

We may evaluate $g_2(x_0)$ in a similar way. From (4.11)

$$g_2(x_0) \equiv 1 - \frac{2}{x_0^2} \int_0^\infty \left\{ X[1 - 2f(X)] - \frac{x_0^2}{2x} [1 - 2f(x)] - x[1 - 2f(x)] \right\} dx$$

$$\cong 1 - \int_0^{\beta_c \hbar \omega} \left[\frac{2X}{x_0^2} - \frac{1 - 2f(x)}{x} - \frac{2x}{x_0^2} \right] dx$$

$$+ \frac{4}{x_0^2} \int_0^\infty [Xf(X) - xf(x)] dx. \quad (C3)$$

We again expand $f(X)$ in powers of e^{-X}

$$\frac{4}{x_0^2} \int_0^\infty Xf(X) dx = \frac{4}{x_0^2} \sum_{n=1}^\infty (-1)^{n+1} \times \int_0^\infty \exp \{ -n[(x^2 + x_0^2)]^{1/2} \} [(x^2 + x_0^2)]^{1/2} dx.$$

Substituting $x = x_0 \sinh y$

$$\frac{4}{x_0^2} \int_0^\infty Xf(X) dx = 4 \sum_{n=1}^\infty (-1)^{n+1} \times \int_0^\infty \exp(-nx_0 \sinh y) (1 + \sinh^2 y) dy$$

$$= 4 \sum_{n=1}^\infty (-1)^{n+1} \left[K_0(nx_0) + \frac{K_1(nx_0)}{nx_0} \right],$$

where $K_1(x)$ is the Hankel function of order one. The

remaining integrals of (C3) are easily evaluated. We find

$$g_2(x_0) = \frac{1}{2} + \ln(x_0/\beta_c \Delta_0) - 2\zeta(x)/x_0^2$$

$$= 4 \sum_{n=1}^\infty (-1)^{n+1} \left[K_0(nx_0) + \frac{K_1(nx_0)}{nx_0} \right], \quad (C4)$$

where $\zeta(x)$ is the Riemann zeta function.²⁷ The Hankel functions $K_\nu(x)$ are related to the Bessel functions of the third kind²⁸ $H_\nu(x)$ by

$$K_\nu(x) = (\pi i/2) e^{\nu\pi i/2} H_\nu^{(1)}(ix).$$

The Hankel functions decrease exponentially for large values of the argument allowing the summations to be truncated at $n \sim 5/x_0$. The functions $g_1(x_0)$ and $g_2(x_0)$, calculated from (C2) and (C4) are given in Figs. 1 and 2. Using these functions and (4.13), we can calculate the free energy as a function of Δ in the absence of external fields or currents. The free energy as a function of Δ for $N(0)V = 0.3$ is given in Fig. 3. Finally, we can find the free energy as a function of Δ when both a magnetic field and current flow are present, and minimize this free energy with respect to Δ to determine the gap Δ in the presence of the field and current. The energy gap as a function of the field has been determined, for $N(0)V = 0.3$, with the free energy given by (4.13) and (5.1), and is given by the solid lines in Fig. 5.

²⁷ E. Jahnke and F. Emde, *Tables of Functions* (Dover Publications, Inc., New York, 1945), p. 236.

²⁸ These functions are tabulated in reference 27, p. 236 and elsewhere.

Note on the Interactions between the Spins of Magnetic Ions or Nuclei in Metals

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THE coupling between spins of magnetic ions, or of nuclei, which results indirectly from the interaction of such spins with those of conduction electrons in metals has been the subject of a number of papers. Zener¹ proposed that this indirect mechanism is the cause of ferromagnetism. The corresponding calculation for nuclear spins was made still earlier

by Fröhlich and Nabarro.² The resulting nuclear coupling is, of course, very weak, but capable of detection in some metals by nuclear resonance. Calculations of the Zener-Fröhlich-Nabarro (ZFN) type are incomplete because they neglect the effect, essentially a second-order or polarization one, of the matrix elements which are nondiagonal in the

¹ C. Zener, *Phys. Rev.* **81**,440 (1951).

² H. Fröhlich and F.R.N. Nabarro, *Proc. Roy. Soc. (London)* **A175**, 382 (1940).

quantum numbers of the conduction electrons. The inadequacy is, in fact, apparent from the fact that such calculations give the physically unreasonable result of a coupling which is independent of distance. The proper calculations inclusive of both diagonal and nondiagonal effects were given by Kasuya³ for the electronic case, and a little later by Yosida⁴ in an illuminating paper which treated both electronic and nuclear moments. Prior to Yosida's paper, exactly the same formula for nuclear coupling was obtained by Ruderman and Kittel⁵ (RK) using a different order of integration over the coordinates of the conduction electrons. However, there was the apparent difference that the Yosida expression resulted from the inclusion of both the nondiagonal or polarization effect, and the static one, resulting from the redistribution of spins to minimize the energy in the ZFN manner. Ruderman and Kittel obtained the complete answer by apparently including only polarization effects. Consequently, from a too superficial examination of their paper, one might be naively inclined to add the ZFN terms to the RK expression, thus obtaining an erroneous result. The main purpose of the present note is to examine mathematically why Ruderman and Kittel obtained the complete answer in their simple procedure. Our analysis does not yield any new physical results, and serves instead as a review and critique of how the integration has been performed by the previous authors.

Ostensibly, we will treat the diagonal and nondiagonal contributions to the energy of interaction between ions or nuclei, and how these depend on distance. A closely related problem is that of the corresponding contributions to the spin density of the conduction electrons, and its spatial distribution. The integrals encountered in either problem are essentially the same, as is obvious from the fact that the final energy of the magnetic ion, or nucleus, is proportional to the local density of magnetic moment of the conduction electrons after they have been polarized and redistributed. Consequently, the reader should have no difficulty in transcribing our discussion to spin densities and how the polarization of the spin moment of the conduction electrons oscillates and drops off as the distance from the polarizing ion increases. We will assume for simplicity that in the electronic case, the exchange coupling between the spin of an ion and that of a conduction electron is isotropic, and that in the nuclear one, the coupling of the nuclear spin to that of the conduction electron

is of the Fermi contact type. We will further assume that the conduction electrons can be described by plane waves, and that the variation in the phase of the wave is negligible across the diameter of an atom (or, trivially, a nucleus).

We denote by \mathbf{s}_k the spin of a conduction electron whose orbital wave function is $e^{i\mathbf{k}\cdot\mathbf{r}}/V^{1/2}$ if the conductor occupies a volume V . The Hamiltonian function for our problem can be written as

$$\mathcal{H} = V^{-1} \sum_n \sum_{k,k'} e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}_n} a_k^* a_k C_n \mathbf{I}_n \cdot \mathbf{s}_k, \quad (1)$$

where a_k, a_k^* are creation and destruction operators for the orbital state k . In the nuclear case \mathbf{I}_n signifies, as usual, the nuclear spin of atom n . Our calculations apply equally well to the electronic case if, instead, we let \mathbf{I}_n denote the spin of a magnetic ion. The cross coupling between the electronic spin of a magnetic ion and the nuclear spin of another atom can be treated by using the corresponding different definitions of \mathbf{I} at the respective lattice sites.

If one uses the simple or naive theory that does not allow for the fact that the field at the nucleus is modified by polarization of inner shells by the conduction electrons, the explicit value of C_n in the nuclear case is

$$C_n = 16\beta_N\beta g_I/3.$$

Here β_N is the nuclear Bohr magneton, g_I the nuclear g factor, and β the usual Bohr magneton. The corresponding "naive" formula for C_n in the electronic case is

$$C_n = -2e^2 \int \dots \int \varphi_a^*(2) r_{12}^{-1} \varphi_a(1) d\tau_1 d\tau_2,$$

Here φ_a is the orbital wave function of one of the electrons with free spin. For simplicity we assume that all the electrons in closed shells are equivalent except for spatial orientation, which does not enter in our calculations as long as we neglect the modulation of the phase of the conduction electron across the atom.

Actually, polarization or screening effects make the effective values of C_n quite different from what one calculates with simple theory. In fact, experiments on the Knight shift show that sometimes even the sign of C_n is different. However, our calculation does not utilize the explicit values of C_n and merely requires that the Hamiltonian function have the general structure (1).

The various simplifying assumptions made above are introduced so we can exhibit as succinctly and simply as possible the complementary role of the diagonal and nondiagonal elements in the ensuing

³ T. Kasuya, Progr. Theoret. Phys. (Kyoto) 16, 45 (1956).

⁴ K. Yosida, Phys. Rev. 106, 893 (1957).

⁵ M. A. Ruderman and C. Kittel, Phys. Rev. 96, 99 (1954).

calculation. These calculations can, in principle, be readily extended to include such complications as anisotropic exchange or dipolar interaction, variation in phase of the conduction electron's wave function over an atomic distance or of its effective mass with velocity, overlap between the wave functions of different atoms, etc. We do not mean to imply that in these more complicated situations, one can necessarily obtain explicit formulas for the final coupling energy, but rather that the same general type of consideration as in the present paper applies to, and elucidates, the relative roles of the diagonal and non-diagonal members.

Fröhlich and Nabarro, or Zener, consider only what we call the diagonal part of the Hamiltonian function, or, in other words, in place of (1) they take

$$\mathcal{H} = \sum_n \sum_k C_n I_{z_n} s_{z_k} / V. \quad (2)$$

Equation (2) assumes that the direction of spatial quantization of the spin is along the z axis, as is, for instance, the case if a magnetic field is applied to lift the degeneracy, or if we imagine the coupling energy resulting from the model itself to give spontaneous magnetization in some direction. Actually, an applied field may not be present, and so use of (2) may well seem to introduce an ambiguity in direction at the outset. However, as we see later, the ambiguity disappears when the complete calculation is made in the Ruderman-Kittel or Kasuya-Yosida fashion.

The Hamiltonian function (2) is a purely static or diagonal one, and the same as though the conduction electrons were exposed to an effective magnetic field

$$H_{\text{eff}} = \sum_n C_n I_{z_n} / 2\beta V \quad (3)$$

independent of \mathbf{k} .

The density of allowed orbital states in \mathbf{k} space is $V/(2\pi)^3$, and the Fermi-Dirac statistics tell us that the number of electrons of given spin in a volume element of this space is

$$V(2\pi)^{-3} f(E_k \mp \beta H_{\text{eff}}) dk_x dk_y dk_z,$$

where the sign choice relates to the two spin orientations, E_k is the translational kinetic energy and

$$f(E) = 1/[1 + e^{(E-\epsilon)/kT}], \quad (4)$$

with ϵ the Fermi threshold. The magnetic moment is

$$M = V(2\pi)^{-3} \beta \iiint [f(E_k - \beta H_{\text{eff}}) - f(E_k + \beta H_{\text{eff}})] \times dk_x dk_y dk_z.$$

If we neglect higher order effects in H_{eff} the integrand is $-2\beta H_{\text{eff}} f'$ where f' denotes df/dE evaluated at $H_{\text{eff}} = 0$, $E = E_k$. Inasmuch as magnetic moment is generally connected with the free energy by the relation $M = -\partial F/\partial H$, giving $F = F_0 - \frac{1}{2}MH$, the change in energy⁶ caused by the effective field (3) is

$$\Delta F_{\text{diag}} = \frac{1}{2}V^{-1}(2\pi)^{-3} \sum_{n>m} C_n C_m I_{z_n} I_{z_m} \times \iiint f'(E_k) dk_x dk_y dk_z. \quad (5)$$

Here, and throughout the balance of the paper, we omit the terms $n = m$ in the double sum over the lattice sites, as these terms are an uninteresting additive constant or "self-energy."⁷ A subscript is attached to ΔF to emphasize that only the diagonal part (2) of Eq. (1) has been utilized.

If we introduce polar coordinates, integrate over the angles, and change variables from k to $E_k = \frac{1}{2}\hbar^2 k^2/m$, the triple integral in (5) reduces to

$$4\pi m \hbar^{-2} \int_0^\infty f' k dE_k.$$

At $T = 0$, and in fact at ordinary temperatures, f is appreciable only near the Fermi threshold $k = k_0$, so that k can be taken outside the integral. Then (5) becomes

$$\Delta F_{\text{diag}} = -V^{-1}(2\pi)^{-2} m \hbar^{-2} k_0 \sum_{n>m} C_n C_m I_{z_n} I_{z_m}. \quad (6)$$

The result (6) can also, of course, be obtained by the usual elementary argument⁸ in which one turns over electrons near the Fermi threshold until the change in Zeeman energy is just counterbalanced by the increase in translational energy for the last electron turned over. We derive (6) the way we do, because the intermediate form (5) is needed for comparison with our subsequent calculation.

The expression (6) gives an energy coupling the spins I_n and I_m . However, this energy is seen to be independent of the distance r_{nm} between sites n and m , but dependent on the bulk volume V of the metal, whereas one's physical intuition tells one that the

⁶ General thermodynamical considerations show that the statistical means taken in our various formulas such as (5), (7), etc. give the displacement in free rather than intrinsic energy due to the perturbation being considered. However, at ordinary temperatures with the Fermi-Dirac statistics, $T\partial F/\partial T$ is negligible compared with F , and so we generally use the word "energy" without a qualifying adjective.

⁷ Actually, the second-order perturbation theory which we subsequently use does not converge adequately to handle the "self" terms, as the expression (11) becomes infinite for $r_{nm} = 0$.

⁸ See, for instance, J. H. Van Vleck, *The Theory of Electric and Magnetic Susceptibilities* (Oxford University Press, New York, 1932), p. 350.

reverse should be true. It is thus clear that something has been left out, and this is the nondiagonal part of (1). This gives rise to a second-order perturbed energy

$$\Delta E_{k, s_k} = \sum_{k', s_{z_k}'} |\langle \mathbf{k} s_{z_k} | \mathcal{H} | \mathbf{k}' s_{z_k}' \rangle|^2 / (E_k - E_{k'})$$

for the state \mathbf{k}, s_{z_k} . The corresponding change in free energy is obtained by summing over all the \mathbf{k}, s_{z_k} states weighted by the Fermi-Dirac distribution. Summing over the different spin orientations has the effect of replacing $(\mathbf{I}_n \cdot \mathbf{s}_k)(\mathbf{I}_m \cdot \mathbf{s}_k')$ by $\frac{1}{2} \mathbf{I}_n \cdot \mathbf{I}_m$. When we remember that in the continuum model each orbital state corresponds to a volume $V/(2\pi)^3$ in \mathbf{k} space, we obtain

$$\Delta F = (2\pi)^{-6} \sum_{n>m} C_n C_m \mathbf{I}_n \cdot \mathbf{I}_m \Phi(r_{nm}), \quad (7)$$

where

$$\Phi(r_{nm}) = \int \dots \int \frac{\cos [(\mathbf{k} - \mathbf{k}') \cdot \mathbf{r}_{nm}] f(E_k)}{E_k - E_{k'}} dk_x \dots dk'_z \quad (8)$$

with \mathbf{r}_{nm} denoting the radius vector joining sites n and m . In principle, the integrand of (8) should contain a factor $[1 - f(E_{k'})]$ to allow for the fact that no transitions are possible to filled states, but this factor can safely be omitted, as the extra term which it adds to the integrand is an odd function of $(\mathbf{k} - \mathbf{k}')$ and so integrates to zero.

Ruderman and Kittel evaluate the sextuple integral (8) by using polar coordinates separately in \mathbf{k} and \mathbf{k}' space. When this is done, and the angular integrations are performed, (8) becomes at $T = 0$

$$\Phi(r_{nm}) = (2\pi)^2 r_{nm}^{-2} \times \int_{-k_0}^{k_0} k dk \int_{-\infty}^{\infty} \frac{e^{i(k-k')r_{nm}}}{(1/2)m^{-1}\hbar^2(k^2 - k'^2)} k' dk' \quad (9)$$

No physical significance can be attached to the negative values of k or k' in (9), but it is a mathematical convenience to express the results in terms of paths which are symmetrical about the origin, as exponential rather than trigonometric functions then appear in the integrand.

Ruderman and Kittel avoid the singularities of the integral in (9) by using principal values. If this is done, the fundamental theorem of contour integration shows us immediately that the integral over k' is equal to the negative of the sum of two integrals over two semi-circles of infinitesimal radius in the

complex k' plane centered at $k' = \pm k$. Thus (9) becomes

$$\Phi(r_{nm}) = -\frac{1}{2} (2\pi)^3 m \hbar^{-2} r_{nm}^{-2} \int_{-k_0}^{k_0} k \sin(2kr_{nm}) dk \quad (10)$$

On performing the elementary remaining integration there follows the final result

$$\Phi(r_{nm}) = \frac{1}{4} (2\pi)^3 m \hbar^{-2} r_{nm}^{-4} \times [2k_0 r_{nm} \cos(2k_0 r_{nm}) - \sin(2k_0 r_{nm})] \quad (11)$$

We shall not attempt to discuss the applicability of Eq. (11) to actual materials. Our attention is instead focused on the fact that one might naively suppose that since diagonal contributions should be included in addition to the nondiagonal ones, (6) should be added to (7). This is incorrect. From the form in which we have presented the calculations, it is easy to see why Ruderman and Kittel obtained the right answer inclusive of the diagonal terms even though they appear to have been omitted. We have only to write the integral (8) in the form

$$\Phi(r_{nm}) = \frac{1}{2} \int \dots \int \frac{[f(E_k) - f(E_{k'})] \cos [(\mathbf{k} - \mathbf{k}') \cdot \mathbf{r}_{nm}]}{E_k - E_{k'}} \times dk_x \dots dk'_z \quad (12)$$

The part of (7) attributable to diagonal terms should be stricken out and replaced by (5). The terms diagonal in \mathbf{k} correspond to a small volume element of size $(2\pi)^3/V$ enclosing the point $\mathbf{k}' = \mathbf{k}$ in k' space. (Actually we have a discrete sum over translational energy states, but with the continuum approximation each discrete state is identified with a cell of volume $(2\pi)^3/V$ in k or k' space.) In this small volume element the integrand of (12) is virtually equal to $f'(E_k)$, and so the part of (12) attributable to diagonal terms is $\frac{1}{2}(2\pi)^3/V$ times the triple integral entering in (5). Furthermore diagonality in s_z implies that the stricken portion of (7) involves only a factor $I_{z_n} I_{z_m}$ out of $\mathbf{I}_n \cdot \mathbf{I}_m$. Thus the part of (7) to be replaced by (5) is the same as (5). In other words, the contributions which Ruderman and Kittel, in a sense, improperly include as a nondiagonal term is nothing but the effect (5) of the diagonal terms computed in the ZFN fashion, and it is now clear why Ruderman and Kittel obtained the correct answer.

Those familiar with the general formalism of the theory of magnetic susceptibilities will recognize that our demonstration that the RK formula, in fact, includes properly both the diagonal and nondiagonal

effects is very similar to the proof⁹ that with ordinary Boltzmann distributions diagonal and nondiagonal matrix elements make exactly the same contribution to the susceptibility if the "line strength" is the same, and the energy transition associated with the off-diagonal element is small compared with kT . In our case we are dealing with Fermi-Dirac rather than Boltzmann statistics, and the contribution of the diagonal or near-diagonal elements is practically independent of temperature rather than proportional to $1/T$. Consequently the pairing of terms involved in transforming (8) into (12) can be profitably used right down to $T = 0$, whereas with Boltzmann statistics, where $f \sim e^{-E/kT}$, the replacement of a difference quotient by a derivative ceases to be valid for a near-diagonal element if the temperature is reduced sufficiently.

Of course at $T = 0$ the derivative f' becomes infinite at $k = k_0$ even in formulas such as (5), which we have used, but this fact causes no difficulty in the calculation, as then f' can be treated as a Dirac delta function of E . The susceptibility or free energy will approach continuously the limiting values at $T = 0$, and will differ but little from these values at ordinary temperatures. The Ruderman-Kittel procedure of taking f as either 0 or 1 is hence quite warranted.

The fact that the diagonal contribution just pieces out what is missing when the nondiagonal terms are rigorously handled is very clear in the way that Kasuya and Yosida (KY) perform the integration, which they do to bring out just this point. We believe, however, that the physical reason for the equivalent behavior of diagonal and nondiagonal terms of equal line strength is more apparent from the pairing procedure involved in (12) and in comparison with (5), than in the KY type of integration, in which the equivalence seems somewhat accidental, though it is perhaps quibbling to labor the point at all. Also, our proof of the equivalence is not specialized to $T = 0$.

What Kasuya, or Yosida, does is to change variables from \mathbf{k}, \mathbf{k}' to \mathbf{k}, \mathbf{q} with $\mathbf{q} = \mathbf{k}' - \mathbf{k}$. They integrate first over \mathbf{k} space, holding \mathbf{q} fast. This is most easily done in cylindrical coordinates, with the z axis parallel to \mathbf{q} . After the trivial integrations over k_ρ, k_z , Eq. (8) becomes at $T = 0$.

$$\Phi(r_{nm}) = -2\pi m\hbar^{-2} \iiint \cos(\mathbf{q} \cdot \mathbf{r}_{nm}) F(q) dq_x dq_y dq_z, \quad (13)$$

with

$$F(q) = \int_{-k_0}^{k_0} \frac{(k_0^2 - k_z^2)}{2qk_z + q^2} dk_z. \quad (14)$$

This integral diverges if $q \leq 2k_0$, and in this case the principal value is used; if this is done, then integration of (14) gives for all values of q

$$F(q) = \frac{1}{2} k_0 + \frac{1}{2q} (k_0^2 - \frac{1}{4} q^2) \ln \left| \frac{q + 2k_0}{q - 2k_0} \right|. \quad (15)$$

Actually, because the states are quantized, we should replace the integral (13) by a sum over the discrete permitted values of q . The term of type $q = 0$ multiplying the part $I_{z_n} I_{z_m}$ of $\mathbf{I}_n \cdot \mathbf{I}_m$ should be excluded, as it represents a diagonal rather than nondiagonal effect. As $F(0) = k_0$, and as each discrete term corresponds to a volume element $(2\pi)^3/V$ in the continuum approximation, the portion of (7) so excluded has precisely the value (6). So Kasuya and Yosida observe that one can use (13) in (7) without exclusion and forget (6).

After polar coordinates are introduced and the angular integrations are performed, (13) becomes

$$\Phi(r_{nm}) = (2\pi)^2 m\hbar^{-2} i^{-1} r_{nm}^{-1} \int_{-\infty}^{\infty} e^{i\mathbf{q} \cdot \mathbf{r}_{nm}} F(q) q dq. \quad (16)$$

The integral in (16) can be evaluated in terms of elementary functions by straightforward quadrature, as was done by Yosida, but this procedure is somewhat tedious because the path of integration must be split up into several sectors because of the absolute value sign in the argument of the logarithm entering in (15). However, this complication can be avoided, and the integration greatly simplified by a nice little application of contour integration. This observation is the final contribution of the present paper. The integral in (16) is only infinitesimally changed if we deform the path to go infinitesimally above a cut along the real axis extending from $q = -2k_0$ to $q = 2k_0$ in the complex q plane. Were there no absolute value signs, the integral would then be zero. This one sees by completing the contour with an infinite semicircle in the upper half of the q plane; the resulting contour incloses or contains no singularities since with our slightly deformed path the branch points of the logarithm in (15) are avoided, and there is no contribution from the infinite arc since $qF(q)$ vanishes like $1/q$ for large $|q|$. The integral entering in (16) is thus the same as the difference between the integral as it stands and the integral with the absolute value sign removed from the argument of the logarithm in (15). After this removal, the imaginary

⁹ See reference 8, p. 191.

part of the logarithm is πi for the part of the path just above the cut. The expression (16) is consequently.

$$\Phi(r_{nm}) = -\frac{1}{4} (2\pi)^3 m \hbar^{-2} r_{nm}^{-1} \int_{-2k_0}^{2k_0} (k_0^2 - \frac{1}{4} q^2) e^{iqr_{nm}} dq. \quad (17)$$

This integral is easy to evaluate. In fact, one sees immediately by changing the variable of integration

by a factor 2 and making a partial integration that (17) is equivalent to (10) and hence to (11). The final result is thus independent of the order of integration, as one expects.

The present paper was written while I was Eastman Visiting Professor at Oxford University, and the staff of the Clarendon Laboratory join me in extending heartiest congratulations to Professor Wigner on his sixtieth birthday.

Energy Spectrum of Elementary Excitations in Helium II*

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I. INTRODUCTION

THE elementary excitations in helium II have been the object of extensive study in the past twenty years. The phonon-roton type dispersion curve¹ was first introduced to account for superfluid properties and thermodynamic behavior of liquid helium below the λ transition line. Experiment² has confirmed the general dependence of excitation energy on momentum postulated on phenomenological grounds by Landau.¹ The direct observation of single excitations generated by inelastic neutron scattering yields the experimental dispersion curve shown in Fig. 1.

A quantum theory of the excitations exhibiting both the phonon and roton aspects of the phenomenological dispersion curve was first derived by Bijl³ and later with great clarity and simplicity by Feynman.⁴ Further development of the theory by Feynman and Cohen⁵ led to fair agreement with the phenomenological dispersion curve. In these calculations physically plausible trial wave functions are used to com-

pute the expectation value of the energy. A somewhat different type of calculation by Kuper,⁶ based on the evaluation of phonon-phonon interaction using the Rayleigh-Schrödinger perturbation formalism, gives similar results at the one point where the numerical evaluation was carried to completion. However, Kuper regarded the agreement as partly fortuitous and pointed out several deficiencies in the calculation, some unavoidable considering the state of the theory at that time and others due to the practical limitations of a hand calculation.

The theoretical description of a single excitation developed in references 3 and 4 can be extended in a systematic manner to an arbitrary number of excitations, provided that real and virtual processes in which excitations split and coalesce and scatter are neglected.⁷ In this approximation, the theory gives a "free phonon" description of the excitations with the energy formula

$$\epsilon_0(k) = \hbar^2 k^2 / 2MS(k) \quad (1)$$

plotted in Fig. 1 as the B-F curve. Here $\epsilon_0(k)$ is the energy of an excitation with momentum $\hbar\mathbf{k}$. The function $S(k)$ is the liquid structure factor derived from x-ray scattering data extrapolated to absolute zero.

We report in this paper on the evaluation of phonon-phonon interaction in the approximation of

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[†] National Science Foundation Predoctoral Fellow.

¹ L. Landau, *Phys. Rev.* **60**, 356 (1941).

² D. G. Henshaw and A. D. B. Woods, *Phys. Rev.* **121**, 1266 (1961); D. G. Henshaw and A. D. B. Woods, *Proceedings of Seventh International Conference on Low Temperature Physics* (University of Toronto Press, Toronto, 1961).

³ A. Bijl, *Physica* **7**, 869 (1940).

⁴ R. P. Feynman, *Phys. Rev.* **94**, 262 (1954).

⁵ R. P. Feynman and M. Cohen, *Phys. Rev.* **102**, 1189 (1956).

⁶ C. G. Kuper, *Proc. Roy. Soc. (London)* **A233**, 223 (1955).

⁷ H. W. Jackson and E. Feenberg, *Ann. Phys. (N. Y.)* **15**, 266 (1961).