THE ENERGY SPECTRUM OF THE EXCITATIONS IN LIQUID HELIUM

Thesis by

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ABSTRACT

Feynman has used the wave function $\phi \sum_i e^{i\underline{k}\cdot\underline{r}_i}$ to represent an excitation (phonon or roton) of momentum $\hbar\underline{k}$ in liquid helium. ϕ is the ground state wave function, and the sum runs over all the atoms in the liquid. The resultant energy spectrum is correct for phonons ($k \lesssim 0.5$ Å^{-1}) and has the qualitatively correct feature of exhibiting a minimum at $k = 2$ Å^{-1} (roton region). Landau and subsequent workers have shown that the specific heat and second sound velocity data require the value $\Delta/k = 9.6^\circ$K, where Δ is the minimum roton energy and k is Boltzmann's constant. Feynman's energy spectrum locates the minimum correctly but gives $\Delta/k = 19.1^\circ$K.

A wave function of the form $\phi \sum_j e^{i\underline{k}\cdot\underline{r}_j} \exp\left(i \sum_{k\neq j} g(\underline{r}_{kj})\right)$ is proposed here to represent an excitation of momentum $\hbar\underline{k}$. The function g represents the fact that the neighbors of a moving atom execute some smooth pattern of backflow around it; g is taken as the potential function for a dipole velocity field, the strength of the dipole being left arbitrary until the end of the computation. To facilitate computation, it proves useful to replace $\exp(i\sum g(\underline{r}_{kj})$ by $1 + i\sum g(\underline{r}_{kj})$. This procedure is mathematically legitimate, not only because $\sum g(\underline{r}_{kj})$ is small, but because the wave function is inserted into a variational principle for the energy and is guaranteed to yield an overestimate. The strength of the dipole is finally chosen to minimize the energy, yielding the new value $\Delta/k = 11.5^\circ$. The optimal value for the dipole strength is very close to the "classical" value which one would expect on the basis of a current conservation argument.

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INTRODUCTION

In analogy with the ideal Bose gas, which condenses when the temperature is low enough, a Bose liquid might be expected to demonstrate some remarkable quantum-mechanical properties at very low temperatures. But with the single exception of helium, all Bose liquids freeze before they have a chance to manifest their extreme quantum-mechanical properties.* Liquid helium is consequently an attractive subject of investigation for both the experimenter and the theorist. The latter is in an especially comfortable position, since he can, without the risk of embarrassment, make statements which presumably apply not only to helium but also to the general imperfect Bose liquid.

Liquid helium undergoes a thermodynamic transition of the second kind (i.e. the specific heat is discontinuous) at 2.19°K.** Below this temperature, many of the properties of the liquid are explained by Tisza's phenomonological two-fluid model, which is described in greater detail below. Landau realized that the macroscopic properties of the liquid would resemble those of a mixture of two fluids, provided that a certain form is assumed for the energy-momentum curve of the elementary excitations in the liquid. Starting from first principles, Feynman has recently computed an energy-momentum curve which is based on certain ideas about the nature of the wave functions representing the excitations. The shape of the curve is in qualitative agreement with Landau's, but

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* The low mass and consequent high zero-point motion of He atoms melt any lattice structure which might try to form. On the basis of this argument, one might also expect molecular hydrogen to remain liquid at very low temperatures; but the high polarizability of the molecules (as contrasted with He atoms) creates strong intermolecular forces which make the formation of a regular structure energetically advantageous despite the high kinetic energy involved.

** The transition is known as the "lambda transition" because of the shape of the specific heat curve near 2.19°K. The resemblance is not close.

some serious quantitative discrepancies exist. In the present thesis we pursue Feynman's ideas somewhat further and construct a more complicated wave function to represent an excitation. The energy-momentum curve computed with this wave function will prove to be in better agreement with Landau's.

The first section of this thesis describes the two-fluid model, as put forth by Tisza, and the subsequent work of Landau. The second section deals with Feynman's work, and the third section with our refinements of it. In addition to the actual computations, the third section contains discussion of approximate methods which may be useful in other work of this sort.

I. THE TWO-FLUID MODEL

Tisza [1], [2], [3] found that many aspects of the behavior of liquid helium below the λ-point can be understood by regarding the liquid as a mixture of two fluids, a normal and a superfluid. The two fluids, though completely mixed together, are assumed capable of flowing with different velocities. The superfluid flows with no viscosity along surfaces and through thin tubes. The proportion of the liquid which is in the superfluid state is assumed to decrease monotonically with increasing temperature; the proportion is unity at absolute zero and decreases until the superfluid component vanishes at some temperature which is identified with the lambda temperature. At least at temperatures above 1°K, the normal fluid carries all the entropy of the liquid. The major quantitative success of Tisza's theory was his prediction of temperature waves ("second sound") and his calculation of their velocity in terms of thermodynamic data. Tisza made no serious attempt to justify his model from a microscopic theory based on first principles. Hence the theory does not predict such numbers as the proportion of superfluid at a given temperature; but it does give relations among various measurable quantities.

Landau [4] made considerable progress toward an explanation of the behavior of liquid helium from first principles. He argued that there are only two kinds of low-energy excitations of the liquid: "phonons" and "rotons". The phonons are ordinary longitudinal sound waves; the energy of a phonon with momentum p is

$$E = cp \qquad (1)$$

where c is the velocity of sound (about 240 m/sec). Any vortex motion of the fluid must be carried by the rotons. Landau introduced quantum-mechanical operators to represent the current, density, and velocity at a given point in the fluid; he found that the operators corresponding to different components of curl $\underline{v}$ do not commute, and by analogy with the theory of angular momenta concluded that vorticity is quantized.* Consequently, "no states can exist in which curl $\underline{v}$ would be non-zero, but arbitrarily small over the whole volume of the liquid." A roton must therefore have a certain minimum energy Δ. Landau originally assumed that the energy** of a roton with momentum p is

$$E = \Delta + p^2/2\mu$$

where μ is some kind of "effective mass".

At sufficiently low temperatures only a few phonons and rotons are present, and the interference among them is negligible. Phonons are known to obey Bose statistics; the statistics of the rotons proves to be unimportant because at temperatures of interest Δ/kT is so large as to make all kinds of statistics equivalent. Knowing the spectra and statistics of the excitations, one can treat them as an ideal gas (neglecting interference) and thus obtain the partition function for the liquid at low temperatures. In this way Landau obtained a formula for the specific heat, and found that he could fit the data of Keesom and

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* Landau's argument on this point is vague. He points out that the commutation relation $M_iM_j - M_jM_i = i\hbar M_k$ implies that the angular momentum $\underline{M}$ cannot be arbitrarily small, since the left side is quadratic and the right side linear. He does not, however, derive an analogous inhomogeneous commutation relation for the components of curl $\underline{v}$.

** We always measure energies relative to the energy of the liquid in its ground state.

Miss Keesom [5] in the range 1.2°-1.5°K by choosing

$$\Delta/k = 8\text{-}9^\circ\mathrm{K} \qquad \mu = 7\text{-}8m_{\mathrm{He}} .$$

By considering the equilibrium of a gas of phonons and rotons in a rotating vessel, Landau found that the angular momentum of the fluid is proportional to the angular velocity of the vessel, but with a coefficient smaller than the moment of inertia which one would compute under the assumption that the entire mass of fluid is rotating. The coefficient of proportionality increases from zero at absolute zero to unity at the λ -point (but the picture of independent excitations breaks down at temperatures somewhat lower than T_λ). Hence it is possible to regard the liquid as

> "... a mixture of two liquids, one of which is superfluid having no viscosity and not carried along by the walls of the vessel and the other — a 'normal' one which is carried along by the moving walls and behaves like a normal liquid. It is most essential that 'there is no friction' between these two liquids moving through each other.... If there can be some sort of relative motion in the state of statistical equilibrium ... it cannot be accompanied by friction."

In this way Landau showed that the two-fluid picture follows from his form for the energy spectrum of the elementary excitations.

The details of the energy spectrum in Landau's theory have changed somewhat since he proposed it in 1941, but with the best spectrum the theory is in good agreement with all the experimental data accumulated since then.* Discrepancies between the predicted values of the velocity of second sound and the values measured by Peshkov led Landau [6] to propose that low-energy rotons have their momenta centered about some

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* We refer, of course, only to experiments which measure quantities for which the theory predicts a value. Many quantities, such as the critical velocity for superfluid flow in thin tubes, have not yet been unambiguously computed from Landau's theory.

non-zero value p_o, with the resultant spectrum

$$E = \Delta + (p - p_o)^2/2\mu \ . \qquad (2)$$

The specific heat and second sound velocity data available at that time (1947) could be fitted with the values

$$\Delta/k = 9.6^\circ \ , \qquad p_o/\hbar = 1.95 \times 10^8 \ \mathrm{cm}^{-1}, \qquad \mu = 0.77 \ m_{He} \ . \qquad (3)$$

This new form for the energy of the rotons led Landau to believe that the energy spectrum of the excitations does not have two branches, one for phonons and one for rotons, but consists rather of one continuous curve (Fig. 1) which rises linearly for small momenta and goes through a minimum at some momentum p_o. At low temperatures, only the linear portion of the spectrum (phonons) and the portion near the minimum (rotons) are excited. The formulas resulting from this spectrum are therefore the same as those arising from the two-branch spectrum, with the energy of the branches given by (1) and (2).

Subsequent measurements of the specific heat [7] down to 0.25°K (which is well below the temperature at which the T^3 phonon contribution dominates the $\exp(-\Delta/kT)$ roton contribution) and the velocity of second sound [8] down to 0.015°K confirm the value $\Delta/k = 9.6^\circ$. This number is well determined (to within less than 0.2 degrees*) because it enters into formulas exponentially. The specific heat depends on μ and p_o through the combination $\mu^{1/2} p_o^2$. Since Landau's values (3) fit the full range of specific heat data very well, de Klerk et al. [8] conclude that any modification of μ and p_o should leave the product $\mu^{1/2} p_o^2$ unchanged. Observing this restriction, they find that the second

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* I am indebted to Dr. J.R. Pellam for committing himself on this point.

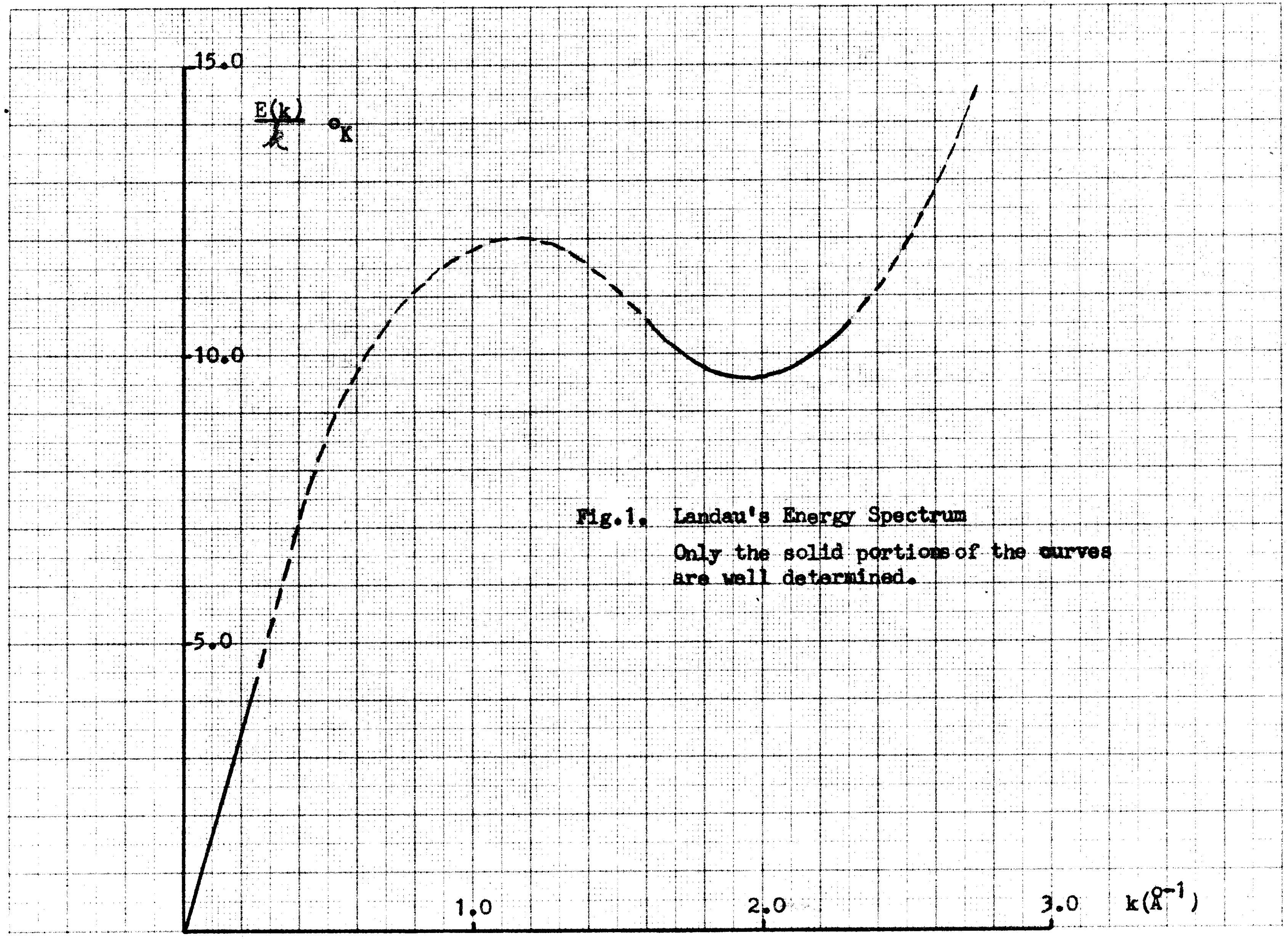

Fig.1. Landau's Energy Spectrum

Only the solid portions of the curves are well determined.

sound data below 1°K are fitted best with the values

$$\Delta/k = 9.6^\circ , \qquad p_o/\hbar = 2.30 \times 10^8 \text{ cm}^{-1}, \qquad \mu = 0.40\ m_{He} , \quad (4)$$

although Landau's values (3) also fit quite well. The differences between (3) and (4) are probably a fair measure of the present uncertainty in the values of μ and p_o.

Landau's theory is very successful in showing how the macroscopic properties of liquid helium follow from certain assumptions about the energy spectrum. It is possible to question the conceptual grounds of his quantum hydrodynamics, and in particular it is disturbing* that the reasoning by which he infers the form of the spectrum makes no reference to the Bose statistics of the atoms. A complete microscopic theory ought to start with Schrodinger's equation and deduce the form of the spectrum, including the values of Δ, p_o, and μ.

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* Especially in view of the experimental fact, now quite well established, that the isotope He^3 does not demonstrate superfluidity.

II. FEYNMAN'S WAVE FUNCTION FOR THE EXCITATIONS

In several recent papers ([9], [10], and especially [11]) Feynman has explained many properties of helium from first principles by analyzing solutions of the Schrodinger equation for a large number of Bose particles with strong short-range mutual repulsions. He arrives at a theoretical form for the energy spectrum of the excitations which is in qualitative agreement with the later curve proposed by Landau (Fig. 1). The quantitative disagreement between the Feynman and Landau energy spectra is serious, but the present thesis was motivated by the idea that Feynman's arguments are essentially correct and, if refined, would lead to a spectrum in better agreement with Landau's. Consequently, we shall review some of these arguments with an eye toward refining them.

Since the excited states represent modifications imposed on the ground state, one ought first to have a picture of the ground state. The wave function for the ground state is non-degenerate and has no nodes,* and may therefore be taken as real and positive for all configurations. These statements apply to the ground state of a collection of particles when no symmetry requirements are imposed on the wave function. Since the Hamiltonian for a collection of identical particles is unchanged by any interchange of the names, it follows that the wave function of a non-degenerate level must be odd or even under the interchange of any pair of variables. But since the ground state has no nodes, it cannot be odd under any interchange and must therefore be even under all interchanges. Hence, the ground state is the same for Bose or (if there were such a thing) Boltzmann helium atoms. For atoms of Fermi helium, the ground state is

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* These statements are proved in Appendix A.

quite different and higher in energy, since the antisymmetrization of a symmetric function yields zero.

In the ground state the amplitude is largest for configurations in which the atoms are spaced as well apart as possible, with none of the repulsive potentials being violated. Each atom may be pictured as sitting in a cage* formed by its neighbors; the amplitude falls off as an atom moves toward the edge of its cage, and goes strongly to zero if any of the repulsive potentials is violated.

One possible excited state of low energy is a sound wave; the density fluctuations in such an excitation are periodic in space and time, and have wavelengths which are large compared with the interatomic spacing. Standing or running sound waves of nearly the same wave number (and direction) can be superposed to form localized packets which travel through the fluid like particles. These are the so-called "phonons", though we shall use the term to refer sometimes to the elementary excitation and sometimes to the packet.

Classically, the normal coordinate for a sound wave of wave number $\underline{k}$ is $q_{\underline{k}} = \int \rho(\underline{r})\, e^{i\underline{k}\cdot\underline{r}}\, d\underline{r}$, where $\rho(\underline{r})$ is the number or mass density at $\underline{r}$. Quantum mechanically, $\rho(\underline{r})$ is replaced by the operator $\sum_i \delta(\underline{r} - \underline{r}_i)$, where the index i runs over all the atoms; $q_{\underline{k}}$ then goes over into the quantum-mechanical normal coordinate $\sum e^{i\underline{k}\cdot\underline{r}_i}$. When expressed in terms of these normal coordinates, the Hamiltonian for the phonon field becomes simply a sum of harmonic oscillator

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* But escape from the cage is possible, because the mean distance between neighbors is greater than the size of the atoms.

Hamiltonians,[*] one oscillator of frequency $\omega = c|\underline{k}|$ being present for each wave number $\underline{k}$ which fits the box. When one phonon of wave number $\underline{k}$ is present, the corresponding oscillator is in its first excited state; since the wave function for an oscillator in its first excited state is $q\phi$, where ϕ is the ground state wave function, the wave function for a single phonon of wave number $\underline{k}$ is

$$q_{\underline{k}}\,\phi = \sum e^{i\underline{k}\cdot\underline{r}_i}\,\phi \tag{5}$$

where ϕ is the wave function for the liquid in its ground state.[**] The energy of a phonon is just the energy difference between the ground state and first excited state of the corresponding oscillator, namely

$$E = \hbar\omega = \hbar ck\ . \tag{5a}$$

For configurations in which the density is almost uniform throughout the liquid, ϕ has a large amplitude, but $\sum e^{i\underline{k}\cdot\underline{r}_i}$ has just about as many positive as negative terms; hence the cancellation is almost complete and the wave function (5) has a small amplitude for such configurations. But for configurations with a periodic density fluctuation of wave number $\underline{k}$ the terms in $\sum e^{i\underline{k}\cdot\underline{r}_i}$ add up in phase. Hence (5) picks out such configurations and assigns a large amplitude to them.

To understand the T^3 behavior of the specific heat at very low temperatures,[***] one must not only believe that there are phonons,

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[*] Appendix B shows the equivalence of longitudinal sound waves with a set of harmonic oscillators.

[**] The wave function (5) and energy (5a) are exact only if $k \ll 2\pi/a$ where a is the interatomic spacing. When the wavelength of a density fluctuation becomes comparable with the interatomic spacing, it is no longer correct to treat the liquid as a continuous medium.

[***] The T^3 behavior is to be expected of a "gas" composed exclusively of phonons. The theoretical coefficient is predictable from the velocity of sound and agrees with the observed one.

but must also understand why no other excitations of very low energy are possible. Feynman's argument on this point, though lacking mathematical rigor, is physically convincing, especially since it makes explicit reference to the Bose statistics of the atoms.* The main point is that any wave function takes on its maximum positive** amplitude for some configuration α and its maximum negative amplitude for some other configuration β. If the two configurations are far apart, then the wave function can keep its derivatives small while making the transition from α to β, and the energy is low. If α and β are close to each other in configuration space, then the gradients of the wave function must be large and the energy is high. With distinguishable particles it is easy to make the α and β configurations remote from each other. One way is to let the sites at which atoms are located in the β configuration be the same as the sites where atoms were located in the α configuration, but with a different atom now at each site. One can assign the atoms to the sites in such a way that each atom in the β configuration is far from where it was in the α configuration; hence the energy can be made arbitrarily small. For Bose atoms this scheme fails, since the wave function must be unchanged when the atoms are permuted among the sites, and hence must be the same for the α and β configurations.

As long as a finite fraction of the atoms have to travel a long distance in getting from the α to the β configuration, it is possible to keep all gradients small and thus to construct a wave function of low energy which is maximum for α and minimum for β. With distinguishable atoms, the sites where atoms are located in the α and β

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* Measurements of the specific heat of the Fermi isotope He^3 down to 0.57°K (Ref. [12]) seem to indicate the presence of terms much larger than T^3.

**The wave function can be taken real. In order to be orthogonal to the ground state it must be somewhere positive and somewhere negative.

configurations could be those indicated in Fig. 2 by the solid and dotted circles respectively. An arrow between a solid and a dotted site means that the atom which was on the solid site in configuration α is on the dotted site in configuration β. The existence of the long arrows ensures that the energy can be made low by appropriate choice of the wave function. This scheme also fails if the atoms obey Bose statistics, since the wave function must not depend on which atom is on which site, and hence the arrows could be redrawn as in Fig. 3 without changing the value of the wave function for the β configuration. Thus, the α and β configurations are really quite close, and consequently the energy cannot be very small. As long as the density distribution of the atoms is uniform in both the α and β configurations, it is impossible to keep the two configurations far apart if the atoms obey Bose statistics. If the α and β configurations do not have a uniform number density of atoms, and if the regions of high density in the α configuration are remote from the nearest regions of high density in the β configuration, then, regardless of statistics, a finite fraction of the atoms must travel long distances in going from α to β and the energy is low. This type of state is a phonon (or superposition of phonons).

On the basis of the preceding arguments, it seems reasonable to believe that in He^4 any excited state other than a phonon must have an energy greater than some minimum value Δ. Feynman [11] computes a value for Δ, and in fact computes an entire energy spectrum for the excitations, by manufacturing an approximate wave function and putting it into a variational principle for the energy. If the wave function

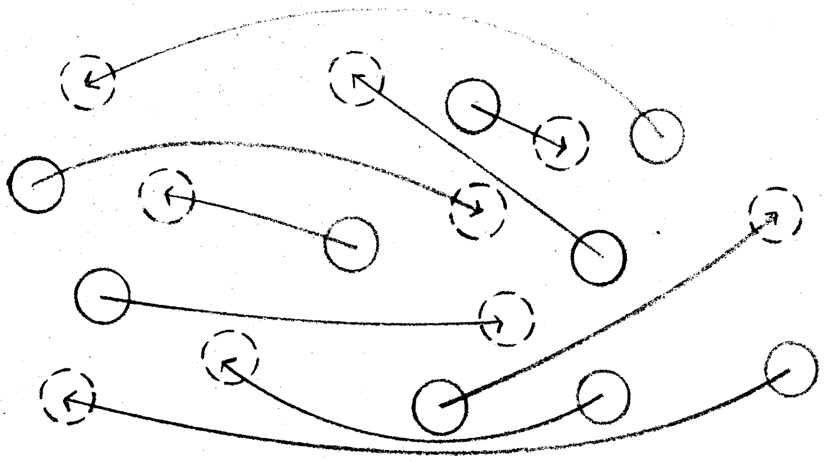

Fig.2. α- and β- sites for a low-energy wave function with distinguishable atoms.

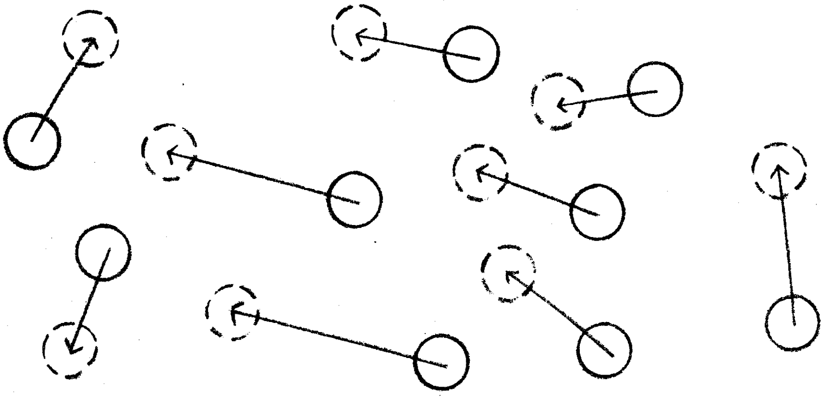

Fig.3. The same α- and β-sites no longer represent a low energy for Bose atoms.

for an excited state is written in the form $\Psi = F\phi$, where ϕ is the ground state wave function, and if energies are measured relative to the ground state energy E_o (so that $H\phi = 0$), then

$$H\Psi = \left(\frac{-h^2}{2m} \sum \nabla_i^2 \right) F\phi + (V - E_o)\, F\phi$$

$$= FH\phi - \frac{h^2}{2m} \sum (\phi \nabla_i^2 F + 2 \nabla_i F \cdot \nabla_i \phi)$$

$$= \phi^{-1} \left(\frac{-h^2}{2m} \right) \sum \nabla_i \cdot (\phi^2 \nabla_i F) \quad .$$

The energy of the state is

$$E = \mathcal{E}/\mathcal{J} \tag{6}$$

where

$$\mathcal{E} = \int \Psi^* H\Psi\, d^N\underline{r} = \frac{h^2}{2m} \sum \int \nabla_i F \cdot \nabla_i F^* \phi^2\, d^N\underline{r} \tag{7}$$

and

$$\mathcal{J} = \int \Psi^* \Psi\, d^N \underline{r} = \int F^* F \phi^2\, d^N \underline{r} \quad . \tag{8}$$

If we assume that ϕ has the same value in the α and β configurations (i.e. both configurations have the atoms well-spaced), then F should be a function whose real part has its maximum positive value when all the atoms are on α-sites, and its maximum negative value when all the atoms are on β-sites, and varies smoothly between the two configurations. The simplest such function is

$$F = \sum f(\underline{r}_i) \tag{9}$$

where $f(\underline{r})$ is a function whose real part varies smoothly from +1 when $\underline{r}$ is on an α-site to -1 when $\underline{r}$ is on a β-site. This function also satisfies the symmetry requirements for Bose atoms. We require that the wave function

$$\Psi = \sum f(\underline{r}_i)\,\phi \tag{10}$$

be an eigenfunction of the total momentum operator*

$$\underline{P} = \frac{\hbar}{i}\sum \nabla_i$$

with eigenvalue $\hbar\underline{k}$. Since $\underline{P}\phi = 0$, it follows that $f(\underline{r}) = e^{i\underline{k}\cdot\underline{r}}$ and hence

$$\Psi = \sum e^{i\underline{k}\cdot\underline{r}_i}\,\phi\ . \tag{11}$$

For each value of $\underline{k}$, substitution of (11) into (6) gives an upper limit for the energy of the lowest state of momentum $\underline{k}$.** The numerator is $N\hbar^2k^2/2m$, where N is the number of atoms in the liquid. The normalization integral is

$$I = \sum_{i,j}\int e^{i\underline{k}\cdot\underline{r}_{ij}}\,\phi^2\, d^N\underline{r}\ . \tag{12}$$

For fixed i and j, integration of ϕ^2 over all the other atomic coordinates yields the probability (in the ground state) that the i^{th} atom is at $\underline{r}_i$ and the j^{th} atom is at $\underline{r}_j$. This is a function only

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* If the liquid were confined to a box of side L, with fixed walls, then the walls could absorb momentum and the energy eigenstates would not be momentum eigenstates. Instead, we control the density by requiring the wave function to be periodic in all variables with period L. With this boundary condition, $\underline{P}$ commutes with H and the energy eigenstates can also be taken as momentum eigenstates.

** Eigenfunctions of $\underline{P}$ belonging to different eigenvalues $\hbar\underline{k}$ are orthogonal. Hence, for different $\underline{k}$, the trial functions (11) are orthogonal to each other and also to the true wave functions which minimize (6). The entire spectrum $E(k)$ therefore lies above the true spectrum. In footnote 3 of [11] Feynman mentions that the wave function $\phi \exp i\hbar N^{-1}\underline{k}\cdot\sum\underline{r}_i$ which represents translational motion of the whole liquid, has momentum $\underline{k}$ and energy $\hbar^2k^2/2mN$, which is certainly lower than any energy we shall compute from (11). The periodic boundary condition, however, rules out such states unless k is as large as $N^{2/3}$.

of r_{ij} (except for the negligible region where one of the two atoms is near the surface of the liquid); holding r_{ij} fixed, the sum over indices yields the probability that there are atoms at two sites separated by a distance r (we replace r_{ij} by r). This probability is $\rho_o p(r)$, where ρ_o is the number density of atoms and $p(r)$ is the probability per unit volume that there is an atom centered at r if there is an atom centered at the origin. When $r = 0$, $p(r)$ has a delta-function singularity (this accounts for terms in (12) where $i = j$); $p(r)$ is zero out to twice the "radius" of a helium atom, then rises to a maximum and oscillates with decreasing amplitude to the asymptotic value ρ_o at $r = \infty$ (Fig. 4). The oscillations are due to the existence of some local order in the liquid.*

In (12) we are left with an integral over the coordinates of two atoms; since the integrand depends only on the relative coordinate $\underline{r}$, the answer is proportional to V. Thus (12) becomes

$$\mathcal{J} = \rho_o V \int e^{i\underline{k}\cdot\underline{r}} p(r)\, d\underline{r}$$

and finally, since $V\rho_o = N$, (6) gives

$$E(k) = \hbar^2 k^2/2mS(k) \tag{13}$$

where $S(k)$ is the Fourier transform of the correlation function $p(r)$,

$$S(k) = \int e^{i\underline{k}\cdot\underline{r}} p(r)\, d\underline{r} \quad . \tag{14}$$

$S(k)$ depends only on k because $p(\underline{r})$ depends only on r.

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* One way to understand the order is to think first of the limiting case of classical hard spheres packed very densely; if the volume per sphere is small enough, the only way the spheres can fit into the box is by forming a lattice. If we now allow more volume per sphere and give all the spheres a zero-point motion, the regular structure begins to disappear, but some remains.

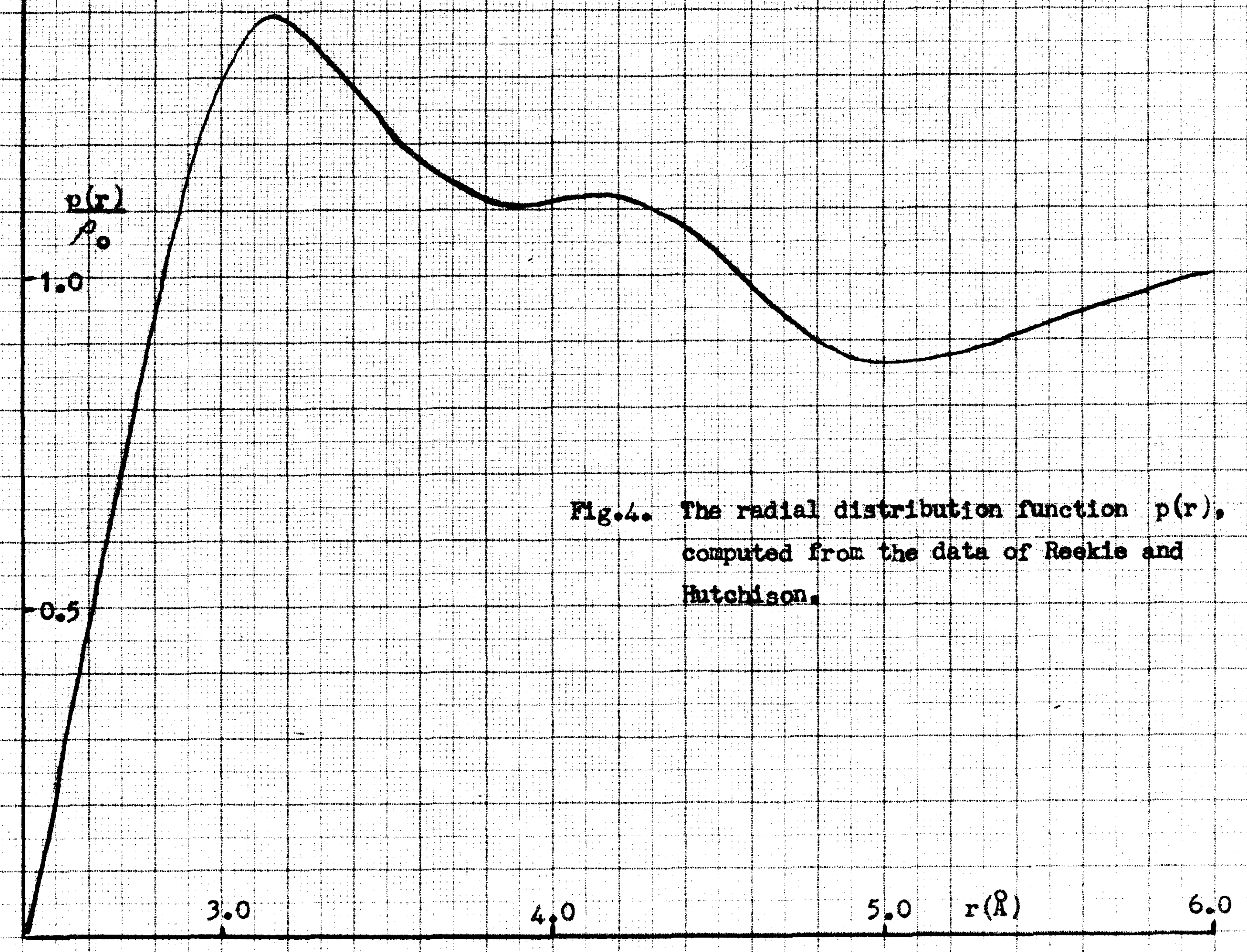

Fig.4. The radial distribution function p(r), computed from the data of Reekie and Hutchison.

S(k) can be determined experimentally* from the scattering of x-rays [14] or neutrons [15]. For large k it approaches unity because p(r) contains a delta-function. When $2\pi/k$ is of the order of interatomic spacings, S(k) oscillates, reflecting the structure of p(r). The highest maximum of S(k) occurs at a wavelength approximately equal to the radius where p(r) has its first and highest maximum. For small k, (5) shows that S(k) is just 1/N times the expectation value of $q_{\mathbf{k}}^2$ in the ground state, where $q_{\mathbf{k}}$ is the normal coordinate for sound of wave number $\mathbf{k}$. In Appendix B the constants are treated carefully and it is shown (eq. (77)) that the energy of the phonon field is

$$\frac{1}{2}\sum_{\mathbf{k}} m_{\mathbf{k}} [\dot{q}(\mathbf{k},t)\, \dot{q}^*(\mathbf{k},t) + \omega_{\mathbf{k}}^2\, q(\mathbf{k},t)\, q^*(\mathbf{k},t)]$$

where $\omega_{\mathbf{k}} = ck$ and $m_{\mathbf{k}} = m/Nk^2$. Since the average potential energy of an oscillator is equal to half the total energy, the average of $\frac{1}{2} m_{\mathbf{k}} \omega_{\mathbf{k}}^2 q_{\mathbf{k}}^2$ in the ground state must be $\frac{1}{4}\hbar\omega_{\mathbf{k}}$. The average of $q_{\mathbf{k}}^2$ is therefore $N\hbar k/2mc$; consequently, for small k

$$S(k) = \hbar k/2mc \tag{14a}$$

and (13) gives for phonons (small k)

$$E(k) = \hbar ck$$

which is in agreement with (5a). The agreement of (13) and (5a) at low energies is of course to be expected, since the wave function (11) is

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* It is possible to derive theoretical curves for p(r) and S(k) from an approximate integral equation (see [13]). In order to get an unequivocal test of our ideas about the nature of excited states, however, we use experimental values for S(k).

the same as (5), and the latter is exact for small k. We now see, however, that (6) also has some significance when k is not so small.

The data which we have used for $S(k)$ is essentially that of Reekie, and is given in Fig. 5. Reekie's data was taken at a finite temperature and therefore does not go to zero as $k \to 0$.* We have extrapolated it linearly to zero and have renormalized it slightly. Fig. 6 gives the spectrum $E(k)$ resulting from (13) with the data of Fig. 5. Energies are measured in temperature units (i.e. all energies are divided by Boltzmann's constant $\mathcal{k}$). The curve has the form of Landau's curve (Fig. 1) and the minimum is correctly located, but the value of Δ ($\sim 19.1^\circ$) is twice too high. The need for an improved wave function in the roton** region is evident.

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* Appendix C contains discussions of the behavior of $S(k)$ for small k at finite temperatures, our method of normalizing Reekie's data, and an important identity satisfied by $p(r)$.

** It is not at all obvious that the wave function (11) represents some type of rotational motion when k is in the region 2Å^{-1}. We call the excitations in this region "rotons" simply because that is the common terminology.

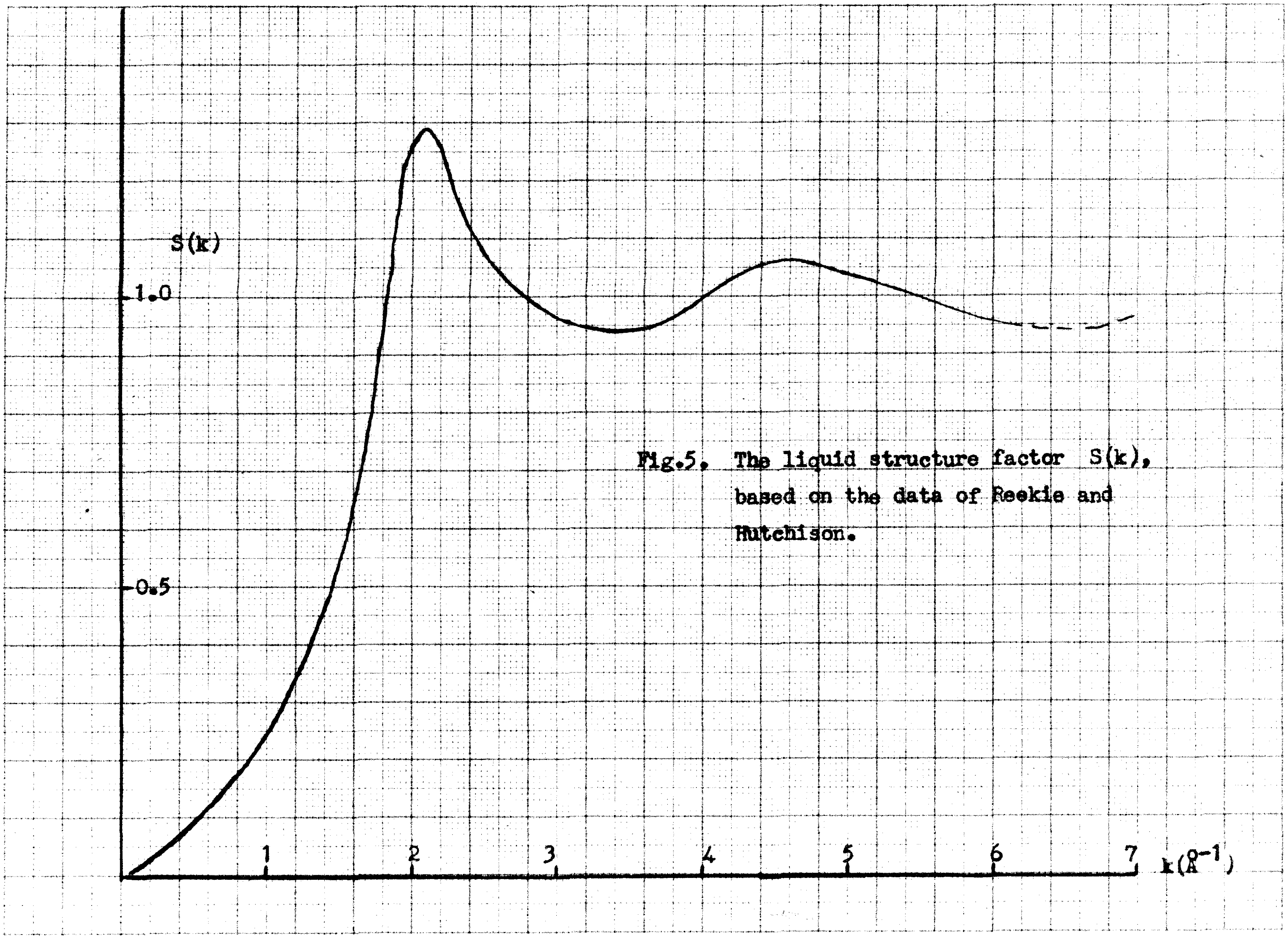

Fig.5. The liquid structure factor S(k), based on the data of Reekie and Hutchison.

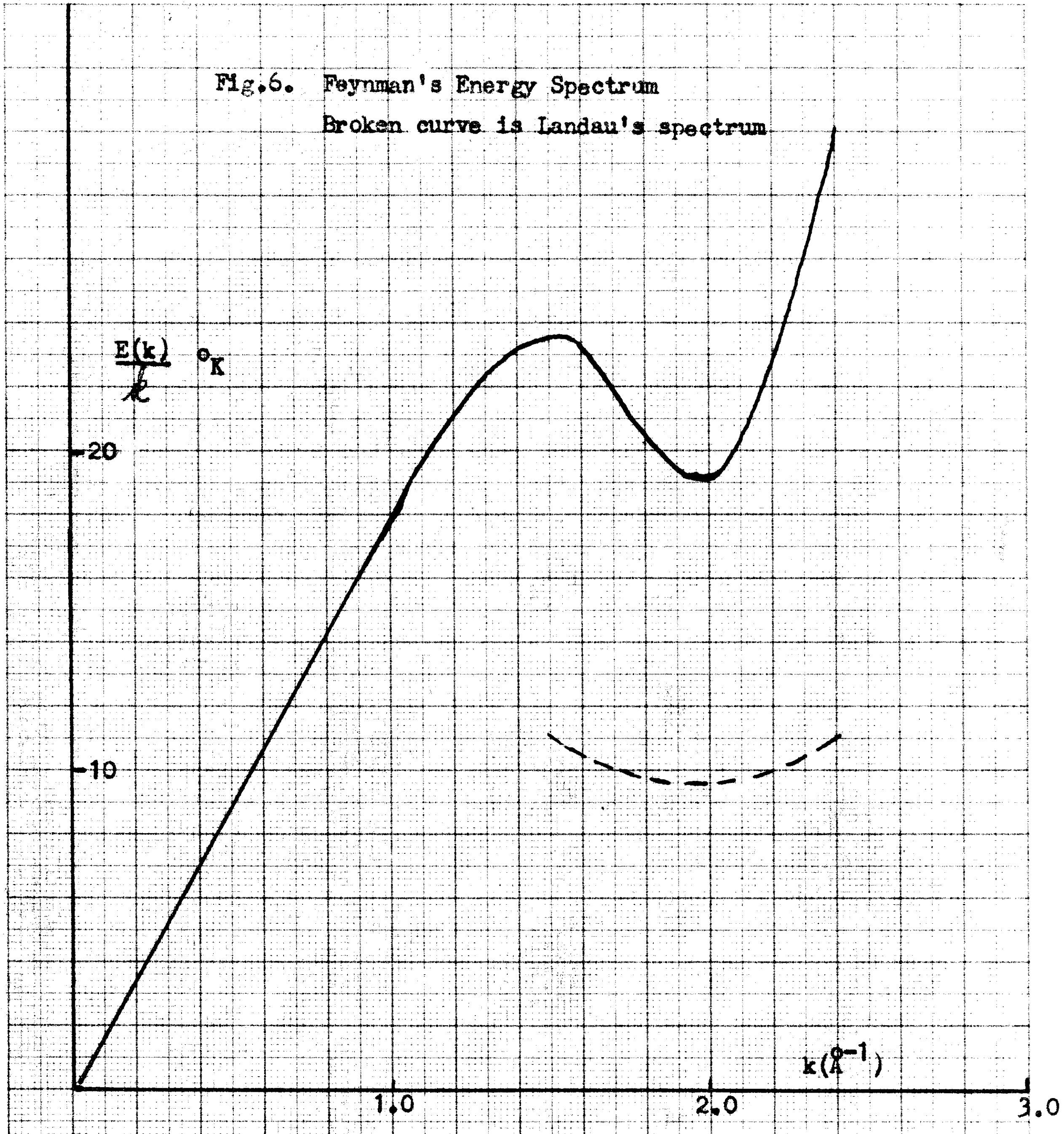

Fig. 6. Feynman's Energy Spectrum
Broken curve is Landau's spectrum

For $k < 1.2$Å^{-1}, curve is adjusted to have the theoretically correct slope $\hbar c$, rather than the incorrect slope from Fig. 5. (See Appendix C.)

III. AN IMPROVED ENERGY SPECTRUM

III.1. ARGUMENTS FOR A NEW WAVE FUNCTION

The excitation (11) can be localized in a definite region by the formation of a wave packet. If $h(\underline{r})$ is a function, like a Gaussian, which is peaked about some location in the liquid and falls off smoothly in a distance large compared with $2\pi/k$ but small compared with the size of the box, then the wave function

$$\Psi = \sum h(\underline{r}_i)\, e^{i\underline{k}\cdot\underline{r}_i}\, \phi \tag{15}$$

represents a localized excitation. The packet will spread in time, and will drift with velocity $\frac{1}{\hbar} \nabla_{\underline{k}} E(\underline{k})$. Feynman [11] has computed the current and density associated with (15). The number density is very close to ρ_0, even in the region of the packet, and the current at a point $\underline{a}$ is $\underline{j}(\underline{a}) = \frac{\hbar \underline{k}}{m} |h(\underline{a})|^2$. The wave function (15) therefore leads to the picture of a total current $\hbar\underline{k}/m$ (assume $\int |h(\underline{a})|^2 \, d\underline{a} = 1$) distributed over a small region and having everywhere the same direction, with no appreciable change in the number density anywhere. Such a picture clearly cannot represent anything like a stationary state, since in a stationary state the current is divergence-free and there would necessarily be a return flow directed oppositely to $\underline{k}$.

One way to incorporate such a backflow into (15) is to multiply the wave function by $\exp(i\sum g(\underline{r}_i))$, obtaining

$$\Psi = \exp(i \sum g(\underline{r}_i)) \sum h(\underline{r}_i)\, e^{i\underline{k}\cdot\underline{r}_i} \phi \quad . \tag{15a}$$

Application of the velocity operator $\frac{\hbar}{im} \nabla_i$ shows that, in addition to whatever velocity it had in (15), the i^{th} atom now has an extra velocity

$\frac{\hbar}{m} \nabla g(\underline{r}_i)$. Feynman computes the energy of (15a) and finds that the energy is minimized if $g(\underline{r})$ satisfies

$$\nabla \cdot \left(\underline{j} + \frac{\hbar \rho_o}{m} \nabla g\right) = 0 \tag{15b}$$

where $\underline{j}$ is the current computed from the old wave function (15). Furthermore, the current arising from (15a) is $\underline{J} = \underline{j} + \frac{\hbar \rho_o}{m} \nabla g$, so that (15b) states that the best backflow g is that which conserves current. Equation (15b), with the physically reasonable boundary condition that $g \to 0$ as $r \to \infty$, completely determines g. At large distances g has the form of the velocity potential for dipole flow, namely $\underline{\mu} \cdot \underline{r}/r^3$; the dipole moment is

$$\underline{\mu} = \frac{1}{4\pi} \frac{m}{\hbar \rho_o} \int \underline{a} \, \nabla \cdot \underline{j}(\underline{a}) \, d\underline{a} = - \frac{1}{4\pi} \frac{m}{\hbar \rho_o} \int \underline{j}(\underline{a}) d\underline{a} = -\frac{1}{4\pi \rho_o} \, \underline{k} \, . \tag{15c}$$

The negative sign of $\underline{\mu}$ indicates that the direction of the backflow is opposite to that of $\underline{k}$, as expected. We shall refer to the value of $\underline{\mu}$ given by (15c) as the "classical value", since it is derivable from the equation of conservation of current plus the assumption that the momentum density is equal to the current density times the mass. Feynman shows that the energy of (15a) is only slightly lower than that of (15), the difference being of the order of the reciprocal of the volume of the packet. The important point to be learned from his calculation is that the energy is lowered if the wave function conserves current.

The solution of a somewhat different problem tends to support the same idea. Suppose we want to find the energy of a state in which a foreign atom moves through the liquid with momentum $\hbar \underline{k}$. The foreign atom is assumed to have the same mass as He atoms, and also to experience the same forces, but it is not subject to Bose statistics. Feynman [11] computed the energy of this situation, using at first the trial wave function

$$\Psi = e^{i\underline{k}\cdot\underline{r}_A} \phi \quad ; \tag{16}$$

$\underline{r}_A$ is the coordinate of the foreign atom, and ϕ is the wave function for the ground state of the entire system (which is the same as if all the atoms obeyed Bose statistics). With this wave function, equation (6) gives $E = \hbar^2 k^2/2m$. A possible way of lowering the energy would be to let the neighbors of the moving atom execute some pattern of flow around it, leaving space in front of it and filling in the hole behind it. Some such pattern is already contained in (16), since the ground state wave function ϕ prohibits atoms from overlapping. But in the ground state, readjustments are made by pushing a few immediate neighbors of the foreign atom out of the way; these neighbors are crowded into less than their usual volumes, causing (16) to have a high kinetic energy. If, instead, room could be made for the moving atom by the simultaneous motion of many atoms, each being crowded only slightly, the kinetic energy of the state would be lower. In fact, there is no reason why the crowding cannot be eliminated entirely since the amount of matter in the system remains constant. Roughly, speaking, the requirement of no crowding means that the current is divergence-free, and the no-crowding argument shows physically why it is energetically advantageous to conserve current. The argument is vague, however, and the exact form of the backflow will be determined by more accurate methods.

A wave function of momentum $\hbar \underline{k}$ which includes a pattern of backflow around the foreign atom is

$$\Psi = \phi \, e^{i\underline{k}\cdot\underline{r}_A} \exp(i \sum_{i \neq A} g(\underline{r}_i - \underline{r}_A)) \quad . \tag{17}$$

When (17) is substituted into the expression (6) for the energy, minimization of E leads to a differential equation which determines $g(\underline{r})$. The solution at large $\underline{r}$ is proportional to $\underline{k} \cdot \underline{r}/r^3$. Feynman then sets the differential equation aside (its accurate numerical solution is simple but uncertain because of uncertainty in the values of $p(r)$) and takes $g(\underline{r}) = A\underline{k} \cdot \underline{r}/r^3$. Substitution of (17) into the variational principle (6) gives

$$E = \frac{\hbar^2 k^2}{2m} (1 + I_1 A + (I_4 + I_{5a})A^2) \tag{17a}$$

where I_1 and I_4 are integrals defined by equation (23) and I_{5a} is an integral defined by (69). The integrals are evaluated further on; only the answer interests us here. Equation (17a) becomes

$$E = \frac{\hbar^2 k^2}{2m} (1 + .186A + .0246A^2) \tag{17b}$$

with A measured in Å^3. The energy is minimum when $A = -3.8\text{Å}^3$; the "classical" value predicted by (15c) is $A = -1/4\pi\rho_o = -3.6\text{Å}^3$. The close agreement of the two values seems to indicate that the reduction in energy is due to the physical effects we have mentioned, and is not simply the result of allowing an extra degree of freedom in the wave function. The improved value for the energy is

$$E = .648\ \hbar^2 k^2/2m \quad .^{*} \tag{17c}$$

Since the wave function (11) for a phonon or roton is just what would result from symmetrizing (16), one might hope to lower the energy of (11) by adding terms to represent a backflow around each moving atom. The resulting wave function would be the symmetrization of (17), i.e.

$$\Psi = \phi \sum_i e^{i\underline{k}\cdot\underline{r}_i} \exp(i \sum_{j\neq i} g(\underline{r}_{ji})). \tag{18}$$

For large k, when this wave function is substituted into the energy and normalization integrals, there is little interference between terms with different i; the energy is therefore given by (17c) and is a definite improvement over (13). For small k, (18) cannot lead to a lower energy than (11), because (11) is exact for phonons. At intermediate k, one might thus expect to lower the energy by a factor between 1.00 and .65. In fact, we do better than this.

The attempt to find the function $g(\underline{r})$ which gives the lowest energy when (18) is substituted into (6) leads to an intractable equation. We therefore take $g(\underline{r}) = A\underline{k} \cdot \underline{r}/r^3$, where A will be chosen to minimize the energy. The difficulty of handling integrals which

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[*] This is somewhat higher than the value obtained by Feynman in [11]. He used a rather inaccurate approximation for I_4. With our value for I_4 we find that the effective mass of a He^3 atom moving through He^4 is 5.0 atomic mass units, instead of Feynman's 5.8. In the calculation it is assumed that the distribution of atoms around the He^3 atom is the same as that around an He^4 atom. The higher zero-point motion of the lighter atom actually pushes its neighbors further away. If this effect is taken into account, the effective mass is raised and comes closer to the experimental value of 8 or 9 mass units.

involve e^{ig} leads one to consider the possibility of replacing $e^{i\Sigma g}$ by $1 + i\Sigma g$. The average value of $\sum_{j\neq i} g(\underline{r}_{ji})$ is $\int_{0^+}^{\infty} p(r)\, g(\underline{r})\, d\underline{r}$, which is zero because $g(\underline{r})$ is an odd function. The mean-square value of $\sum_{j\neq i} g(\underline{r}_{ji})$ is $\frac{1}{\rho_0} \int \rho_3(\underline{r}_1, \underline{r}_2, \underline{r}_3)\, g(\underline{r}_{21})\, g(\underline{r}_{31})\, d\underline{r}_2\, d\underline{r}_3$, where $\rho_3(\underline{r}_1, \underline{r}_2, \underline{r}_3)$ is the probability in the ground state of finding atoms at the sites $\underline{r}_1$, $\underline{r}_2$, and $\underline{r}_3$.* The integral is evaluated further on; with the classical value for A (which is close to the optimal value throughout the interesting range of k) the root-mean-square value of $\sum g(\underline{r}_{ji})$ turns out to be $0.25k$, where k is measured in inverse Angstroms. Even when $k = 2Å^{-1}$, replacement of $e^{i\Sigma g}$ by $1 + i\Sigma g$ is not unreasonable,** and we shall work with the wave function

$$\Psi = \phi \sum_{i} e^{i\underline{k}\cdot\underline{r}_i} \left(1 + i \sum_{j\neq i} g(\underline{r}_{ji})\right) \qquad (19)$$

where $g(\underline{r}) = A\underline{k} \cdot \underline{r}/r^3$.

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* We can forget the restriction that $j \neq i$ by imagining $g(\underline{r})$ to become zero when r is very small; otherwise one must remember that in this integral $\rho_3(\underline{r}_1, \underline{r}_2, \underline{r}_3)$ contains a term $\rho_0 p(\underline{r}_{12})\, \delta(\underline{r}_{23})$ but does not contain similar terms involving $\delta(\underline{r}_{12})$ and $\delta(\underline{r}_{13})$.

** Of course it would be mathematically legitimate to insert $1 + i\Sigma g$ into the variational principle (6) even if Σg were not small, but there would be little physical reason to expect a good answer. If $\exp(i\Sigma g(\underline{r}_i - \underline{r}_A))$ is replaced by $1 + i\Sigma g(\underline{r}_i - \underline{r}_A)$ in the foreign atom problem, the resulting integrals are among the ones defined and evaluated further on. The energy is given by

$$E = \frac{\hbar^2 k^2}{2m} \, \frac{1 + .186A + (.0217 + .0045k^2)A^2}{1 + .0045k^2A^2} \; .$$

When $k = 2Å^{-1}$, the fraction has the minimum value .684, which is 5.5 per cent higher than the value given by (17c). The associated value of A is $-3.5Å^3$. When $k = 2.5Å^{-1}$, the fraction is .710, corresponding to $A = -3.0Å^3$. We conclude that for $k < 2Å^{-1}$, replacement of $e^{i\Sigma g}$ by $1 + i\Sigma g$ does not seriously raise the energy.

The wave function (19) can also be understood in terms of Feynman's argument about α and β sites. The most obvious trouble with a wave function of the form $\Psi = \phi \sum f(\underline{r}_i)$ is that it rises just as much when several atoms move toward the same α site as when they move toward different α sites (of course ϕ will ultimately cause the amplitude to fall when the atoms begin to encroach on each other, but, as has already been pointed out, a high kinetic energy is involved if we count on ϕ to do all the work of keeping the atoms apart). The easiest way to straighten out the trouble is to replace $f(\underline{r}_i)$ by $f(\underline{r}_i)\,(1 + \sum_{j \neq i} h(\underline{r}_{ji}))$. When all the atoms change their positions, the change in the wave function due to the motion of the i^{th} atom now involves a factor which takes into account the correlation between the displacement of the i^{th} atom and the displacements of all its neighbors. The function $h(\underline{r})$ should go to zero for large r, since correlations between well-separated atoms are unimportant. If an atom i happens to have no near neighbors, the change in the wave function due to its motion should be just the change in $f(\underline{r}_i)$; hence the extra "1". It is difficult in this picture to see why $h(\underline{r})$ is pure imaginary and is the potential function for dipole flow. The requirement that Ψ be an eigenfunction of the total momentum operator implies that $f(\underline{r}) = e^{i\underline{k}\cdot\underline{r}}$.

If one tries to construct a wave function having the next degree of complexity beyond (10), namely

$$\Psi = \phi \sum_{i,j} f(\underline{r}_i, \underline{r}_j)$$

the requirement that Ψ be an eigenfunction of $\underline{P}$ implies that $f(\underline{r}_i, \underline{r}_j) = e^{i\underline{k}\cdot\underline{r}_i} s(\underline{r}_{ij})$, and we are again led to the form (19). Further arguments, however, are needed to determine the function $s(\underline{r})$.

III.2. COMPUTATIONS WITH THE NEW WAVE FUNCTION

We substitute (19) into (7) and (8), remembering that g is odd. This implies the vanishing of some integrals, like $\int g(\underline{r}_{12})\,\rho_2(\underline{r}_1, \underline{r}_2)\,d\underline{r}_1\,d\underline{r}_2$. The result is $E = \epsilon/\mathcal{J}$ where

$$\begin{aligned}
\frac{2m\epsilon}{\hbar^2} = {} & Nk^2 + k^2\int g(\underline{r}_{21})\,g(\underline{r}_{31})\,\rho_3(1,2,3)\,d\underline{r}_1\,d\underline{r}_2\,d\underline{r}_3 \\
& + \int \nabla g(\underline{r}_{21})\cdot\nabla g(\underline{r}_{31})\,\rho_3(1,2,3)\,d\underline{r}_1\,d\underline{r}_2\,d\underline{r}_3 \\
& + \int e^{i\underline{k}\cdot\underline{r}_{23}}\,\nabla g(\underline{r}_{12})\cdot\nabla g(\underline{r}_{13})\,\rho_3(1,2,3)\,d\underline{r}_1\,d\underline{r}_2\,d\underline{r}_3 \\
& - 2\underline{k}\cdot\int \nabla g(\underline{r}_{21})\,\rho_2(1,2)\,d\underline{r}_1\,d\underline{r}_2 \\
& + 2\int e^{i\underline{k}\cdot\underline{r}_{12}}\,\underline{k}\cdot\nabla g(\underline{r}_{12})\,\rho_2(1,2)\,d\underline{r}_1\,d\underline{r}_2 \\
& + 2i\int e^{i\underline{k}\cdot\underline{r}_{13}}\,g(\underline{r}_{21})\,\underline{k}\cdot\nabla g(\underline{r}_{13})\,\rho_3(1,2,3)\,d\underline{r}_1\,d\underline{r}_2\,d\underline{r}_3 \\
& - 2\int e^{i\underline{k}\cdot\underline{r}_{13}}\,\nabla g(\underline{r}_{21})\cdot\nabla g(\underline{r}_{13})\,\rho_3(1,2,3)\,d\underline{r}_1\,d\underline{r}_2\,d\underline{r}_3
\end{aligned} \tag{20}$$

$$\begin{aligned}
\mathcal{J} = {} & \int e^{i\underline{k}\cdot\underline{r}_{12}}\,\rho_2(1,2)\,d\underline{r}_1\,d\underline{r}_2 - 2i\int e^{i\underline{k}\cdot\underline{r}_{12}}\,g(\underline{r}_{32})\,\rho_3(1,2,3)\,d\underline{r}_1 d\underline{r}_2 d\underline{r}_3 \\
& + \int e^{i\underline{k}\cdot\underline{r}_{12}}\,g(\underline{r}_{31})\,g(\underline{r}_{42})\,\rho_4(1,2,3,4)\,d\underline{r}_1\,d\underline{r}_2\,d\underline{r}_3\,d\underline{r}_4 \; .
\end{aligned} \tag{21}$$

In all of the above integrals, the integrand is a function only of the relative coordinates $\underline{r}_{ij}$. Integration over the last coordinate can therefore be replaced by a factor V. If the density functions ρ_2, ρ_3, and ρ_4 are divided by ρ_0, a factor $\rho_0 V = N$ then appears in front of each integral. Writing $g(\underline{r}) = Akg_1(\underline{r})$, we finally obtain

$$\frac{2m\mathcal{E}}{N\hbar^2} = k^2\left[1 + A(I_1 + I_2) + A^2(k^2 I_3 + I_4 + I_5 + kI_6 + I_7)\right] \tag{22a}$$

$$\frac{\mathcal{J}}{N} = I_8 + AkI_9 + A^2k^2I_{10} \tag{22b}$$

where

$$I_1 = \frac{-2}{\rho_o}\frac{\underline{k}}{k}\cdot\int\nabla g_1(\underline{r}_{21})\,\rho_2(1,2)\,d\underline{r}_{21}$$

$$I_2 = \frac{2}{\rho_o}\int e^{i\underline{k}\cdot\underline{r}_{12}}\,\frac{\underline{k}}{k}\cdot\nabla g_1(\underline{r}_{12})\,\rho_2(1,2)\,d\underline{r}_{21}$$

$$I_3 = \frac{1}{\rho_o}\int g_1(\underline{r}_{21})\,g(\underline{r}_{31})\,\rho_3(1,2,3)\,d\underline{r}_{21}\,d\underline{r}_{31}$$

$$I_4 = \frac{1}{\rho_o}\int\nabla g_1(\underline{r}_{21})\cdot\nabla g_1(\underline{r}_{31})\,\rho_3(1,2,3)\,d\underline{r}_{21}\,d\underline{r}_{31}$$

$$I_5 = \frac{1}{\rho_o}\int e^{i\underline{k}\cdot\underline{r}_{23}}\,\nabla g_1(\underline{r}_{12})\cdot\nabla g_1(\underline{r}_{13})\,\rho_3(1,2,3)\,d\underline{r}_{21}\,d\underline{r}_{31}$$

$$I_6 = \frac{2i}{\rho_o}\int e^{i\underline{k}\cdot\underline{r}_{13}}\,g_1(\underline{r}_{21})\,\frac{\underline{k}}{k}\cdot\nabla g_1(\underline{r}_{13})\,\rho_3(1,2,3)\,d\underline{r}_{21}\,d\underline{r}_{31}$$

$$I_7 = \frac{-2}{\rho_o}\int e^{i\underline{k}\cdot\underline{r}_{13}}\,\nabla g_1(\underline{r}_{21})\cdot\nabla g_1(\underline{r}_{13})\,\rho_3(1,2,3)\,d\underline{r}_{21}\,d\underline{r}_{31}$$

$$I_8 = \int e^{i\underline{k}\cdot\underline{r}}\,p(r)\,d\underline{r} = S(k) \qquad \text{(see eqn. (14))}$$

$$I_9 = \frac{-2i}{\rho_o}\int e^{i\underline{k}\cdot\underline{r}_{12}}\,g_1(\underline{r}_{32})\,\rho_3(1,2,3)\,d\underline{r}_{21}\,d\underline{r}_{31}$$

$$I_{10} = \frac{1}{\rho_o}\int e^{i\underline{k}\cdot\underline{r}_{12}}\,g_1(\underline{r}_{31})\,g_1(\underline{r}_{42})\,\rho_4(1,2,3,4)\,d\underline{r}_{21}\,d\underline{r}_{31}\,d\underline{r}_{41} \tag{23}$$

I_1, I_3, and I_4 are independent of k. In the other integrals it will prove possible to extract most of the k-dependence rather simply when k is in the roton region, the remaining complicated terms being very small.

This means that the computation of the entire roton spectrum will not be much more difficult than the computation of one point on it.

Some further definitions are helpful. It was noted earlier that $\rho_2(\underline{r}_1, \underline{r}_2) = \rho_o p(r_{12})$. We now define

$$p(r) = \delta(\underline{r}) + p_1(r) \tag{24}$$

$$p_1(r) = \rho_o(1 + p_2(r)) \tag{25}$$

where p_1 and p_2 have no singularities and $p_2(r) \to 0$ as $r \to \infty$. Strictly speaking, in the definition of I_1 we should replace $\rho_2(\underline{r}_1, \underline{r}_2)$ by $\rho_2(\underline{r}_1, \underline{r}_2) - \rho_o \delta(\underline{r}_{12})$ since g is always a function of the relative coordinates of two <u>distinct</u> atoms. To avoid unnecessary confusion, however, it is easier to think of $g(\underline{r})$ as becoming zero for sufficiently small r. Similar remarks apply to ρ_3 and ρ_4 when they occur in $I_2, \dots, I_{10}$. If one does not wish to think of $g(\underline{r})$ as being modified near the origin, then the ρ's should be understood as containing delta functions of all coordinate differences except those which appear as arguments of g in the same integral. The non-singular part of ρ_3, which we call ρ_3', is defined by

$$\rho_3(\underline{r}_1, \underline{r}_2, \underline{r}_3) = \rho_3'(\underline{r}_1, \underline{r}_2, \underline{r}_3) + \rho_o p_1(r_{12}) \delta(\underline{r}_{23}) + \rho_o p_1(r_{13}) \delta(\underline{r}_{12})$$
$$+ \rho_o p_1(\underline{r}_{23}) \delta(\underline{r}_{13}) + \rho_o \delta(\underline{r}_{12}) \delta(\underline{r}_{23}) . \tag{26}$$

No experimental data for ρ_3' is available. If any of the mutual distances, say r_{12}, is large, then $\rho_3'(\underline{r}_1, \underline{r}_2, \underline{r}_3) = \rho_o p_1(r_{13})\, p\, (r_{23})$. If any of the interatomic distances becomes less than 2.4Å, then $\rho_3' = 0$.

The approximation*

$$\rho_3'(\underline{r}_1, \underline{r}_2, \underline{r}_3) \simeq p_1(r_{12})\, p_1(r_{13})\, p_1(r_{23}) \tag{27}$$

has these correct limiting features. Much has been written about the validity of this approximation; for some, but not all purposes, (27) is quite sufficient. We shall see that our answer is only slightly sensitive to the difference between the right and left sides of (27).

I_1 can be done exactly. We integrate by parts over a volume bounded by two concentric surfaces, one lying inside the radius where $p(r) = 0$ and the other very far from the origin. The inner surface contributes nothing, but the integrand $g_1(\underline{r})\, p_1(r)$ falls off only as r^{-2}, with the result that the outer surface makes a finite contribution, which is easily computed to be $\frac{-8}{3}\pi\rho_0$. We eliminate this contribution by redefining $g(\underline{r})$ to have a small decay factor, say $e^{-\varepsilon r}$, which makes surface terms vanish at infinity. This procedure is mathematically legitimate, since we are free to use any wave function we want in the variational principle, and is in accord with the physical idea that all the momentum of the backflow should be contained in a finite volume. It will generally not be necessary to represent ε explicitly; the convergence factor will be used only to justify certain operations. After the parts integration, there remains

$$I_1 = \frac{2\underline{k}}{k} \cdot \int g_1(\underline{r}) \nabla p_1(r)\, d\underline{r} = \frac{8\pi\rho_0}{3} \int_0^\infty \frac{dp_1(r)}{dr}\, dr = \frac{8\pi\rho_0}{3}\,. \tag{28}$$

In the last integral, the integrand should really be $e^{-\varepsilon r}\,\frac{dp_1}{dr}$, but if ε is small enough the convergence factor will be unity out to

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* This is sometimes called the Kirkwood approximation or the superposition approximation.

radii where dp_1/dr becomes negligible.

After performing the angular integrations in I_2, we find

$$I_2 = 16\pi\rho_o \int_{r_o}^{\infty} j_2(kr) \frac{(1 + p_2(r))}{r} dr = 16\pi\rho_o \left[\frac{j_1(kr_o)}{kr_o} + F(k)\right] \equiv 16\pi\rho_o I_{2a}(k) \tag{29}$$

where r_o is any radius inside the region where $p_1(r) = 0$ (we take $r_o = 2.4Å$, the radius where $p_1(r)$ first becomes positive) and

$$F(k) \equiv \int_{r_o}^{\infty} j_2(kr) \frac{p_2(r)}{r} dr \quad . \tag{30}$$

The spherical Bessel functions j_1 and j_2 are expressible in terms of trigonometric functions, and are related to the ordinary Bessel functions of half-integral order by the equation

$$j_n(x) = \sqrt{\pi/2x} \; J_{n+1/2}(x).$$

There is no problem of a convergence factor in I_2, since the oscillations of $e^{i\underline{k}\cdot\underline{r}}$ provide a natural convergence factor. In order to do integrals like I_4 and I_5, we shall need to know the value of $I_{2a}(k)$ for all k. Using tabulated [18] values for j_2, we have evaluated $F(k)$ by numerical integration for 23 values of k between 0 and $7Å^{-1}$. The values are given in Table 1 and are shown as crosses in Fig. 7 and Fig. 7a; it is evident from the graphs that the 23 crosses fully determine the curve for $F(k)$, except in the region of small k, where $F(k)$ is so small as to be unimportant compared with $j_1(kr_o)/kr_o$. The integrand in (30) was evaluated at intervals of $0.1Å$ for $2.4Å \leq r \leq 4.4Å$, and at intervals of $0.2Å$ for $4.6Å \leq r \leq 6Å$. A simple trapezoidal rule was used

Table 1.

Table of $F(k) = \int_{2.4}^{\infty} j_2(kr)\, p_2(r)\, \frac{dr}{r}$

$k(\text{Å}^{-1})$	$F(k)$
0.5	.0012
0.8	.0037
1.0	.0036
1.2	.0002
1.4	-.0082
1.6	-.0152
1.8	-.0207
2.0	-.0203
2.2	-.0134
2.4	-.0038
2.6	.0058
2.8	.0124
3.0	.0146
3.4	.0078
3.8	-.0031
4.2	-.0096
4.6	-.0066
5.0	.0023
5.4	.0073
5.8	.0044
6.2	-.0017
6.6	-.0046
7.0	-.0030

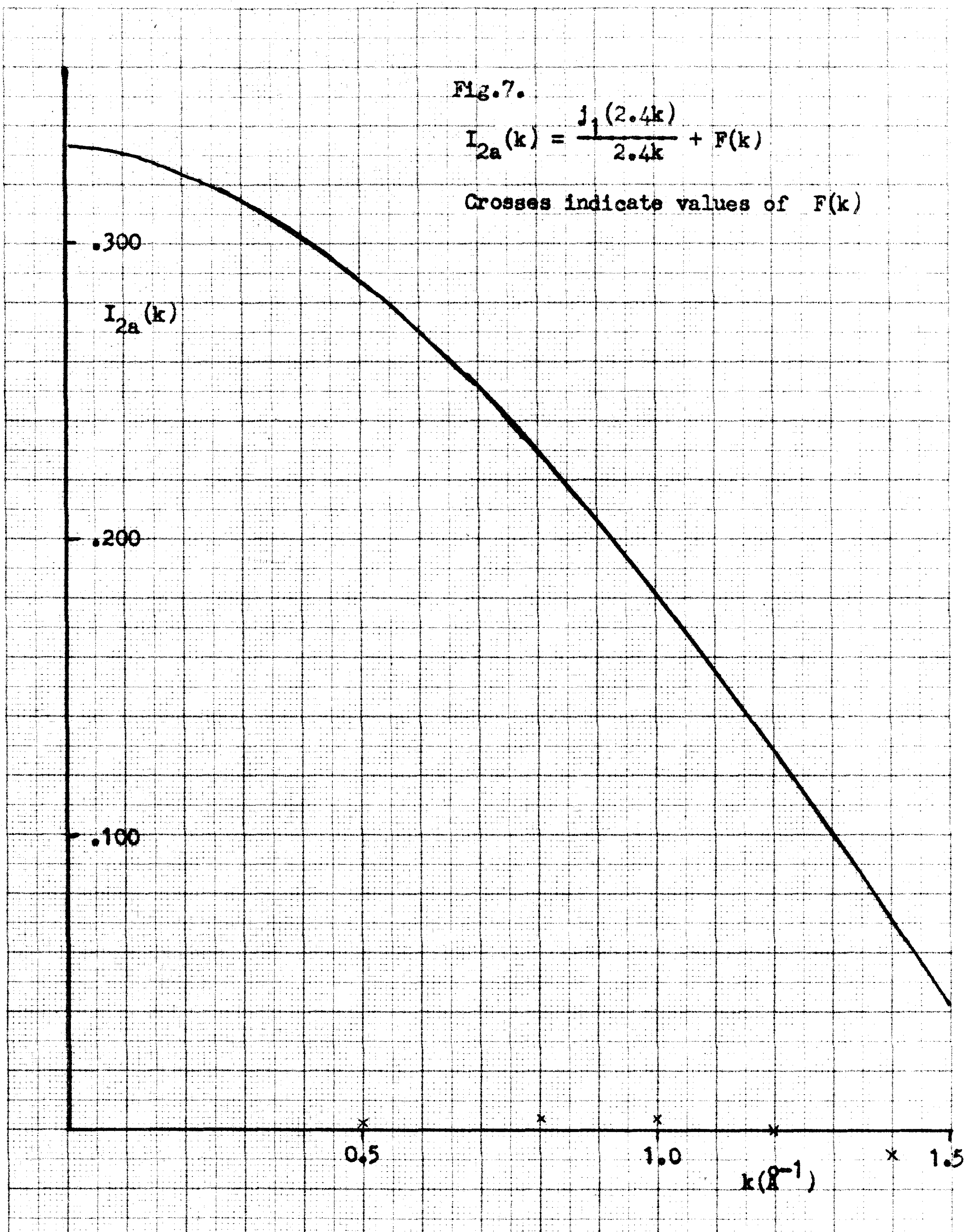
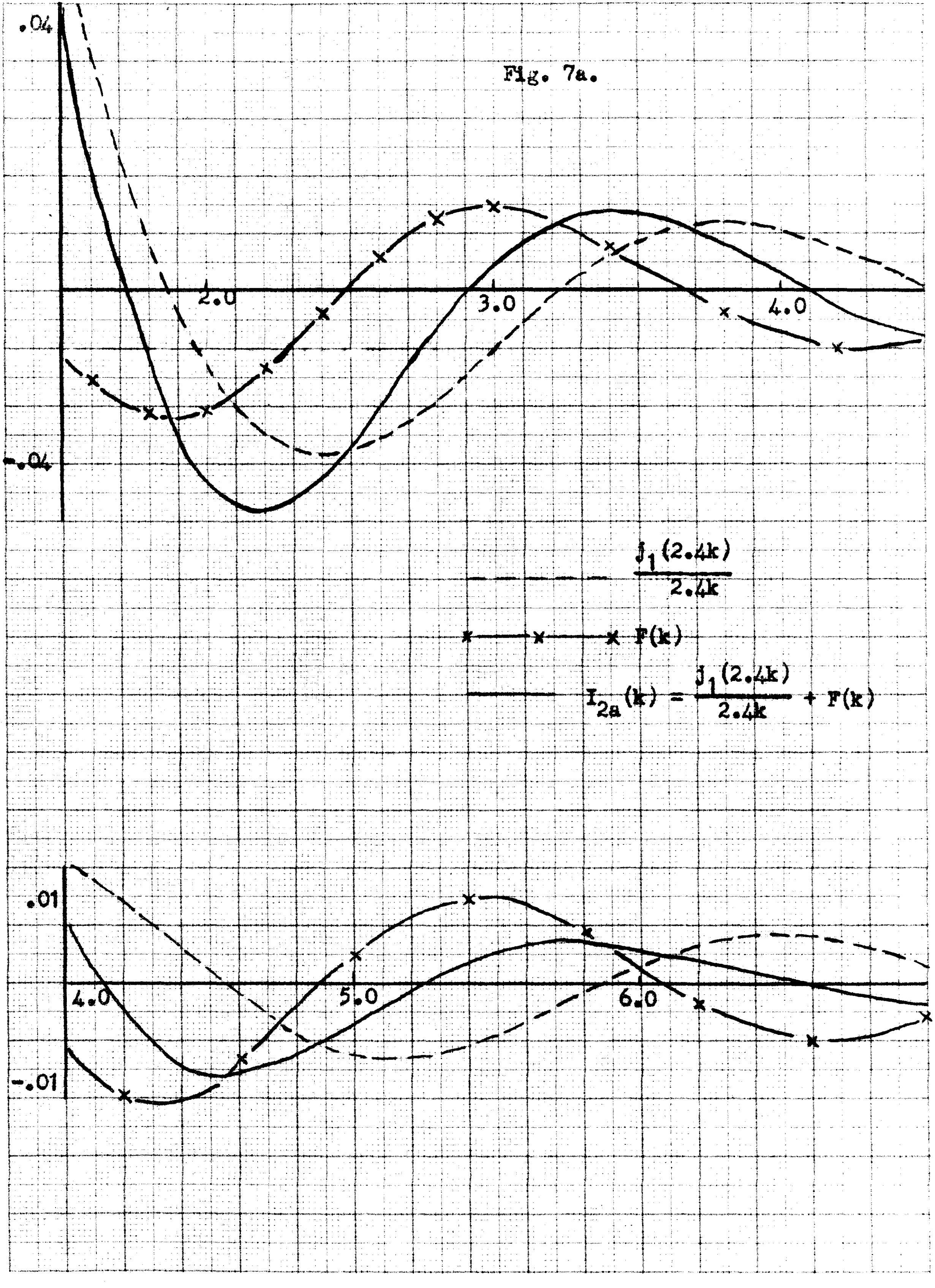


Fig.7.

$$I_{2a}(k) = \frac{j_1(2.4k)}{2.4k} + F(k)$$

Crosses indicate values of F(k)

Fig. 7a.


.04
-.04
2.0
3.0
4.0
$\frac{J_1(2.4k)}{2.4k}$
F(k)
$I_{2a}(k) = \frac{J_1(2.4k)}{2.4k} + F(k)$
.01
-.01
4.0
5.0
6.0

for the numerical integrations. The general philosophy used throughout the numerical work is that the methods should be sufficient to make full use of the accuracy in the available data for p(r) and S(k); when the numerical methods become more accurate than this, time is probably being wasted. The convergence of (30) is best for large k, since the range of r where $j_2(kr)$ is appreciable becomes smaller as k increases. The convergence is good for $k > 1\text{Å}^{-1}$.

One might expect from (23) that $\lim_{k \to 0} I_2 = -I_1$. As k approaches zero, $F(k)$ approaches zero and $j_1(kr_o)/kr_o$ approaches $1/3$. Comparison of (28) and (29) thus shows that I_2 approaches $2I_1$ instead of $-I_1$. The reason for the discrepancy is that (29) is wrong when k is very small, of the same order of magnitude as ε; in this case we must take account of the term $\nabla e^{-\varepsilon r}$ in ∇g, and there will be a correction term which will cause I_2 to change from $16\pi \rho_o/3$ to $-8\pi \rho_o/3$ as k decreases from ε to 0.

I_2 can also be evaluated in momentum space, using data for S(k) rather than p(r). In momentum space the integrals converge well for small k rather than large k. The results are not very important because (29) is useful down to $k = 0$ for reasons already mentioned; but they do provide a check of our numerical work and also of the consistency of the data for p(r) with that for S(k). Starting with

$$\int e^{-i\underline{k}_1 \cdot \underline{r}} g_1(\underline{r})\, d\underline{r} = -4\pi i \frac{\underline{k} \cdot \underline{k}_1}{k\, k_1^2} \qquad (31)$$

and using Fourier's theorem, we obtain

$$g_1(\underline{r}) = (2\pi)^{-3} (-4\pi i) \int e^{i\underline{k}_1 \cdot \underline{r}_i} \frac{\underline{k} \cdot \underline{k}_1}{k\, k_1^2}\, d\underline{k}_1 \,. \qquad (32)$$

Taking the gradient of both sides with respect to $\underline{r}$, and assuming that g_1 has convergence factors for large and small r, we find

$$\nabla g_1(\underline{r}) = (2\pi)^{-3} \int e^{i\underline{k}_1 \cdot \underline{r}} \, \underline{A}(\underline{k}_1) \, d\underline{k}_1 \tag{33}$$

where

$$\underline{A}(\underline{k}_1) = 4\pi \frac{\underline{k} \cdot \underline{k}_1}{k \, k_1} \frac{\underline{k}_1}{k_1} \quad . \tag{34}$$

$S(k)$ was defined by (14) as the Fourier transform of $p(r)$, where $p(r)$ includes a delta function at the origin and a constant term ρ_o at infinity. Therefore $S(k) \to 1$ as $k \to \infty$ and $S(k)$ includes a term $(2\pi)^3 \rho_o \delta(\underline{k})$. We define

$$S_1(k) = S(k) - 1 - (2\pi)^3 \rho_o \delta(\underline{k}). \tag{35}$$

Since $\rho_o p_2(r) = (2\pi)^{-3} \int e^{i\underline{k}\cdot\underline{r}} \, S_1(k) \, d\underline{k}$, we find

$$\begin{aligned} I_2 &= 8\pi \rho_o + (2\pi)^{-6} \, \frac{2\underline{k}}{k} \cdot \int e^{i(\underline{k}+\underline{k}_1+\underline{k}_2)\cdot\underline{r}} \, \underline{A}(\underline{k}_1) \, S_1(\underline{k}_2) \, d\underline{k}_1 \, d\underline{k}_2 \, d\underline{r} \\ &= 8\pi \rho_o + (2\pi)^{-3} \, \frac{2\underline{k}}{k} \cdot \int \underline{A}(\underline{k} - \underline{k}_2) \, S_1(\underline{k}_2) \, d\underline{k}_2 \end{aligned}$$

where we have used the identity $\delta(\underline{k}) = (2\pi)^{-3} \int e^{i\underline{k}\cdot\underline{r}} \, d\underline{r}$ and the evenness of $\underline{A}$ and S_1. Taking $\underline{k}$ as the polar axis, we obtain

$$\begin{aligned} I_2 &= 8\pi\rho_o + \frac{2}{\pi} \int_0^\infty \int_0^\pi S_1(k_2) \, k_2^2 \, \frac{(k/k_2 - \cos\theta)^2}{1 + (\frac{k}{k_2})^2 - 2\frac{k}{k_2}\cos\theta} \sin\theta \, d\theta \, dk_2 \\ &= 8\pi\rho_o + \frac{2}{\pi} \int_0^\infty S_1(k_2) \, k_2^2 \, a(\tfrac{k_2}{k}) \, dk_2 \end{aligned} \tag{37}$$

where

$$a(x) = \int_{-1}^{1} du \, \frac{(\frac{1}{x} - u)^2}{1 + \frac{1}{x^2} - \frac{2u}{x}} = \frac{3}{2} - \frac{x^2}{2} - \frac{1}{4x}(1 - x^2)^2 \log\left|\frac{1-x}{1+x}\right|$$

$$a(0) = 2 \qquad\qquad a(\infty) = 2/3 \; .$$

The convergence of the numerical integral in (37) is speeded by defining

$$b(x) = a(x) - 2/3 = 5/6 - x^2/2 - \frac{1}{4x}(1-x^2)^2 \log\left|\frac{1-x}{1+x}\right| . \qquad (38)$$

One easily verifies that

$$b(0) = 4/3 \qquad b(x) \sim \frac{4}{15}\frac{1}{x^2} \qquad \text{(large } x\text{)}.$$

Fig. 8 is a graph of $b(x)$. Taking $\underline{r} = 0$ in (36), we find

$$-\rho_0 = (2\pi)^{-3} \int_0^\infty S_1(k)\, 4\pi k^2\, dk \qquad (39)$$

and finally

$$I_2 = \frac{16}{3}\pi\rho_0 + \frac{2}{\pi}\int_0^\infty S_1(k_1)\, k_1^2\, b(\frac{k_1}{k})\, dk_1 . \qquad (40)$$

The numerical integral in (40) converges faster than that in (37) because $b(x) \to 0$ for large x. The integrand was evaluated at intervals of $0.2Å^{-1}$ for $0 \leq k_1 \leq 1.4Å^{-1}$ and $2.4Å^{-1} \leq k_1 \leq 5.4Å^{-1}$; in the region $1.5Å^{-1} \leq k_1 \leq 2.4Å^{-1}$, where S_1 varies rapidly, the integrand was evaluated at intervals of $0.1Å^{-1}$. The integral was evaluated for $k = 0.5, 1.0, 1.5, 2.0Å^{-1}$. Convergence is good, and the values are accurate to within a few per cent. Nevertheless, (40) does not give accurate values of I_2 when $k > 1.5A^{-1}$, because for large k the cancellation between the two terms of (40) is almost complete (as it must be because $I_2 \to 0$ as $k \to \infty$), and hence a 3 per cent error in the numerical integral may cause a 30 per cent error in I_2. We take the volume per atom of liquid helium as $45Å^3$.* Table 2 compares the value of $I_2(k)$ obtained from (29) with those obtained from (40).

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* The atomic volume of liquid He under its own saturated vapor pressure at 0 K is $46Å^3$, but $45Å^3$ is closer to the value at 2.06K, where the structure factor data was taken. Internal inconsistencies would develop if ρ_0 and $S(k)$ were taken at different temperatures. One might ask where the theory takes account of the external pressure. The pressure determines the values of ρ_0 and, more important, $S(k)$. An increase in pressure sharpens the maxima and minima of $p(r)$ and $S(k)$.

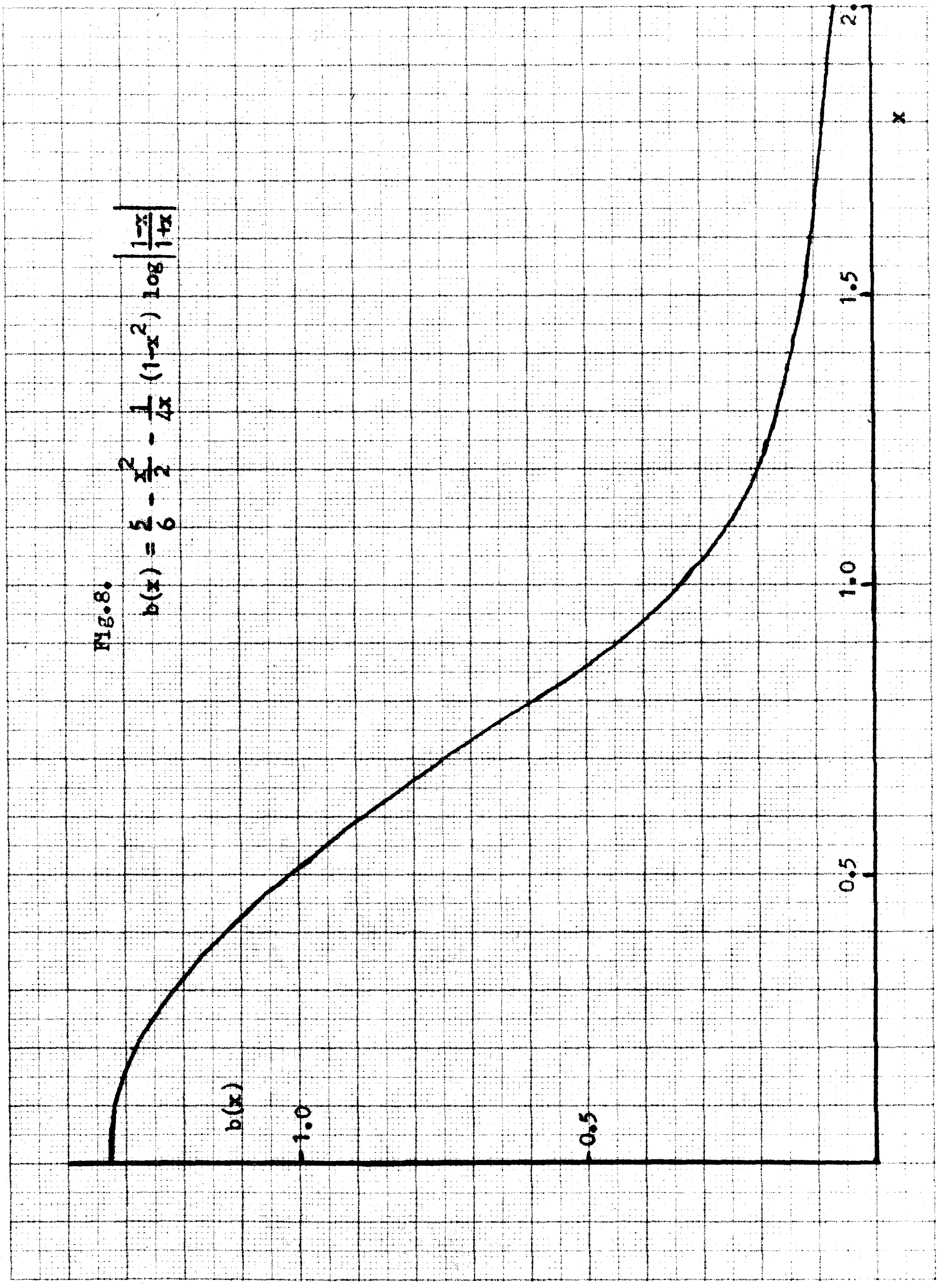

Fig.8.

$$b(x) = \frac{5}{6} - \frac{x^2}{2} - \frac{1}{4x}\,(1-x^2)\,\log\left|\frac{1-x}{1+x}\right|$$

Table 2.

k (Å^{-1})		0	0.5	1.0	1.5	2.0	∞
$I_2(k)$ (Å^{-3})	from (29)	.372	.322	.194	.054	-.036	0
	from (40)	.372	.326	.200	.050	-.060	0

The discrepancy at $k = 2$Å^{-1} is not serious, for the reasons just mentioned, and the agreement elsewhere is sufficiently close for our purposes. The values derived from (29) are used throughout our work.

I_4 presents no problem if $I_{2a}(k)$ is known for all k. Using (25) and (26), and Fourier analyzing $p_2(r_{23})$ with (36), we obtain

$$I_4 = \int p_1(r)\,(\nabla g_1(\underline{r}))^2\,d\underline{r} + \left(\int p_1(r)\,\nabla\, g_1(\underline{r})\,d\underline{r}\right)^2 + \frac{1}{(2\pi)^3\rho_o}\int d\underline{k}_1\,S_1(\underline{k}_1)\,\left[\int e^{i\underline{k}_1\cdot\underline{r}_2}\nabla g_1(\underline{r}_2)\,p_1(r_2)\,d\underline{r}_2\right]^2 . \tag{41}$$

The integral in square brackets is a generalization of I_2 to the case where the $\underline{k}$ in the exponential has a different direction from the $\underline{k}$ in g_1. The angular integrations are easily performed, yielding

$$\int e^{i\underline{k}_1\cdot\underline{r}_2}\,\nabla\, g_1(\underline{r}_2)\,p_1(r_2)\,d\underline{r}_2 = 8\pi\rho_o\,I_{2a}(k_1)\left[\frac{\underline{k}_1}{k_1}\cos\theta - \frac{1}{2}\,\underline{e}_1\sin\theta\right] \tag{42}$$

where $\frac{\underline{k}_1}{k_1}\cos\theta$ and $\underline{e}_1\sin\theta$ are the components of $\underline{k}/k$ parallel and perpendicular to $\underline{k}_1$ (see Fig. 9); $\underline{e}_1$ is a unit vector, and θ is the angle from $\underline{k}_1$

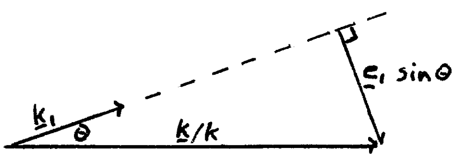

Fig.9. Definition of the vectors in (42).

to $\underline{k}$. The equation

$$\underline{e}_1 \sin \theta = \frac{(k_1 \times \underline{k}) \times \underline{k}_1}{k_1^2 k}$$

is true but not useful. Since the average over angles of $\cos^2 \theta + \frac{1}{4} \sin^2 \theta$ is $\frac{1}{2}$, (41) becomes

$$I_4 = 8\pi \rho_o \int_{r_o}^{\infty} (1 + p_2(r))\, r^{-4}\, dr + (\tfrac{4}{3} \pi \rho_o)^2$$

$$+ 16 \rho_o \int_0^{\infty} k_1^2\, S_1(k_1)\, (I_{2a}(k_1))^2\, dk_1$$

$$= .01190 + .00867 - .00790 = .01267 \text{Å}^{-6} . \qquad (43)$$

The convergence in both numerical integrals is very good; $\int p_2(r)\, r^2\, dr$ and $\int k_1^2\, S_1(k_1)\, dk_1$ are already convergent, and r^{-6} and $[I_{2a}(k_1)]^2$ provide very strong damping factors. The answer may be in error by several per cent due to uncertainties in ρ_o, $p_2(r)$, and $S_1(k_1)$, but the single numerical integrations are so easy that no time is lost by retaining an insignificant figure. The magnitude of $\int_{r_o}^{\infty} p_2(r)\, r^{-4}\, dr$ is only 1/10 that of $\int_{r_o}^{\infty} r^{-4}\, dr$; also, Fig. 7 shows that in the important range of k_1, $I_{2a}(k_1)$ is the same as would result if we took

$$p_1(r) = \begin{cases} 0 & r < 2.4\text{Å} \\ \rho_o & r > 2.4\text{Å} \end{cases} .$$

The important point to be learned from this discussion is that the values of I_4, and of the other integrals which contribute significantly to the coefficient of A^2 in (22a), depend mainly on the gross features of $p(r)$ (i.e. its delta function at the origin, its vanishing for $r < 2.4\text{Å}$, and its quick rise to the asymptotic value ρ_0) and not on the details of its behavior. The coefficients of A are more sensitive to the detailed behavior of $p(r)$; it is the detailed behavior which determines the location of the minimum in the energy spectrum. The insensitivity of the quadratic coefficients to the exact form of $p(r)$ can be similarly verified in the computations which follow, and will not be pointed out explicitly. A rough way of estimating the error due to the approximation (27) is to imagine $p_2(r_{23})$ replaced by some other function of r_{23} which is -1 for $r_{23} < r_0$ and approaches zero as $r_{23} \to \infty$. Of course, in the actual case this function would also depend on r_{12} and r_{13}, since the true ρ_3' is not factorable; but the argument still ought to give orders of magnitude correctly. The result of this change would be to replace $S_1(k_1)$ in (43) by some other function which is -1 when $k_1 = 0$, has the slope $\hbar/2mc$ at the origin, and first becomes zero near $k_1 = 2\text{Å}^{-1}$. But 90 per cent of the contribution to $\int_0^\infty k_1^2 \, S_1(k_1) \, (I_{2a}(k_1))^2 \, dk_1$ comes from the region $k_1 < 1.2\text{Å}^{-1}$, where the behavior of S_1 is pretty well determined by its value and slope at the origin. With any reasonable function in place of $S_1(k_1)$, the integral would probably not be changed by more than 10 per cent; hence the error in I_4 due to the approximation (27) is almost certainly less than 10 per cent, and probably less than 5 per cent. More generally, one can argue that the two sides of (27) must differ by zero whenever any of the mutual distances is less than 2.4Å or greater than about 4Å. This region includes so much of phase space that even if the difference develops sufficiently high derivatives to become significantly different from zero, it can do so only over a small region.

The value of I_4 and the size of the various terms which contribute to it can be understood fairly well in terms of some simple approximations for integrals involving the coordinates of three atoms. With the help of these approximations we can understand the sizes of all the remaining integrals; if we know that an integral is small, it will not be necessary to waste time in evaluating it very accurately.

Suppose we want to do an integral of the form

$$\int f(\underline{r}_{21})\, f(\underline{r}_{31})\, \rho_3(1,\ 2,\ 3)\, d\underline{r}_2\, d\underline{r}_3$$

(in this integral we shall understand ρ_3 to include a delta function on coordinates 2 and 3, but not on any other pairs). If the positions of 1 and 2 are fixed and 3 is not too close to 2, then $\rho_3(1,\ 2,\ 3)$ can be approximated very closely by $\rho_o p_1(r_{21})\, p_1(r_{31})$. We write

$$\rho_3(1,2,3) \simeq \rho_o p_1(r_{21})\, p_1(r_{31}) \quad . \qquad (44)$$

When 3 approaches 2, this is wrong because ρ_3 goes to zero but $p_1(r_{21})\, p_1(r_{31})$ keeps a finite value (assuming, of course, that $r_{21} > 2.4Å$; otherwise both expressions are zero). When 2 and 3 coincide, however, ρ_3 exhibits a delta function and far exceeds $\rho_o p_1(r_{21})\, p_1(r_{31})$. The strength of the delta function is such that if we integrate the difference between the two sides of (44) over the positions of 3, the result is exactly zero, i.e.

$$\int [\rho_3(1,2,3) - \rho_o p_1(r_{21})\, p_1(r_{31})]\, d\underline{r}_3 = 0 \quad . \qquad (45)$$

The result is easily understood for small or large values of r_{12}. If $r_{12} < 2.4\text{Å}$, both sides of (44) are identically zero for all $\underline{r}_3$. If 1 and 2 are far apart, then ρ_3 can be written as

$$\rho_o p_1(r_{31})\, p_1(r_{32}) + \rho_o^2\, \delta(\underline{r}_{32})$$

and the right side becomes $\rho_o^2 p_1(r_{31})$. If 3 is far from 2, then both sides are equal. Hence the only contribution to the integral comes when 3 is near 2; but then we can set $p_1(r_{31}) = \rho_o$ and we are left with $\int d\underline{r}_{32}\, \rho_o^2 (p_1(r_{32}) + \delta(\underline{r}_{32}) - \rho_o)$ which vanishes as a result of the identity

$$\int_{o^+}^{\infty} (p(r) - \rho_o)\, 4\pi r^2\, dr = -1 \qquad (46)$$

which is proved in Appendix C. At the present time we are unable to supply a rigorous proof of (45) for all values of r_{12}. In Appendix C we discuss our reasons for believing (45); its physical interpretation is essentially the same as that of the proven identity (46). Even if (45) is not rigorously true for intermediate values of r_{12}, it cannot fail badly; for when r_{12} is greater than 2.4Å, but not very large, then for any fixed radius r_{32} the solid angle in which 3 interferes with 1 is small (less than one quarter of the total solid angle available to $\underline{r}_{23}$).

If $f(\underline{r})$ is a slow-varying function, i.e. $f(\underline{r})$ does not change much when $\underline{r}$ changes by 2.4Å, then for a fixed value of $\underline{r}_{12}$ the value of $f(\underline{r}_{31})$ is almost constant over the region where the two sides of (44) differ appreciably. Using (45), we see that the integral

$$\int f(\underline{r}_{31}) \, [\rho_3(1,2,3) - \rho_o p_1(r_{21}) \, p_1(r_{31})] \, d\underline{r}_3$$

is very close to zero. We therefore find

$$\int f(\underline{r}_{31}) \, \rho_3(1,2,3) \, d\underline{r}_3 \simeq \rho_o p_1(r_{21}) \int f(\underline{r}_{31}) \, p_1(r_{31}) \, d\underline{r}_3$$

(unless both integrals are very close to zero) and finally

$$\int f(\underline{r}_{21}) \, f(\underline{r}_{31}) \, \rho_3(1,2,3) \, d\underline{r}_2 \, d\underline{r}_3 \simeq \rho_o \left[\int f(\underline{r}) \, p_1(r) \, d\underline{r} \right]^2 . \tag{47}$$

Similarly, if f <u>or</u> g is slowly-varying,

$$\int f(\underline{r}_{21}) \, g(\underline{r}_{31}) \, \rho_3(1,2,3) \, d\underline{r}_2 \, d\underline{r}_3 \simeq$$

$$\simeq \rho_o \left(\int f(\underline{r}) \, p_1(r) \, d\underline{r} \right) \left(\int g(\underline{r}) \, p_1(r) \, d\underline{r} \right) . \tag{48}$$

Actually, our criterion for a slowly-varying function is too stringent. The behavior of $f(\underline{r})$ for $r < 2.4$Å is of no importance, since $p_1(r)$ is zero in that range; hence f may be singular at the origin. The important question is, how much does $f(\underline{r}_1 + \underline{r}_2)$ differ from $f(\underline{r}_1)$ when $\underline{r}_1$ and $\underline{r}_2$ are any two vectors of length 2.4Å? And even if the difference is large compared with $f(\underline{r}_1)$, (47) is still good if $f(\underline{r})$ is such that the major contribution to $\int f(\underline{r}) \, p_1(r) \, d\underline{r}$ comes from $r > 3$ or 4Å.

Another type of integral which interests us is

$$\int f(\underline{r}_{21}) \, g(\underline{r}_{31}) \, h(\underline{r}_{23}) \rho_3(1,2,3) \, d\underline{r}_2 \, d\underline{r}_3 ,$$

where f and g are smooth and $h(\underline{r})$ oscillates so rapidly that it produces almost complete cancellation when integrated against $p_1(r)$.

ρ_3 is still understood to contain a delta function on 2 and 3, and on no other pair. In this case, if 1 and 2 are held fixed and 3 is allowed to vary, the oscillations in $h(\underline{r}_{23})$ make the contribution to the integral small. The major contribution comes when 3 and 2 are tied together by the delta function and we find

$$\int f(\underline{r}_{21})\, g(\underline{r}_{31})\, h(\underline{r}_{23})\, \rho_3(1,2,3)\, d\underline{r}_2\, d\underline{r}_3$$

$$\simeq h(0) \int f(\underline{r})\, g(\underline{r})\, p_1(r)\, d\underline{r} \quad . \tag{49}$$

If $\nabla\, g_1(\underline{r})$ is sufficiently smooth, (47) can be used to estimate I_4. The answer thus obtained is $(\frac{4}{3}\pi\rho_0)^2 = .00867\text{Å}^{-6}$, which is the middle term of (43); if ∇g_1 were very smooth, the first and third terms would cancel completely. The first term $(.01190\text{Å}^{-6})$ is larger than the third term $(-.00790\text{Å}^{-6})$ because $\nabla g_1(\underline{r})$ is proportional to r^{-3} and therefore quite strongly peaked for small r; hence the delta function more than compensates for the "hole" in ρ_3. The answer given by (47) is 2/3 the correct answer.

With the aid of (47)-(49) we can discuss the remaining integrals more intelligently. If Landau's energy spectrum is even qualitatively correct, then the most important points to compute are those in the neighborhood of the roton minimum. The phonon spectrum is guaranteed to be correct; and when the temperature is high enough to excite the portion of the spectrum lying appreciably above the roton minimum, then the picture of the liquid as a gas of independent excitations has broken down. Thus, even if we knew the exact form of the high part of the spectrum, we would not know how to do the thermodynamics. Furthermore, the high-momentum end of the spectrum computed with (18) or (19) is certainly wrong, since the slope dE/dp exceeds the velocity of sound when $k \geq 2.2Å^{-1}$; whenever $|dE(p)/dp| > c$, there obviously exist states with two excitations, one of which is a phonon, which have total momentum p but energy less than $E(p)$. We shall compute the energy at several points in the region $1.6Å^{-1} \leq k \leq 2.4Å^{-1}$, and also at $k = 1.2Å^{-1}$ in order to estimate the height of the hump between the phonon and roton regions.

Since g_1 is smoother than ∇g_1, I_3 is a good candidate for the approximation (47), which predicts $I_3 = 0$ because $\int p_1(r)\, g_1(\underline{r})\, d\underline{r} = 0$. We infer that I_3 is small; but it is important to know <u>how</u> small, because the factor k^2 which multiplies I_3 in (22) is fairly large. The exact value of I_3 (i.e. no approximations beyond (27)) can be computed by the method used for I_4. The result is

$$\begin{aligned}
I_3 &\equiv I_{3a} + I_{3b} \\
&= \int [g_1(\underline{r})]^2\, p_1(r) d\underline{r} + \int g_1(\underline{r}_{21}) g_1(\underline{r}_{31}) p_1(\underline{r}_{21}) p_1(r_{31}) p_2(r_{23}) d\underline{r}_{21}\, d\underline{r}_{31} \\
&= \rho_0 [\tfrac{4\pi}{3} \int_0^\infty (1 + p_2(r))\, r^{-2}\, dr + \tfrac{8}{3} \int_0^\infty S_1(k_1) [I_{9a}(k_1)]^2 dk_1] \\
&= \frac{1}{45} (1.707 - 1.470) = .0053Å^{-4}.
\end{aligned}$$

The integral $I_{9a}(k_1)$ is defined by equation (56). The approximation (47) is based on the idea that I_{3a} and I_{3b} should cancel each other. Since $I_{3a} - I_{3b}$ is only 14 per cent of I_{3a}, the idea behind (47) is good, but (47) tells us nothing about the size of I_3 because

$$\int g_1(\underline{r})\, p_1(r)\, d\underline{r} = 0\ .^{*}$$

If $I_3 = .0053\,\text{Å}^{-4}$, then in the roton region the term $k^2 I_3$ contributes about half of the total coefficient of A^2 in (22a). Any possibility of serious error in I_3 ought therefore to be investigated carefully. The idea that I_3 is almost zero is based on the approximation (47), which in turn is based on the identity (45). Actually, the approximate form which we have used for ρ_3 does not satisfy (45) exactly. Slight departures from (45) ordinarily would not affect the validity of (47), were it not for the fact that $\int p_1(r)\, g_1(\underline{r})\, d\underline{r} = 0$. In this case the question arises: how much of the non-zeroness of I_3 is real, and how much is due to the fact that the approximate ρ_3 does not satisfy (45)? I_{3b} is only an approximation to the exact expression

$$I_{3c} \equiv \frac{1}{\rho_o} \int g_1(\underline{r}_{21}) g_1(\underline{r}_{31}) [\rho_3'(1,2,3) - \rho_o p_1(r_{21}) p_1(r_{31})]\, d\underline{r}_{21}\, d\underline{r}_{31}$$

where ρ_3' is defined by (26). In I_{3b} we have replaced $\rho_3'(1,2,3)$ by $p_1(r_{21})\, p_1(r_{31})\, p_1(r_{32})$. An exact expression for I_3 is

$$\begin{aligned} I_3 &= I_{3a} + I_{3c} = I_{3a} + I_{3b} - (I_{3b} - I_{3c}) \\ &= .0053 - \frac{1}{\rho_o} \int g_1(\underline{r}_{21}) g_1(\underline{r}_{31}) [p_1(r_{21}) p_1(r_{31}) p_1(r_{23}) \\ &\qquad\qquad - \rho_3'(1,2,3)]\, d\underline{r}_{21}\, d\underline{r}_{31} \\ &\equiv .0053 - I_{3d} \end{aligned} \tag{50}$$

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[*] It is worth noting that if

$$p_1(r) = \begin{cases} 0 & r < r_o \\ \rho_o & r > r_o \end{cases}$$

then I_3 can be computed analytically. One finds that the difference of the two terms is 3/16 of the larger term. Analytic computations with this artificial form for $p_1(r)$ may occasionally be useful in estimating small terms whose more exact computation is laborious. To satisfy (46), we must take $\frac{4}{3}\pi \rho_o r_o^3 = 1$.

If any of the mutual distances is less than 2.4Å or more than about 4Å, then $p_1(r_{21})\, p_1(r_{31})\, p_1(r_{23}) - \rho_3^{!}(1,2,3)$ is very close to zero. Consequently, the integrand of I_{3d} is appreciable only if r_{21} and r_{31} are almost the same and the angle between $\underline{r}_{21}$ and $\underline{r}_{31}$ is such that $2.4Å \leq r_{23} \lesssim 4Å$. Since the angular variation of g_1 is slow, we do not change I_{3d} much if we replace $g_1(\underline{r}_{21})\, g_1(\underline{r}_{31})$ by $[g_1(\underline{r}_{31})]^2$; we obtain

$$I_{3d} \simeq I_{3e}$$

where

$$I_{3e} \equiv \frac{1}{\rho_o} \int [g_1(\underline{r}_{31})]^2 [p_1(r_{21})\, p_1(r_{31})\, p_1(r_{23}) - \rho_3^{!}(1,2,3)]\, d\underline{r}_{21}\, d\underline{r}_{31}.$$

Making use of the fact that the true ρ_3 satisfies (45) and p_1 satisfies (46), we obtain

$$I_{3e} = \rho_o \int p_2(r_{23})\, p_2(r_{12})\, p_1(r_{13}) [g_1(\underline{r}_{13})]^2\, d\underline{r}_2\, d\underline{r}_3$$

$$= \frac{2}{3\pi \rho_o} \int_{2.4}^{\infty} r^{-2}\, p_1(r)\, I_{3f}(r)\, dr \tag{51}$$

where

$$I_{3f}(r) \equiv \int_0^{\infty} \frac{\sin(kr)}{kr} [S_1(k)]^2 k^2\, dk \tag{52}$$

$I_{3f}(r)$ was computed for 19 values of r between 2.4Å and 5.6Å. the numerical integrals converge well, and the results are shown in Fig. 10. Performing the final numerical integration in (51), we find $I_{3c} = .00081Å^{-4}$ and finally

$$I_3 = .0045Å^{-4} \quad . \tag{53}$$

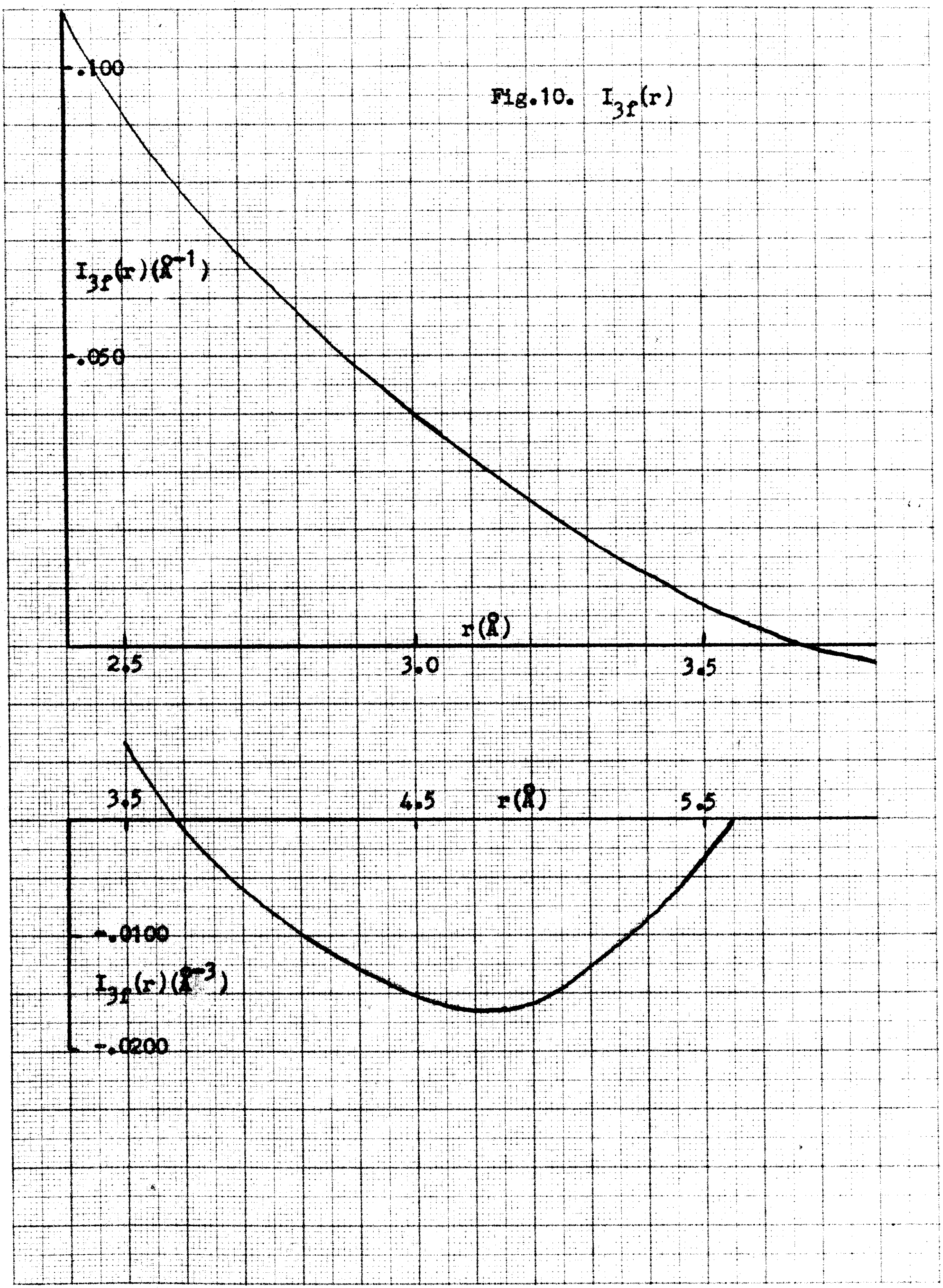


Fig.10. $I_{3f}(r)$

.100
$I_{3f}(r)(\mathring{A}^{-1})$
.050
r(Å)
2.5
3.0
3.5
3.5
4.5
r(Å)
5.5
-.0100
$I_{3f}(r)(\mathring{A}^{-3})$
-.0200

The smallness of the correction to I_3 shows that the slight failure of (45) does not cause a significant error in I_3. This fact was not intuitively obvious, however, and needed verification.

I_9 occurs in (22b) as a coefficient of A, rather than A^2, and ought therefore to be treated as accurately as is possible. In I_9, ρ_3 includes delta functions on $\underline{r}_{12}$ and $\underline{r}_{13}$. Using (27), we write

$$\begin{aligned}\rho_3(1,2,3) &= p_1(1,2)p_1(1,3)p_1(2,3) + \rho_o p_1(2,3)\delta(1,2) + \rho_o p_1(2,3)\delta(1,3)\\ &\equiv \rho_o(1 + p_2(1,3))\, p_1(1,2)p_1(2,3) + \rho_o p_1(2,3)\,\delta(1,2)\\ &\quad + \rho_o p_1(2,3)\,\delta(1,3).\end{aligned}$$

Several terms are zero because of the oddness of g_1, and we obtain

$$\begin{aligned}I_9 &= -2i \int e^{i\underline{k}\cdot\underline{r}_{12}}\, g_1(\underline{r}_{32})\, p_2(r_{13})\, p_1(r_{12})\, p_1(r_{23})\, d\underline{r}_{21}\, d\underline{r}_{31}\\ &\quad - 2i \int e^{i\underline{k}\cdot\underline{r}_{12}}\, g_1(\underline{r}_{12})\, p_1(r_{12})\, d\underline{r}_{21} \quad .\end{aligned} \tag{54}$$

First we consider the second integral, since we must know its value for all $\underline{k}$ in order to do the first integral. The integral, like I_2, can be performed in coordinate or momentum space; after the angular integrations are done, the result is

$$\int e^{i\underline{k}_1\cdot\underline{r}}\, g_1(\underline{r})\, p_1(r)\, d\underline{r} = \frac{\underline{k}_1\cdot\underline{k}}{k_1^2\, k}\, 4\pi\rho_o\, i\, I_{9a}(k_1) \tag{55}$$

where

$$I_{9a}(k) = \frac{\sin(2.4k)}{2.4k} + k \int_{2.4}^{\infty} p_2(r)\, j_1(kr)\, dr \tag{56}$$

$$= 1 + (4\pi^2\rho_o)^{-1} \int_0^{\infty} k_1^2\, S_1(k_1)\, c(k_1/k)\, dk_1 \tag{57}$$

and

$$c(x) = 1 + \frac{1}{2}\,(x - \frac{1}{x})\,\log\left|\frac{1-x}{1+x}\right|$$

$$c(0) = 2 \qquad c(x) \simeq \frac{2}{3x^2}\ (\text{large}\ \ x).^{*}$$

Fig. 11 is a graph of $c(x)$.

We define

$$I_{9b}(k) = \int_{2.4}^{\infty} p_2(r)\, j_1(kr)\, dr \tag{58}$$

$$I_{9c}(k) = \int_{0}^{\infty} dk_1\, k_1^2\, S_1(k_1)\, c(k_1/k)\ . \tag{59}$$

As before, the coordinate space formula (56) proves sufficient over the entire range of k. For small k, when the numerical integral $I_{9b}(k)$ cannot be done accurately, its value is so small as to be unimportant compared with $\sin(2.4k)/2.4k$. $I_{9b}(k)$ was computed for 16 points between $k = 1Å^{-1}$ and $k = 7Å^{-1}$. The integrand was evaluated at intervals of 0.1Å for $2.4Å \le r \le 4.4Å$, and at intervals of 0.2Å for $4.4Å \le r \le 6Å$. The results are given in Table 3. The values of $I_{9a}(k)$ computed from (56) are given in Figs. 12 and 12a and are accurate within less than .02 for k in the neighborhood of $2Å^{-1}$; for large k, the

---

[*] Since $\int g_1(\underline{r})\, p_1(r)\, d\underline{r} = 0$, one might expect the right side of (55) to approach zero as k_1 becomes small. But $I_{9a}(k_1)$ aproaches unity for small k_1, and consequently the right side of (55) approaches $\pm\infty$, depending on the angle between $\underline{k}$ and $\underline{k}_1$. The trouble, as before, is resolved by noting that (55) and (56) are wrong for $k_1 < \varepsilon$ (g_1 should really have a factor $e^{-\varepsilon r}$ in it). In the correct version of (56) the term $\sin(2.4k)/2.4k$ is replaced by zero when $k \ll \varepsilon$; hence $I_{9a}(k_1)$ goes as k_1^2 when $k_1 \ll \varepsilon$, and the right side of (55) approaches zero. The "error" in (55) and (56) has no effect on our computations, but it is worth mentioning lest the reader discover it and develop a distrust of the formulas.

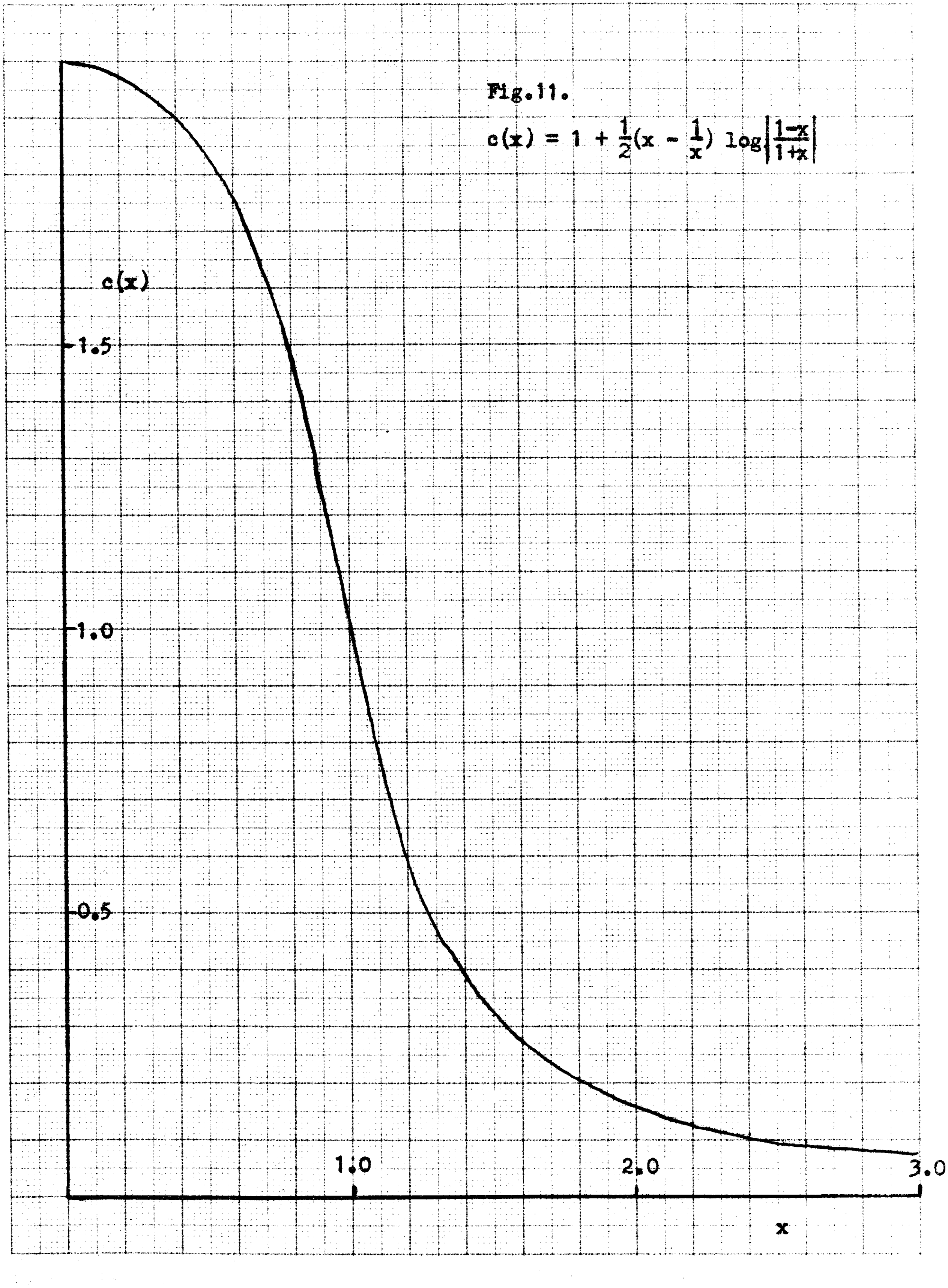


Fig.11.

$c(x) = 1 + \frac{1}{2}(x - \frac{1}{x}) \log\left|\frac{1-x}{1+x}\right|$

Table 3

Table of $I_{9b}(k) = \int_{2.4}^{\infty} j_1(kr)\, p_2(r)\, dr$

$k(\AA^{-1})$	$I_{9b}(k)(\AA)$
0.5	.0142
1.0	.0040
1.3	-.0430
1.7	-.0609
2.0	-.0119
2.3	.0400
2.5	.0517
3.0	.0123
3.5	-.0230
4.0	-.0225
4.5	.0084
5.0	.0226
5.5	.0005
6.0	-.0152
6.5	-.0062
7.0	.0065

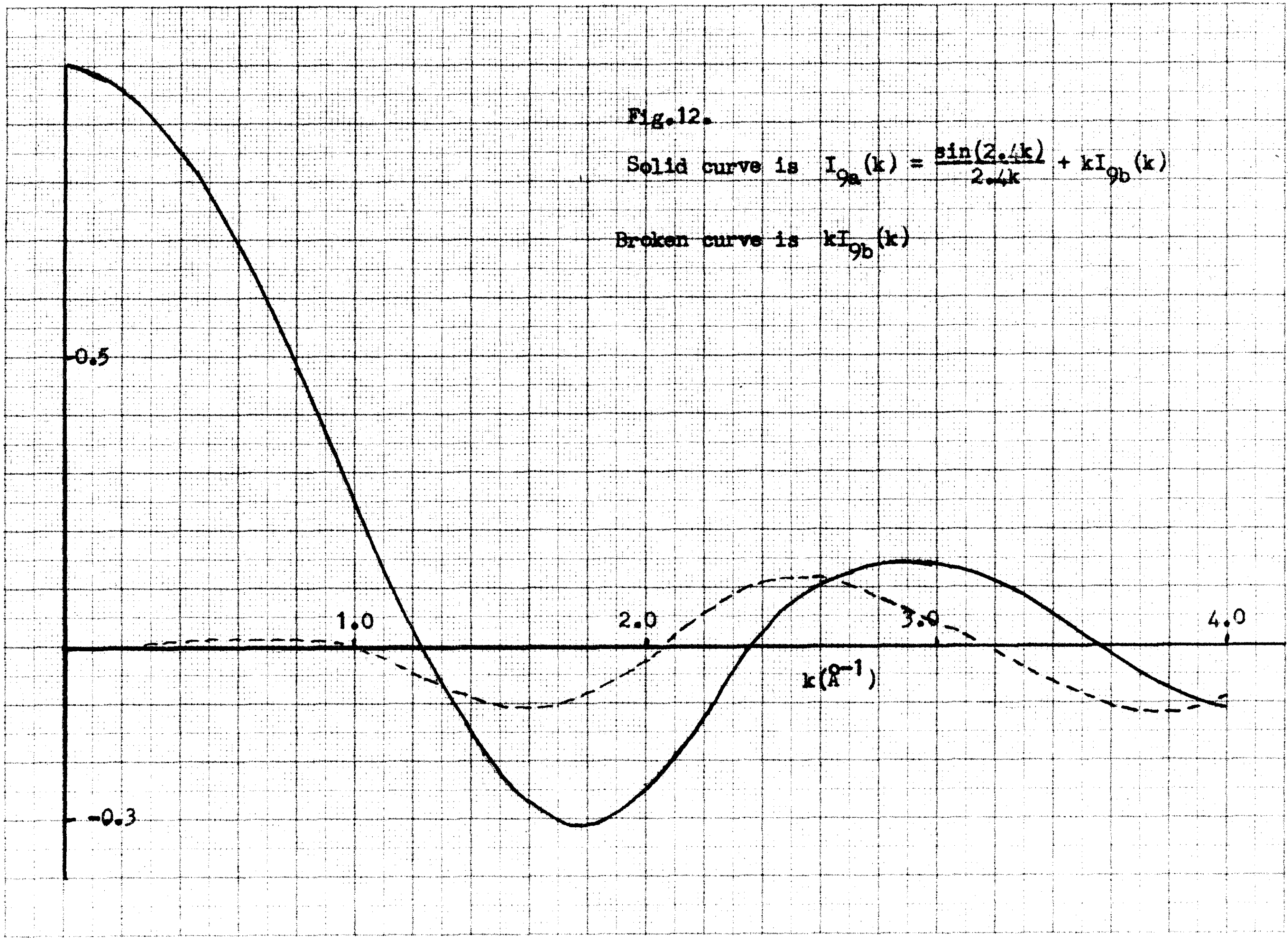


Fig.12.

Solid curve is $I_{9a}(k) = \frac{\sin(2.4k)}{2.4k} + kI_{9b}(k)$

Broken curve is $kI_{9b}(k)$

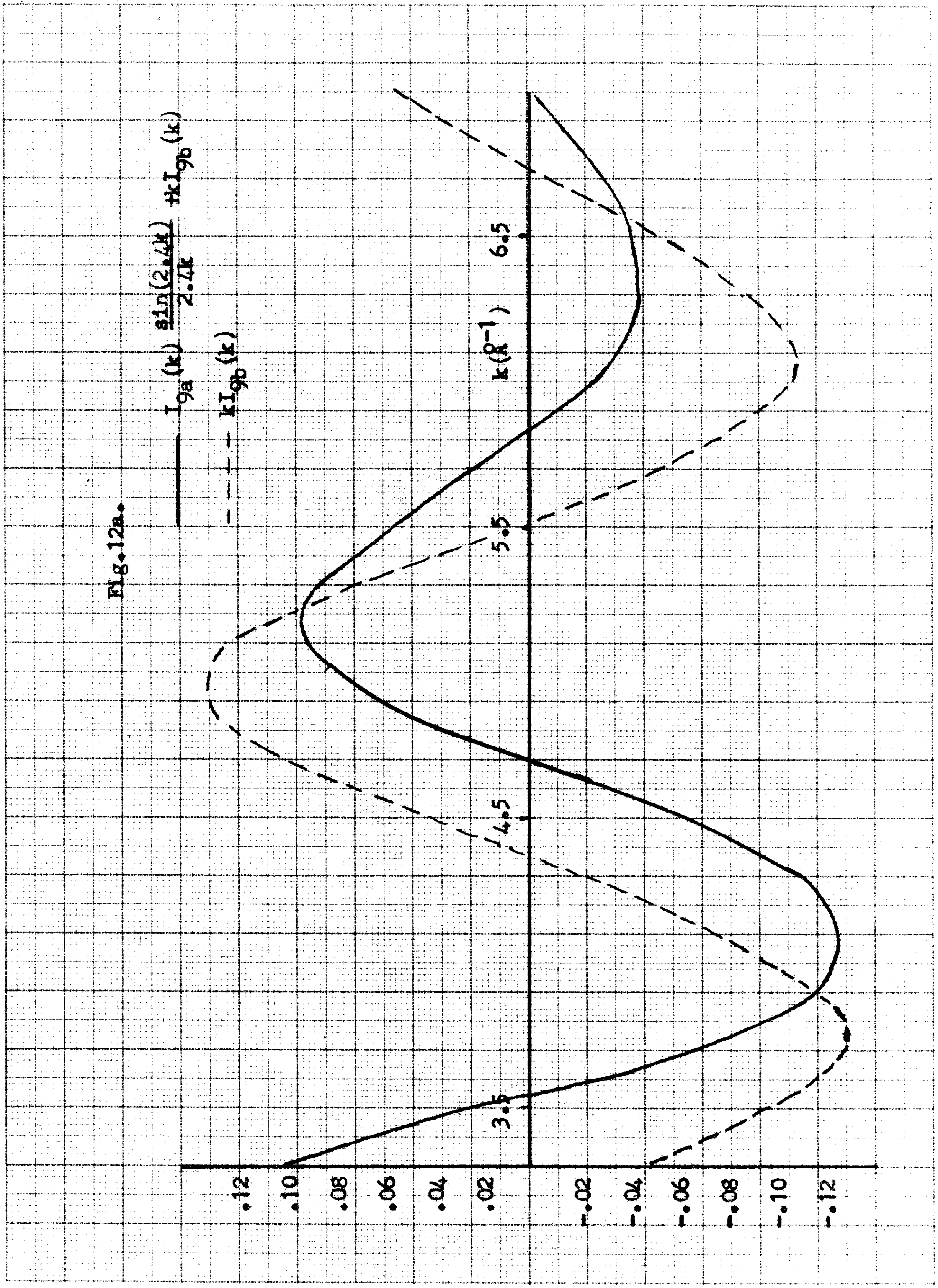


Fig.12a.

$I_{9a}(k)\,\frac{\sin(2.4k)}{2.4k} + kI_{9b}(k)$
$kI_{9b}(k)$
$k(\text{Å}^{-1})$
3.5
4.5
5.5
6.5
.12
.10
.08
.06
.04
.02
-.02
-.04
-.06
-.08
-.10
-.12

more rapid convergence of the integral $I_{9b}(k)$ gives an accuracy of 0.1 or less. For our purposes, the most important region of k is near 2Å^{-1}. Although the fractional error in $I_{9b}(k)$ is sizable here, $I_{9a}(k)$ is probably accurate within 5 per cent. For $k > 1\text{A}^{-1}$, formula (57) suffers from the same disease as (40). Although the numerical integral can be done to within five or ten per cent accuracy, it almost cancels the constant term; therefore the fractional error is large, and is magnified if the value of ρ_0 is not exactly consistent with the data for $S_1(k_1)$. In order to check the data computed from (56), $I_{9c}(k)$ was computed for $k = .5, 1, 1.5, 2, 2.5$, and 3Å^{-1}. The values of $I_{9a}(k)$ derived from (56) and (57) are compared in Table 4.

Table 4

k (Å^{-1})		0	0.5	1.0	1.5	2.0	2.5	3.0
$I_{9a}(k)$	(56)	1.000	.782	.285	-.223	-.240	.082	.145
$I_{9a}(k)$	(57)	1.000	.788	.245	-.222	-.251	-.005	.142

The discrepancy at $k = 1.0\text{Å}^{-1}$ is slightly disturbing, since I_{9c} converges well there and I_{9b} is very small. The sign and magnitude of the error, which is probably in the value derived from (57), can be accounted for by the fact that our curve for S_1 does not have the correct slope at the origin (see Appendix C). The agreement at $k = 1.5$, 2.0, and 3.0Å^{-1} is much better than we have a right to expect; the disagreement at $k = 2.5\text{A}^{-1}$ could easily arise from the fact that the integral (59) was cut off at a finite value of k_1. We adopt the values given by (56).

Since $p_1(r_{12}) = \rho_o(1 + p_2(r_{12}))$, the first integral in (54) becomes

$$\rho_o \int e^{i\underline{k}\cdot\underline{r}_{12}}\, g_1(\underline{r}_{32})\, p_1(r_{32})\, (1 + p_2(r_{12}))\, p_2(r_{13})\, d\underline{r}_{21} d\underline{r}_{31}$$

$$= \rho_o \int e^{i\underline{k}\cdot\underline{r}_{12}}\, g_1(\underline{r}_{32}) p_1(r_{32}) p_2(r_{13})\, d\underline{r}_{21}\, d\underline{r}_{31}$$

$$+ \rho_o \int e^{i\underline{k}\cdot\underline{r}_{12}}\, g_1(\underline{r}_{32}) p_1(r_{32}) p_2(r_{12})\, p_2(r_{13})\, d\underline{r}_{21}\, d\underline{r}_{31} \,. \qquad (60)$$

The first integral on the right in (60) can be done by writing $e^{i\underline{k}\cdot\underline{r}_{12}} = e^{i\underline{k}_1\cdot\underline{r}_{13}}\, e^{i\underline{k}\cdot\underline{r}_{32}}$ and using the new integration variables $\underline{r}_{31}$ and $\underline{r}_{32}$. The result is

$$\int e^{i\underline{k}\cdot\underline{r}_{12}}\, g_1(\underline{r}_{32}) p_1(r_{32}) p_2(r_{13})\, d\underline{r}_{21}\, d\underline{r}_{31} = \frac{4\pi\rho_o i}{k}\, S_1(k)\, I_{9a}(k). \qquad (61)$$

In the second integral on the right in (60) we use the integration variables $\underline{r}_{21}$ and $\underline{r}_{32}$; Fourier analyzing $p_2(r_{13})$ we obtain

$$\int e^{i\underline{k}\cdot\underline{r}_{12}}\, g_1(\underline{r}_{32}) p_1(r_{23}) p_2(r_{12}) p_2(r_{13})\, d\underline{r}_{21}\, d\underline{r}_{31}$$

$$= \frac{-i}{\pi\rho_o} \int_o^\infty \int_o^\pi dk_1\, d\theta\, k_1\, S_1(k_1)\, S_1(|\underline{k} + \underline{k}_1|)\, I_{9a}(k_1) \cos\theta \sin\theta \qquad (62)$$

where θ is the angle between $\underline{k}$ and $\underline{k}_1$. If we let

$$u = |\underline{k} + \underline{k}_1| = (k^2 + k_1^2 + 2k\, k_1 \cos\theta)^{1/2}$$

the right side of (62) becomes

$$\frac{-i}{2\pi\rho_o}\, \frac{1}{k^2} \int_o^\infty \frac{dk_1}{k_1}\, I_{9a}(k_1)\, S_1(k_1) \int_{|k-k_1|}^{k+k_1} S_1(u)(u^2-k^2-k_1^2)u\, du \qquad (63)$$

Since

$$\int_0^\infty dk_1\ f(k_1) \int_{|k-k_1|}^{k+k_1} g(u)\ du = \int_0^\infty du\ g(u) \int_{|k-u|}^{k+u} f(k_1) dk_1 ,$$

a numerical integral like (63) can be done in several different ways. One should look for the way which converges fastest, is least sensitive to information which we do not know (like the value of $S_1(u)$ for large u), and does not involve small differences of big terms. For example, one should avoid dealing with the indefinite integral of $S_1(u)\, u^3$, since it oscillates badly for large u; hence (63) is not convenient to use as it stands. Probably the best form of (63) is

$$\frac{-i}{2\pi \rho_o k^2} \left[\int_0^\infty u S_1(u)(u^2-k^2)\ du \int_{|u-k|}^{u+k} \frac{dk_1}{k_1}\ I_{9a}(k_1)\ S_1(k_1) \right.$$

$$\left. - \int_0^\infty u S_1(u)\ du \int_{|u-k|}^{u+k} dk_1\ k_1\ I_{9a}(k_1)\ S_1(k_1) \right]$$

$$\equiv \frac{-i}{2\pi \rho_o k^2} \left[I_{9f}(k) - I_{9g}(k) \right] \tag{64}$$

In this form, the inside integral acts as a convergence factor for the integrand of the outside integral, and the answer is not sensitive to the values of $S_1(u)$ for large u. The inside integral can be tabulated once and for all as an indefinite integral; thus, the evaluation of (64) involves only a single numerical integration for each value of k.

We define

$$I_{9d}(x) \equiv \int_{0.2}^{x} \frac{dk}{k}\ I_{9a}(k)\ S_1(k)$$

$$I_{9e}(x) \equiv \int_0^x dk\ k\ I_{9a}(k)\ S_1(k) \quad . \tag{65}$$

I_{9d} and I_{9e} are tabulated in Tables 5 and 6. In evaluating $I_{9d}(k)$ for $0 < k \leq 0.6\text{Å}^{-1}$, $S_1(k)$ was taken as $-1 + .212k$ and $I_{9a}(k)$ was taken as $\sin(2.4k)/2.4k$. From (58) and (59) there follow immediately

$$I_{9f}(k) = \int_0^\infty S_1(u)\, u(u^2-k^2)\, du\, [I_{9d}(u+k) - I_{9d}(|u-k|)$$

$$I_{9g}(k) = \int_0^\infty S_1(u)\, udu[I_{9e}(u+k) - I_{9e}(|u-k|)] \qquad . \qquad (66)$$

The integrand of I_{9f} is perfectly well-behaved as $u \to k$, since $\lim_{\varepsilon \to 0} \varepsilon \log \varepsilon = 0$. The integrand of I_{9f} was evaluated at intervals of 0.1Å^{-1}, except for $k - 0.2 \leq u \leq k + 0.2$, where intervals of 0.04Å^{-1} were used. Intervals of 0.1Å^{-1} were used in evaluating I_{9g}. Both integrals converge very well, and their values are given in Table 7.

Table 7

k (Å^{-1})	1.2	1.6	1.8	2.0	2.2	2.4
$I_{9f}(k)$ (Å^{-4})	-.019	-.387	-.406	-.364	-.086	.155
$I_{9g}(k)$ (Å^{-4})	.172	.089	.031	-.017	-.048	-.054

If (48) were used to estimate $I_9\ (k)$, the result would be

$$I_9\ (k) \simeq -2i \int e^{i\underline{k}\cdot\underline{r}}\, p_1(r)\, d\underline{r} \int g_1(\underline{r})\, p_1(r)\, d\underline{r} = 0.$$

As in the case of I_3, the question arises: how much of the non-zeroness of $I_9(k)$ is real, and how much is due to the failure of our approximate ρ_3 to satisfy (45)? The analysis proceeds exactly as with I_3, and we find that the quantity

Table 5

Table of $I_{9d}(x) = \int_{0.2}^{x} \frac{dk}{k} I_{9a}(k)\, S_1(k)$

$x(\text{Å}^{-1})$	$I_{9d}(x)$
0.04	1.5608
0.08	0.8757
0.12	0.4822
0.16	0.2083
0.2	0.0000
0.3	-0.3618
0.4	-0.5984
0.5	-0.7635
0.6	-0.8810
0.7	-0.9675
0.8	-1.0286
0.9	-1.0710
1.0	-1.0985
1.1	-1.1145
1.2	-1.1214
1.3	-1.1215
1.4	-1.1173
1.5	-1.1111
1.6	-1.1049
1.7	-1.0999
1.8	-1.0973
1.9	-1.0977
2.0	-1.1002
2.1	-1.1031
2.2	-1.1051
2.3	-1.1059
2.4	-1.1060
2.5	-1.1058
2.6	-1.1056
2.7	-1.1054
2.8	-1.1054
2.9	-1.1054
3.0	-1.1055
3.1	-1.1057
3.2	-1.1059
3.3	-1.1061
3.4	-1.1062
3.5	-1.1063
3.6	-1.1063
3.7	-1.1062
3.8	-1.1061
3.9	-1.1061
4.0	-1.1061
4.1	-1.1061
4.2	-1.1062
4.3	-1.1063
4.4	-1.1064
4.5	-1.1065
4.6	-1.1066
4.7	-1.1066
4.8	-1.1066
4.9	-1.1065
5.0	-1.1065
5.1	-1.1064
5.2	-1.1064
5.3	-1.1064
5.4	-1.1064
5.5	-1.1064
5.6	-1.1064
5.7	-1.1064
5.8	-1.1064
5.9	-1.1064
6.0	-1.1063
6.1	-1.1063
6.2	-1.1063
6.3	-1.1063
6.4	-1.1062
6.5	-1.1062
6.6	-1.1062
6.7	-1.1062
6.8	-1.1062
6.9	-1.1062
7.0	-1.1062

Table 6

Table of $I_{9e}(x) = \int_0^x dk\, k\, I_{9a}(k)\, S_1(k)$

$X(\AA^{-1})$	$I_{9e}(x)(\AA^{-2})$	$X(\AA^{-1})$	$I_{9e}(x)(\AA^{-2})$
0.0	.00000	3.6	-.27344
0.1	-.00488	3.7	-.27282
0.2	-.01901	3.8	-.27182
0.3	-.04125	3.9	-.27090
0.4	-.06992	4.0	-.27073
0.5	-.10340	4.1	-.27151
0.6	-.13944	4.2	-.27292
0.7	-.17525	4.3	-.27297
0.8	-.20898	4.4	-.27680
0.9	-.23895	4.5	-.27860
1.0	-.26327	4.6	-.27975
1.1	-.28037	4.7	-.28014
1.2	-.28907	4.8	-.27978
1.3	-.28896	4.9	-.27879
1.4	-.28108	5.0	-.27748
1.5	-.26798	5.1	-.27622
1.6	-.25296	5.2	-.27254
1.7	-.23949	5.3	-.27456
1.8	-.23192	5.4	-.27346
1.9	-.23372	5.5	-.27265
2.0	-.24334	5.6	-.27271
2.1	-.25532	5.7	-.27285
2.2	-.26439	5.8	-.27296
2.3	-.26847	5.9	-.27290
2.4	-.26896	6.0	-.27257
2.5	-.26785	6.1	-.27191
2.6	-.26631	6.2	-.27092
2.7	-.26515	6.3	-.26973
2.8	-.26470	6.4	-.26846
2.9	-.26502	6.5	-.26724
3.0	-.26600	6.6	-.26612
3.1	-.26761	6.7	-.26522
3.2	-.26948	6.8	-.26461
3.3	-.27119	6.9	-.26430
3.4	-.27257	7.0	-.26423
3.5	-.27339		

$$I_{9h}(k) = -2i\rho_o \int e^{i\underline{k}\cdot\underline{r}_{32}} g_1(\underline{r}_{32})\, p_1(r_{32})\, p_2(r_{31})\, p_2(r_{12})\, d\underline{r}_{32}\, d\underline{r}_{12}$$

$$= \frac{4}{\pi\rho_o} \int_0^\infty p_1(r)\, j_1(kr)\, I_{3f}(r)\, dr \qquad (67)$$

should be subtracted from (54). Table 8 gives values of $I_{9h}(k)$.

Table 8

k $(\mathring{A}^{-1})$	1.2	1.6	1.8	2.0	2.2	2.4
$I_{9h}(k)$ $(\mathring{A}^{-2})$	.0153	-.0005	-.0069	-.0094	-.0079	-.0041

Combining equations (54) - (67) we obtain

$$I_9(k) = \frac{8\pi\rho_o}{k} I_{9a}(k)\, S(k) + \frac{1}{\pi k^2}\left[I_{9g}(k) - I_{9f}(k)\right] - I_{9h}(k). \qquad (68)$$

Table 9 gives values of $I_9(k)$.

Table 9

k $(\mathring{A}^{-1})$	1.2	1.6	1.8	2.0	2.2	2.4
$I_9(k)$ $(\mathring{A}^{-2})$	.0367	-.0051	-.0352	-.0471	-.0267	-.0023

Comparison of Tables 8 and 9 shows that the correction I_{9h} is not negligible. The size of the correction term at $k = 2.4\mathring{A}^{-1}$ indicates that the fractional error in $I_9(2.4)$ is large. For $k > 2.2A^{-1}$, however, the energies which we shall compute are so high as to make that portion of the spectrum physically uninteresting.

Using (27), we can write I_5 as

$$I_5 = \int_0^\infty p_1(r)\,[\nabla g_1(\underline{r})]^2\,d\underline{r} + \left[\int_0^\infty e^{i\underline{k}\cdot\underline{r}}\,p_1(r)\,\nabla g_1(\underline{r})\,d\underline{r}\right]^2$$

$$+ \int e^{i\underline{k}\cdot\underline{r}_{23}}\,\nabla g_1(\underline{r}_{21})\cdot\nabla g_1(\underline{r}_{31})\,p_1(r_{21})p_1(r_{31})p_2(r_{23})\,d\underline{r}_{21}\,d\underline{r}_{31}$$

$$\equiv I_{5a} + I_{5b} + I_{5c} \quad . \qquad (69)$$

The oscillatory factor $e^{i\underline{k}\cdot\underline{r}_{23}}$ makes I_5 a likely candidate for (49), which says $I_5 \simeq I_{5a}$[*] . Since I_5 is independent of the direction of $\underline{k}$, we can average it over the directions; then the exponential is replaced essentially by $(kr_{23})^{-1}$ times some trigonometric function of r_{23}. If 2 and 3 do not coincide, then r_{23} must be at least 2.4Å, and the most important value of r_{23} is about 3Å because $p_1(r_{23})$ is maximum there. Therefore, when $k = 2\text{Å}^{-1}$, the term I_{5a}, which arises from the delta function in ρ_3, ought to be at least six times as large as $I_{5b}(k)+I_{5c}(k)$. In fact the estimate is a pessimistic one, since the radial oscillations of the trigonometric function further decrease the size of $I_{5b} + I_{5c}$. Even when $k = 1.2\text{Å}^{-1}$, we probably do not commit an important error if we neglect $I_{5b} + I_{5c}$. At the cost of considerable labor we shall compute $I_{5b} + I_{5c}$ when $k = 2\text{Å}^{-1}$ and verify that it can indeed be neglected.

I_{5a} has been evaluated in connection with I_4. From (29) and (23) we obtain

$$I_{5b}(k) = [8\pi\rho_0\, I_{2a}(k)]^2 \quad .$$

$I_{5c}(k)$ can be evaluated by the same methods used for I_9. The result is

---

[*] Compare (49) with the definition of I_5 in (23).

$$I_{5c}(k) = \frac{1}{(2\pi)^3\rho_o} \int d\underline{k}_1\, S_1(\underline{k}_1) \left| \int e^{i(\underline{k}+\underline{k}_1)\cdot\underline{r}}\, p_1(r) \quad g_1(\underline{r})\, d\underline{r} \right|^2$$

$$= 4\rho_o \Big[\frac{1}{k} \int_0^\infty S_1(u)\, u\, du \int_{|k-u|}^{k+u} x(I_{2a}(x))^2\, dx$$

$$+ \frac{3}{4k^3} \Big\{ \int_0^\infty S_1(u)\, u\, du (u^2-k^2)^2 \int_{|k-u|}^{k+u} (I_{2a}(x))^2\, dx/x$$

$$+ \int_0^\infty S_1(u)\, u\, du \int_{|k-u|}^{k+u} (I_{2a}(x))^2\, x^3\, dx$$

$$- 2 \int_0^\infty S_1(u)\, u\, du (u^2-k^2) \int_{|u-k|}^{u+k} (I_{2a}(x))^2\, x\, dx \Big\} \Big] \qquad (70)$$

The indefinite integrals

$$I_{5d}(y) \equiv \int_{0.1}^{y} [I_{2a}(x)]^2\, dx/x$$

$$I_{5e}(y) \equiv \int_{0}^{y} x[I_{2a}(x)]^2\, dx$$

$$I_{5f}(y) \equiv \int_{0}^{y} x^3[I_{2a}(x)]^2\, dx$$

are tabulated in Tables 10, 11, and 12. For $k = 2Å^{-1}$, I_{5c} was evaluated and is equal to $-.0013Å^{-6}$. Inserting values for I_{5a} and I_{5b} we find

$$I_5(2Å^{-1}) = .0119 + .0003 - .0013 = .0109Å^{-6} .$$

The smallness of I_{5b} and I_{5c} compared with I_{5a} confirms our previous statement that for values of k in the roton region, we can neglect I_{5b} and I_{5c}.

I_6 is estimated by (48) as zero. As in the case of I_3, it is important to find out whether I_6 is really small enough to be neglected. To obtain a more accurate estimate, we write

$$I_6 = I_{6a} + I_{6b}$$

where

$$I_{6a} = 2i \int e^{-i\underline{k}\cdot\underline{r}} g_1(r) \frac{\underline{k}}{k} \cdot \nabla g_1(\underline{r})\, p_1(r)\, d\underline{r}$$

$$I_{6b} = 2i \int e^{i\underline{k}\cdot\underline{r}_{13}} g_1(\underline{r}_{21}) \frac{\underline{k}}{k} \cdot \nabla g_1(\underline{r}_{13})\, p_1(r_{31}) p_1(r_{21}) p_2(r_{23}) d\underline{r}_{31} d\underline{r}_{21}$$

According to the discussion preceding (48), I_{6a} and I_{6b} will cancel each other almost completely, so I_6 is some fraction (probably about one fourth) of I_{6a}. Performing the angular integrations in I_{6a}, we obtain

$$I_{6a} = 8\pi \rho_o \int_0^\infty \frac{dr}{r^3} [1 + p_2(r)] [\frac{-2 \cos kr}{kr} + \frac{8 \sin kr}{(kr)^2} + \frac{18 \cos kr}{(kr)^3} - \frac{18 \sin kr}{(kr)^4}] \quad .$$

A rough numerical integration gives

$$I_{6a}(2Å^{-1}) \simeq -.003Å^{-5} \quad .$$

Hence $I_6(2Å^{-1}) \simeq -.001Å^{-5}$, and $kI_6 \simeq -.002Å^{-6}$ when $k = 2Å^{-1}$. Since $k^2 I_3 + I_4 + I_5 \simeq .040Å^{-6}$ near $k = 2Å^{-1}$, we can neglect kI_6 without much error.

Table 10

Table of $I_{5d}(x) = \int_{0.1}^{x} [I_{2a}(k)]^2 \frac{dk}{k}$

There may be a constant error in the entries, but differences are accurate within several per cent.

$X(\text{Å}^{-1})$	$I_{5d}(x)$	$X(\text{Å}^{-1})$	$I_{5d}(x)$
0.1	.0000000	3.6	.22330346
0.2	.0815563	3.7	0420
0.3	.1249223	3.8	0671
0.4	.1533629	3.9	0815
0.5	.1734620	4.0	0883
0.6	.1880746	4.1	0899
0.7	.1988190	4.2	0905
0.8	.2066684	4.3	0937
0.9	.2123168	4.4	1024
1.0	.2163147	4.5	1146
1.1	.2190579	4.6	1274
1.2	.2208564	4.7	1400
1.3	.2219375	4.8	1512
1.4	.2225223	4.9	1599
1.5	.2228040	5.0	1650
1.6	.2229109	5.1	1670
1.7	.2229347	5.2	1673
1.8	.2229398	5.3	1689
1.9	.2229578	5.4	1750
2.0	.2229996	5.5	1885
2.1	.2230593	5.6	2090
2.2	.2231261	5.7	2328
2.3	.2231826	5.8	2562
2.4	.2232237	5.9	2781
2.5	.2232392	6.0	2973
2.6	.2232591	6.1	3115
2.7	.2232690	6.2	3211
2.8	.2232729	6.3	3269
2.9	735	6.4	3298
3.0	7392	6.5	3304
3.1	7559	6.6	3307
3.2	7934	6.7	3324
3.3	8426	6.8	3352
3.4	8978	6.9	3407
3.5	9524	7.0	3462

Table 11

Table of $I_{5e}(x) = \int_0^x [I_{2a}(k)]^2 \, k \, dk$

$X(\text{Å}^{-1})$	$I_{5e}(x)(\text{Å}^{-2})$	$X(\text{Å}^{-1})$	$I_{5e}(x)(\text{Å}^{-2})$
0.0	.00000000	3.6	.04383225
0.1	.00054962	3.7	.04388444
0.2	.00216305	3.8	.04391964
0.3	.00473620	3.9	.04394113
0.4	.00811275	4.0	.04395141
0.5	.01208723	4.1	.04395398
0.6	.01642052	4.2	.04395478
0.7	.02088145	4.3	.04396085
0.8	.02522106	4.4	.04397681
0.9	.02923726	4.5	.04400090
1.0	.03278674	4.6	.04402794
1.1	.03576189	4.7	.04405489
1.2	.03809786	4.8	.04408049
1.3	.03975150	4.9	.04410139
1.4	.04079331	5.0	1408
1.5	.04136930	5.1	1899
1.6	.04161596	5.2	1980
1.7	.04167813	5.3	2021
1.8	.04169464	5.4	2198
1.9	.04175836	5.5	2603
2.0	.04191975	5.6	3236
2.1	.04217258	5.7	3997
2.2	.04247595	5.8	4774
2.3	.04279443	5.9	5525
2.4	.04308585	6.0	6200
2.5	.04330232	6.1	6714
2.6	.04343134	6.2	7080
2.7	.04350026	6.3	7305
2.8	.04352817	6.4	7417
2.9	.04353312	6.5	7449
3.0	.04353649	6.6	7465
3.1	.04355232	6.7	7536
3.2	.04358839	6.8	7661
3.3	.04364186	6.9	7925
3.4	.04370407	7.0	8198
3.5	.04376895		

Table 12

Table of $I_{5f}(x) = \int_0^x [I_{2a}(k)]^2 k^3 \, dk$

$x(\text{Å}^{-1})$	$I_{5f}(x)$ (Å^{-4})
0.0	.0000000
0.1	.0000055
0.2	.0000536
0.3	.0002364
0.4	.0006751
0.5	.0015008
0.6	.0028289
0.7	.0047254
0.8	.0072096
0.9	.0101470
1.0	.0133334
1.1	.0165891
1.2	.0196456
1.3	.0221909
1.4	.0240563
1.5	.0252398
1.6	.0258128
1.7	.0259810
1.8	.0260408
1.9	.0262662
2.0	.0268916
2.1	.0279617
2.2	.0293684
2.3	.0309810
2.4	.0325853
2.5	.0338725
2.6	.0347024
2.7	.0351803
2.8	.0353865
2.9	.0354251
3.0	.0354556
3.1	.0356055
3.2	.0359672
3.3	.0365341
3.4	.0372332
3.5	.0380053
3.6	.0388028
3.7	.0394949
3.8	.0399869
3.9	.0403033
4.0	.0404616
4.1	.0405027
4.2	.0405172
4.3	.0406283
4.4	.0409334
4.5	.0414120
4.6	.0419721
4.7	.0525547
4.8	.0431322
4.9	.0436220
5.0	.0439303
5.1	.0440542
5.2	.0440754
5.3	.0440870
5.4	.0441381
5.5	.0442595
5.6	.0444538
5.7	.0446979
5.8	.0449542
5.9	.0452114
6.0	.0454497
6.1	.0456379
6.2	.0457751
6.3	.0458628
6.4	.0459080
6.5	.0459212
6.6	.0459289
6.7	.0459601
6.8	.0460246
6.9	.0461415
7.0	.0462726

Estimation of I_7 by (48) gives

$$I_7 \simeq - 2(- \tfrac{4}{3} \pi \rho_o)\, 8\pi\rho_o\, I_{2a}(k) = \tfrac{1}{3} (8\pi\rho_o)^2\, I_{2a}(k) \quad . \qquad (71)$$

Considerations similar to those used in estimating I_6 show that (71) is accurate within about 25 per cent except when k is very near 1.7Å^{-1}, where $I_{2a}(k) = 0$. Since I_7 is small (about $.003\text{Å}^{-6}$) in the roton region, (71) is sufficiently accurate.

When k is in the roton region, the major portion of I_{10} comes from the term $\delta(\underline{r}_{12})\rho_3(2,3,4)$, which is contained in $\rho_4(1,2,3,4)$. When $r_{12} \neq 0$, the oscillations of $e^{i\underline{k}\cdot\underline{r}_{12}}$ make the contribution to the integral very small.* If we neglect all of ρ_4 except $\delta(\underline{r}_{12})\rho_3(2,3,4)$, we are making essentially the approximation which was used in I_5 and was shown to be very accurate there. We then obtain

$$I_{10} \simeq I_3 \qquad (72)$$

and our evaluation of the integrals in (23) is completed.

---

* If the integral

$$J(\underline{r}_{12}) = \frac{1}{\rho_o^2} \int \rho_4(1,2,3,4)\, g_1(\underline{r}_{31})\, g_1(\underline{r}_{42})\, d\underline{r}_3\, d\underline{r}_4$$

were to become large compared with I_3 as r_{12} grows large, then the growth of J might offset the oscillations of $\exp(i\underline{k}\cdot\underline{r}_{12})$ and (72) would be wrong. It is easy to see, however, that as 1 and 2 go farther apart, $J(\underline{r}_{12})$ approaches $[\int p_1(r)\, g_1(\underline{r})\, d\underline{r}]^2$, which is zero. Since the factorization of J into a product of two integrals becomes more nearly exact as r_{12} increases, it is very plausible that J decreases with increasing r_{12} and is largest when 1 and 2 coincide. In the latter case J is equal to I_3.

If one is skeptical about the accuracy of (72), there is a more rigorous way of dealing with I_{10}. $\mathcal{J}$ is a normalization integral and must therefore be positive for any real value of A. In (22b), $\mathcal{J}$ is expressed as a second degree polynomial in A. The requirement that this polynomial have no real root is

$$I_9^2 < 4 I_8 \, I_{10} \quad .$$

Since I_{10} and I_8 are positive, it follows that

$$I_{10} > I_9^2 / 4 I_8 \quad . \tag{72a}$$

If the right side of (72a) were used as an estimate of I_{10}, $\mathcal{J}$ would be lowered below its true value and the energy would be raised. The value of Δ resulting from (72a) is about 1.3° higher than that resulting from (72). In the roton region we believe (72) to be much more accurate than (72a), although a numerical demonstration of this fact would be very laborious. For very small k, (72) is very inaccurate; not only does the oscillation argument fail, but I_3 becomes much smaller than the right side of (72a).

For $k \geq 1.2 \text{Å}^{-1}$, the coefficient of A^2 in (22a) is estimated well by

$$k^2 \, I_3 + I_4 + I_{5a} + \frac{1}{3} \, (8\pi \rho_0)^2 \, I_{2a}(k) \quad .$$

We have omitted I_{5b}, I_{5c}, and kI_6, and have approximated I_7 by (71). I_{5c} and kI_6 have both been shown to be very small, and are both difficult to compute; omission of these terms simplifies the computation of the energy spectrum, and does not significantly change the location of the minimum. I_{5b} has been omitted for the sake of consistency, since it is even smaller than I_{5c}. After locating the minimum, we shall reinstate the omitted terms in our final computation of Δ. We estimate I_{10} by (72).

With the omissions and approximations mentioned in the preceding paragraph, we obtain

$$\frac{E(k)}{E_F(k)} < \frac{1 + A(I_1 + I_2) + A^2(k^2 I_3 + I_4 + I_{5a} + \frac{1}{3}(8\pi \quad {}_o)^2 I_{2a})}{1 + A\frac{kI_9}{I_8} + A^2k^2 \; \frac{I_3}{I_8}}$$

$$= \frac{1 + A(.186 + 1.117 I_{2a}(k)) + A^2(.0246 + .0045k^2 + 108 I_{2a}(k))}{1 + A\,\frac{kI_9(k)}{S(k)} + \frac{.0045k^2A^2}{S(k)}}$$

$$= \frac{E'(k)}{E_F(k)} \tag{73}$$

$E(k)$ is the true lowest energy of a state having momentum $\hbar \underline{k}$; $E_F(k)$ is Feynman's spectrum; i.e., $E_F(k) = \hbar^2k^2/2mS(k)$; $E'(k)$ is the spectrum we have computed, subject to the omission and approximations noted above.

For $k = 2Å^{-1}$, (73) becomes

$$\frac{E(k)}{E_F(k)} < \frac{1 + .149A + .0390A^2}{1 - .0753A + .0143A^2} \tag{74}$$

The first attractive feature of (74) is that the coefficients of A in the numerator and denominator have opposite signs, so that the denominator increases while the numerator decreases. The optimal value of A is $-3.4Å^3$, which is very close to the classical value $A_{c1} = -3.6Å^3$. The minimum value of $E'(2)/E(2)$ is .664, corresponding to $\frac{E'(2Å^{-1})}{k} = 12.7°K$.

Computation of the coefficients in (73) and minimization of the resulting expressions yields the results given in Table 13.

Table 13

k ($Å^{-1}$)	1.2	1.6	1.8	2.0	2.2	2.4
A($Å^3$)	-3.7	-3.8	-3.6	-3.4	-3.0	-2.5
$E'(k)/E_F(k)$	.504	.575	.595	.664	.736	.796
$E'(k)/k$ (°K)	12.5	13.4	12.0	12.7	17.0	31.0

We estimate the minimum value of $\frac{E'(k)}{k}$ as 12.0°K, corresponding to $k = 1.85\ Å^{-1}$. If we estimate $I_{5c}(1.85Å^{-1})$ and $I_6(1.85Å^{-1})$ by the values of the corresponding integrals at $k = 2Å^{-1}$, we find that the coefficient of A^2 in the numerator of (73) should be diminished by $.003Å^{-6}$ when $k = 1.85Å^{-1}$. This change lowers the energy by 0.5°K and we obtain as the final result of this computation

$$\frac{p_o}{\hbar} = 1.85Å^{-1} \qquad \frac{\Delta}{k} = 11.5°K \quad . \tag{75}$$

One might challenge the correctness of the results in Table 13 because $\frac{E'(k)}{E_F(k)}$ appears to decrease with decreasing k. In any correct theory $E'(k)/E_F(k)$ must approach unity for very small k because we cannot lower the energy of a phonon. By studying the behavior of the integrals in (23) for very small k, we have verified that our spectrum does indeed have the correct limiting behavior.* A more direct way of seeing the result is to look at (19)(or (18)) when k is very small. The correlation term $g(\underline{r}_{ij})$ is significant only when i and j are fairly close. But in this case $e^{i\underline{k}\cdot\underline{r}_i}$ and $e^{i\underline{k}\cdot\underline{r}_j}$ are almost equal because k is small, and hence the correlation terms cancel almost completely because g is odd. Thus, (19) is almost the same as (11) for small k, and leads to the same energy. The value of k where (19) and (11) become almost the same, however, is much smaller than 1.2Å^{-1}, where Table 13 stops.

For high k, $E'(k)/E_F(k)$ approaches unity because the approximation $\exp(i\Sigma\, g(\underline{r}_{ji})) \simeq 1 + i\,\Sigma\, g(\underline{r}_{ji})$ fails badly. We noted earlier that if we could compute with the wave function (18), the interference between terms with different i would vanish when k is large. If $E''(k)$ is the energy arising from (18), we should find that for large k

$$E''(k)/E_F(k) = .65$$

as in the foreign atom problem. It is amusing to conjecture on how much $E''(k)$ might lie below $E'(k)$ when $k = 1.8\text{Å}^{-1}$. In view of the accuracy of the approximation $\exp(i\,\Sigma\, g) = 1 + i\,\Sigma g$ in the foreign atom problem when $k < 2\text{Å}^{-1}$ (see footnote following our discussion of that problem), we do not believe that the difference would be appreciable.

The energy spectrum $E'(k)$ is shown in Fig. 13 as curve A.

---

* If $g(\underline{r})$ falls off sharply at large r, the analysis is simple. In our case the analysis is complicated by the slowness with which $\underline{k}\cdot\underline{r}/r^3$ falls off, but the ultimate result is the desired one.

We have also plotted

B: Feynman's spectrum $E_F(k)$,

C: de Klerk, Hudson, and Pellam's spectrum (eqn.(4)),

D: spectrum of the form (2), with $p_0/\hbar = 1.85Å^{-1}$ and μ chosen so that $\mu^{1/2} p_0^2$ has the same value as in C.

From the curvatures A, C, and D it is clear that our spectrum $E'(k)$ predicts too small a value of μ. In a computation of this sort, however, it is doubtful that the curvature has much significance.

Curve A brings out the fact that the "hump" between the phonon and roton regions is not nearly so high as one might expect. Consequently, when computing the specific heat or normal fluid density at temperatures high enough to excite rotons, it is probably also necessary to take into account the deviations of the phonon spectrum from linearity (and also the deviations of the roton spectrum from pure parabolic behavior). Qualitatively, it appears that such corrections might improve the agreement between the theoretical spectrum and the specific heat and second sound data.

The two major sources of error in our computation are

a) the absence of information about the true form of $\rho_3(1,2,3)$

and

b) the uncertainties in the data for $S_1(k)$ at large k (see Appendix C).

The most important uncertainty occasioned by (a) is in the value of I_9. Inclusion of the term I_{9h}, which is 20 per cent of I_9 when $k = 1.8Å^{-1}$, compensates for most of theerror caused by the approximation,

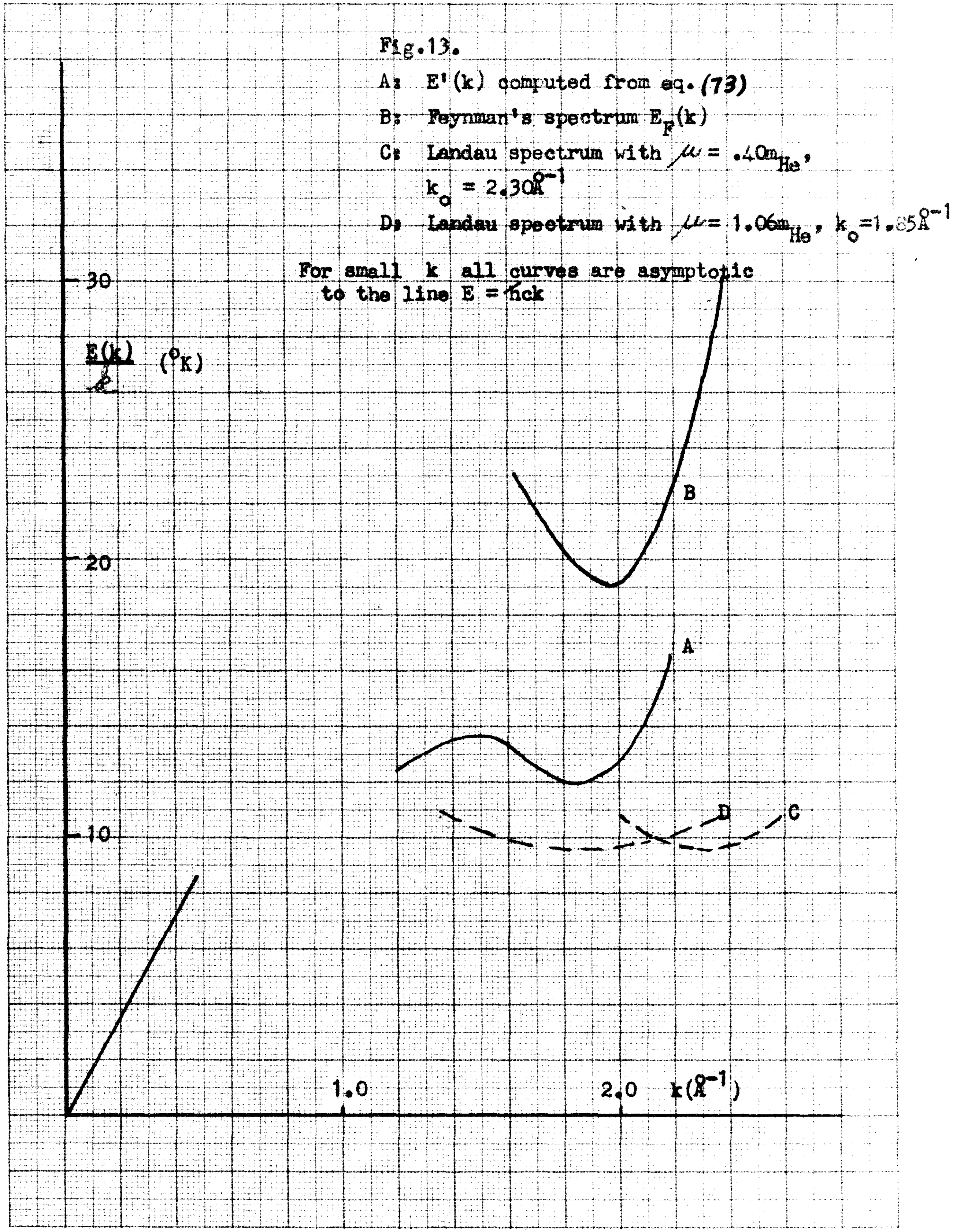


Fig.13.

A: $E'(k)$ computed from eq. (73)

B: Feynman's spectrum $E_F(k)$

C: Landau spectrum with $\mu = .40 m_{He}$, $k_o = 2.30 Å^{-1}$

D: Landau spectrum with $\mu = 1.06 m_{He}$, $k_o = 1.85 Å^{-1}$

For small k all curves are asymptotic to the line $E = \hbar ck$

(27). If I_{9h} were omitted completely, the value of Δ/k would be 0.7° lower. We believe, therefore, that the error in Δ/k due to (a) is less than 0.3°.

Considerable pains were taken to arrange the numerical work in such a way that the answers are insensitive to the behavior of $S_1(k)$ for large k. The residual error due to (b) is found mainly in the coefficient of A^2 in the numerator of (73). This coefficient may be in error by 5 per cent, and the resulting error in Δ/k might be as much as 0.5°.

We consider the value $\Delta/k = 11.5^{\circ}$ to be accurate within 0.6°, i.e. the lowest energy computable with the wave function (19) is between 10.9° and 12.1°. In the opinion of the author, the reduction of Δ/k from 19.1°K to 11.5° removes the major quantitative objection to Feynman's ideas about the nature of rotons. It is also the author's opinion that the labor involved in computing with a wave function more complicated than (19) would be unwarranted until something can be done to eliminate the errors (a) and (b).

APPENDIX A: PROOF OF NON-DEGENERACY OF THE GROUND STATE

It seems to be generally known that the ground state of any system is non-degenerate, provided the system is described by Schrodinger's equation and has no coordinates, such as spin, which do not appear in the equation. Although proofs of this theorem undoubtedly exist in the literature, the difficulty of finding them justifies the inclusion of a proof here.

If we can prove that the ground state wave function never assumes the value zero, then it must be non-degenerate. For if $\Psi_1(\underline{r})$ and $\Psi_2(\underline{r})$ both have energy E_o and are linearly independent, then we can construct a wave function $\Psi_2(\underline{r}_o)\,\Psi_1(\underline{r}) - \Psi_1(\underline{r}_o)\,\Psi_2(\underline{r})$ which vanishes at any desired position $\underline{r}_o$.

We work with the one-dimensional Schrodinger equation

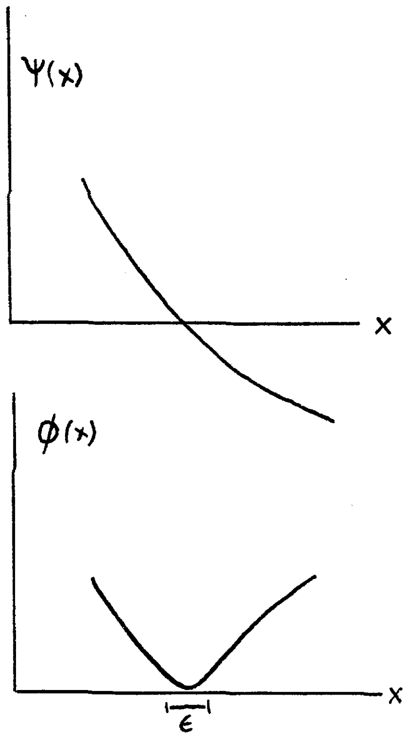
$$- \frac{h^2}{2m} \frac{d^2\Psi}{dx^2} + V(x)\,\Psi = E\Psi$$

Generalization to three dimensions and many particles is thoroughly straightforward. It is also assumed that V is finite. The lowest energy is the minimum value of

$$\frac{\mathcal{E}}{\mathcal{J}} = \frac{\frac{h^2}{2m} \int \left|\frac{d\Psi}{dx}\right|^2 dx + \int \Psi\,\Psi^*\,V(x)\,dx}{\int \Psi\,\Psi^*\,dx} .$$

Since the real part of the wave function satisfies Schrodinger's equation, we may assume that $\mathcal{E}/\mathcal{J}$ takes on its minimum value for some real Ψ. We now show that if Ψ has a zero, a new function can be constructed which will give a lower value of $\mathcal{E}/\mathcal{J}$.

If Ψ has a zero at x_0, we construct the function $\phi(x)$, which is equal to $|\Psi(x)|$ except in a region of length ε near x_0, where ϕ is rounded off to give it a smooth derivative. $\Psi'(x_0)$ is not zero, since Ψ is assumed to satisfy Schrodinger's equation and would be identically zero if it vanished simultaneously with its derivative. The normalization and potential energy integrals are changed by a quantity of order ε^3 when ϕ is used instead of Ψ. However, the average value of $|\phi'(x)|^2$ over the interval $(x_0 - \frac{\varepsilon}{2}, x_0 + \frac{\varepsilon}{2})$ is some finite fraction of $|\Psi'(x_0)|^2$ (the exact fraction depends on the shape of the round-off); hence the kinetic energy integral is decreased by a term of order ε, and ϕ would have a lower energy than Ψ.



APPENDIX B: EQUIVALENCE OF LONGITUDINAL SOUND WAVES WITH A SET OF OSCILLATORS

A continuous medium can be described by a vector field $\underline{x}(\underline{r},t)$, where $\underline{r} + \underline{x}(\underline{r},t)$ is the position at time t of the mass element which was at $\underline{r}$ at time $t = 0$. If the gradients of $\underline{x}$ are small, computation of the Jacobian of the transformation $\underline{r} \rightarrow \underline{r} + \underline{x}$ shows that the mass element which originally occupied a volume dV at $\underline{r}$ occupies a volume $dV' = dV(1 + \operatorname{div} \underline{x})$ at time t. If the mass density $\mu(\underline{r})$ originally had the equilibrium value μ_o everywhere, then $\mu_o dV = \mu(\underline{r})\ (1 + \operatorname{div} \underline{x})\ dV$, or

$$\frac{\mu(\underline{r})}{\mu_o} = 1 - \operatorname{div} \underline{x} \tag{76}$$

($\operatorname{div} \underline{x}$ is assumed small, so we can write $(1 + \operatorname{div} \underline{x})^{-1} = 1 - \operatorname{div} \underline{x}$). If the compressibility is given by $dp/d\mu = c^2$, then the work done in compressing (or expanding) dV into dV' is

$$\frac{1}{2} c^2(\mu - \mu_o)\ (dV - dV') = \frac{1}{2}\mu_o c^2(\operatorname{div} \underline{x})^2 dV$$

and the potential energy of the medium is $\frac{1}{2}\mu_o c^2 \int d\underline{r}(\operatorname{div} \underline{x}(\underline{r},t))^2$. In the same approximation the kinetic energy is given by $\frac{1}{2}\mu_o \int \dot{\underline{x}}^2(\underline{r},t) d\underline{r}$.

If periodic boundary conditions are imposed on the liquid in a box of volume V, $\underline{x}(\underline{r},t)$ can be expanded in a Fourier series

$$\underline{x}(\underline{r},t) = \sum_{\underline{k}} \underline{g}(\underline{k},t)\ e^{i\underline{k}\cdot\underline{r}}$$

where $\underline{k}$ runs over all the wave vectors which fit the box and

$$\underline{g}(\underline{k},t) = \frac{1}{V} \int \underline{x}(\underline{r},t)\ e^{-i\underline{k}\cdot\underline{r}} d\underline{r} = \underline{g}^*(-\underline{k},t).$$

In terms of these new coordinates, the kinetic and potential energies assume the forms

$$\text{K.E.} = \frac{1}{2}\mu_o V \sum_{\underline{k}} |\dot{\underline{g}}(\underline{k},t)|^2$$

$$\text{P.E.} = \frac{1}{2}\mu_o V c^2 \sum_{\underline{k}} |\underline{k} \cdot \underline{g}(\underline{k},t)|^2 \quad .$$

We can write $\underline{x} = \underline{x}_1 + \underline{x}_2$ where curl $\underline{x}_1 = 0$ and div $\underline{x}_2 = 0$. Correspondingly, $\underline{g} = \underline{g}_1 + \underline{g}_2$ where $\underline{k} \times \underline{g}_1 = 0$, $\underline{k} \cdot \underline{g}_2 = 0$, $\underline{g}_1 \cdot \underline{g}_2 = 0$. The energy can be expressed as

$$E = \frac{1}{2}\mu_o V \sum \dot{g}_1 \cdot \dot{g}_1^* + \frac{1}{2}\mu_o Vc^2 \sum k^2 g_1 \cdot g_1^* + \frac{1}{2}\mu_o V \sum \dot{g}_2 \cdot \dot{g}_2^* \, .$$

No potential energy is associated with the displacement field $\underline{x}_2$, which represents pure shear. In section II of this thesis we have reproduced Feynman's "proof" that in a Bose liquid any excitation which does not involve large-scale changes of density must have an energy greater than some minimum value. Consequently, at very low temperatures the shear modes can be omitted from the Hamiltonian. This argument does not apply to the Fermi or classical liquid.

With the omission of the shear modes, the energy is the same as that of a collection of oscillators. For future reference, we re-express the energy in terms of the coordinates $q_{\underline{k}}$ which are used in section II. If $\rho(\underline{r})$ is the number density of atoms at $\underline{r}$, then $\mu(\underline{r}) = m\rho(\underline{r})$. If we define

$$q(\underline{k},t) = \int \rho(\underline{r},t)\, e^{i\underline{k}\cdot\underline{r}}\, d\underline{r},$$

then (76) implies, for $\underline{k} \neq 0$,

$$\frac{1}{\rho_o V} q^*(\underline{k},t) = -i\underline{k}\cdot\underline{g}(\underline{k},t).$$

The energy then takes the form

$$E = \frac{1}{2}\sum_{\underline{k}} m_{\underline{k}}[\dot{q}(\underline{k},t)\ \dot{q}^*(\underline{k},t) + \omega_{\underline{k}}^2\ q(\underline{k},t)\ q^*(\underline{k},t)] \tag{77}$$

where $\omega_{\underline{k}} = ck$ and $m_{\underline{k}} = m/\rho_o Vk^2 = m/Nk^2$.

APPENDIX C: DISCUSSION OF S(k) and p(r)

The curve for $S(k)$ given in Fig. 5 is essentially that obtained from x-ray scattering by Reekie and Hutchison.* The proper normalization of the data can, in principle, be determined from the fact that $S(k) \to 1$ as $k \to \infty$. According to Goldstein and Reekie [14], "limitations inherent in the very low scattering cross section of liquid helium and the experimental technique have prevented effective exploration (of the range $k > 6\text{Å}^{-1}$)". Since $S(k)$ is still oscillating strongly at $k = 6\text{Å}^{-1}$, the normalization of $S(k)$ is uncertain by a few per cent. For $k \gtrsim 2.5\text{Å}^{-1}$, the per cent error in $S(k) -1$ is large, and our computations would be totally unreliable if the integrals had not been set up in such a way as to be insensitive to the behavior of $S(k) - 1$ for large k. We feel intuitively that $S(k)$ ought to oscillate about its asymptotic value, and have therefore taken $S(k) = 1$ at a point whose ordinate is the average of the values of $S(k)$ at the minimum near 3.4Å^{-1} and the maximum near 4.6Å^{-1}. With Reekie's normalization, $S(k)$ is unity at an ordinate much nearer to the minima of the oscillations. Our normalization maximizes the cancellation at large k when we are performing integrals whose integrand contains $S(k) - 1$ as a factor. Since $S(k)$ is the Fourier transform of $p(r)$, we find (see (36) and (39))

$$-2\pi^2 \rho_0 = \int_{0^+}^{\infty} k^2 (S(k) - 1)\, dk \qquad (78)$$

The relation (78) might serve as a test of the normalization of $S(k)$,

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* Their conclusions about $p(r)$ are given in Ref. [16], which does not include their data on $S(k)$. We are indebted to Dr. Reekie for sending us the data, which is now generally available in Ref. [14].

were it not for the fact that the numerical integral gives no sign of converging if we cut it off at $k = 6\text{Å}^{-1}$. The left side of (78) is equal to $-.43\text{Å}^{-3}$. With our normalization, integration of the right side out to $k = 6\text{Å}^{-1}$ gives $+.44A^{-3}$, but the integrand is still oscillating wildly and there is a chance of ultimately converging to a correct answer. With Reekie's normalization, integration of the right side out to $k = 6\text{Å}^{-1}$ gives a positive value much larger than $+.44\text{Å}^{-3}$, and the contribution from $k > 6\text{Å}^{-1}$ will also be positive unless the successive minima of $S(k)$ cease to be closer and closer to the asymptotic value of unity. At any rate, the consistency of the results which we have obtained by performing the same integral in coordinate and momentum space (see, for example, Table 2) convinces us that our $S(k)$ is sufficiently accurate for the present computations.

Most of the curve in Fig. 5 represents data taken at 2.06°K. According to [14], there is very little change in the values of $S(k)$ for $k > 0.9\text{Å}^{-1}$ as the temperature decreases from 2.5°K to 1.25°K. Therefore, in the range $k > 0.9\text{Å}^{-1}$, it is probably safe to represent the zero-temperature structure factor $S(k)$ by the data taken at 2.06°K. For $k < 0.9\text{Å}^{-1}$, the temperature dependence of $S(k)$ is more important, and it is necessary to extrapolate $S(k)$ linearly to zero by using (14a). We have done this, using a slope about 20 per cent higher than the theoretical value in order to join the experimental data smoothly. The error thus introduced is small.

The argument used to derive (14a) also yields the behavior of $S(k)$ for small k when $T \neq 0$. In the latter case, the oscillator representing phonons of wave number $\underline{k}$ is no longer necessarily in its ground state, but may be in its n^{th} excited state with probability proportional to exp $(-E_n/k\,T)$. It follows that $(\beta \equiv 1/k\,T)$

$$S(k) = \frac{\hbar k}{2mc} \coth \frac{1}{2} \beta \hbar ck \tag{79}$$

$$= \frac{1}{\beta\, mc^2} + \frac{1}{12} \beta \frac{\hbar^2 k^2}{m} - \dots \tag{79a}$$

From (79) there follows immediately the famous formula

$$\lim_{k \to 0} S(k) = \rho_o k\, T\, X_T$$

where ρ_o is the number density and X_T the isothermal compressibility of the liquid. When $\hbar ck$ becomes greater than $k\,T$, (79) becomes essentially linear in k. Strictly speaking, however, $S(k)$ starts quadratically from a non-zero value except when $T = 0$. The possibility of a linear behavior of $S(k)$ for small k, as predicted by (14a) when $T = 0$, has been sometimes questioned on the basis of (14). From (14) it follows that

$$S(k) - 1 = 4\pi \int_{0^+}^{\infty} (p(r) - \rho_o) \frac{\sin(kr)}{kr} r^2\, dr \tag{81}$$

Since $p(r) - \rho_o$ approaches zero for large r, it is argued that it is legitimate to expand $\sin(kr)/kr$ as $1 - \frac{(kr)^2}{6} + \cdots$. Integrating term by term, one finds

$$S(k) - 1 = C_1 + C_2 k^2 + \cdots \tag{81a}$$

where $C_1 = 4\pi \int_{0^+}^{\infty} (p(r) - \rho_o)\, r^2\, dr$ and $C_2 = -\frac{4\pi}{6} \int_{0^+}^{\infty} (p(r) - \rho_o) r^4 dr$.

Hence it appears that $S(k)$ always starts quadratically in k. The fallacy in the argument lies in the fact that $p(r)$ may not approach its asymptotic value fast enough, and the expansion may be meaningless. For example, if $p(r) - \rho_o$ decreases as r^{-3} for large r, (81) converges perfectly well but C_1 and C_2 are infinite. When $T = 0$, $p(r) - \rho_o$ falls off slowly enough to invalidate the expansion, and (14a) is correct; at any finite temperature $p(r) - \rho_o$ ultimately falls off exponentially and the expansion (81a) is legitimate. One might think that all the coefficients of (81a) can be determined by comparison with (79a); this is incorrect because (79) is wrong for large k. Using (80) and (81), however, we do obtain the important result

$$1 + 4\pi \int_{0^+}^{\infty} (p(r) - \rho_o)\, r^2\, dr = \rho_o k T X_T \quad , \qquad (82)$$

and when $T = 0$

$$1 + 4\pi \int_{0^+}^{\infty} (p(r) - \rho_o)\, r^2\, dr = 0 \quad . \qquad (83)$$

The result (82) can be obtained by rather simple classical arguments. Suppose we have a very large volume V of the liquid, and we consider a large sub-volume V_1 in the interior of the liquid. If ρ_o is the mean density of the liquid, the average number of atoms in V_1 is $\bar{N} = \rho_o V_1$. We are interested in computing the fluctuation of N, the number of atoms in V_1. This is $\overline{(N-\bar{N})^2} = \overline{N^2} - \bar{N}^2$ (a bar denotes "average value"). The volume V_1 can be subdivided into many small volumes Δ_i, each so small that there is no chance of finding two atoms both with their centers in the same Δ_i . For the i^th volume we can define a random variable X_i which is 1 if there is an atom centered in Δ_i, and zero otherwise. The average value of X_i is $\bar{X}_i = \rho_o \Delta_i$. If the cells Δ_i are small enough, the distance between an atom in cell i and an atom in cell j can be taken as the distance r_{ij} between the centers of the cells, and the definition of p(r) implies $\overline{X_i X_j} = \Delta_i \Delta_j \rho_o p(r_{ij})$. Since $N = \sum X_i$, it follows that

$$\frac{\overline{(N-\bar{N})^2}}{\bar{N}} = 1 + 4\pi \int_{0^+}^{\infty} (p(r) - \rho_o) r^2 \, dr \quad . \qquad (84)$$

The largeness of V_1 is invoked when extending the r-integration to infinity. Thus we see that (82) is really a theorem about density fluctuations in a large sub-volume of a liquid; the latter can be treated by statistical mechanics. Suppose that the liquid is bounded by a rigid closed cylinder of volume V with heat-conducting walls, the entire container being immersed in a heat bath at temperature T. If V is very large, we can mentally divide the cylinder into two volumes V_1 and V_2, both large but with $V_2 >> V_1$. The expected number of atoms in V_1 is $\bar{N}_1 = \rho_o V_1$. Any deviation of N_1 from $\bar{N}_1$ represents potential energy, for when we see such a deviation we can insert a thin piston between the two volumes and hold it in place while thermal equilibrium is re-established on both sides of the piston. Since the density of atoms is no longer the same on both sides, there is a resultant force on the piston and work can be extracted from it by allowing it to move slowly toward its new equilibrium position. If $V_2 >> V_1$, a fluctuation n in the number of atoms in V_1 produces no density or pressure change in V_2. The potential energy contained in such a fluctuation is easily computed to be $\frac{1}{2} \frac{n^2}{\bar{N}_1 \rho_o \chi_T}$, and Gibbsian statistics states that the probability of such a fluctuation is proportional to exp $(-\frac{1}{2}n^2/\bar{N}_1\,\rho_o\,X_T\,k\,T)$. One readily obtains

$$\frac{\overline{n^2}}{\bar{N}_1} = \rho_o k\,TX_T \qquad , \qquad (85)$$

and (82) then follows from (84). The result (85) was obtained by Smoluchowski [17] in 1908.

A casual observer might think that (83) is a simple consequence of the definition of $p(r)$. For if an atom is known to be at $\underline{r}_1$, the probability that there is an atom at $\underline{r}_2$ is $\frac{\rho_2(\underline{r}_1,\underline{r}_2)}{\rho_1(\underline{r}_1)}$. If $\underline{r}_1$ is not near the surface of the liquid, then $\rho_1(\underline{r}_1) = \rho_o$; if $\underline{r}_1$ and $\underline{r}_2$ are both far from the surface, then $\rho_2(\underline{r}_1, \underline{r}_2) = \rho_o p(r_{12})$. If we integrate $\frac{\rho_2(\underline{r}_1,\underline{r}_2)}{\rho_1(\underline{r}_1)}$ over all locations $\underline{r}_2$, excluding the point $\underline{r}_1$, the answer must be exactly N-1. But if we integrate $\rho_1(\underline{r})$ over all positions of $\underline{r}$, the answer is exactly N. Consequently

$$\int_{\underline{r}_2\neq\underline{r}_1} [\rho_2(\underline{r}_1,\underline{r}_2)/\rho_1(\underline{r}_1) - \rho_1(\underline{r}_2)]\, d\underline{r}_2 = -1 \; . \qquad (86)$$

If we take $\underline{r}_1$ far from the surface, $\rho_1(\underline{r}_1)$ can be replaced by ρ_o. Furthermore, the integrand is appreciable only when $\underline{r}_2$ is near $\underline{r}_1$, in which case $\frac{\rho_2(\underline{r}_1\underline{r}_2)}{\rho_1(\underline{r}_1)} - \rho_1(\underline{r}_2) = p(r_{12}) - \rho_o$ (there are no complications at the surface of the liquid since the surface corrections to both terms of the integrand are identical). Then (86) reduces exactly to (83).

Something must be wrong with the preceding argument at finite temperatures, since (83) is false if $T \neq 0$. The difficulty lies in the fact that, at finite T, the limiting value of $\frac{\rho_2(\underline{r}_1,\underline{r}_2)}{\rho_o}$ for large $\underline{r}_{12}$ is not ρ_o, but is slightly lower by an amount of order $1/N$. At high T, if there is known to be an excess density of atoms in a certain region, it is most likely that the excess was caused by a flux of atoms coming from far away; the most likely configuration of the far away atoms is one in which the density is uniform, but infinitesimally lowered to account for the atoms which have flowed into the region of excess density. At high T it is permissible to think of the atoms as classical hard spheres. If r_o is the radius of a sphere, then the centers of the spheres must always be at least $2r_o$ apart; the forbidden volume around an atom is $v_o = \frac{4}{3}\pi(2r_o)^3$. The actual volume per atom of the liquid, which we call v_A, is greater than v_o. If an atom is known to be at the origin, then an additional volume $v_A - v_o$ is available for the motions of the other atoms; hence the density far away is lowered by $\frac{v_A - v_o}{N}$. Actually, the atoms are not merely classical hard spheres, but have quantum-mechanical zero-point motions; in a classical picture the zero-point motion is equivalent to a soft repulsive potential outside the hard core. At high temperatures the soft potential is easily penetrated and can be ignored. As the temperature is lowered, the soft repulsive potential becomes more effective in keeping other atoms away, and the forbidden volume around an atom is greater than v_o by an amount $v_z(T)$. If an atom is known to be at the origin, the density far away is lowered by $\frac{v_A - v_o - v_z(T)}{N}$. When $T = 0$ the atomic volume of the liquid is completely determined by the zero-point motion (there is no other kinetic energy) and we have

$v_A = v_o + v_z(0)$. Then the asymptotic value of ρ_2/ρ_o is exactly ρ_o and (86) reduces to (83). When $T \neq 0$, however, there is a finite negative contribution to (86) from the region of very large r_{12} (i.e. the region where $\frac{\rho_2(\underline{r}_1,\underline{r}_2)}{\rho_o}$ has reached its asymptotic value, which is not necessarily equal to ρ_o). Since (86) is rigorously true, the integral $4\pi \int_{0^+}^{\infty} (p(r) - \rho_o)\, r^2\, dr$, which represents the contribution to the left side of (86) from the region where r_{12} is not very large, must be greater than -1; thus we arrive at (82) instead of (83).*

The simple counting argument which the "casual observer" used to prove (83) is actually correct when $T = 0$, because there is no change in the density far away when we localize an atom at the origin. For the same reason, we believe that any identity based on a counting argument becomes correct when $T = 0$. We therefore believe in the truth of the identity

$$\int_{\underline{r}_3 \neq \underline{r}_2, \underline{r}_1} d\underline{r}_3 \left[\frac{\rho_3(\underline{r}_1,\underline{r}_2,\underline{r}_3)}{\rho_o p(r_{12})} - \rho_o \right] = -2 \qquad (87)$$

although we cannot give a rigorous proof of it. Eqns. (83) and (87) are easily combined to give eqn. (45), which we have used in our work (one must remember that in (45) ρ_3 is defined to include a delta function on $\underline{r}_{23}$).

Reekie and Hutchison [16] have computed $p(r)$ for $r \leq 6$Å by inverting their data for $S(k)$. The curve for $p(r)$ which we have given in Fig. 4 is obtained from one of their graphs and, as has been previously mentioned, seems consistent with our curve for $S(k)$. The numerical inversion of diffraction data is not unambiguous, since the

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* The argument in this paragraph is due to R.P. Feynman. See also ref. [11], p. 266.

integrand of the relevant numerical integral is not small at the cut-off value $k = 6\text{Å}^{-1}$. Furthermore, an arbitrary cut-off procedure must be used to make $p(r)$ vanish for $r < 2.4\text{Å}$. More recently, Goldstein and Reekie [14] have employed an IBM 701 calculator to compute $p(r)$ out to 20Å, using the data of Reekie and Hutchison. Their article was not published until after the completion of the present calculation; the authors state that the results out to 6Å "fully confirm" the results of [16]. Goldstein and Reekie apply the integral test (82) to their curves for $p(r)$ and find satisfactory results. Since the integrands do not become small until $r \gtrsim 13\text{Å}$, we found it impossible to apply the test to the curve in Fig. 4.

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