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Properties of Liquid He^3 at Low Temperature

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The properties of liquid He^3 have been determined at low temperature by using a procedure previously applied to the study of nuclear matter. The interactions considered are the de Boer and Yntema-Schneider potentials. The values predicted for the equilibrium density, energy, compressibility, specific heat, magnetic susceptibility (and its density variation) are in semiquantitative agreement with experiment.

I. INTRODUCTION

In the preceding paper (to be referred to in the following as I) a theory of the many-body system has been applied to the determination of the properties of nuclear matter. In this paper we apply the theory to the study of liquid He^3 at low temperatures. For brevity we take the necessary formulas from I and give details only where the difference between the two systems makes this necessary.

We consider a very large number N of He^3 atoms in a volume Ω so that the density is $\rho=N/\Omega$. The interaction between pairs of atoms has been determined theoretically by Kirkwood and Slater[1] and also derived from the second virial coefficient. The two potentials which we have considered are

$$V(r)=V_0[(R/r)^{12}-(R/r)^6],\qquad V_0=40.88°\text{K},\quad R=2.55\text{ A},\tag{1}$$

and

$$V(r)=V_0\left[1200e^{-4.82r}-\frac{1.24}{r^6}-\frac{1.89}{r^8}\right],\qquad V_0=7250°\text{K},\quad r\text{ in A.}\tag{2}$$

(For convenience, we express potentials and energies in units of degrees Kelvin = ergs/k, where k is Boltzmann's constant.) The former was fitted by de Boer[2] to the low-temperature virial coefficients and the latter by Yntema and Schneider[3] to the virial coefficients up to 1000°K. These potentials are given in Fig. 1; they are very similar in the attractive region but the Yntema-Schneider potential rises less rapidly in the repulsive region. Because of this difference their potential gives considerably more binding than the de Boer potential. The results we give in the following are for the Yntema-Schneider potential. The failure of the de Boer potential to give the high-density properties correctly is not surprising; the disagreement of the predictions of this potential with the observed high-temperature virial coefficients is primarily due to the excessively steep rise of the region of repulsion in the potential.

We give here for convenience some additional parameters of the system. We define a mean volume per particle with radius r_0 by the equation

$$\Omega/N=\tfrac{4}{3}\pi r_0^3.\tag{3}$$

At normal density, which corresponds to 0.082 g/cm^3,[4] $r_0=2.43$ A. At this density the experimentally determined mean energy per particle at absolute zero is 5.04 calories per mole or 2.53 degrees per particle.[5]

The energy and maximum momentum of an ideal Fermi gas will also be needed; the Fermi momentum p_F is given by

$$2\Omega\tfrac{4}{3}\pi p_F^3/(2\pi\hbar)^3=N.\tag{4}$$

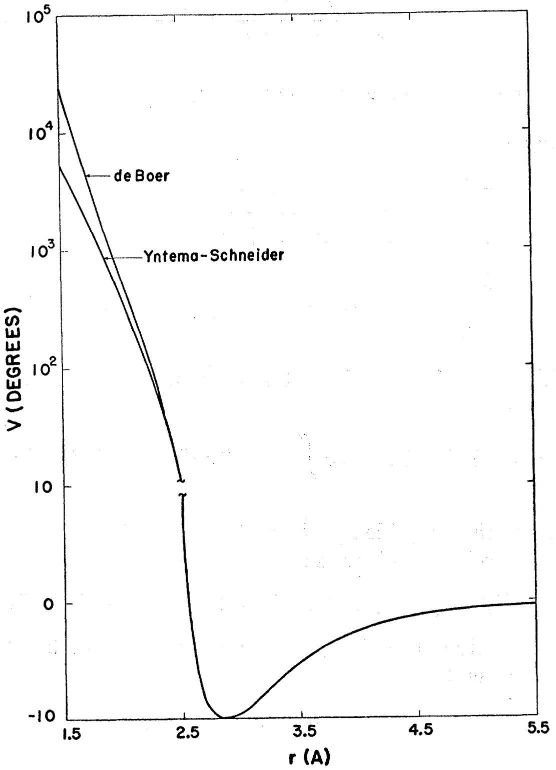

FIG. 1. He^3 potentials. Note change from linear to logarithmic scale at 10 degrees.

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[1] J. C. Slater and J. G. Kirkwood, Phys. Rev. **37**, 682 (1931).

[2] J. de Boer and A. Michels, Physica **5**, 945 (1938).

[3] J. L. Yntema and W. G. Schneider, J. Chem. Phys. **18**, 641 (1950).

[4] E. C. Kerr, Phys. Rev. **96**, 551 (1954).

[5] S. G. Sydoriak and T. R. Roberts, Phys. Rev. **106**, 175 (1957).

The factor of two comes from two spin states per momentum state. This gives

$$p_F=(9\pi/4)^{\frac{1}{3}}(\hbar/r_0)=1.918(\hbar/r_0). \tag{5}$$

The average kinetic energy of the Fermi gas per particle then is

$$(T_F)_{\text{Av}}=\tfrac{3}{5}(p_F{}^2/2M). \tag{6}$$

It is convenient here to introduce the energy unit $\hbar^2/[M(1\text{ A})^2]=16.36$ deg. The average kinetic energy per particle of the Fermi gas then is

$$(T_F)_{\text{Av}} \text{ in deg}=18.0/(r_0 \text{ in A})^2. \tag{7}$$

At normal density for example, with $r_0=2.43$ A, $(T_F)_{\text{Av}}$ is equal to 3.04 degrees.

II. SUMMARY OF FORMALISM

The properties of He^3 are determined from the solution for the elements of the reaction matrix (for details, see I)

$$K_{ij,kl}=V_{ij,kl}+\sum_{mn} V_{ij,mn}[E_0(k)+E_0(l) -E_1(m,\Sigma)-E_1(n,\Sigma)]^{-1}K_{mn,kl}, \tag{8}$$

where $V_{ij,kl}$ is a matrix element of the potential taken with respect to the plane wave eigenstates of the unperturbed system. The indices specify the spin and momentum states. The sum over m and n is to be taken over the states above the Fermi surface. The energies appearing in the energy denominator of Eq. (8) are determined by the diagonal elements of K. The energy of an unexcited particle is

$$E_0(k)=(k^2/2M)+\textstyle\sum_s(K_{ks,ks}-K_{ks,sk}), \tag{9}$$

where the second term comes from exchange of spin and momentum coordinates. The sum over s runs over the states of the Fermi gas. The energies of excitation are given by a similar equation; for a particle excited from momentum k to m while at the same time the state l has been emptied is

$$E_1(m,\Sigma)=(m^2/2M)+\textstyle\sum_s[K(\Sigma)_{ms,ms}-K(\Sigma)_{ms,sm}], \tag{10}$$

where the excited state K matrix is

$$K(\Sigma)_{ij,ms}=V_{ij,ms}+\sum_{u,v} V_{ij,uv}[\Sigma-E_1(u,\Sigma) -E_1(v,\Sigma)-\Delta]^{-1}K(\Sigma)_{uv,ms}, \tag{11}$$

and

$$\Sigma=E_0(k)+E_0(l). \tag{12}$$

The parameter Δ appearing in the equation for $K(\Sigma)$ is an approximation to the excitation energy of other particles simultaneously excited. The results are very insensitive to Δ which can be reasonably chosen to be the mean excitation energy of the Fermi gas.

We shall not give the formal justification of these equations here since they are discussed exhaustively in I and elsewhere. We also shall not discuss the corrections from the linked-cluster expansion; these have been shown to be negligible in the nuclear problem and are estimated to have a small effect in this system.

We follow a procedure very similar to that outlined in I in obtaining solutions to the coupled equations given by Eqs. (8)–(11). We first make the angular momentum reduction of the K-matrix equation, which allows us to write the diagonal elements of K for the angular momentum l and relative momentum k as

$$(k|K_l|k)=4\pi\int drr^2 j_l(kr)v(r)u_l(r). \tag{13}$$

In this equation we have not indicated explicitly the dependence on the total momentum P or on Σ [see Eq. (12)] although these must be taken into account in computing the energies. For Eq. (13), $j_l(kr)$ is the usual spherical Bessel function and the radial function $u_l(r)$ is defined by the integral equation

$$u_l(r)=j_l(kr)+4\pi\int r'^2dr'G_l(r,r')V(r')u_l(r'). \tag{14}$$

The Green's function is determined by the equation

$$G_l(r,r')=4\pi\int k'^2dk'\frac{j_l(k'r)j_l(k'r')f_P(k')}{\Sigma-E(k_+)-E(k_-)}, \tag{15}$$

where the effect of the exclusion principle enters through

$$\begin{aligned} f_P(k)&=0, \quad k<(k_{F^2}-\tfrac{1}{4}P^2)^{\frac{1}{2}} \\ &=\frac{k^2-k_{F^2}+P^2/4}{kP}, \quad (k_{F^2}-\tfrac{1}{4}P^2)^{\frac{1}{2}}<k<k_F+\tfrac{1}{2}P \\ &=1, \quad k>k_F+\tfrac{1}{2}P, \end{aligned} \tag{16}$$

and

$$k_{\pm}{}^2=k^2+\tfrac{1}{4}P^2\pm 3^{-\frac{1}{2}}kPf_P(k)^2. \tag{17}$$

The introduction of the function $f_P(k)$ and the averaged momenta $k+$ and $k-$ is discussed in detail in I.

In obtaining solutions to Eq. (14) for the radial function $u_l(r)$, we have not made a separation of the region of repulsion as was done in the nuclear case where the respulsion was treated as an infinitely-repulsive core. This was not done since the exact structure of the potential near the point at which it becomes repulsive turns out to be important. In addition the product of the Fermi momentum and core radius is in this case about equal to two, invalidating the treatment made in the nuclear problem where k_Fa is considerably smaller.

To treat the very strong repulsion, we have solved the integral equation directly starting for sufficiently small values of r to insure the vanishing of $V(r)u(r)$. Detailed investigation showed that a satisfactory starting point was 1.40 A where the repulsion is several thousand degrees.

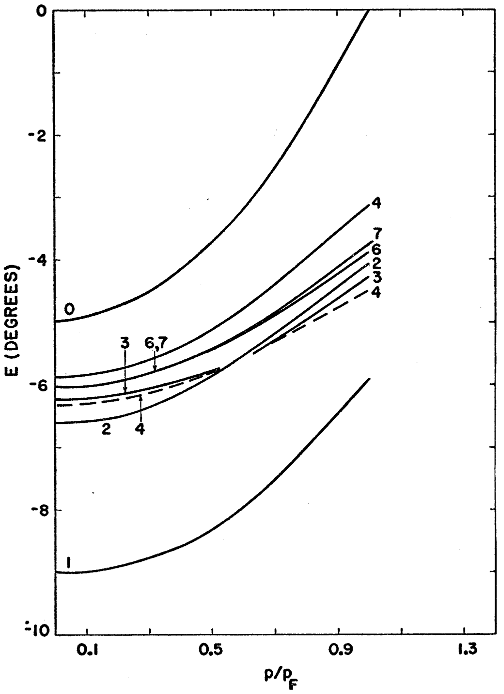

FIG. 2. Iteration sequence at $r_0=2.45$ A. The first input marked zero is the kinetic energy alone. $E(p)$ is not given for $p>p_F$.

After the solution to Eq. (14) has been obtained, the necessary elements of the K matrix can be determined from Eq. (13). The energy of a particle moving on the energy shell with momentum k_i then is [see Eq. (9)].

$$E(k_i)=\frac{k_i^2}{2M}+\sum_j(K_{ij,ij}-K_{ij,ji})$$

$$=\frac{k_i^2}{2M}+2\times2\times\sum_{k_j}\Big[\tfrac{1}{4}\sum_{l\text{ even}}(2l+1)(k_{ij}|K_l|k_{ij})+\tfrac{3}{4}\sum_{l\text{ odd}}(2l+1)(k_{ij}|K_l|k_{ij})\Big]. \quad (18)$$

In the interaction term the first factor of 2 comes from 2 spin states per momentum state, the second factor of 2 from the exchange term. The factors of $\frac{1}{4}$ and $\frac{3}{4}$ are the *a priori* weights of singlet and triplet spin states. The sum over k_j runs over the Fermi gas.

The computations were carried out for l values from 0 to 6 for states below the Fermi surface and for l from 0 to 3 for excited states. In the latter case the higher values of l were included by replacing the K-matrix elements by those appropriate for free scattering, i.e.,

$$(k_{ij}|K_l|k_{ij})\rightarrow(-4\pi/M\Omega)\lambda_{ij}\delta_l(K_{ij}) \quad \text{(free scattering limit).} \quad (19)$$

These equations have been solved numerically by iteration, starting with a first guess for $E(k_i)$ (usually the kinetic energy alone) and then iterating until the input spectrum for $E(k)$ agreed with the output spectrum (for details, see I). A typical iteration sequence at $r_0=2.45$ A is shown in Fig. 2.

III. RESULTS

A. Binding Energy and Compressibility

The procedure of the last section (described more fully in I) has been carried out as a function of density. The results for the binding energy are given in Fig. 3. The self-consistent excitation spectrum is also shown in Fig. 4 for several values of the density. The energy minimum of -0.96 degree per particle occurs at $r_0=2.60$ A. This value of the energy is only about one-half the observed value. The discrepancy may be due to the approximation method we use, although we feel that our method in this case tends to overestimate the energy slightly since the neglected cluster corrections probably give some repulsion. It is to be emphasized that the value we have obtained is extremely sensitive to the potential used, since the binding energy is actually the difference between the large repulsive and attractive effects. The repulsion comes from the large repulsive region in the potential and the high zero-point Fermi energy and is only very slightly overcompensated by the attractive part of the potential. A few percent increase in the attraction or a very slight decrease in the radius of repulsion in the potential would be sufficient to correct our value for the energy to the observed value. This slight effect may also rise from quite weak 3-body van der Waals forces.

It is also possible to obtain an approximate value for

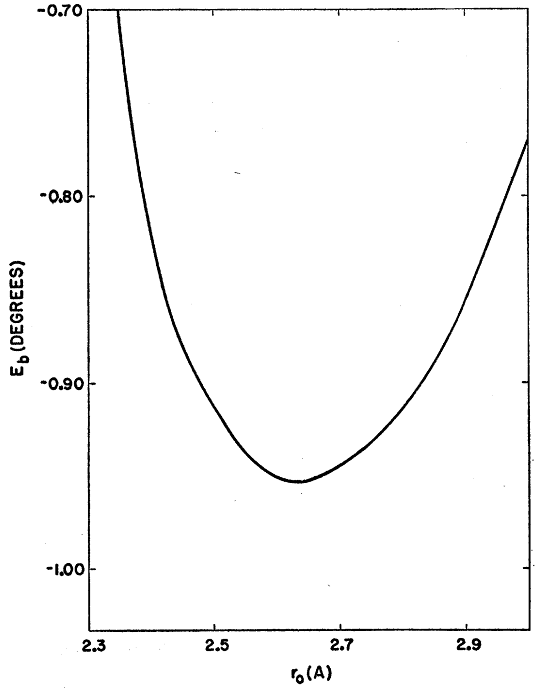

FIG. 3. Binding energy as a function of the mean radius per particle, defined in Eq. (3).

the compressibility from these results; Fig. 3 shows that if r_0 is decreased from 2.60 to 2.40, the energy rises by about 0.18 degree per particle. Assuming a quadratic dependence of energy on density over this region, it is then easy to show that the pressure-density relation is $p=18.9(\rho/\rho_0-1)$ atmospheres or that the volume change is 5.3% per atmosphere. This result is to be compared with the experimental value obtained at 1.2 degrees by Walters and Fairbanks[6] who found that the compressibility was about 3% per atmosphere. These values should perhaps not be compared directly since they refer to different temperatures, the theoretical value being for the ground state at 0°K. The comparison is close enough to show, however, that the theory does make a semiquantitative prediction of the remarkably high compressibility of liquid He³.

B. Specific Heat

Another result of considerable interest is the specific heat of the He³ liquid. We are able to determine this from our results only in the vicinity of absolute zero. The anomaly in the specific heat may be determined most easily by writing the excitation energy near the Fermi surface as

$$\begin{aligned} E(k) &= (k^2/2M)+V(k) \\ &= (k^2/2M^*)+V(k_F), \end{aligned} \tag{20}$$

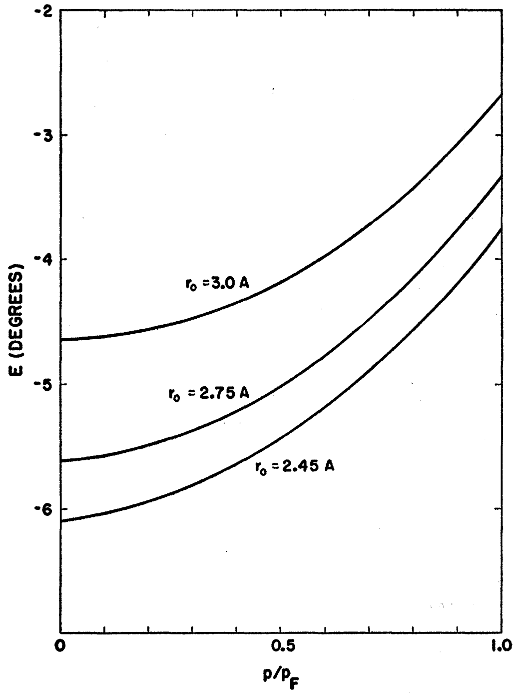

FIG. 4. Self-consistent spectra for several densities.

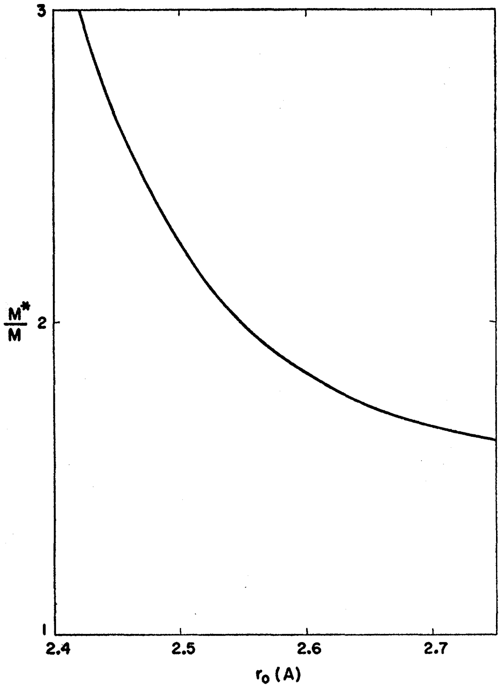

FIG. 5. Effective mass (at the Fermi surface) as a function of density.

where the effective mass M^* is given by

$$\frac{M^*}{M}=\left[1+\frac{M}{k_F}\frac{dV(k_F)}{dk_F}\right]^{-1}. \tag{21}$$

The values determined by our results are shown in Fig. 5; at the energy minimum the value is $M^*/M=1.84$. This considerable increase in the effective mass or equivalently in the flatness of the excitation spectrum is due to the rapid increase in the potential energy as the Fermi surface is approached. This increase is due to the effect of the exclusion principle on the particle interactions. A slow particle near the bottom of the Fermi distribution interacts with other particles primarily in *s*-states of orbital angular momentum. In these states the repulsive core acts most strongly. The effect of the repulsion is further enhanced by the exclusion principle which acts to increase the effects of the repulsive region and to decrease the effects of the attraction. For the more rapidly moving particles near the Fermi surface, the interaction in states of higher angular momentum, particularly the *P* states, becomes more effective. For these states the repulsive core and the exclusion effect both act less strongly while the attractive potential has almost full strength at the impact parameters typical of *P* states; thus the net effect of the interaction in these states is attractive and considerably larger than in the *S* states. The potential energy of interaction thus increases as the particle momentum increases, giving rise to the large effective mass.

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[6] G. K. Walters and W. M. Fairbanks, Phys. Rev. **103**, 263 (1956).

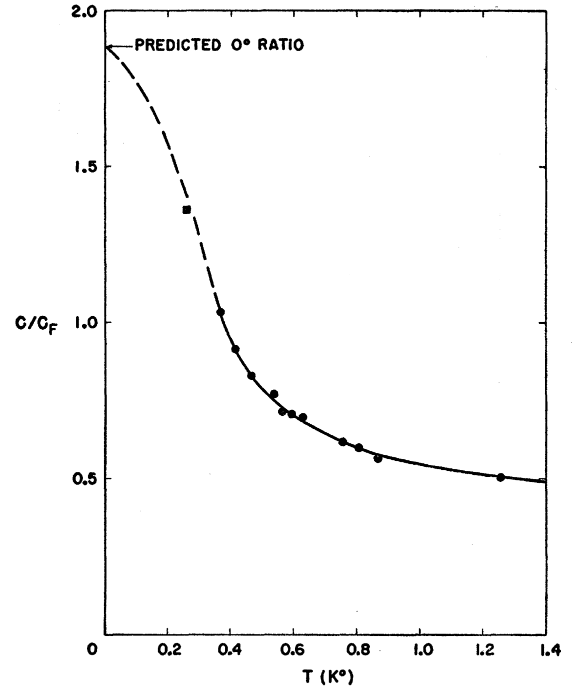

FIG. 6. Specific heat as a function of temperature as taken from Roberts and Sydoriak (reference 7). The point indicated by an open square is from unpublished work by D. Osborne. The dashed curve is an extrapolation to the computed value at $T=0$.

The alteration of the specific heat is easy to determine; a simple consideration shows that the effect of the flat excitation spectrum is to alter the specific heat compared to that of a Fermi gas by the factor M^*/M, i.e.,

$$C=C_F M^*/M. \tag{22}$$

The specific heat this is 1.84 times that of a Fermi gas. This result is shown in Fig. 6 together with the experimental values obtained at low temperatures.[7] It is clear that the predicted specific heat agrees with a reasonable extrapolation of the experimental data.

Our results also show that the specific heat should rise if the liquid is compressed, the change being given by the density variation of M^*/M shown in Fig. 5. There is at present no experimental evidence on this point.

C. Magnetic Susceptibility

Another property of He^3 of great interest is the magnetic susceptibility. This is a measure of the energy required to produce a net spin alignment in a given direction. It is easily determined from the elements of the K matrix, at least in the limit of small spin alignment. We let the number of atoms with spin up and spin down be

$$N_+=\tfrac{1}{2}N+\epsilon,\quad N_-=\tfrac{1}{2}N-\epsilon. \tag{23}$$

The kinetic energy then is simply shown to be, to lowest order in ϵ,

$$T_F(\epsilon)=\frac{3}{5}\frac{p_F^2}{2M}\left[1+\frac{20}{9}\frac{\epsilon^2}{N^2}\right]. \tag{24}$$

To determine the change in the interaction energy, we separate the sum over k which gives the total interaction energy into sums over spin up and spin down, neglecting for the present any variation of the interactions as the spins are polarized. The result is

$$V(\epsilon)=\left(\sum_{k_i=0}^{k_+}\sum_{k_j=0}^{k_+}+\sum_{k_i=0}^{k_-}\sum_{k_j=0}^{k_-}\right)a_0(k_i,k_j)$$
$$+\sum_{k_i=0}^{k_+}\sum_{k_j=0}^{k_-}[a_0(k_i,k_j)+a_e(k_i,k_j)], \tag{25}$$

where the even- and odd-state contributions are

$$a_e(k_i,k_j)=\sum_{l\text{ even}}(2l+1)(k_{ij}|K_l|k_{ij}),$$
$$a_o(k_i,k_j)=\sum_{l\text{ odd}}(2l+1)(k_{ij}|K_l|k_{ij}). \tag{26}$$

Equation (25) can readily be brought to the form (again retaining only leading terms in ϵ)

$$V(\epsilon)=V(0)+\left(\sum_{k_j=k_F}^{k_+}-\sum_{k_j=k_-}^{k_F}\right)\sum_{k_i=0}^{k_F}[3a_0(k_i,k_j)+a_e(k_i,k_j)]$$
$$+\sum_{k_i=k_F}^{k_+}\sum_{k_j=k_F}^{k_+}[a_o(k_i,k_j)-a_e(k_i,k_j)]. \tag{27}$$

The second term in this equation can be written in simpler form. We recognize the sum over k_i as the single particle potential

$$V(k_j)=\sum_{k_i=0}^{k_F}[3a_o(k_i,k_j)+a_e(k_i,k_j)]. \tag{28}$$

Therefore, for small ϵ, we have

$$\left(\sum_{k_j=k_F}^{k_+}-\sum_{k_j=k_-}^{k_F}\right)V(k_j)=\frac{4\pi\Omega}{(2\pi)^3}(k_+-k_F)^2k_F^2\frac{dV(k_F)}{dk_F}. \tag{29}$$

Upon using Eqs. (4), (20), and (23), this gives

$$N\left(\frac{2\epsilon}{N}\right)^2\frac{k_F^2}{6}\left(\frac{1}{M^*}-\frac{1}{M}\right).$$

The last term in Eq. (27) can also be written more simply as

$$\sum_{k_i=k_F}^{k_+}\sum_{k_j=k_F}^{k_+}[a_o(k_i,k_j)-a_e(k_i,k_j)]$$
$$=N\frac{k_F^3}{3\pi^2}\left(\frac{\epsilon}{N}\right)^2\Omega[a_o(k_F,k_F)_{\text{Av}}-a_e(k_F,k_F)_{\text{Av}}], \tag{30}$$

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[7] T. R. Roberts and S. G. Sydoriak, Phys. Rev. 98, 1672 (1955).

where we have made explicit use of Eq. (4) and defined

$$a(k_F,k_F)_{\mathrm{Av}}=\left[\int\frac{d\Omega_i}{4\pi}\int\frac{d\Omega_j}{4\pi}a(k_i,k_j)\right]_{k_i=k_j=k_F}. \quad (31)$$

One additional effect arises from the variation of the K matrix as the spins are polarized. This contribution is evaluated in the Appendix.

Collecting these results we find for the spin symmetry energy, taking for convenience the ratio to that of an ideal Fermi gas,

$$\frac{E_s}{E_s(F)}=\frac{M}{M^*}+p_F\frac{M\Omega}{\partial\pi^2}[a_0(k_F,k_F)_{\mathrm{Av}}-a_e(k_F,k_F)_{\mathrm{Av}}]$$
$$+\frac{2Mp_F\Omega}{\pi^2}\left\{\int\frac{d\mathbf{k}_i}{4\pi k_F^3}k_F\frac{\partial}{\partial k_F}[a_0(\mathbf{k}_i,\mathbf{k}_j)]_{k_j=k_F}\right.$$
$$+\frac{1}{8}\int\frac{d\mathbf{k}_i}{4\pi k_F^3}\int\frac{d\mathbf{k}_j}{4\pi k_F^3}k_F\frac{\partial}{\partial k_F}$$
$$\left.\times[5a_0(\mathbf{k}_i,\mathbf{k}_j)+a_e(\mathbf{k}_i,\mathbf{k}_j)]\right\}. \quad (32)$$

The first term is the same as that determining the specific heat anomaly. The second term results from the spin dependence of the interactions which is brought about by the operation of the exclusion principle. The third term results from the variation of the amplitudes with the Fermi momentum, this resulting from the spin polarization.

The amplitudes a_0 and a_e as determined from the solutions to the integral equations give a value of -0.390 for the second term in Eq. (32). The third term as evaluated in the Appendix has a value of 0.289. Inserting the value of $M^*/M=0.543$ at the equilibrium density, we find

$$E_s/E_s(F)=0.083=(12.0)^{-1}. \quad (33)$$

Thus the energy required to polarize the spins is very small compared to a Fermi gas, or correspondingly the magnetic susceptibility is very large, 12.0 times that of a Fermi gas. It is to be emphasized here that the specific heat and magnetic susceptibility are not directly related as for an ideal Fermi gas since the large value of the susceptibility is due to the large spin dependence terms in Eq. (32).[8] These nearly cancel the combined effects of the kinetic energy and velocity dependence of the potential which together determine the specific heat.

The actual value of 12.0 which we obtain is of course very sensitive to the precise values of M^* and the even-odd amplitude difference, particularly since these effects very nearly cancel. Thus we can safely conclude from our results only that the susceptibility is very large and that it is markedly different from the value suggested by the specific heat.

Another property clearly indicated by our results is that since the effective mass increases with increasing density, there is a tendency for the magnetic susceptibility to increase with increasing density.[9] Our results in fact suggest that the system may become unstable against spin alignment at high density, i.e., that the energy is lowered if the spins become polarized. This effect is very sensitive to the details of the calculations, however, so that we cannot safely predict the value of the density at which this transition might occur, if at all.

D. Indications of Solidification

In our calculations it is not clear if and how the procedure used will break down as the solid density is approached. It is, however, interesting to note that the iteration procedure which we used in solving the reaction-matrix equations showed signs of instability at the highest density point, $r_0=2.35$ A. The difficulty was the result of the very flat excitation spectrum at that density. This can be interpreted to be an indication that the lowest energy state of the system is no longer a degenerate Fermi gas but instead a state of higher spatial order and consequently, lower momentum order. Our methods are not suitable without basic modification for further investigation of this difficulty.

IV. ACKNOWLEDGMENTS

The authors are indebted to Professor Michael Buckingham and Professor William Fairbanks for very helpful discussions on the contents of this paper.

APPENDIX. DENSITY VARIATION OF THE K MATRIX AND ITS EFFECT ON THE MAGNETIC SUSCEPTIBILITY

As the fermion liquid is polarized, the shift in spin population causes a change in the K matrices through the alteration of the Fermi momentum. To determine the magnitude of this effect, we write the dependence of the amplitudes on the Fermi momentum as

$$a(\mathbf{k}_i,\mathbf{k}_j;\,k_F). \quad (\mathrm{A1})$$

In the odd states, as the system is polarized the Fermi momentum of the states with spin-up shifts to k_+, and with spin-down to k_-. In the even states a particle with spin-up interacts with a particle with spin-down. In the approximation we use in calculating the K matrix, only the average value of the new Fermi momenta in the states of spin-up and down enters into the calculation for the even states. The average is

$$k'=\frac{[k_+^2+k_-^2]^{\frac{1}{2}}}{2}. \quad (\mathrm{A2})$$

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[8] This point has also been emphasized by M. Buckingham, *Proceedings of the Conference on Low Tempertaure Physics, Paris, 1955* (Centre National de la Recherche Scientifique and UNESCO, Paris, 1956).

[9] This prediction is borne out by the experimental results of W. Fairbanks (private communication).

Returning now to Eq. (25), we rewrite it, indicating explicitly the dependence on the shifted Fermi momenta, as

$$V(\epsilon)=\sum_{k_i=0}^{k_+}\sum_{k_j=0}^{k_+} a_0(\mathbf{k}_i,\mathbf{k}_j;\,k_+)+\sum_{k_i=0}^{k_-}\sum_{k_j=0}^{k_-} a_0(\mathbf{k}_i,\mathbf{k}_j;\,k_-)$$

$$+\sum_{k_i=0}^{k_+}\sum_{k_j=0}^{k_-} [a_0(\mathbf{k}_i,\mathbf{k}_j;\,k')+a_e(\mathbf{k}_i,\mathbf{k}_j;\,k')]. \quad \text{(A3)}$$

We now carry out an expansion of the amplitudes around k_+, k_-, and $k'=k_F$. Keeping terms to second order in the small parameter ϵ of Eq. (23) and dropping the second derivative of the amplitudes with respect to k_F, we find the result given as the third term of Eq. (32).

To evaluate the integrals in this term, we first make the approximation of setting $\partial a_e/\partial k_F=\partial a_0/\partial k_F$, which can have only a very small effect on the result since $\partial a_e/\partial k_F$ appears with a small coefficient. We also assume (as is true to a good approximation) that a_0 depends only on $|\mathbf{k}_i-\mathbf{k}_j|$. We then can bring the third term in Eq. (32) to the form

$$\frac{4Mp_F}{\pi}\int_0^1 \frac{x^2dx}{k_F{}^3}\left(4-\frac{2x}{k_F}-\frac{2x^3}{k_F{}^3}\right)k_F\frac{\partial}{\partial k_F}a_0(x,k_F), \quad \text{(A4)}$$

where x is the relative momentum.

To carry out the indicated differentiation of a_0 with respect to k_F, we assume a linear dependence of a_0 on k_F and write

$$a_0(x,k_F)=a_0(x,0)+k_Ff(x). \quad \text{(A5)}$$

This linear dependence is verified to a good approximation by the results of the calculations. The function $f(x)$ is then determined by the difference between $a_0(x,0)$, which is the amplitude for zero density or for free particles, and $a_0(x,k_F)$ at the equilibrium density. These amplitudes have been taken from the computed results; evaluation of the integral of Eq. (A4) then gives the value of 0.289 for the third term of Eq. (32).

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Measurement of Lattice Vibrations in Vanadium by Neutron Scattering*

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The energy spectrum of slow neutrons inelastically scattered by vanadium metal has been measured by the time-of-flight technique. The neutrons gain energy by absorbing quanta of lattice vibration energy (phonons). As the nuclear scattering amplitude of vanadium is incoherent, the energy distribution of scattered neutrons is directly related to the frequency distribution of lattice vibrations. The measured neutron energy spectrum, as well as the derived frequency distribution, shows a clearly resolved double peak. This structure, which is distinctly different from the simple Debye distribution, but expected on the basis of detailed calculations, has heretofore not been amenable to direct measurement. The measured frequency distribution is compared with calculations for a body-centered cubic lattice by the Born-von Kármán theory and qualitative agreement is obtained. A more exact comparison awaits measurement of the elastic constants of vanadium.

I. INTRODUCTION

MANY theoretical and experimental studies of the influence of crystal dynamics on the scattering of slow neutrons have been made in recent years. The general theory is discussed by Placzek and Van Hove,[1] who give expressions for the angular and energy distribution of neutrons inelastically scattered by crystals. In this process, phonons (the quanta of lattice vibration energy) may be gained or lost by the neutrons.

The case of single phonon gain by scattering in a cubic crystal is of special interest if the nuclei scatter incoherently (spin-dependent scattering), as the energy gain is simply connected with the frequency distribution of the lattice vibrations of the crystal. Thus a measurement of the emergent energy of slow incident neutrons can be used to obtain the vibration spectrum with little ambiguity. For incoherent inelastic scattering, phonon and neutron properties are related only through the energy conservation condition

$$\hbar^2|k^2-k_0{}^2|/2m=\hbar\omega_j(\mathbf{q}), \quad (1)$$

with no need to satisfy interference (momentum) conditions, as is true for the more frequent case of coherent inelastic scattering. In Eq. (1), $\mathbf{k}$ and $\mathbf{k}_0$ are the scattered and incident neutron wave vectors respectively, m is the neutron mass, and $\omega_j(\mathbf{q})$ the angular frequency of the absorbed or emitted phonon with wave vector $\mathbf{q}$ and polarization index j.

The intensity formula, used to obtain the frequency

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‡ On leave from Weizmann Institute, Rehovoth, Israel, and the Atomic Energy Commission of Israel.

[1] G. Placzek and L. Van Hove, Phys. Rev. 93, 1207 (1954).