \nabla \cdot \vec{E} - e\rho$, becomes

$$\mathbf{G} = \vec{k} \cdot \frac{\delta}{\delta \vec{a}(\vec{k})} - e \sum_{r, r'=1}^4 \int \frac{d^3p}{(2\pi)^{\frac{3}{2}}} \left(\frac{m^2}{E_{\vec{p}+\vec{k}} E_{\vec{p}}} \right)^{\frac{1}{2}} w^\dagger(\vec{p}+\vec{k}, \tau') w(\vec{p}, \tau) \frac{\delta}{\delta b(\vec{p}+\vec{k}, \tau')} b(\vec{p}, \tau) \quad (3.12)$$

$\Psi_{\vec{q}}^{(0)}$ satisfies $(H_\gamma + H_e) \Psi_{\vec{q}}^{(0)} = E_{\vec{q}}^{(0)} \Psi_{\vec{q}}^{(0)}$.

We seek the functional, $\Psi_{\vec{q}}^{(0)} + e \Psi_{\vec{q}}^{(1)}$, that satisfies the Schrödinger equation and Gauss's Law to first order in e . For notational convenience we will write $\Psi_{\vec{q}}^{(0)} = \eta \Omega_{\vec{q}}^{(0)} \exp(R)$ so that

$$R = -\frac{1}{2} \int \frac{(\vec{k} \times \vec{a}(\vec{k})) \cdot (\vec{k} \times \alpha(-\vec{k}))}{|\vec{k}|} d^3k \quad (3.13)$$

and $\Omega_{\vec{q}}^{(0)}$ is given by eq. (3.8). Let us assume that $\Psi_{\vec{q}}^{(1)}$ has the form

$$\Psi_{\vec{q}}^{(1)} = F[\mathbf{a}, \mathbf{b}] \exp(R).$$

Since H_I contains one factor of $\vec{a}(\vec{k})$ we expect that $F[\mathbf{a}, \mathbf{b}]$ will be similar. Including $\exp(R)$ in the form for $\Psi_{\vec{q}}^{(1)}$ will allow us to insert the Gauss's Law constraint in the functional differential equation at the appropriate place. We then solve the new functional differential equation. The solution will satisfy both the original differential equation and the Gauss's Law constraint. To insert Gauss's Law, however, we must assume that $\vec{a}(\vec{k})$ in R is no longer purely transverse. Gauss's Law to zeroth order tells us otherwise.

In summary, the technique we will use to solve the functional differential equation and satisfy Gauss's Law will be to place the assumed form for $\Psi_{\vec{q}}^{(1)}$ in the differential equation, separate out the terms to order e , assume that $\vec{a}(\vec{k})$ in R contains a longitudinal component, insert the Gauss's Law constraint in the equation where it is needed, and solve the resulting new functional differential equation.

Letting H operate on $\Psi_{\vec{q}}^{(0)} + e \Psi_{\vec{q}}^{(1)}$, we find that the zeroth order terms disappear as they should. Keeping terms to order e only we find that

$$-\frac{1}{2} \int d^3k \frac{\delta}{\delta \vec{a}(-\vec{k})} \cdot \frac{\delta F}{\delta \mathbf{a}(\vec{k})} + 2 \frac{\delta R}{\delta \mathbf{a}(-\vec{k})} \cdot \frac{\delta F}{\delta \mathbf{a}(\vec{k})} \quad (3.14a)$$

$$+ \sum_{r=1}^4 \int d^3p \ -\varepsilon_r \omega_p b(\vec{p}, r) \cdot \frac{\delta}{\delta b(\vec{p}, r)} F[\mathbf{a}, \mathbf{b}] \quad (3.14b)$$

$$\begin{aligned} - \sum_{r'=1}^4 \sum_{r=1}^4 \int \frac{d^3k d^3p}{(2\pi)^{\frac{3}{2}}} \left(\frac{m^2}{E_{p+k} E_p} \right)^{\frac{1}{2}} w^\dagger(\vec{p}+\vec{k}, r') \alpha \cdot \vec{a}(\vec{k}) w(\vec{p}, r) \frac{\delta}{\delta b(\vec{p}+\vec{k}, r')} b(\vec{p}, r) \Omega_q^{(0)} \\ = E_q^{(1)} \Omega_q^{(0)} + E_q F[\mathbf{a}, \mathbf{b}] . \end{aligned} \quad (3.14c)$$

We expect that $E_q^{(1)}$ will be zero, so for now we will assume it. We also expect $F[\mathbf{a}, \mathbf{b}]$ to contain one factor of $\vec{a}(\vec{k})$ so that

$$\frac{\delta}{\delta \vec{a}(-\vec{k})} \cdot \frac{\delta F}{\delta \mathbf{a}(\vec{k})} = 0 . \quad (3.15)$$

Another way to arrive at eq. (3.15) is to note that $\frac{\delta R}{\delta \mathbf{a}(-\vec{k})}$ contains one factor of $\vec{a}(\vec{k})$ so the only term that could give a pure number (no $\vec{a}(\vec{k})$'s or $b(\vec{p}, r)$'s) would be the left-hand side of eq. (3.15). So if $E_q^{(1)}$ is assumed to be zero, we must set eq. (3.15) to zero.

Let us examine the remaining term in eq. (3.14a). Since

$$\frac{\delta R}{\delta \mathbf{a}(-\vec{k})} = \frac{\vec{k} \times (\vec{k} \times \vec{a}(\vec{k}))}{|\vec{k}|} \quad (3.16)$$

this term becomes

$$\int d^3k \frac{(\vec{k} \times \vec{a}(\vec{k})) \cdot (\vec{k} \times \frac{\delta F}{\delta \mathbf{a}(\vec{k})})}{|\vec{k}|} . \quad (3.17)$$

Now we assume that $\vec{a}(\vec{k})$ is no longer purely transverse even though Gauss's Law to lowest order tells us that it should be. Applying a vector identity, eq. (3.17) becomes

$$\int d^3k |\vec{k}| (\vec{a}(\vec{k}) \cdot \frac{\delta F}{\delta \alpha(\vec{k})}) - \frac{(\vec{k} \cdot \vec{a}(\vec{k})) \cdot (\vec{k} \cdot \frac{\delta F}{\delta \alpha(\vec{k})})}{|\vec{k}|}. \quad (3.18)$$

Now we note that

$$\int d^3k (\vec{a}(\vec{k}) \cdot \frac{\delta F}{\delta \alpha(\vec{k})}) = F[\mathbf{a}, \mathbf{b}].$$

We do not know, however, what the second term in eq. (3.18) is. We cannot set it to zero because of Gauss's Law. But Gauss's Law dictates the exact form of $\vec{k} \cdot \frac{\delta F}{\delta \alpha(\vec{k})}$ in terms of known functionals. Thus, since $\Psi_q^{(1)}$ must satisfy the Gauss's Law constraint, we can use the constraint to rewrite the second term in eq. (3.18) in terms of known functionals. Gauss's Law to first order in e states that

$$\vec{k} \cdot \frac{\delta F}{\delta \alpha(\vec{k})} - \sum_{r,r'=1}^4 \int \frac{d^3p}{(2\pi)^{\frac{3}{2}}} \left(\frac{m^2}{E_{p+k} E_p} \right)^{\frac{1}{2}} \omega^\dagger(\vec{p}+\vec{k}, r') \omega(\vec{p}, r) \frac{\delta}{\delta b(\vec{p}+\vec{k}, r')} b(\vec{p}, r) \Omega_q^{(0)} = 0. \quad (3.19)$$

We insert this into the functional differential equation. Next we rewrite eqs. (3.14) with the unknown functional, $F[\mathbf{a}, \mathbf{b}]$ on the left-hand side and known functionals on the right. We obtain

$$\int d^3k |\vec{k}| (\vec{a}(\vec{k}) \cdot \frac{\delta F}{\delta \alpha(\vec{k})}) - \sum_{r=1}^4 \varepsilon_r \omega_k b(\vec{k}, r) \frac{\delta}{\delta b(\vec{k}, r)} F[\mathbf{a}, \mathbf{b}] - E_q F[\mathbf{a}, \mathbf{b}] \quad (3.20a)$$

$$= \sum_{r,r'=1}^4 \int \frac{d^3k d^3p}{(2\pi)^{\frac{3}{2}}} \left(\frac{m^2}{E_{p+k} E_p} \right)^{\frac{1}{2}} \omega^\dagger(\vec{p}+\vec{k}, r') (\alpha \cdot \vec{a}(\vec{k}) + \frac{\vec{k} \cdot \vec{a}(\vec{k})}{|\vec{k}|}) \omega(\vec{p}, r) \frac{\delta}{\delta b(\vec{p}+\vec{k}, r')} b(\vec{p}, r) \Omega_q^{(0)}. \quad (3.20b)$$

Notice that H_I and Gauss's Law operating on $\Omega_q^{(0)}$ give the same form, namely,

$$\frac{\delta}{\delta b(\vec{p}+\vec{k}, r')} b(\vec{p}, r) \Omega_{\vec{q}}^{(0)}. \quad (3.21)$$

This is the only place where the fermionic variables occur on the right-hand side of eq. (3.20) so $F[\mathbf{a}, \mathbf{b}]$ must have the same form as eq. (3.21)

$$F[\mathbf{a}, \mathbf{b}] \sim f[\mathbf{a}] \sum_{r, r'=1}^4 \frac{\delta}{\delta b(\vec{p}+\vec{k}, r')} b(\vec{p}, r) \Omega_{\vec{q}}^{(0)}.$$

This observation allows us to determine the contribution of the second term in eq. (3.20a).

$$\begin{aligned} & \sum_{r, r'=1}^4 \sum_{s=1}^4 \varepsilon_r \omega_k b(\vec{k}', s) \frac{\delta}{\delta b(\vec{k}', s)} \left(\frac{\delta}{\delta b(\vec{p}+\vec{k}, r')} b(\vec{p}, r) \Omega_{\vec{q}}^{(0)} \right) \\ &= \sum_{r'=1}^2 \sum_{r=3}^4 (\omega_{p+k} + \omega_p + \omega_q) \frac{\delta}{\delta b(\vec{p}+\vec{k}, r')} b(\vec{p}, r) \Omega_{\vec{q}}^{(0)} \\ & \quad + \sum_{r'=1}^2 \omega_{q+k} \frac{\delta}{\delta b(\vec{q}+\vec{k}, r')} b(\vec{q}, 1) \Omega_{\vec{q}}^{(0)}. \end{aligned}$$

Thus eq. (3.20a) becomes ($\omega_k = E_k$)

$$\begin{aligned} & \sum_{r=3}^4 \sum_{r'=1}^2 \int d^3k d^3p (|\vec{k}| + E_{p+k} + E_p) f[\mathbf{a}] \frac{\delta}{\delta b(\vec{p}+\vec{k}, r')} b(\vec{p}, r) \Omega_{\vec{q}}^{(0)} \\ & \quad + \sum_{r'=1}^2 \int d^3k (|\vec{k}| + E_{q+k} - E_q) f[\mathbf{a}] \frac{\delta}{\delta b(\vec{q}+\vec{k}, r')} b(\vec{q}, 1) \Omega_{\vec{q}}^{(0)}. \quad (3.22) \end{aligned}$$

The factors multiplying the two terms of $F[\mathbf{a}, \mathbf{b}]$ above can be recognized as the "energy denominator" in eq. (3.4). To bring it over to the right-hand side of eq. (3.20), we take the functional derivative of eq. (3.20), using eq. (3.22) for eq. (3.20a), with respect to $\vec{d}(\vec{k})$, divide matching fermion terms on both sides by their energy denominator, dot with $\vec{d}(\vec{k})$ and integrate over \vec{k} . The result is

$$\begin{aligned}
F[a, b] = & \sum_{r=3r'=1}^2 \sum_{r'=1}^2 \int \frac{d^3k d^3p}{(2\pi)^{\frac{3}{2}}} \left(\frac{m^2}{E_{p+k} E_p} \right)^{\frac{1}{2}} \frac{1}{|\vec{k}| + E_p + E_{p+k}} \omega^\dagger(\vec{p} + \vec{k}, r') (\alpha \cdot \vec{a}(\vec{k}) + \frac{\vec{k} \cdot \vec{a}(\vec{k})}{|\vec{k}|}) \omega(\vec{p}, r) \\
& \exp(R) b(\vec{p}, r) \prod_{s=1}^2 \prod_{\substack{\vec{p}' \\ (\vec{p} + \vec{k}, r') \text{ and } (\vec{q}, 1)}} b(\vec{p}', s) \\
- & \sum_{r'=1}^2 \int \frac{d^3k}{(2\pi)^{\frac{3}{2}}} \left(\frac{m^2}{E_{q+k} E_q} \right)^{\frac{1}{2}} \frac{1}{E_q - E_{q+k} - |\vec{k}|} \omega^\dagger(\vec{q} + \vec{k}, r') (\alpha \cdot \vec{a}(\vec{k}) + \frac{\vec{k} \cdot \vec{a}(\vec{k})}{|\vec{k}|}) \omega(\vec{q}, 1) \\
& \exp(R) \prod_{s=1}^2 \prod_{\substack{\vec{p}' \\ (\vec{q} + \vec{k}, r')}} b(\vec{p}', s) .
\end{aligned} \tag{3.23}$$

The first term in eq. (3.23) is essentially independent of \vec{q} and represents a disconnected vacuum process. A term almost identical to this appears in the vacuum wave functional to first order. The second term in eq. (3.23) represents the interaction of the electron with momentum \vec{q} with a photon of momentum \vec{k} .

We may easily verify that F given by eq. (3.23) does indeed satisfy the Gauss's Law constraint, eq. (3.12), and the Schrödinger equation (3.14) if we note the identity

$$\omega^\dagger(\vec{p} + \vec{k}, r') (\vec{k} \cdot \alpha) \omega(\vec{p}, r) = (\varepsilon_r \cdot E_{p+k} - \varepsilon_r \cdot E_p) \omega^\dagger(\vec{p} + \vec{k}, r') \omega(\vec{p}, r) . \tag{3.24}$$

Now that we have the correct $\Psi_{\vec{q}}^{(1)}$ we may compare it with eq. (3.4). We can see that eq. (3.4) would give us the $\alpha \cdot \vec{a}$ term in eq. (3.23) but would miss the $\vec{k} \cdot \vec{a}$ term. Eq. (3.4) would give the correct form if we modified the Hamiltonian, eq. (3.1), by adding the term

$$- e \int \frac{(\vec{\nabla} \cdot \vec{A}(\vec{x})) \cdot \frac{\delta}{\delta \psi(\vec{y})} \psi(\vec{y})}{|\vec{x} - \vec{y}|^2} d^3x d^3y , \tag{3.25}$$

assumed that the vector potential everywhere contains a longitudinal component, and did the functional integrals over all configurations (including gauge equivalent ones). The added interaction to the Hamiltonian, eq. (3.25), is not gauge invariant.

Since we know how to repair eq. (3.4) we may wonder if the same procedure will cure eq. (3.5). We will see that it does. To do this we will calculate to second-order correction to the energy by computing part of the second order perturbed wave functional, the part that contributes to the energy. We will compute this portion using the same procedure that worked for the first-order functional. We then obtain the energy by functionally differentiating this term twice.

To determine what part of the second-order functional contributes to the computation of the energy we examine the Schrödinger equation to second order. We write

$$\Psi_{\vec{q}}^{(2)} = S[\mathbf{a}, \mathbf{b}] \exp(R).$$

Then the second-order piece of the Schrödinger equation gives

$$-\frac{1}{2} \int (2 \frac{\delta S}{\delta \mathbf{a}(\vec{k})} \cdot \frac{\delta R}{\delta \mathbf{a}(-\vec{k})} + \frac{\delta}{\delta \mathbf{a}(\vec{k})} \cdot \frac{\delta S}{\delta \mathbf{a}(-\vec{k})}) d^3k + \mathbf{H}_e S + \mathbf{H}_I F = \omega_{\vec{q}} S + E_{\vec{q}}^{(2)} \Omega_{\vec{q}}^{(0)}. \quad (3.26)$$

Since the energy, $E_{\vec{q}}^{(2)}$, is a pure number it cannot contain any factors of $\vec{d}(\vec{k})$. The form of Gauss's Law and $\mathbf{H}_I F$ indicates that all of the terms in S will contain two factors of \vec{d} , say $\vec{d}(\vec{k})$ and $\vec{d}(\vec{k}')$, and fermion wavefunctionals for states containing 1, 3, and 5 electrons and positrons. The only term on the left-hand side of eq. (3.26) that may possibly contain no factors of \vec{d} is

$$\frac{\delta}{\delta a(\vec{k})} \cdot \frac{\delta S}{\delta a(-\vec{k})}$$

We also see that $E_{\vec{q}}^{(2)}$ multiplies $\Omega_{\vec{q}}^{(0)}$ in eq. (3.26), a state with one electron. Thus the terms in $\Psi_{\vec{q}}^{(2)}$ that contribute to $E_{\vec{q}}^{(2)}$ are those with fermion wavefunctionals that describe states with one electron.

Sparing the reader of most of the details, we solve eq. (3.26) for the terms we want by inserting Gauss's Law into the first term of eq. (3.26) after we have expanded this term into transverse and longitudinal parts. We can then read off the fermion dependence from Gauss's Law and the term $H_I F$. It is

$$S \sim_S [a] \sum_{s,s'=1}^4 \frac{\delta}{\delta b(\vec{p}'+\vec{k}',s')} b(\vec{p}',s) \left(\sum_{r=3r'=1}^4 \sum_{r'=1}^2 b(\vec{p}',r) \prod_{r''=1}^2 \prod_{\substack{\vec{p}'' \\ (\vec{p}+\vec{k}',r') \text{ and } (\vec{q},1)}} b(\vec{p}'',r'') + \sum_{r'=1}^2 \prod_{r''=1}^2 \prod_{\substack{\vec{p}'' \\ (\vec{q}+\vec{k}',r')}} b(\vec{p}'',r'') \right). \quad (3.27)$$

When $s = r'$, $\vec{p}' = \vec{p} + \vec{k}'$, $s' = r$, and $\vec{p}' + \vec{k}' = \vec{p}$, the first term in eq. (3.27) will be proportional to $\Omega_{\vec{q}}^{(0)}$. When $s = 1$, $\vec{p}' = \vec{q}$, $s' = r$, and $\vec{p}' + \vec{k}' = \vec{p}$, the first term will be proportional to $\Omega_{\vec{p}+\vec{k}}^{(0)}$. When $s = r'$, $\vec{p}' = \vec{q} + \vec{k}'$, and $s' = 1$, the second term above will be proportional to $\Omega_{\vec{p}+\vec{k}}^{(0)}$. These conditions determine the remaining factors in the desired terms of S to be

$$S_v = \sum_{r=3r'=1}^4 \sum_{r'=1}^2 \int \frac{d^3 k}{|\vec{k}|} \frac{d^3 p}{(2\pi)^3} \left[\frac{m^2}{E_{p+k} E_p} \right] w^\dagger(\vec{p}, r) (\alpha \cdot \vec{a}(-\vec{k}) - \frac{\vec{k} \cdot \vec{a}(-\vec{k})}{|\vec{k}|}) w(\vec{p} + \vec{k}, r')$$

$$\frac{1}{|\vec{k}| + E_p + E_{p+k}} w^\dagger(\vec{p} + \vec{k}, r') (\alpha \cdot \vec{a}(\vec{k}) + \frac{\vec{k} \cdot \vec{a}(\vec{k})}{|\vec{k}|}) w(\vec{p}, r) \Omega_{\vec{q}}^{(0)}$$

$$S_1 = \sum_{r=3r'=1}^4 \sum_{r'=1}^2 \int \frac{d^3 k d^3 p}{(2\pi)^3} \left[\frac{m^2}{E_{p+k} E_p} \right]^{\frac{1}{2}} \left[\frac{m^2}{E_p E_q} \right]^{\frac{1}{2}} \frac{1}{|\vec{k}| + E_p + E_{p+k}} \frac{1}{|\vec{p} - \vec{q}| + E_{p+k} - E_q}$$

$$\begin{aligned}
& \omega^\dagger(\vec{p}, r) \left(\alpha \cdot \vec{d}(\vec{p}-\vec{q}) + \frac{(\vec{p}-\vec{q}) \cdot \vec{d}(\vec{p}-\vec{q})}{|\vec{p}-\vec{q}|} \right) \omega(\vec{q}, 1) \omega^\dagger(\vec{p}+\vec{k}, r') \left(\alpha \cdot \vec{d}(\vec{k}) + \frac{\vec{k} \cdot \vec{d}(\vec{k})}{|\vec{k}|} \right) \omega(\vec{p}, r) \Omega_{\vec{p}+\vec{k}}^{(0)} \\
S_2 &= \sum_{s'=1}^2 \sum_{r'=1}^2 \int \frac{d^3k d^3k'}{(2\pi)^3} \left[\frac{m^2}{E_{q+k} E_q} \right]^{\frac{1}{2}} \left[\frac{m^2}{E_{q+k+k'} E_{q+k}} \right]^{\frac{1}{2}} \frac{1}{|\vec{k}| + E_{q+k} - E_q} \frac{1}{|\vec{k}'| + E_{q+k+k'} - E_q} \\
& \omega^\dagger(\vec{q}+\vec{k}+\vec{k}', s') \left(\alpha \cdot \vec{d}(\vec{k}') + \frac{\vec{k}' \cdot \vec{d}(\vec{k}')}{|\vec{k}'|} \right) \omega(\vec{q}+\vec{k}, r') \omega^\dagger(\vec{q}+\vec{k}, r') \left(\alpha \cdot \vec{d}(\vec{k}) + \frac{\vec{k} \cdot \vec{d}(\vec{k})}{|\vec{k}|} \right) \omega(\vec{q}, 1) \Omega_{\vec{q}+\vec{k}+\vec{k}'}^{(0)}.
\end{aligned} \tag{3.28}$$

When we take the second functional derivative of the last two terms, we find $\vec{p}+\vec{k}=\vec{q}$ in S_1 and $\vec{p}'+\vec{k}'=\vec{q}$ in S_2 . Upon differentiation, these terms become proportional to $\Omega_{\vec{q}}^{(0)}$.

The second-order correction to the energy is half the second derivative with respect to $\vec{d}(\vec{k})$ of the previous expression.

$$\begin{aligned}
E_{\vec{q}}^{(2)} &= E_0^{(2)} + E_1^{(2)} + E_2^{(2)} = \sum_{r=3}^4 \sum_{r'=1}^2 \int \frac{d^3k d^3p}{|\vec{k}| (2\pi)^3} \left[\frac{m^2}{E_{p+k} E_p} \right] \frac{1}{|\vec{k}| + E_p + E_{p+k}} \\
& \omega^\dagger(\vec{p}, r) \left(\alpha_j - \frac{k_j}{|\vec{k}|} \right) \omega(\vec{p}+\vec{k}, r') \omega^\dagger(\vec{p}+\vec{k}, r') \left(\alpha_j + \frac{k_j}{|\vec{k}|} \right) \omega(\vec{p}, r) \\
& + \sum_{r=3}^4 \int \frac{d^3k}{(2\pi)^3} \left[\frac{m^2}{E_{q+k} E_q} \right] \frac{1}{|\vec{k}|} \frac{1}{|\vec{k}| + E_{q+k} + E_q} \\
& \omega^\dagger(\vec{q}+\vec{k}, r) \left(\alpha_j + \frac{k_j}{|\vec{k}|} \right) \omega(\vec{q}, 1) \omega^\dagger(\vec{q}, 1) \left(\alpha_j - \frac{k_j}{|\vec{k}|} \right) \omega(\vec{q}+\vec{k}, r) \\
& + \sum_{r'=1}^2 \int \frac{d^3k}{|\vec{k}| (2\pi)^3} \left[\frac{m^2}{E_{q+k} E_q} \right] \frac{1}{|\vec{k}| + E_{q+k} - E_q} \\
& \omega^\dagger(\vec{q}, 1) \left(\alpha_j - \frac{k_j}{|\vec{k}|} \right) \omega(\vec{q}+\vec{k}, r') \omega^\dagger(\vec{q}+\vec{k}, r') \left(\alpha_j + \frac{k_j}{|\vec{k}|} \right) \omega(\vec{q}, 1)
\end{aligned} \tag{3.29}$$

The first term in eq. (3.29) is just the vacuum energy at second order. The second and third terms are more interesting. Using the projection operator

$$w^\dagger(\vec{p}, \tau)(E_p - \varepsilon_\tau(\alpha \cdot \vec{p} + \gamma_0 m)) = 0 \quad (3.30)$$

and completeness

$$\sum_{\tau=1}^4 w_\alpha(\vec{p}, \tau) w_\beta^\dagger(\vec{p}, \tau) = \frac{E_p}{m} \delta_{\alpha\beta} \quad (3.31)$$

it is easy to reduce the second and third terms in eq. (3.29) to

$$E_{\vec{q}}^{(2)} = \left(\frac{m}{E_q} \right) \int \frac{d^3k}{|\vec{k}|} \frac{1}{(2\pi)^3} \frac{1}{E_q - E_{q+k} - |\vec{k}|} \left(\frac{2E_q}{m} \right). \quad (3.32)$$

For $\vec{q} \rightarrow 0$, $E_{\vec{q}}^{(0)} + e^2 E_{\vec{q}}^{(2)}$ is the mass of the electron to second order.

$$m_{e^-} = m + 2e^2 \int \frac{d^3k}{|\vec{k}|} \frac{1}{(2\pi)^3} \frac{1}{m - E_k - |\vec{k}|}. \quad (3.33)$$

The mass to second order is divergent.

The computation of the S matrix in the Schrödinger representation is conceptually straight forward. If the initial state is $|i\rangle$ and the final state is $|f\rangle$, then the S matrix element for the process is $S_{fi} = \langle f | i \rangle$. The initial and final states are represented by wave functionals derived from the functional Schrödinger equation and the matrix element is a functional integral.

As an example let us calculate the S matrix for electron-proton scattering to second order (tree level). For this we need the wave functional representing a state with one electron of momentum \vec{q} and one proton of momentum \vec{Q} to first order. To compute this functional we follow the same technique as we did for the single electron case. The Hamiltonian now contains terms for the

proton. We will use capital letters for the coordinates representing the proton. The relevant part of the first-order functional is

$$\begin{aligned}
 F_2 = & \sum_{r'=1}^2 \int \frac{d^3k}{(2\pi)^{\frac{3}{2}}} \left(\frac{m^2}{E_{q+k}E_q} \right)^{\frac{1}{2}} \frac{1}{|\vec{k}| + E_{q+k} - E_q} \omega^\dagger(\vec{q}+\vec{k}, r') (\alpha \cdot \vec{a}(\vec{k}) + \frac{\vec{k} \cdot \vec{a}(\vec{k})}{|\vec{k}|}) \omega(\vec{q}, 1) \Omega_{\vec{q}+\vec{k}}^{(\sigma)} \Omega_{\vec{q}}^{(\sigma)} \\
 & + \sum_{r'=1}^2 \int \frac{d^3k}{(2\pi)^{\frac{3}{2}}} \left(\frac{M^2}{E_{q+k}E_Q} \right)^{\frac{1}{2}} \frac{1}{|\vec{k}| + E_{q+k} - E_Q} W^\dagger(\vec{Q}+\vec{k}, r') (\alpha \cdot \vec{a}(\vec{k}) + \frac{\vec{k} \cdot \vec{a}(\vec{k})}{|\vec{k}|}) W(\vec{Q}, 1) \Omega_{\vec{q}}^{(\sigma)} \Omega_{\vec{Q}+\vec{k}}^{(\sigma)}
 \end{aligned} \tag{3.34}$$

Let the initial state be an electron with momentum \vec{q} and a proton with momentum \vec{Q} , and let the final state be an electron with momentum \vec{q}' , and a proton with momentum \vec{Q}' . Suppose all are spin up. Let the momentum transferred by the photon be \vec{k} . The matrix element at second order is $S_{ff}^{(2)} = \langle F_f^{(\sigma)}(\vec{q}', \vec{Q}', \vec{k}') | F_f^{(\sigma)}(\vec{q}, \vec{Q}, \vec{k}) \rangle$. When we do this functional integral, the integral over the vector potential, $\vec{a}(\vec{k})$, will be proportional to $\delta(\vec{k}-\vec{k}')$. The fermionic functional integrals will be proportional to $\delta(\vec{q}-\vec{q}'-\vec{k}) \delta(\vec{Q}+\vec{k}-\vec{Q}') \delta_{r_1} \delta_{r_1'}$. The delta functions provide momentum conservation. The result for the functional integral is

$$\begin{aligned}
 S_{ff}^{(2)} = & 3 \int \frac{d^3k}{(2\pi)^{\frac{3}{2}}} \frac{1}{|\vec{k}|} \left(\frac{m^2}{E_q E_{q-k}} \right)^{\frac{1}{2}} \left(\frac{M^2}{E_{q+k} E_Q} \right)^{\frac{1}{2}} \frac{1}{|\vec{k}| + E_q - E_{q-k}} \frac{1}{|\vec{k}| + E_{q+k} - E_Q} \\
 & \omega^\dagger(\vec{q}, 1) (\alpha_j) \omega(\vec{q}-\vec{k}, 1) W^\dagger(\vec{Q}+\vec{k}, 1) (\alpha_j) W(\vec{Q}, 1) .
 \end{aligned} \tag{3.35}$$

This expression agrees with the standard result computed with the propagator formalism [7], once the k_0 momentum integral is done in [7].

C. Regularization and Renormalization

We will regularize in a gauge invariant, nonperturbative way by using a functional directional derivative [8]. The directional derivative of a functional $F[A]$ in the direction of the function ξ is defined as [9]

$$\frac{\delta_\xi}{\delta_\xi A} F[A] = \lim_{\varepsilon \rightarrow 0} \frac{F[A + \varepsilon \xi(\mathbf{x})] - F[A]}{\varepsilon}. \quad (3.36)$$

The functional derivatives $\frac{\delta}{\delta A_i(\vec{x})}$, and $\frac{\delta}{\delta \psi(\vec{x})}$ appearing in the previous section are just directional functional derivatives in the direction of the δ - function, $\frac{\delta}{\delta A(\mathbf{x})} \equiv \frac{\delta_{\delta(\mathbf{x})}}{\delta_{\delta(\mathbf{x})} A(\mathbf{x})}$. Since $\frac{\delta}{\delta A(\vec{x})} A(\vec{y}) = \delta(\vec{x} - \vec{y})$, the meaning of (3.36) is then, $\frac{\delta_\xi}{\delta_\xi A(\vec{x})} A(\vec{y}) = \xi(\vec{x} - \vec{y})$.

We will regularize the theories by replacing some of the functional derivatives that appear in the Schrödinger representation by directional functional derivatives, and by modifying the fermionic part of the Hamiltonian. We choose $\xi(\vec{x})$ in eq (3.36) to be a sequence of functions, $\delta_\lambda(\vec{x})$, where $\delta_\lambda(\vec{x}) \rightarrow \delta(\vec{x})$ as $\lambda \rightarrow 0$, and denote these directional derivatives as $\frac{\delta_\lambda}{\delta_\lambda A(\vec{x})}$.

In the momentum representation, the replacement above implies that we replace $\frac{\delta}{\delta \vec{a}(\vec{k})}$ with $\frac{\delta_\lambda}{\delta_\lambda \vec{a}(\vec{k})}$ where $\frac{\delta_\lambda}{\delta_\lambda \vec{a}(\vec{k})} = f_\lambda(\vec{k}) \frac{\delta}{\delta \vec{a}(\vec{k})}$ and $f_\lambda(\vec{k})$ is the Fourier transform of $\delta_\lambda(\vec{x})$ so that $f_\lambda(\vec{k}) \rightarrow 1$ as $\lambda \rightarrow 0$.

We could replace all the functional derivatives appearing in the Hamiltonian and Gauss's Law as we have done earlier [10]. The eigenfunctionals in the regulated theory will depend on λ and will be a solution to $H_\lambda \Psi_\lambda = E_\lambda \Psi_\lambda$ where H_λ is the Hamiltonian with functional derivatives $\frac{\delta_\lambda}{\delta_\lambda A(\vec{x})}$ and $\frac{\delta_\lambda}{\delta_\lambda \psi(\vec{x})}$. We will

regularize here in a slightly different way by only replacing the functional derivatives in H_γ , eq. (3.9), and by modifying $\vec{\alpha}$ in H_e and H_f . Thus H_γ becomes

$$H_{\gamma\lambda} = \frac{1}{2} \int -f_\lambda^2(k) \frac{\delta}{\delta \vec{\alpha}(\vec{k})} \cdot \frac{\delta}{\delta \vec{\alpha}(-\vec{k})} + (\vec{k} \times \vec{\alpha}(\vec{k})) \cdot (\vec{k} \times \vec{\alpha}(-\vec{k})) d^3k . \quad (3.37)$$

In the fermionic parts of the Hamiltonian we replace $\vec{\alpha}$ with

$$\vec{\alpha}(\nu) = \begin{bmatrix} \nu \vec{\sigma} & \vec{\sigma} \\ \vec{\sigma} & \nu \vec{\sigma} \end{bmatrix} . \quad (3.37a)$$

For $\nu = 0$ we recover the original Hamiltonian. To regularize, we will take $\nu = 1$ for spin up and $\nu = -1$ for spin down solutions of the free Hamiltonian. The reason that this will regularize fermion loops is that this modification to the free Dirac Hamiltonian modifies the energy eigenvalues to be

$$E(\nu) = \pm((p^2 + m^2)^{\frac{1}{2}} - |\nu| |\vec{p}|)$$

and $E(\pm 1) \rightarrow 0$ as $|\vec{p}| \rightarrow \infty$. Since we are modifying only $\vec{\alpha}$, we preserve gauge invariance.

The eigenfunctionals, Ψ_λ now satisfy

$$(H_{\gamma\lambda} + H_{e\nu} + H_{f\nu}) \Psi_{\lambda\nu} = E_\lambda(\nu) \Psi_{\lambda\nu} . \quad (3.38)$$

The Gauss Law operator is unchanged and it is easy to check that the modification to H preserves gauge invariance, $[G, H_\lambda] = 0$.

Consider the state with one electron with momentum \vec{q} again. To lowest order the wave functional obeying eq. (3.38) is

$$\Psi_{\lambda 0 \vec{q}}^{(0)} = \eta_f \exp\left(-\frac{1}{2} \int \frac{(\vec{k} \times \vec{\alpha}(\vec{k})) \cdot (\vec{k} \times \vec{\alpha}(-\vec{k}))}{f_\lambda(k) |\vec{k}|} d^3k\right) \prod_{r=1}^2 \prod_{\substack{\vec{p} \\ (\vec{p}=\vec{q}, r=1)}} b(p, s) \quad (3.39)$$

where $\eta_f = \left(\frac{|\vec{k}|}{f_\lambda(k)\pi}\right)^{\frac{1}{4}}$. That is, R , eq. (3.13) becomes

$$R_\lambda = -\frac{1}{2} \int \frac{(\vec{k} \times \vec{a}(\vec{k})) \cdot (\vec{k} \times \vec{a}(-\vec{k}))}{f_\lambda(k) |\vec{k}|} d^3k . \quad (3.40)$$

It still satisfies Gauss's Law to lowest order. $E_{\vec{q}\lambda}^{(0)} = E_{\vec{q}}$ still, but a single photon of momentum \vec{k} now has energy $f_\lambda(k) |\vec{k}|$ above the ground state. We may solve the functional differential equation, eq.(3.38) for the first-order regulated functional in the same manner we used earlier for F . The result is

$$\begin{aligned} F_\lambda[a, b] &= \sum_{r=3}^4 \sum_{r'=1}^2 \int \frac{d^3k d^3p}{(2\pi)^{\frac{3}{2}}} \left[\frac{m^2}{E_{p+k}(\nu) E_p(\nu)} \right]^{\frac{1}{2}} \frac{1}{f_\lambda(k) |\vec{k}| + E_p(\nu) + E_{p+k}(\nu)} \\ & w_{\downarrow}(\vec{p}+\vec{k}, r') (\alpha(\nu) \cdot \vec{a}(\vec{k}) + \frac{f_\lambda(k) \vec{k} \cdot \vec{a}(\vec{k})}{|\vec{k}|}) w_{\nu}(\vec{p}, r) \exp(R_\lambda) b(\vec{p}, r) \prod_{s=1}^2 \prod_{\vec{p}'} b(\vec{p}', s) \\ & \quad \text{except } (\vec{p}+\vec{k}, r') \text{ and } (\vec{q}, 1) \\ & - \sum_{r'=1}^2 \int \frac{d^3k}{(2\pi)^{\frac{3}{2}}} \left[\frac{m^2}{E_{q+k}(\nu) E_q(\nu)} \right]^{\frac{1}{2}} \frac{1}{E_q(\nu) - E_{q+k}(\nu) - f_\lambda(k) |\vec{k}|} \\ & w_{\downarrow}(\vec{q}+\vec{k}, r') (\alpha(\nu) \cdot \vec{a}(\vec{k}) + \frac{f_\lambda(k) \vec{k} \cdot \vec{a}(\vec{k})}{|\vec{k}|}) w_{\nu}(\vec{q}, 1) \exp(R_\lambda) \prod_{s=1}^2 \prod_{\vec{p}'} b(\vec{p}', s) \quad (3.41) \\ & \quad \text{except } (\vec{q}+\vec{k}, r') \end{aligned}$$

It is easy to check that eq. (3.41) still obeys the Gauss's Law constraint. (This is equivalent to checking that the Ward identities are still satisfied in other formalisms.) This shows that the regularization preserves gauge invariance.

S_λ requires the same replacement in eq. (3.28) as $F \rightarrow F_\lambda$ and the factor $\frac{1}{|\vec{k}|}$ multiplying everything becomes $\frac{1}{f_\lambda(k) |\vec{k}|}$. To find the energy to second order we compute $\frac{\delta_\lambda}{\delta_\lambda \vec{A}} \frac{\delta_\lambda}{\delta_\lambda \vec{A}} S_\lambda$. The result is

$$E_q^{(2)} = \left(\frac{m}{E_q} \right) \int \frac{d^3k}{(2\pi)^3} \frac{1}{|\vec{k}|} \frac{f_\lambda(k)}{E_q - E_{q+k} - f_\lambda(k) |\vec{k}|} \left(\frac{2E_q}{m} \right) \quad (3.42)$$

where we have already taken the limit $\nu \rightarrow 0$ since the mass will still be regulated.

The mass is

$$m_{e^-} = m + 2e^2 \int \frac{d^3k}{(2\pi)^3} \frac{1}{|\vec{k}|} \frac{f_\lambda(k)}{m - E_k - f_\lambda(k) |\vec{k}|}. \quad (3.43)$$

We are free to choose $f_\lambda(k)$ at this point. For example, the choice $f_\lambda(k) = e^{-\lambda^2 k^2}$ will make the mass finite. We may also use $f_\lambda(k)$ as a cutoff.

The reason that the energy is regulated by this method is that the wave functionals pick up only one factor of $f_\lambda^{-1}(k)$ so that the potential terms will be canceled by $f_\lambda \frac{\delta \Psi_\lambda}{\delta a} f_\lambda \frac{\delta \Psi_\lambda}{\delta a}$. The eigenvalues arise from the term $f_\lambda^2 \frac{\delta^2 \Psi_\lambda}{\delta a^2}$, so there is an extra factor of $f_\lambda(k)$ left over. For matrix elements, the functional integral introduces $f_\lambda^2(k)$ because of the gaussian nature of R_λ .

To complete mass renormalization we introduce a counter term in the Hamiltonian that looks like $\delta m \frac{\delta}{\delta \psi(\vec{x})} \psi(\vec{x})$ where δm is equal to

$$-2e^2 \int \frac{d^3k}{(2\pi)^3} \frac{1}{|\vec{k}|} \frac{f_\lambda(k)}{m - E_k - f_\lambda(k) |\vec{k}|}$$

(throw away the finite part). We now interpret the quantity m wherever it appears to be the physical mass. The mass to second order is now $m_{e^-} = m$. We renormalize ψ and $\frac{\delta}{\delta \psi}$ by rescaling the $w(\vec{p}, \tau)$'s. They are rescaled to remove the infinite part of eq. (3.42) after subtracting the mass (and throwing away any finite part). We can rescale the charge in a similar manner.

Another way to carry out renormalization would be to compute the effective action. The effective action is the minimum of $\langle H \rangle$ in a state such that $\langle A \rangle = A_b$, $\langle \psi \rangle = \psi_b$ [11]. A way to calculate this is to find the perturbed vacuum wave functional. (We have essentially done that. It is very similar to the first term in F .) Then replace A with $A + A_b$, ψ with $\psi + \psi_b$, and $\frac{\delta}{\delta \psi}$ with $\frac{\delta}{\delta \psi} + \psi_b^\dagger$. Then compute $\langle H \rangle$ in this state. Alternatively, we could quantize in a background field, $(A_b, \psi_b, \psi_b^\dagger)$ and find $\langle H \rangle$ in the normal vacuum state. Either way the renormalized mass is found by $m = \frac{\delta^2 \langle H \rangle}{\delta \psi_b \delta \psi_b^\dagger} \Big|_{\psi_b = \psi_b^\dagger = A_b = 0}$ and the renormalized charge

by $\frac{\delta^2 \langle H \rangle}{\delta A_b \delta \psi_b \delta \psi_b^\dagger} \Big|_{\psi_b = \psi_b^\dagger = A_b = 0}$.

We may regularize in the same way as above.

Chapter 4. The Abelian Higgs Model

A. The Temporal Gauge and Choice of Coordinates

One advantage of working with the functional Schrödinger representation is that we have available a nonperturbative technique. We can construct trial wave functionals with parameters to be varied and compute the expectation of say, the energy, and minimize. This is a natural way to compute the effective action nonperturbatively. As an example to show that the application of the technique is unrestrictive, we show how to compute the string tension of a magnetic flux tube in the Abelian Higgs model. There is no restriction on whether the coupling is large or small.

The Lagrangian density used by Nielsen and Olesen [12],

$$L = -\frac{1}{4}F^{\mu\nu}F_{\mu\nu} + \frac{1}{2}|(\partial_\mu + ieA_\mu)\varphi|^2 + c_2|\varphi|^2 + c_4|\varphi|^4 \quad (4.1)$$

yields the following Hamiltonian in the temporal gauge ($A_0=0$),

$$\begin{aligned} H = \int d^3x & \frac{1}{2}E^2 + \frac{1}{2}B^2 + \frac{1}{2}(\dot{\varphi}^* \varphi) \\ & + \frac{1}{2}((\partial_i - ieA_i)\varphi^*(\partial_i + ieA_i)\varphi) - c_2|\varphi|^2 + c_4|\varphi|^4. \end{aligned} \quad (4.2)$$

Canonical quantization implies that at equal times

$$\begin{aligned} [\Pi_A^i(\vec{x}), A^j(\vec{y})] &= -i \delta^{ij} \delta(\vec{x}-\vec{y}) \\ [\Pi_\varphi(\vec{x}), \varphi(\vec{y})] &= -i \delta(\vec{x}-\vec{y}) \\ [\Pi_{\varphi^*}(\vec{x}), \varphi^*(\vec{y})] &= -i \delta(\vec{x}-\vec{y}). \end{aligned} \quad (4.3)$$

For the Lagrangian, eq (4.1), $\Pi_A^i = -E^i$, $\Pi_\varphi = \dot{\varphi}^*$, and $\Pi_{\varphi^*} = \dot{\varphi}$. In the Schrödinger

representation we represent the conjugate momenta as the functional derivatives,

$$E_i(\vec{x}) = i \frac{\delta}{\delta A_i(\vec{x})}, \quad \dot{\varphi}^*(\vec{x}) = -i \frac{\delta}{\delta \varphi(\vec{x})}, \quad \text{and} \quad \dot{\varphi}(\vec{x}) = -i \frac{\delta}{\delta \varphi^*(\vec{x})}. \quad (4.4)$$

Stationary states represented by the wave functionals, $\Psi[A, \varphi, \varphi^*]$ satisfy the functional equation

$$\int d^3x -\frac{1}{2} \frac{\delta}{\delta \vec{A}(\vec{x})} \cdot \frac{\delta}{\delta \vec{A}(\vec{x})} + \frac{1}{2} \frac{\delta}{\delta \varphi(\vec{x})} \frac{\delta}{\delta \varphi^*(\vec{x})} + \frac{1}{2} ((\partial_j - ieA_j(\vec{x}))\varphi^*(\vec{x}) (\partial_j + ieA_j(\vec{x}))\varphi(\vec{x})) \\ + \frac{1}{2} \vec{B}(\vec{x}) \cdot \vec{B}(\vec{x}) - C_2 |\varphi|^2 + C_4 |\varphi|^4 \Psi[A, \varphi, \varphi^*] = E \Psi[A, \varphi, \varphi^*]. \quad (4.5)$$

As usual, in the temporal gauge we must add Gauss's Law as a constraint. Using eq. (4.4), the wave functionals $\Psi[A, \varphi, \varphi^*]$ must also satisfy

$$\nabla \cdot \frac{\delta}{\delta \vec{A}(\vec{x})} - \frac{e}{2} (\varphi^* \frac{\delta}{\delta \varphi^*(\vec{x})} - \varphi \frac{\delta}{\delta \varphi(\vec{x})}) \Psi[A, \varphi, \varphi^*] = 0. \quad (4.6)$$

Since Gauss's Law generates infinitesimal time-independent gauge transformations, eq. (4.6) implies that $\Psi[A, \varphi, \varphi^*]$ must be gauge invariant under time-independent transformations. The first term alone in eq. (4.6) simply means that the wave functional cannot depend on the longitudinal component of $\vec{A}(\vec{x})$. The second term alone tells us that φ and φ^* must appear "locally" symmetric in $\Psi[A, \varphi, \varphi^*]$. Thus $\int \varphi^*(\vec{x}) \varphi(\vec{x}) d^3x$ is gauge invariant but $\int \varphi^*(\vec{x}) \varphi(\vec{y}) d^3x d^3y$ is not. We want to construct realistic trial wave functionals for a variational calculation and these functionals should involve "nonlocal" functionals of φ and φ^* . One way would be to combine the longitudinal part of \vec{A} with the gauge-dependent part of a nonlocal functional of φ and φ^* so that eq. (4.6) is satisfied. For example, one way to do this is to parallel transport $\varphi(\vec{y})$ to \vec{x} and combine with

$\varphi^0(\vec{x})$.

$$\Psi \sim \exp\left(\int \varphi^0(\vec{x}) \exp\left(ie \int \vec{A} \cdot d\vec{\tau}\right) \varphi(\vec{y}) d^3x d^3y\right). \quad (4.7)$$

This form, however, is impractical and requires us to choose a path over which to transport. In short, construction of gauge invariant trial functionals which are fairly easy to use in calculations yet realistic is difficult with φ, φ^0 coordinates, especially if you want a gaussian trial functional that gives $\langle \varphi \rangle \neq 0$.

To overcome this difficulty we will change coordinates. Ideally, we want a coordinate system where some of the coordinates are gauge invariant. This is easy to accomplish in this case. We will use "polar" coordinates, $(\xi(\vec{x}), \chi(\vec{x}))$, where

$$\varphi(\vec{x}) = \xi(\vec{x}) e^{i\chi(\vec{x})}. \quad (4.8)$$

Under a gauge transformation, $\varphi(\vec{x}) = e^{ie\Lambda(\vec{x})} \varphi(\vec{x})$, ξ is invariant and $\chi \rightarrow \chi + e\Lambda(\vec{x})$.

For our purposes it will be convenient to quantize in a background field. Thus we write

$$\begin{aligned} \xi &\rightarrow \xi_b(\vec{x}) + \xi(\vec{x}) \\ \vec{A} &\rightarrow \vec{A}_b(\vec{x}) + \vec{A}(\vec{x}) \end{aligned} \quad (4.9)$$

where $\xi_b(\vec{x})$ and $\vec{A}_b(\vec{x})$ are background fields and $\xi(\vec{x})$ and $\vec{A}(\vec{x})$ fluctuate.

The Hamiltonian reexpressed in these coordinates becomes

$$\begin{aligned} H = \int d^3x & -\frac{1}{2} \frac{\delta}{\delta \vec{A}(\vec{x})} \cdot \frac{\delta}{\delta \vec{A}(\vec{x})} \left[\frac{\delta}{\delta \xi(\vec{x})} \right]^2 - \frac{1}{2} \frac{1}{(\xi + \xi_b)^2} \left[\frac{\delta}{\delta \chi(\vec{x})} \right]^2 + \frac{1}{2} (\vec{B} + \vec{B}_b)^2 \\ & + \frac{1}{2} (\nabla_i(\xi + \xi_b))^2 + \frac{1}{2} (\xi + \xi_b)^2 (\nabla_i \chi)^2 + e (A_i + A_{bi})(\xi + \xi_b)^2 (\nabla_i \chi) \end{aligned}$$

$$+ \frac{1}{2} e^2 (\vec{A} + \vec{A}_0)^2 (\xi + \xi_0)^2 - C_2 (\xi + \xi_0)^2 + C_4 (\xi + \xi_0)^4 \quad (4.10)$$

where we have represented $\Pi_\xi = \dot{\xi}$ by $-i \frac{\delta}{\delta \xi}$ and $\Pi_\chi = \xi^2 \dot{\chi}$ by $-i \frac{\delta}{\delta \chi}$. The Gauss's Law constraint now becomes transparent

$$\left(\nabla \cdot \frac{\delta}{\delta \vec{A}(\vec{x})} - e \frac{\delta}{\delta \chi(\vec{x})} \right) \Psi[A, \xi, \chi] = 0. \quad (4.11)$$

If Ψ does not depend on \vec{A}_L or χ , then it will be gauge invariant. We may construct wave functionals that do depend on \vec{A}_L and χ and still satisfy Gauss's Law but they will not be useful for our present purposes.

When we compute matrix elements in the Schrödinger representation, we must compute functional integrals. For example, the norm of a state $\Psi[A, \xi, \chi]$ is

$$\langle \Psi | \Psi \rangle = \int DA D\xi D\chi \Psi^*[A, \xi, \chi] \Psi[A, \xi, \chi]. \quad (4.12)$$

Once again, if Ψ satisfies Gauss's Law, then this integral will not be finite; the states satisfying Gauss's Law are not normalizable. What we really want to do is only integrate over gauge inequivalent configurations. In the present situation this is easily accomplished by inserting a δ -functional for χ and \vec{A}_L , the longitudinal component. When we compute expectation values, we now assume that these δ -functionals are present.

Now it is a simple task to construct gauge invariant wave functionals that are realistic and gaussian.

B. Trial Wave Functionals and Magnetic Flux Tubes

The choice of trial wave functionals is, of course, the heart of the matter for a variational calculation of this kind. We are limited in our choice by our ability to solve functional differential equations, even approximately, and by evaluating functional integrals. Since we only know how to exactly integrate gaussians and δ functionals we will choose our trial states here to be gaussian so that we may evaluate the functional integrals without approximation.

For our trial state we will take

$$\Psi_{AH} = \eta e^{-\frac{1}{2} \int h(k) \tilde{a}^2(\vec{k}) d^3k} e^{-\frac{1}{2} \int g(k) \xi^2(\vec{k}) d^3k} \quad (4.12)$$

where η is the normalization, $\prod_k \frac{1}{2} \left(\frac{\pi}{h(k)} \right)^{\frac{1}{2}} \frac{1}{g(k)}$.

The expectation of the Hamiltonian in the background fields, eq. (4.10), is now readily evaluated. When we minimize it with respect to the variational parameters, we have an effective action [11]. In practice we do this by first minimizing with respect to $h(k)$ and $g(k)$, and then with respect to A_0, ξ_0 .

We can carry out renormalization in a manner similar to Ref. [8]. First we vary $\langle H \rangle$ with respect to $h(k)$, solve for $h(k)$, and note that the form of $h(k)$ is similar to the free field case, namely, $h^2(k) = k^2 + m^2$. The constant, m^2 (which depends on the other variational parameters) is interpreted as the renormalized mass of the vector particle. Next we vary $g(k)$ and look for the same behavior. For the case above, however, $g(k)$ does not look like the free field case. This is not a surprise since we are dealing with a nonperturbative calculation. Instead we define the scalar mass to be $g(k=0)$. Inverting the above expressions for the mass will require regularization which we can, with directional functional derivatives as in Chapter 3.

To renormalize the charge we take the second derivative of $\langle H \rangle$ with respect to A_0 followed by the second derivative with respect to ξ_0 , $\frac{\delta^2 \langle H \rangle}{\delta \xi_0^2 \delta A_0^2}$. This represents the renormalized charge as a function of A_0 and ξ_0 . We determine A_0 and ξ_0 by minimizing $\langle H \rangle$ with respect to them and insert the results into the expression for e .

If we want to treat magnetic flux tubes, then all we have to do is to constrain A_0 such that $\int (\nabla \times A_0) dx dy$, the magnetic flux in the z direction, is equal to unity (in terms of e).

If we want to see if flux tubes attract or repel (depending on our choice of parameters), then we can compare the energy when we constrain A_0 so that two units of flux are present and compare it to twice the energy when one unit of flux is present. If the energy for two units is larger than twice the energy for one unit, then they repel.

The above program is difficult analytically to carry out in practice but is possible on a computer. Nothing restricts the size of the couplings so we have a method of studying the behavior of nontrivial theories in nonperturbative regions.

Chapter V. Yang-Mills

A. Temporal Gauge

The Lagrangian for SU(2) Yang-Mills theory is given by

$$L = -\frac{1}{4} \text{tr} \int d^4x F^{\mu\nu} F_{\mu\nu} \quad (5.1)$$

where

$$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu + g[A_\mu, A_\nu] \quad (5.2)$$

and

$$A_\mu = A_\mu^\alpha \frac{\tau^\alpha}{2i} \quad (5.3)$$

where τ^α is the usual Pauli matrix. α, β, γ will always be used as color indices which may take on the values a, b, c for the color axes a, b, c. If we choose the temporal gauge, $A_0 = 0$, the Hamiltonian is

$$H = \frac{1}{2} \int d^3x (\vec{E}^\alpha \cdot \vec{E}^\alpha + \vec{B}^\alpha \cdot \vec{B}^\alpha) \quad (5.4)$$

where

$$E_i^\alpha(\vec{x}) = -\dot{A}_i^\alpha(\vec{x}) \quad (5.5)$$

and

$$\vec{B}^\alpha(\vec{x}) = \vec{\nabla} \times \vec{A}^\alpha(\vec{x}) + \frac{g}{2} \varepsilon^{\alpha\beta\gamma} \vec{A}^\beta(\vec{x}) \times \vec{A}^\gamma(\vec{x}) \quad (5.6)$$

where $\varepsilon^{abc} = 1$. Canonical quantization gives the equal time commutator

$$\left[E_i^{\mathbf{p}}(\vec{x}), A_j^{\mathbf{p}}(\vec{y}) \right] = i \delta^{ab} \delta_{ij} \delta(\vec{x}-\vec{y}) . \quad (5.7)$$

We will work in the $\vec{A}^{\alpha}(\vec{x})$ representation so we may take

$$E_i^{\mathbf{p}}(\vec{x}) = i \frac{\delta}{\delta A_i^{\mathbf{p}}(\vec{x})} . \quad (5.8)$$

The ground state wave functional, $\Psi_0[A]$, is the vacuum state in the $A_i^{\mathbf{p}}(\vec{x})$ representation and satisfies the functional Schrödinger equation

$$\frac{1}{2} \int d^3x \left[- \frac{\delta}{\delta \vec{A}^{\alpha}(\vec{x})} \cdot \frac{\delta}{\delta \vec{A}^{\alpha}(\vec{x})} + \vec{B}^{\alpha} \cdot \vec{B}^{\alpha} \right] \Psi_0[A] = E_0 \Psi_0[A] . \quad (5.9)$$

As in QED, there is no Hamiltonian equation of motion for Gauss's Law in the temporal gauge. Gauss's Law must be added as a constraint on the wave functional. So the wave functional that satisfies eq (5.9) must also satisfy

$$(D \cdot E)^{\alpha} \Psi_0[A] = 0 \quad (5.10)$$

where $D_i = \partial_i + g[A_i, \cdot]$ is the covariant derivative. The operator $(D \cdot E)^{\alpha}$ is also the generator of time-independent gauge transformations so the Gauss's Law constraint amounts to requiring $\Psi_0[A]$ to be gauge invariant under time-independent gauge transformations.

Since $\Psi_0[A]$ satisfies the Gauss's Law constraint, it is gauge invariant under time-independent gauge transformations, so $\Psi_0[A]$ will not be normalizable. We may still find the vacuum expectation values for operators gauge invariant under time-independent gauge transformations by integrating only over gauge inequivalent configurations of $\vec{A}^{\alpha}(\vec{x})$.

B. The Vacuum Wave Functional to First Order in g

The structure of the ground state of Yang-Mills is generally thought of as bringing about confinement. The determination of the ground state, however, is not a trivial problem. Part of the difficulty lies in that the true ground state is not reachable by perturbative calculations [13]. Presently, no one knows how to do reliable nonperturbative approximations.

Even though the perturbative vacuum may not confine, its structure is still interesting since it antiscreens and it is a result of a nonlinear field theory. The perturbative ground state is taken to be the vacuum inside the "bag" defining a hadron [14]. The perturbative wave functional may also be used as the "short distance" limit of the true ground state [15]. With a suitable choice for a long-distance wave functional [16], a functional that interpolates between the limits may be used as a starting point for a variational trial functional for the nonperturbative vacuum.

Once again we find that the standard formula for the perturbed wave functionals fail. We instead will solve the functional Schrödinger equation directly using the same technique we used in Chapter 3.

If we set $g=0$ we have a system of 3 independent fields that describe free photons. The ground state wave functional for $g=0$, $\Psi_0^{(0)}[A]$, satisfies

$$\begin{aligned} & \frac{1}{2} \int d^3x \left[-\frac{\delta}{\delta \vec{A}^a(\vec{x})} \cdot \frac{\delta}{\delta \vec{A}^a(\vec{x})} \right. \\ & \left. + (\vec{\nabla} \times \vec{A}^a(\vec{x})) \cdot (\vec{\nabla} \times \vec{A}^a(\vec{x})) \right] \Psi_0^{(0)}[A] = E_0^{(0)} \Psi_0^{(0)}[A] \end{aligned} \quad (5.11)$$

and

$$\vec{\nabla} \cdot \frac{\delta \Psi_0^{(0)}[A]}{\delta \vec{A}^a(\vec{x})} = 0 \quad (5.12)$$

and is given by

$$\Psi_0^{(0)}[A] = \exp(R)$$

where

$$R = -\frac{1}{(2\pi)^2} \int \frac{(\vec{\nabla} \times \vec{A}^a(\vec{x})) \cdot (\vec{\nabla} \times \vec{A}^a(\vec{y}))}{|\vec{x} - \vec{y}|^2} d^3x d^3y . \quad (5.13)$$

If we attempt to apply the standard perturbative formulas we run into trouble. Formally, the first-order correction to the vacuum energy, $E_0^{(1)}$, is given by

$$E_0^{(1)} = \int \Psi_0^{(0)*}[A] H_1 \Psi_0^{(0)}[A] DA / \int \Psi_0^{(0)*}[A] \Psi_0^{(0)}[A] DA \quad (5.14)$$

where

$$H_1 = \varepsilon^{\alpha\beta\gamma} \int (\vec{\nabla} \times \vec{A}^{\alpha}(\vec{x})) \cdot (\vec{A}^{\beta}(\vec{x}) \times \vec{A}^{\gamma}(\vec{x})) d^3x. \quad (5.15)$$

Integrating only over gauge inequivalent configurations in eq. (5.14), we find that $E_0^{(1)}$ from equation (5.14) is infinite since $\Psi_0^{(0)}[A]$ only involves the transverse potentials, H_1 contains longitudinal potentials, and we are integrating over both transverse and longitudinal potentials. We expect $E_0^{(1)}$ to be zero.

Similarly, applying perturbative corrections to the wave functional, $\Psi_0^{(0)}[A]$, we find that the first order correction, $\Psi_0^{(1)}[A]$, is also infinite. The first-order correction is given by

$$\Psi_0^{(1)}[A] = \sum_N \frac{\langle N | H_1 | 0 \rangle}{E_N^{(0)} - E_0^{(0)}} \Psi_N^{(0)}[A]$$

where

$$\langle N | H_1 | 0 \rangle = \int \Psi_N^{(0)*}[A] H_1 \Psi_0^{(0)}[A] DA$$

and $\Psi_N^{(0)}[A]$ is a state containing N longitudinal and transverse photons. As before, the functional integration over the longitudinal component of the potentials diverges since $\Psi_0^{(0)}[A]$ does not depend on the longitudinal potentials and $\Psi_N^{(0)}[A]$ depends on the longitudinal components in an oscillatory manner.

To obtain the first-order correction, we will solve the functional Schrödinger equation directly. Since $\Psi_0[A]$ is the lowest energy eigenfunctional of Schrödinger equation, eq. (5.9), we believe that $\Psi_0[A]$ has no nodes [3] so that we may write $\Psi_0[A]$ as $\exp(V[A])$. If we set $g=0$, then

$$V[A]_{g=0} = R.$$

We seek the functional, F , such that the wave functional $\Psi_0[A] = \exp(R+gF)$ will satisfy equations (5.9) and (5.10) to first order in g . Placing $\exp(R+gF)$ into equation (5.9) and keeping terms up to first order in g we find that F must satisfy

$$\begin{aligned} & \frac{1}{2} \int -\frac{\delta}{\delta \vec{A}^\alpha(\vec{x})} \cdot \frac{\delta F}{\delta \vec{A}^\alpha(\vec{x})} - 2 \frac{\delta F}{\delta \vec{A}^\alpha(\vec{x})} \cdot \frac{\delta R}{\delta \vec{A}^\alpha(\vec{x})} \\ & + 2\varepsilon^{\alpha\beta\gamma} (\vec{\nabla} \times \vec{A}^\alpha(\vec{x})) \cdot (\vec{A}^\beta(\vec{x}) \times \vec{A}^\gamma(\vec{x})) d^3x = E_0^{(1)} \end{aligned} \quad (5.16)$$

since R satisfies

$$\begin{aligned} & \frac{1}{2} \int -\frac{\delta R}{\delta \vec{A}^\alpha(\vec{x})} \cdot \frac{\delta R}{\delta \vec{A}^\alpha(\vec{x})} - \frac{\delta}{\delta \vec{A}^\alpha(\vec{x})} \cdot \frac{\delta R}{\delta \vec{A}^\alpha(\vec{x})} \\ & + (\vec{\nabla} \times \vec{A}^\alpha(\vec{x})) \cdot (\vec{\nabla} \times \vec{A}^\alpha(\vec{x})) d^3x = E_0^{(0)}. \end{aligned}$$

To satisfy the Gauss's Law constraint F must also satisfy

$$\vec{\nabla} \cdot \frac{\delta F}{\delta \vec{A}^\alpha(\vec{x})} = -\varepsilon^{\alpha\beta\gamma} \vec{A}^\beta(\vec{x}) \cdot \frac{\delta R}{\delta \vec{A}^\gamma(\vec{x})}. \quad (5.17)$$

To find the functional F , we assume F will be of the form

$$F = \varepsilon^{\alpha\beta\gamma} f[A^\alpha, A^\beta, A^\gamma], \quad (5.18)$$

with $\varepsilon^{abc} = 1$, so that

$$\int \frac{\delta}{\delta \vec{A}^\alpha(\vec{x})} \cdot \frac{\delta F}{\delta \vec{A}^\alpha(\vec{x})} d^3x = 0, \quad (5.19)$$

and

$$E_0^{(1)} = 0.$$

The functional F must then satisfy

$$2 \int \frac{\delta F}{\delta \vec{A}^\alpha(\vec{x})} \cdot \frac{\delta R}{\delta \vec{A}^\alpha(\vec{x})} d^3x + H_1 = 0 \quad (5.20)$$

where H_1 is given by equation (5.15).

It is easier to solve the functional differential equation in the momentum representation. Let, as usual,

$$\vec{A}^\alpha(\vec{x}) = \frac{1}{\sqrt{(2\pi)^3}} \int \vec{a}^\alpha(\vec{k}) e^{i\vec{k}\cdot\vec{x}} d^3k \quad (5.21)$$

so

$$\frac{\delta}{\delta \vec{A}^\alpha(\vec{x})} = \frac{1}{\sqrt{(2\pi)^3}} \int \frac{\delta}{\delta \vec{a}^\alpha(\vec{k})} e^{-i\vec{k}\cdot\vec{x}} d^3k. \quad (5.22)$$

Equation (5.20) then becomes

$$2 \int \frac{\delta F}{\delta \vec{a}^\alpha(\vec{k})} \cdot \frac{\delta R}{\delta \vec{a}^\alpha(-\vec{k})} d^3k + H_1 = 0 \quad (5.23)$$

with

$$H_1 = i\varepsilon^{\alpha\beta\gamma} \int [\vec{k} \times \vec{a}^\alpha(\vec{k})] \cdot [\vec{a}^\beta(\vec{k}') \times \vec{a}^\gamma(-(\vec{k} + \vec{k}'))] d^3k d^3k' \quad (5.24)$$

and

$$\frac{\delta R}{\delta \vec{a}^\alpha(-\vec{k})} = \frac{\vec{k} \times (\vec{k} \times \vec{a}^\alpha(\vec{k}))}{|\vec{k}|}. \quad (5.25)$$

The first term in equation (5.23) may be rewritten using vector identities as

$$-\int [|\vec{k}| \left(\frac{\delta F}{\delta \vec{a}^\alpha(\vec{k})} \cdot \vec{a}^\alpha(\vec{k}) \right) - \frac{(\vec{k} \cdot \vec{a}^\alpha(\vec{k})) (\vec{k} \cdot \frac{\delta F}{\delta \vec{a}^\alpha(\vec{k})})}{|\vec{k}|}] d^3k. \quad (5.26)$$

The second term in equation (5.26) involves the longitudinal part of the vector potential, $\vec{a}^\alpha(\vec{k})$, and the (yet unknown) longitudinal part of the functional derivative of F . However, F must satisfy the Gauss's Law constraint, eq. (5.17). This constraint dictates the exact form of the longitudinal part of the functional derivative of F . By transforming (5.17) we find

$$\vec{k} \cdot \frac{\delta F}{\delta \vec{a}^\alpha(\vec{k})} = i\varepsilon^{\alpha\beta\gamma} \int \vec{a}^\gamma(-(\vec{k} + \vec{k}')) \cdot \frac{(\vec{k}' \times (\vec{k}' \times \vec{a}^\beta(\vec{k}')))}{|\vec{k}'|} d^3k'. \quad (5.27)$$

From the form of (5.27) and (5.24), we can see that F will be an integral over \vec{k} and \vec{k}' .

Now examine the first term in equation (5.26). First observe that

$$F = \int \frac{\delta F}{\delta \vec{a}^\alpha(\vec{k})} \cdot \vec{a}^\alpha(\vec{k}) d^3k \quad (\text{no sum on } \alpha). \quad (5.28)$$

From our assumption of the form of F , equation (5.18), $\frac{\delta F}{\delta \vec{a}^\alpha(\vec{k})}$ will not depend upon $\vec{a}^\alpha(\vec{k})$. So the result of functionally differentiating F with respect to $\vec{a}^\alpha(\vec{k})$, dotting the result with $\vec{a}^\alpha(\vec{k})$, and integrating over \vec{k} returns F as an expression with the momentum space coordinate of \vec{a}^α as \vec{k} . If we differentiate with respect

to $\vec{a}^b(\vec{k})$, dot with $\vec{a}^b(\vec{k})$, and integrate over \vec{k} , we will obtain the same functional as above except that now the momentum space coordinate of \vec{a}^b will be \vec{k} and the momentum space coordinate of \vec{a}^a will be either \vec{k}' or $-(\vec{k}+\vec{k}')$. If we adopt the convention that the momentum coordinate of \vec{a}^a is \vec{k} , the momentum coordinate of \vec{a}^b is \vec{k}' , and that of \vec{a}^c is $-(\vec{k}+\vec{k}')$, then

$$\vec{a}^a(\vec{k}) \cdot \frac{\delta F}{\delta \vec{a}^a(\vec{k})} = \vec{a}^b(\vec{k}') \cdot \frac{\delta F}{\delta \vec{a}^b(\vec{k}')} = \vec{a}^c(-(\vec{k}+\vec{k}')) \cdot \frac{\delta F}{\delta \vec{a}^c(-(\vec{k}+\vec{k}'))} \quad (5.29)$$

where $\frac{\delta F}{\delta \vec{a}^a(\vec{k})}$ will be an integral over \vec{k}' , $\frac{\delta F}{\delta \vec{a}^b(\vec{k}')}$ and $\frac{\delta F}{\delta \vec{a}^c(-(\vec{k}+\vec{k}'))}$ will be integrals over \vec{k} . With this convention we can see that

$$\int |\vec{k}| \vec{a}^b(\vec{k}) \cdot \frac{\delta F}{\delta \vec{a}^b(\vec{k})} d^3k = \int |\vec{k}'| \vec{a}^a(\vec{k}') \cdot \frac{\delta F}{\delta \vec{a}^a(\vec{k}')} d^3k$$

(no sum on a, b) (5.30)

and similarly

$$\int |\vec{k}| \vec{a}^c(\vec{k}) \cdot \frac{\delta F}{\delta \vec{a}^c(\vec{k})} d^3k = \int |\vec{k}+\vec{k}'| \vec{a}^a(\vec{k}) \cdot \frac{\delta F}{\delta \vec{a}^a(\vec{k})} d^3k$$

(no sum on a, c) (5.31)

so the first term in expression (5.26) is

$$\int (|\vec{k}| + |\vec{k}'| + |\vec{k}+\vec{k}'|) \vec{a}^a(\vec{k}) \cdot \frac{\delta F}{\delta \vec{a}^a(\vec{k})} d^3k . \quad (5.32)$$

The factor $(|\vec{k}| + |\vec{k}'| + |\vec{k}+\vec{k}'|)$ is the "energy denominator," $E_{\vec{k}}^{(p)} - E_0^{(0)}$, that appears in the standard formula for the perturbed wave function.

Now substitute expressions (5.24), (5.26), (5.27), and (5.32) into equation (5.23). Solving for the term containing F we obtain

$$\begin{aligned}
& \int (|\vec{k}| + |\vec{k}'| + |\vec{k} + \vec{k}'|) \vec{a}^\alpha(\vec{k}) \cdot \frac{\delta F}{\delta \vec{a}^\alpha(\vec{k})} d^3k = \\
& -\frac{i}{2} \varepsilon^{\alpha\beta\gamma} \int (\vec{k} \times \vec{a}^\alpha(\vec{k})) \cdot (\vec{a}^\beta(\vec{k}') \times \vec{a}^\gamma(-(\vec{k} + \vec{k}')))) d^3k d^3k' \\
& + i \varepsilon^{\alpha\beta\gamma} \int \frac{\vec{a}^\gamma(-(\vec{k} + \vec{k}')) \cdot (\vec{k}' \times (\vec{k}' \times \vec{a}^\beta(\vec{k}')))) [\vec{k} \cdot \vec{a}^\alpha(\vec{k})]}{|\vec{k}| |\vec{k}'|} d^3k d^3k'. \tag{5.33}
\end{aligned}$$

To eliminate the "energy denominator" from the left-hand side of equation (5.33), we differentiate both sides of (5.33) by $\vec{a}^\alpha(\vec{q})$, then by $\vec{a}^\beta(\vec{q}')$, and divide both sides by $(|\vec{q}| + |\vec{q}'| + |\vec{q} + \vec{q}'|)$. To recover F , we dot both sides by $\vec{a}^\beta(\vec{q}')$ and $\vec{a}^\alpha(\vec{q})$ and integrate over \vec{q} and \vec{q}' . The left-hand side will be F . The result is

$$\begin{aligned}
F &= \int \vec{a}^\alpha(\vec{q}) \cdot \frac{\delta F}{\delta \vec{a}^\alpha(\vec{q})} d^3q \\
&= -\frac{i}{2} \varepsilon^{\alpha\beta\gamma} \int \frac{(\vec{q} \times \vec{a}^\alpha(\vec{q})) \cdot (\vec{a}^\beta(\vec{q}') \times \vec{a}^\gamma(-(\vec{q} + \vec{q}')))}{|\vec{q}| + |\vec{q}'| + |\vec{q} + \vec{q}'|} d^3q d^3q' \\
&+ i \varepsilon^{\alpha\beta\gamma} \int \frac{[\vec{a}^\gamma(-(\vec{q} + \vec{q}')) \cdot (\vec{q}' \times (\vec{q}' \times \vec{a}^\beta(\vec{q}')))] [\vec{q} \cdot \vec{a}^\alpha(\vec{q})]}{|\vec{q}| |\vec{q}'| (|\vec{q}| + |\vec{q}'| + |\vec{q} + \vec{q}'|)} d^3q d^3q'. \tag{5.34}
\end{aligned}$$

One may easily check that F satisfies equation (5.23) and constraint (5.27). This justifies the assumptions we made through the calculation. The first term in (5.34) is similar in form to the standard perturbative formula for the wave function except that we are also including the longitudinal component of the potential. The second term must be added to the first to satisfy (5.23) and Gauss's Law.

The correct first-order functional in the temporal gauge, which is only a phase in momentum space, has been found by requiring that the longitudinal part of its functional derivative, $\vec{\nabla} \cdot \frac{\delta F}{\delta A}$, be given by the Gauss's Law constraint, a separate condition. The Gauss's Law constraint is compatible with the

Schrödinger equation to first order in that we may insert the constraint into the functional differential equation, solve the resulting *new* functional differential equation, and obtain a solution that satisfies both the constraint and the original Schrödinger equation. This reflects the fact that the vacuum state should automatically be gauge invariant [15].

The success of inserting Gauss's Law into the Schrödinger equation leads us to suggest that if we write

$$\Psi_0[A] = \exp(R+Q) \quad (5.35)$$

where R is given by (5.13) and Q is a solution of

$$\begin{aligned} & -\frac{1}{2} \int \frac{\delta}{\delta \vec{a}^\alpha(-\vec{k})} \cdot \frac{\delta Q}{\delta \vec{a}^\alpha(\vec{k})} d^3k - \int |\vec{k}| \vec{a}^\alpha(\vec{k}) \cdot \frac{\delta Q}{\delta \vec{a}^\alpha(\vec{k})} d^3k \\ & + \varepsilon^{\alpha\beta\gamma} \int (\vec{k} \cdot \vec{a}^\alpha(\vec{k})) \frac{1}{|\vec{k}|} \int \vec{a}^\gamma(-(\vec{k}+\vec{k}')) \cdot \left[\frac{\vec{k}' \times (\vec{k}' \times \vec{a}^\beta(\vec{k}'))}{|\vec{k}'|} + \frac{\delta Q}{\delta \vec{a}^\beta(-\vec{k}')} \right] d^3k' d^3k \\ & + H_1 + \frac{1}{4} \int (\vec{a}^\alpha(\vec{k}) \times \vec{a}^\beta(\vec{q}-\vec{k})) \cdot (\vec{a}^\alpha(\vec{k}') \times \vec{a}^\beta(-(\vec{q}+\vec{k}'))) d^3k d^3k' d^3q = E_0 - E_0^{(0)}, \end{aligned} \quad (5.36)$$

where H_1 is given by expression (5.24), then $\Psi_0[A]$ will be a solution of the original functional Schrödinger equation (5.9) and $\Psi_0[A]$ will satisfy the Gauss's Law constraint (5.10). We have not proven that if Q satisfies (5.36), then $\Psi_0[A]$ given by (5.35) will be the solution of (5.9) and (5.10). We have shown, however, that this is true to first order in g , so we believe it may hold true to higher orders.

We have used eq. (5.36) to solve for the vacuum functional to second order in g . To do this we note from the terms in eq. (5.36) that the second-order functional, $S[A]$, must contain terms with 4 "a's" in them. $\frac{\delta F}{\delta a^\alpha} \cdot \frac{\delta F}{\delta a^\alpha}$ is an example of one. There must also be terms with 2 only "a's." $\frac{\delta}{\delta \vec{a}^\alpha(-\vec{k})} \cdot \frac{\delta}{\delta \vec{a}^\alpha(\vec{k})}$ on the 4 a

terms will produce some of them. We solve for S by computing the $4a$ terms, using the $4a$ terms to complete the functional equation for the $2a$ terms, compute the $2a$ terms and use these to determine the energy to second order. Since the " $4a$ " part of S contains over 81 terms, we have left out the result.

The form of F , eq. (5.34), suggests that we may repair the perturbative formula

$$\Psi_0^{(1)}[A] = \sum_N \frac{\langle N | H_1 | 0 \rangle}{E_N^{(0)} - E_0^{(0)}} \Psi_N^{(0)}[A]$$

as we did for QED in Chapter 3 by adding to the Hamiltonian a term

$$i \varepsilon^{\alpha\beta\gamma} \int \frac{[\vec{a}^\gamma(-(\vec{k}+\vec{k}')) \cdot (\vec{k}' \times (\vec{k}' \times \vec{a}^\beta(\vec{k}')))] [\vec{k} \cdot \vec{a}^\alpha(\vec{k})]}{|\vec{k}| |\vec{k}'|} d^3k d^3k'$$

and by assuming that $\vec{a}(\vec{k})$ appearing in R contains a longitudinal component. While this change will produce the correct $\Psi_0^{(1)}[A]$, it won't fix higher-order corrections. This is due to the fact that we must add another term to the Hamiltonian proportional to g^2 since the Hamiltonian already contains a g^2 term.

The perturbative wave functional should be a short distance approximation to the true ground state functional [15]. The functional

$$\Psi \sim \exp\left(-\frac{1}{2\mu} \int \vec{B}^\alpha(\vec{x}) \cdot \vec{B}^\alpha(\vec{x}) d^3x\right) \quad (5.37)$$

has been suggested [16] as a long-distance approximation. We may construct a trial variational functional by interpolating between the two limits. The difficulty will be in satisfying the Gauss's Law constraint beyond first order in g . By examining the result for F , equation (5.36), we can see that if we transformed back to x -space, no pair of potentials will be labeled by the same space coordinate. This implies that we will not be able to naturally express the

perturbative functional in terms of the color magnetic fields. Also, it is incorrect perturbatively to replace the $\nabla \times \vec{A}$ (ordinary magnetic field) in R , expression (5.13), by covariant curls, $D \times \vec{A}$ (color magnetic fields), even if we include parallel transport factors to maintain Gauss's Law. It appears that we should instead find a gauge invariant combination of R and $\vec{A}^a(\vec{x})\vec{A}^b(\vec{y})\vec{A}^c(\vec{z})$ that matches the perturbative result when g is small and use this functional for interpolation.

C. Regularization

Up until now, the only nonperturbative gauge invariant regularization of quantum chromodynamics was provided by placing the theory on a lattice. Much progress has been made towards obtaining reliable nonperturbative quantitative results using the lattice[17]. But the lattice formulation has difficulty handling topological effects that depend, for example, on the vacuum angle and suffers from the problem of "fermion doubling." If we regularize in a different fashion, we may be able to avoid these difficulties.

If the fermion doubling is somehow intrinsic and unavoidable, we certainly need to see how it arises with other regulators to understand it.

Recall that in Chapter 3 we used the functional directional derivative defined as [9]

$$\frac{\delta_\xi}{\delta_\xi A} F[A] = \lim_{\epsilon \rightarrow 0} \frac{F[A + \epsilon \xi(\mathbf{x})] - F[A]}{\epsilon} \quad (5.38)$$

to regularize QED. We replaced the kinetic term in the free photon Hamiltonian with directional functional derivatives and chose the derivative to be in the direction of a delta sequence, $\delta_\lambda(\vec{x})$.

To regularize Yang-Mills we could replace every functional derivative with a directional functional derivative [10]. Instead we leave Gauss's Law alone (it is easier to construct trial wave functionals this way) and spread out the kinetic term in the Hamiltonian. In QED, we did this by replacing just the derivatives. For Yang-Mills, however, we must do a little more since the color electric field is gauge covariant, not gauge invariant like the ordinary electric field.

To spread out the kinetic term we parallel transport the electric field at \vec{y} to the point \vec{x} along, say, a straight path between the two points. We then dot the transported electric field with the electric field at \vec{x} . This is a gauge invariant quantity when we take the trace. We then weight this operator by $\delta_\lambda^2(\vec{x}-\vec{y})$ and integrate over \vec{x} and \vec{y} . That is, we replace

$$\int d^3x \frac{\delta}{\delta A^\alpha(\vec{x})} \cdot \frac{\delta}{\delta A^\alpha(\vec{x})}$$

with

$$\text{tr} \int d^3x d^3y \left(\frac{\delta}{\delta A_i(\vec{x})} P(\vec{x}, \vec{y}) \frac{\delta}{\delta A_i(\vec{y})} P(\vec{y}, \vec{x}) \right) \delta_\lambda^2(\vec{x}-\vec{y}) \quad (5.39)$$

where

$$P(\vec{x}, \vec{y}) = P \exp \left(g \int_{\vec{y}}^{\vec{x}} \vec{A}(\vec{z}) \cdot d\vec{z} \right) \quad (5.40)$$

and $A(\vec{z}) = A^\alpha(\vec{z}) \frac{\tau^\alpha}{2i}$.

In the Abelian limit, this reduces to what we did in Chapter 3. The reason it will regularize is the same as for QED. Only one factor of $f_\lambda(k)$ is introduced in the wave functional so that $f_\lambda \frac{\delta \Psi}{\delta A} \cdot f_\lambda \frac{\delta \Psi}{\delta A}$ will cancel the potential term. This leaves an extra factor of f_λ in the eigenvalues, the physical measurements,

from $f_\lambda^2 \frac{\delta^2 \Psi}{\delta A^2}$, or an extra factor of f_λ in expectation values from doing the functional integrals.

D. Do Fluctuations Produce Electric Flux Tubes?

Yang-Mills is supposed to confine. The strong coupling limit of Yang-Mills on the lattice does confine. Numerical simulations indicate that there is no phase transition as $g \rightarrow 0$ but as Shuryak [18] has stated, "an analytic proof is badly needed, as well as a better understanding."

Using the Schrödinger representation we may gain a better understanding of what produces confinement by investigating what types of wave functionals confine. If we had the exact ground state functional, we could see which configurations are most likely and compute the gluon condensate, $\langle B^2 \rangle$. Since we don't have the exact vacuum wave functional we can attempt to find a good approximation by using a variational approach. The variational also allows us to try different features in trial wave functionals and test them, so in the end perhaps we can get a feeling for what the vacuum wave functional looks like. For example, the QCD vacuum has been argued to be a magnetic superconductor composed of color magnetic monopole pairs (color magnetic Cooper pairs). We can build trial functionals that allow magnetic monopoles or we may "cut" them out by disallowing long-range color magnetic fields. We can then test to see which produces better results.

Another approach to constructing trial states is to use the perturbative vacuum functional that we computed in section B. It should be a short- distance approximation to the true ground state. A suitable choice could be made for a long-distance approximation and we could interpolate between the two limits.

The long-distance approximation should at least mimic the low energy properties of Yang-Mills we want. The functional

$$\Psi \sim \exp\left(-\frac{1}{2\mu} \int \vec{B}^a(\vec{x}) \cdot \vec{B}^a(\vec{x}) d^3x\right) \quad (5.41)$$

has been used by many people [19]. It is simple enough so that computations are not immensely difficult. It satisfies Gauss's Law. It gives a nonzero gluon condensate. It also gives area law behavior when used to compute an expectation value of a Wilson loop. This is because there is no correlation between the color magnetic field at two different points in the functional. This permits magnetic disordered configurations to enter with nonzero weight which leads to area law behavior. The functional, eq. (5.41), has been used in some lattice studies where it is called the "independent plaquette" state. It does give behavior as expected for Yang-Mills for long distances but the results do not scale properly for short distances. This is not at all surprising since we know from section B that the perturbed wave functional does not contain the color magnetic field in any simple fashion.

Even though eq. (5.41) is not valid over all distances, it is still useful as a trial functional to test ideas. Since it does give area law behavior, it should produce electric flux tubes. That is, if we looked at the color electric field between two widely separated quarks we should find, using eq. (5.41), that the electric flux does not want to spread out or collapse but instead to be concentrated on a line between the two quarks. Unlike the Abelian Higgs case, the flux tube is not a topological soliton or a solution to the classical field equations. It must be built from quantum fluctuations. The wave functional, eq. (5.41), allows for magnetic disorder and this should produce an electric flux tube.

To try to test this we will do a variational calculation of the energy of a state for pure Yang-Mills with one unit of electric flux in the z direction. This is equivalent to having 2 quarks separated by a large distance. To do the variational calculation we construct a trial wave functional to represent this state in which we incorporate a variational parameter corresponding to the radius of the electric flux tube. We then compute the expectation value of the Hamiltonian in this state and minimize the energy with respect to the variational parameter. If the electric flux wants to spread out, indicating no confinement, then the value of the radius of the tube will be infinite. A nonzero finite value will indicate that a flux tube is present.

Computing the expectation value of the energy involves doing a functional integral which we won't be able to do exactly. We will only try to see if it looks as though a flux tube is present within the approximation we make. The calculation is meant to illustrate how the Schrödinger representation can be used to do nonperturbative calculations to try to understand some of the features of nonlinear theories. We are able to do the Abelian case exactly and we do find that the flux spreads out as we expected.

To begin, we must construct a trial wave functional that represents a state with one unit of electric flux running in the z direction. This will be easy to do if we employ the formalism developed by 't Hooft [20] and work with Yang-Mills in a box with periodic boundary conditions (up to a gauge transformation).

Since the theory is really invariant under transformations from the group $SU(2)$ divided by its center, Z_2 , then there are topologically distinct gauge transformations, different from those associated with instantons, that leave the boundary conditions on the walls of the box invariant. In particular, consider a gauge transformation, $\Omega(\vec{x})$, such that $\Omega(x,y,z=a) = -\Omega(x,y,z=0)$. This gauge

transformation cannot be continuously deformed to the identity. We can associate a winding number in the t-z direction with these Ω .

Now let us transform a state, Ψ , under $\Omega(\vec{x})$. If

$$\Omega\Psi = -\Psi,$$

then there is a unit of electric flux travelling in the z direction through the box. If Ψ is invariant under Ω , then there is no electric flux. Since Ω applied to eq. (5.41) gives (5.41) back again, then eq. (5.41) represents a state with no electric flux. We expected this since we want eq. (5.41) to represent a long-distance approximation to the vacuum.

Next consider Ω applied to the trace of a parallel transport factor, eq. (5.40).

$$\Omega P(\vec{x}, \vec{y}) = \Omega^\dagger(\vec{x}) P(\vec{x}, \vec{y}) \Omega(\vec{y})$$

Thus for \vec{y} on the $z=0$ face of the box and \vec{x} on the $z=a$ face,

$$\Omega P(\vec{x}, \vec{y}) = \Omega^\dagger(z=a) P(\vec{x}, \vec{y}) \Omega(z=0).$$

Taking the trace of both sides we get

$$\text{tr } \Omega P(\vec{x}, \vec{y}) = -\text{tr } P(\vec{x}, \vec{y});$$

thus $P(\vec{x}, \vec{y})$ represents an operator that creates a unit of electric flux running from \vec{y} to \vec{x} . In particular, if we choose the path in eq. (5.40) to be from $(0,0,0)$ to $(0,0,a)$, then

$$L(C) = \text{tr } P \exp\left(-g \int_0^a \vec{A}_z(0,0,z') dz'\right) \quad (5.42)$$

creates a string of unit electric flux along the z axis from one face of the box to the opposite face. We can also see that $L(C)$ creates a unit of flux in the z direction by operating on it with $\int \vec{E} \cdot d\vec{s}$, the electric field normal to a plane (a functional derivative). If the plane is parallel to the z axis, this yields zero. If it is not, then we get g .

So for our trial state we will take $L(C)\Psi_B$ where $L(C)$ is given by eq. (5.42) and Ψ_B is given by eq. (5.41). We want to use eq. (5.41) because far from the flux tube created by $L(C)$ the state should again look like the vacuum, which Ψ_B represents. Ψ_B should also be the confining vacuum to produce finite-sized flux tubes. We have not, however, incorporated any variational parameter representing the width of the flux tube. $L(C)$, eq. (5.42), creates an infinitely narrow tube which will require renormalization. We modify $L(C)$ to be

$$L(C) = \text{tr} P \exp(-g \int f(x',y') A_z(x',y',z') d^3x'). \quad (5.43)$$

Applying $\int \vec{E} \cdot d\vec{s}$ to eq. (5.43) we find that the electric flux flowing in the z direction is $\int f(x,y) dx dy$. We want this to be unity, so $f(x,y)$ must obey the constraint

$$\int f(x,y) dx dy = 1. \quad (5.44)$$

To complete the variational calculation we compute $\langle H \rangle$ using the wave functional $L(C)\Psi_B$ and minimize the result with respect to $f(x,y)$. (The resulting energy will be the string tension.)

Let us first consider the Abelian case. Our trial state is

$$\exp(-ie \int f(x,y) A_z(\vec{x}) d^3x) \Psi_0[A] \quad (5.45)$$

where $\Psi_0[A]$ is eq. (2.7), the vacuum state for free photons. The wave functional, eq. (5.45), represents a state with unit electric flux (in terms of e) travelling in the z direction if $\int f(x,y) dx dy = 1$.

The expectation of the Hamiltonian, H_γ , eq. (3.9), in this state, eq. (5.45), is

$$E[f] = \langle H_\gamma \rangle = \frac{e^2}{2} \int f^2(x,y) dx dy + E_0 \quad (5.46)$$

where E_0 is the usual ground state energy for free photons. The term arising from $\frac{\delta L(C)}{\delta A} \cdot \frac{\delta \Psi_0}{\delta A}$ involves only one factor of $\vec{A}(\vec{x})$ multiplying a gaussian in $\vec{A}(\vec{x})$ and vanishes when we do the functional integral. This term would also vanish if we used

$$\Psi_B \sim \exp\left(-\frac{1}{(2\pi)^2} \int \vec{B} \cdot \vec{B} d^3x\right)$$

instead of $\Psi_0[A]$.

Minimizing $E[f] - \lambda \int f^2(x,y) dx dy$ with respect to $f(x,y)$ gives $f(x,y) = a$ constant. Thus the Abelian flux tube spreads out and disappears as expected.

For Yang-Mills, the expectation value of the Hamiltonian is

$$\langle H \rangle = -\frac{1}{2} \int DA \int \Psi_B^* L^*(C) \frac{\delta^2 L(C)}{\delta A^{\alpha^2}(\vec{x})} \Psi_B d^3x \quad (5.47)$$

$$- \int DA \int \Psi_B^* L^*(C) \frac{\delta L(C)}{\delta A^\alpha(\vec{x})} \cdot \frac{\delta \Psi_B}{\delta A^\alpha(\vec{x})} d^3x \quad (5.48)$$

$$+ \int DA \int \Psi_B^* L^*(C) L(C) \left(-\frac{1}{2} \frac{\delta^2 \Psi_B}{\delta A^{\alpha^2}(\vec{x})} + \vec{B}^\alpha(\vec{x}) \cdot \vec{B}^\alpha(\vec{x})\right) d^3x . \quad (5.49)$$

We can do the first functional integral, eq. (5.47), exactly since

$$\frac{\delta^2 L(C)}{\delta A_4^{\alpha^2}(\vec{x})} = -\frac{3}{4}g^2 f^2(x,y) L(C), \quad (5.50)$$

so eq. (5.47) is

$$\frac{3}{8}g^2 a \int f^2(x,y) dx dy. \quad (5.51)$$

We will approximately compute the remaining two functional integrals, eqs. (5.48) and (5.49), by replacing $L(C)$ with

$$\exp\left(-\frac{g^2}{2}\left(\int f(x',y') A_2^\alpha(\vec{x}') d^3x'\right)^2\right) \quad (5.52)$$

and using the saddle point method. Eq. (5.52) is good through second order in g and sums a number of terms of $L(C)$ at higher orders.

Using eq. (5.52)

$$\frac{\delta L(C)}{\delta A^\alpha(\vec{x})} = -\frac{g^2}{2} f(x,y) \left(\int f(x',y') A_2^\alpha(\vec{x}') d^3x'\right) L(C), \quad (5.53)$$

the term $\frac{\delta L(C)}{\delta A^\alpha(\vec{x})} \cdot \frac{\delta \Psi_B}{\delta A^\alpha(\vec{x})}$ tells us to replace, one at a time, each $A_2^\alpha(\vec{x})$ that appears in $\vec{B}^\alpha \cdot \vec{B}^\alpha$ (the exponent of Ψ_B) by $\int f(x',y') A_2^\alpha(\vec{x}') d^3x'$. When we do the functional integral, eq. (5.48), a δ function, $\delta(\vec{x}-\vec{x}')$ will arise since Ψ_B is gaussian. The integrand for eq. (5.49) is a straightforward computation.

The normalized expectation for the energy determined from eqs. (5.47)-(5.49) divided by a , the length of the box in the z direction, is

$$E[f] = \frac{1}{\mu} \int k^2 d^2k + \frac{3}{8}g^2 \int f^2(k) d^2k$$

$$+ \frac{3}{2} \int \frac{k^2 + \frac{4g^2}{\mu} + 2/\mu(g^2 f^2(k)k^2 + k^4/\mu)}{\left(\frac{k^2}{\mu} + g^2 f^2(k)\right)} + \frac{g^4 f^2(k)}{\left(\frac{k^2}{\mu} + g^2 f^2(k)\right)^2} d^2k$$

$$\begin{aligned}
 & + 3g^2 \int \frac{1}{\left(\frac{k^2}{\mu} + g^2 f^2(k)\right) \left(\frac{(q+k)^2}{\mu} + g^2 f^2(q+k)\right)} + \frac{6k^2}{\left(\frac{k^2}{\mu} + g^2 f^2(k)\right) \left(\frac{q^2}{\mu} + g^2 f^2(q)\right)} d^2k d^2q \\
 & \frac{27g^4}{\mu^2} \int \frac{d^2k d^2q d^2q'}{\left(\frac{k^2}{\mu} + g^2 f^2(k)\right) \left(\frac{(q+k)^2}{\mu} + g^2 f^2(q+k)\right) \left(\frac{(q'+k)^2}{\mu} + g^2 f^2(q'+k)\right)}. \quad (5.54)
 \end{aligned}$$

Now when we vary $E[f]$ we can see that $f(x,y) = \text{constant}$ ($f(\vec{k}) = \text{constant}$ $\delta(\vec{k})$) is no longer a solution. For $\delta(\vec{k})$ to be a solution, then the equation for f must be of the form $f(k) \cdot (\text{something never zero unless } k=0) = 0$. This form cannot result from the expressions above. Thus a large flux tube will want to shrink. It will not completely collapse because $f(k) = \text{constant}$ is also not a solution. $f(k) = \text{constant}$ is too large for large \vec{k} to minimize the energy. Thus a small tube will expand. The net result is that a flux tube has formed whose cross section is approximately given by the function $f(x,y)$.

Chapter 6 Conclusion

We have demonstrated the usefulness of the Schrödinger representation for nonperturbative variational calculations in nonlinear field theory. A large variety of problems can be treated and the formalism is easy to set up. It is clear, however, that even the simplest assumptions lead to complicated answers (analytically). Most numerical calculations will require the computer. The Schrödinger representation may also be regularized with a lattice. The same variational calculations can then be done with traditional lattice techniques. This is an area relatively untouched so far [21]. A balance between numerical computation of functional integrals and analytic approximation for finding the trial wave functionals would be best.

Many improvements could be made in the flux tube calculations we have described. Better trial functionals could be found and, more importantly, a better representation of path order exponentials should be used. We could write $L(C)$ as an integral over fermionic fields [22]. This will improve the evaluation of the functional integrals involved.

There is a strong need to develop techniques in functional calculus to aid in the use of the Schrödinger representation. We have presented one technique to solve functional differential equations but more are badly needed. Variational calculations involve trial wave functionals and functional integrals. If we learn to solve, at least approximately, functional differential equations, then our ability to choose wave functionals greatly increases. If we learn to approximately compute functional integrals better, then we will be able to use a wider variety of forms of trial functionals. Our ability to solve functional differential equations and evaluate functional integrals is presently very limited, so any new techniques would be valuable, not only for the functional Schrödinger

representation, but also for other formalisms and branches of physics.

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