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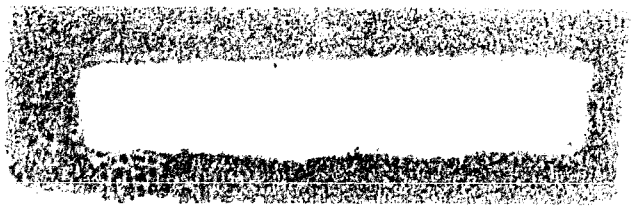

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A POSSIBLE PHASE TRANSITION IN LIQUID He^3

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ABSTRACT

A possible phase transition in liquid He^3 has been investigated theoretically by generalizing the Bardeen, Cooper, and Schrieffer equations for the transition temperature in the manner suggested by Cooper, Mills, and Sessler. The equations are transformed into a form suitable for numerical solution and an expression is given for the transition temperature at which liquid He^3 will change to highly correlated phase.

Following a suggestion of Mottelson, it is shown that the phase transition is a consequence of the interaction of particles in relative D-states.

The predicted value of the transition temperature depends on the assumed form of the effective single-particle potential and the interaction between He^3 atoms. The most important aspects of the single-particle potential are related to the thermodynamic properties of the liquid just above the transition temperature. Two choices of the two-particle interaction,

consistent with experiments, yield a second-order transition at a temperature between approximately ~~0.001~~ 0.06°K and 0.1° K. The highly correlated phase should exhibit enhanced fluidity.

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I. INTRODUCTION

Quantum fluids have been the object of intense experimental and theoretical investigation for many years. At low temperatures, both the boson liquid He^4 and the fermion system of electrons in metals exhibit a phase transition to a superfluid state but, for the rare isotope of helium, He^3, which liquefies at 3.2° K, no phase transition has been observed above 0.085° K - the lowest temperature at which experiments have been performed.

Indeed, Landau and his school[1] describe liquid He^3 as a fluid which has a "Fermi type spectrum," which is tantamount to assuming that the system does not exhibit a phase transition to a highly correlated state.

Recently, an extension[2] of the successful theory of superfluidity of electrons[3,4] indicated that liquid He^3 was unlikely to exhibit a phase transition, although this possibility was not demonstrated conclusively within the scope of the theory. In the present paper, the BCS theory at nonzero temperature is generalized in the manner suggested by CMS and it is shown that this theory does in fact predict a phase transition for liquid He^3 at a temperature which should be attainable

experimentally. The essential point is that the equations, which arise in the theory, possess D-state solutions but not the S-state solutions which had been sought previously without success.

A brief description of the theory and the associated thermodynamics is given in Section II and, in Section III, the problem is expressed in a form suitable for numerical calculation. The results are presented in Section IV and discussed in Section V.

II BASIC EQUATIONS AND THERMODYNAMICS

In the second quantization notation, the Hamiltonian H for a system of fermions may be written as

$$H = \sum_{\underline{k},\underline{\sigma}} \frac{\hbar^2 k^2}{2m} c^{+}(\underline{k},\underline{\sigma})\, c(\underline{k},\underline{\sigma}) + \frac{1}{2} \sum_{\underline{k}_i \underline{\sigma}_i} c^{+}(\underline{k}_1,\underline{\sigma}_1)\, c^{+}(\underline{k}_2,\underline{\sigma}_2)\, (1,2|v|3,4) \times c(\underline{k}_4,\underline{\sigma}_4)\, c(\underline{k}_3,\underline{\sigma}_3), \tag{1}$$

where $c^{+}(\underline{k},\underline{\sigma})$ and $c(\underline{k},\underline{\sigma})$ are respectively the creation and annihilation operators for a particle of momentum $\hbar\,\underline{k}$ and spin direction $\underline{\sigma}$. The thermodynamic properties of the system are to be calculated from the entropy $\underline{S}$ and the free energy $\underline{F}$ of the system.

In the method of BCS, $\underline{F}$ is evaluated in an ensemble of wave functions of the type

$$\underline{\Psi}_{exc} = \prod_{\underline{k}(\mathcal{S})} \left[\underline{\alpha}_{\underline{k}} + \underline{\beta}_{\underline{k}} \, b^{+}_{\underline{k}} \right] \prod_{\underline{k}'(\mathcal{P})} \left[\underline{\alpha}_{\underline{k}'} b^{+}_{\underline{k}'} - \underline{\beta}_{\underline{k}'} \right] \times \prod_{\underline{k}''(\mathcal{A})} c^{+}_{(\underline{k}'')} \; \underline{\Phi}_{VACUUM} . \qquad (2)$$

Here

$$b_{\underline{k}} = c_{-\underline{k}\downarrow} \, c_{\underline{k}\uparrow} \qquad (3)$$

$\mathcal{S}$, $\mathcal{P}$, and $\mathcal{A}$ specify states occupied by ground pairs, excited pairs, and single particles respectively and ($\underline{k}$") indicates either $\underline{k}''\uparrow$ or $\underline{k}''\downarrow$. The wave function Ψ is normalized by requiring

$$\underline{\alpha}_{\underline{k}} = \left(1 - h_{\underline{k}}\right)^{1/2} ,$$
$$\underline{\beta}_{\underline{k}} = h_{\underline{k}}^{1/2} \, e^{i \varphi_{\underline{k}}} , \qquad (4)$$

and $h_{\underline{k}}$, which is real positive and less than unity, is to be determined by minimizing $\underline{F}$. The wave functions of Eq. (2) allow a quite detailed treatment of the interactions between particles of equal and opposite momenta which are thought to be responsible for the phase transition.

Introducing the distribution function, $f_{\underline{k}}$ for the system, it can be shown, in the manner of BCS, that

$$\underline{\underline{S}} = -2k \sum_{\underline{k}'} \left\{ f_{\underline{k}'} \ln f_{\underline{k}'} + (1 - f_{\underline{k}'}) \ln (1 - f_{\underline{k}'}) \right\} \quad (5)$$

and

$$\underline{\underline{F}} = 2 \sum_{\underline{k}} \left[\frac{\hbar^2}{2m} k^2 - \underline{\mu} \right] \left[f_{\underline{k}} + (1 - 2 f_{\underline{k}}) h_{\underline{k}} \right]$$

$$+ \sum_{\underline{k}, \underline{k}'} U_{\underline{k}, \underline{k}'} \left[f_{\underline{k}} + (1 - 2 f_{\underline{k}}) h_{\underline{k}} \right] \left[f_{\underline{k}'} + (1 - 2 f_{\underline{k}'}) h_{\underline{k}'} \right]$$

$$+ \sum_{\underline{k}, \underline{k}'} V_{\underline{k}, \underline{k}'} \left[h_{\underline{k}} (1 - h_{\underline{k}}) h_{\underline{k}'} (1 - h_{\underline{k}'}) \right]^{1/2}$$

$$\times \left[(1 - 2 f_{\underline{k}}) (1 - 2 f_{\underline{k}'}) \right] e^{i (\varphi_k - \varphi_{k'})}$$

$$- T \underline{\underline{S}}, \quad (6)$$

where T is the temperature, k is Boltzmann's constant, $\underline{\mu}$ the chemical potential, and

$$U_{\underline{k}, \underline{k}'} = (\underline{k}\uparrow, \underline{k}'\uparrow | V | \underline{k}\uparrow, \underline{k}'\uparrow) - (\underline{k}\uparrow, \underline{k}'\uparrow | V | \underline{k}'\uparrow, \underline{k}\uparrow)$$
$$+ (\underline{k}\uparrow, -\underline{k}'\downarrow | V | \underline{k}\uparrow, -\underline{k}'\downarrow) - (\underline{k}\uparrow, -\underline{k}'\downarrow | V | -\underline{k}'\downarrow, \underline{k}\uparrow);$$

$$V_{\underline{k}, \underline{k}'} = (\underline{k}\uparrow, -\underline{k}\downarrow | V | \underline{k}'\uparrow, -\underline{k}'\downarrow) - (\underline{k}\uparrow, -\underline{k}\downarrow | V | -\underline{k}'\downarrow, \underline{k}'\uparrow). \quad (7)$$

Introducing the definitions

$$\underline{u}(\underline{k}) = [\underline{\gamma}_{\underline{k}}(1-\underline{\gamma}_{\underline{k}})]^{1/2}(1-2\underline{f}_{\underline{k}})\, e^{i\underline{\varphi}_{\underline{k}}}, \tag{8}$$

$$\underline{F}(\underline{k}) = -\sum_{\underline{k}'} \underline{V}_{\underline{k},\underline{k}'}\, \underline{u}(\underline{k}'), \tag{9}$$

$$\underline{\epsilon}(\underline{k}) = \frac{\hbar^2}{2m}k^2 - \mu + \sum_{\underline{k}'} \underline{V}_{\underline{k},\underline{k}'}\left[\underline{f}_{\underline{k}'} + (1-2\underline{f}_{\underline{k}'})\underline{\gamma}_{\underline{k}'}\right], \tag{10}$$

$$\underline{E}(\underline{k}) = \left[\underline{\epsilon}^2(\underline{k}) + \underline{F}^2(\underline{k})\right]^{1/2}, \tag{11}$$

it is easy to show that on minimizing $\underline{F}$ with respect to $\underline{\varphi}_{\underline{k}}$, $\underline{\gamma}_{\underline{k}}$, and $\underline{f}_{\underline{k}}$, we find that, except for the normal state,

$$\underline{\varphi}_{\underline{k}} = n\pi, \tag{12}$$

$$\underline{f}_{\underline{k}} = \frac{1}{e^{\beta \underline{E}(\underline{k})} + 1}, \tag{13}$$

$$\underline{V}(\underline{k}) = -\tfrac{1}{2}\,\frac{\tanh \tfrac{1}{2}\beta E(\underline{k})}{E(\underline{k})} \sum_{\underline{k}'} V_{\underline{k},\underline{k}'}\,\underline{V}(\underline{k}'), \qquad (14)$$

with $\beta = 1/kT$, and n an integer.

There is a phase transition if there is a value β_c of β for which Eqs. (9), (11), and (14) have a nontrivial solution $\underline{V}(\underline{k})$ whenever $\beta > \beta_c$, and no solution otherwise. $T_c = 1/k\beta_c$ is the transition temperature.

β_c is that value of β for which the equation

$$\underline{V}(\underline{k}) = -\tfrac{1}{2}\,\frac{\tanh \tfrac{1}{2}\beta_c \in(\underline{k})}{\in(\underline{k})} \sum_{\underline{k}'} V_{\underline{k},\underline{k}'}\,\underline{V}(\underline{k}') \qquad (15)$$

has a solution. This equation may be obtained from Eqs. (11) and (14) by putting $F(\underline{k}) = 0$ in $E(\underline{k})$. Equation (15) may then have a nontrivial solution $\underline{V}(\underline{k})$ which is made identically zero by the normalization required by Eq. (9).

It will be seen that Eq. (15), when transformed to coordinate space, can possess solutions if $V_{\underline{k},\underline{k}'}$ is the (formal) Fourier transform of a singular potential. If, however, $U_{\underline{k},\underline{k}'}$ is the (formal) Fourier transform of a singular potential, then $\in(\underline{k})$ defined in Eq. (10) will be infinite in general. A more elaborate theory is necessary to circumvent this difficulty and, in the manner of CMS, we anticipate the

result of such a theory by introducing the single-particle energies $\epsilon(k)$ and writing

$$\underline{\epsilon}(\underline{k}) = \epsilon(k) - \mu, \tag{16}$$

and then $\underline{\mu} = \epsilon(k_F)$ follows from the requirement that the number of particles correspond to a Fermi momentum $\hbar k_F$.

The form of $\epsilon(k)$ is not to be calculated here but is to be determined from other considerations. However, it is clear from Eq. (15) that the value of β_c is strongly dependent on the properties of $\epsilon(k)$, and, indeed, it will be shown in the next section that the derivative of $\epsilon(k)$ at the Fermi surface is of dominant importance in this connection but that the result is insensitive to the other detailed properties of $\epsilon(k)$.

We shall now show that the value of $d\epsilon(k)/dk\,|_{k=k_F}$ is determined by the specific heat of the liquid just above the transition so that, since $V_{\underline{k},\underline{k}'}$ is the only other assumed quantity in Eq. (15), the value of β_c will be made to depend on two empirically determinable factors.

Using Eqs. (5) and (13), the specific heat C is given by

$$C = T\,\frac{d\underline{S}}{dT}$$

$$C = 2k\beta^2 \sum_{\underline{k}'} f_{\underline{k}'}(1-f_{\underline{k}'})\left[E^2(\underline{k}') + \beta\, E(\underline{k}')\frac{dE(\underline{k}')}{d\beta}\right]. \tag{17}$$

Above the transition temperature, $E(k) = \epsilon(k)$, and the right-hand side of Eq. (17) may be evaluated in the usual way (see, e.g., Mayer and Mayer[5]), and it is found that

$$C_n = \frac{k^2 T}{3} k_F^2 \Big/ \left.\frac{d\epsilon(k')}{dk'}\right|_{k'=k_F} + O(T^2) \qquad (18)$$

[C_n is the specified heat for $\beta < \beta_c$ — i.e., for the normal fluid].

Thus, for sufficiently low temperatures, C_n is a linear function of T, and this relationship holds down to the transition temperature. Now, the properties of the normal fluid do not undergo any discontinuous change at β_c, so that

$$\lim_{\beta \to \beta_c^-} \epsilon(k) = \lim_{\beta \to \beta_c^+} \epsilon(k) \qquad \text{for all } k.$$

Consequently we may use the value of $d\epsilon(k)/dk\,|_{k=k_F}$ obtained for $\beta \leq \beta_c$ in the solution of Eq. (15) for $\beta = \beta_c$.

The experiments of Brewer, Daunt, and Sreedhar,[6] which extend down to 0.085° K, show that the specific heat has become a linear function of temperature which extrapolates to zero at absolute zero. If C_F is the specific heat of an ideal Fermi Gas and C_0 is the observed specific heat, then it is found that

$$\frac{C_0}{C_F} = 2.00 \pm .05. \tag{19}$$

If we define the effective mass m^* at the Fermi surface to be given by

$$\frac{\hbar^2}{m^*} = \lim_{k \to k_F} \frac{1}{k} \frac{d\,e(k)}{d\,k}, \tag{20}$$

then it is clear from Eq. (18) that, for small T,

$$\frac{C_n}{C_F} = \frac{m^*}{m} \tag{21}$$

which implies that we must use a single-particle spectrum with effective mass of $2m$ at the Fermi surface.

Finally, Eq. (17) may be used to obtain an expression for the discontinuity of the specific heat which is the difference between the specific heat (c_K) of the highly correlated state (for $\beta > \beta_c$) and that (c_n) of the normal state (for $\beta < \beta_c$).

Neglecting terms of order T^2, we find, at the transition temperature,

$$\frac{C_K - C_n}{C_n} = \frac{3}{\pi^2} \beta_c^3 \mathcal{E}, \qquad (22)$$

where $\mathcal{E}$ is the angular average of $F(\underline{k}) \frac{dF(\underline{k})}{d\beta}$ evaluated at $|\underline{k}| = k_F$ and $\beta = \beta_c$.

III EXPRESSIONS FOR THE TRANSITION TEMPERATURE AND THE SPECIFIC HEAT DISCONTINUITY

1. Rearrangement of the Equations

When $\epsilon(\underline{k})$ has a given form, Eq. (15) becomes a linear integral equation which may be separated into a set of equations each referring to a definite angular momentum l. (The formal manipulation is precisely the same as that used to separate the Schrödinger equation.)

CMS sought $l = 0$ solutions of Eq. (14) (with $\beta \to \infty$) and showed that it was unlikely that such solutions of that equation (and hence of Eq. (15) existed. Indeed this conclusion is confirmed by the numerical work described later.

However, it was suggested by Dr. B. Mottelson (private communication) that there might be an $l = 2$ solution. The plausibility of this suggestion may be seen at once from the results of Emery[7] who showed that a sufficient condition for the existence of a solution of Eq. (15) is that the phase

shift in the solution of the corresponding Schrödinger equation (with angular momentum ℓ and with kinetic energy $\epsilon(k)$) should be positive at the Fermi surface and that the energy gap increases as the phase shift increases.

Now the free-space shifts[8] for the He^3 at k_F are -61° for $\ell = 0$, -2° for $\ell = 1$, $+19^\circ$ for $\ell = 2$ and $+11^\circ$ for $\ell = 3$. Higher angular momentum states show a steady decrease in phase shift as ℓ increases. In $\epsilon(k)$ the effective mass is $2m$ at the Fermi surface and is everywhere greater than or equal to m. This is equivalent to strengthening the potential and suggests that there should be a phase transition for $\ell = 2$ and $\ell = 3$, possibly for $\ell = 1$ but probably not for $\ell = 0$. The largest transition temperature should be obtained for $\ell = 2$. These qualitative conslusions are born out by our numerical results and the predicted transition temperature corresponds to the calculated D-state value. (It should be noted that, since the $\ell = 2$ and $\ell = 3$ phase shifts are so nearly equal, changes in the conventional two-particle potential could result in the largest transition temperature's arising for $\ell = 3$.)

Consequently, we seek a D-state solution of Eq. (15) although for $\beta > \beta_c$, the solution of the nonlinear equation (14) has a much more complicated angular dependence, which becomes more nearly pure D-state as $\beta \to \beta_c$.

In Dirac's notation, the nonangular part, $|\chi\rangle$, of Eq. (15) for $\ell = 2$, satisfies

$$|\chi\rangle = -G v |\chi\rangle, \tag{23}$$

where

$$G = \frac{1}{\pi} \int_0^\infty dk \; |k\rangle\langle k| \; \frac{\tanh \tfrac{1}{2}\beta_c \epsilon(k)}{\epsilon(k)} , \qquad (24)$$

and

$$\langle r|k\rangle = kr \; j_2(kr),$$

$j_2(kr)$ being the spherical Bessel function of order 2.

The most obvious method of solving Eq. (23) would be to introduce an eigenvalue $\lambda(\beta)$ multiplying G and to determine the value β_c of β for which one eigenvalue $\lambda_0(\beta_c) = 1$. It turns out, however, that these are several negative eigenvalues of smaller magnitude than λ_0, and this fact makes it difficult to determine λ_0 with sufficient accuracy. Consequently we rewrite the criterion determining β_c in a more convenient form which also displays in a most striking way the sensitivity of β_c to $\epsilon(k)$ and to the two-particle potential.

Define

$$|\varphi\rangle = |k_F\rangle - G_0 v |\varphi\rangle, \qquad (25)$$

where

$$G_0 = \frac{1}{\pi} \int_0^\infty dk \left[|k\rangle\langle k| - |k_F\rangle\langle k_F| \right] \frac{\tanh \tfrac{1}{2}\beta_c \epsilon(k)}{\epsilon(k)} . \qquad (26)$$

Then from Eqs. (23) and (25)

$$\langle \varphi | v | \chi \rangle = - \langle \varphi | v G_0 v | \chi \rangle$$

$$\langle \varphi | v | \Psi \rangle = \langle k_F | v | \Psi \rangle - \langle \varphi | v G_0 v | \Psi \rangle . \tag{27}$$

Thus, defining

$$L(\beta_c) = \frac{1}{\pi} \int_0^\infty dk \; \frac{\tanh \tfrac{1}{2} \beta \epsilon_k}{\epsilon_k} , \tag{28}$$

we find from Eq. (27) that

$$L(\beta_c) = - \frac{1}{\langle \varphi | v | k_F \rangle} , \tag{29}$$

provided $|\Psi\rangle$ is not identically zero, i.e. a highly correlated state must exist. The evaluation of β_c now rests upon the determination of the integral in Eq. (28) and the solution of the inhomogeneous integral equation (25), which is not beset by the numerical difficulties associated with the solution of the eigenvalue equation (15). The numerical procedures used to obtain $\langle \varphi | v | k_F \rangle$ are described in Appendix I.

2. Evaluation of $L(\beta_c)$

In this section we describe the evaluation of $L(\beta_c)$ in the effective mass approximation. This approximation is quite good, since the integral in Eq. (28) is most sensitive to the values of $\epsilon(k)$ for k

near to k_F. The modifications of the result are quoted in Section IV for the specific forms of $\epsilon(k)$ which are used. Thus we take

$$\epsilon(k) = \frac{\hbar^2 k^2}{2m^*} . \tag{30}$$

Then for β_c large there exists a K such that both

$$\frac{\hbar^2}{2m^*}\beta_c |K^2 - k_F^2| >> 1,$$
$$|K - k_F| << 1, \tag{31}$$

and

so that $L(\beta_c)$ may be approximated by

$$L(\beta_c) = \frac{2m^*}{\pi\hbar^2}\left\{ \int_0^{k_F - K} \frac{dk}{k_F^2 - k^2} + \int_{k_F + K}^{\infty} \frac{dk}{k^2 - k_F^2} \right.$$
$$\left. + \int_{-K}^{K} \frac{\tanh\left(\frac{\hbar^2\beta_c}{2m^*} k_F x\right)}{2k_F x}\, dx \right\} . \tag{32}$$

The third integral on the right-hand side of Eq. (32) has been evaluated by BCS (for large β_c) and it is found that (the value of K not appearing in the result):

$$L(\beta_c) = \frac{2m^*}{\pi \hbar^2 k_F} \ln\left(\frac{2.28\, \hbar^2 k_F^2 \beta_c}{m^*}\right), \qquad (33)$$

so that

$$kT_c = 2.28\, \frac{\hbar^2 k_F^2}{m^*} \exp\left\{ \frac{\pi}{2} \frac{\hbar^2}{m^*} \frac{k_F}{\langle \varphi | v | k_F \rangle} \right\} \qquad (34)$$

in the effective mass approximation. A more careful evaluation of $L(\beta_c)$ shows that the effective mass at the Fermi surface appears in the result just as in Eq. (33), and that a more general form of $\mathcal{C}(k)$ away from k_F merely alters the factor 2.28 slightly, to give a small change in the transition temperature (since as will be seen in Section IV, $\langle \varphi | v | k_F \rangle$ scarcely depends on the finer details of $\mathcal{C}(k)$).

Eq. (34) shows the precise manner in which T_c is determined by m^* (which is an experimentally determined property of $\mathcal{C}(k)$) and by $\langle \varphi | v | k_F \rangle$, which is calculated for the experimentally determined interaction and which is very insensitive to the value of β_c (see Appendix I).

3. Specific-Heat Discontinuity

To calculate the specific-heat discontinuity given by Eq. (22), we rearrange Eq. (14) by the method used in this section to transform Eq. (15). To first order in $F^2(k)$ it is found that

$$\frac{1}{\pi}\int_0^\infty dk\ \frac{\tanh \tfrac{1}{2}\beta \bar{E}(k)}{\bar{E}(k)} = -\frac{1}{\langle \varphi | v | k_F \rangle}, \qquad (35)$$

where

$$\bar{E}(k) = \left[\epsilon^2(k) + \bar{F}^2(k) \right]^{1/2}, \qquad (36)$$

$\bar{F}^2(k)$ being the angular average of $F^2(\underline{k}, \underline{p}^2)$. It is shown in Appendix I that, for β very large, the right-hand side of Eq. (35) is independent of β to a very good approximation. Thus the derivative of the left-hand side of Eq. (35) with respect to β is approximately zero. For $\bar{F}(k)$ small, it makes an appreciable change in $\bar{E}(k)$ for k near to K_F only. Consequently we replace $\bar{F}(k)$ by $\bar{F}(k_F)$ for all k. With these approximations, the expression for $\frac{d}{d\beta}\bar{F}^2(k_F)$ is independent of the form of the interaction v and has been evaluated by BCS. It is found that

$$\lim_{\beta \to \beta_c} \frac{d}{d\beta}\bar{F}^2(k_F) = \frac{10.2}{\beta_c^3}, \qquad (37)$$

provided that $F(\underline{k})$ is not identically zero for $|\underline{k}| = k_F$. [For further discussion see Appendix II.] The left-hand side of Eq. (37) is equal to $\frac{15}{7}\mathcal{E}$ in Eq. (22), so that

$$C_K = \frac{1.71}{2.42} C_n \qquad (38)$$

at the transition temperature.

IV RESULTS

1. One-and Two-Body Potentials

The transition temperature has been evaluated for two choices of $\mathcal{L}(k)$ and of v in order to determine the sensitivity of the result to the assumptions.

The first form of $v(r)$ is a Lennard-Jones 6-12 potential with parameters determined by de Boer,[9]

$$v(r) = V_0 \left[\left(\frac{r_0}{r}\right)^{12} - 2 \left(\frac{r_0}{r}\right)^{6} \right], \qquad (39)$$

with $V_0 = 10.22^{\circ}K$, $r_0 = 2.869\ A^{\circ}$. This potential is presumably the best now available in that it has been fitted to a wide range of experimental data in the low temperature region.[10]

As an alternative, the Yntema-Schneider potential

$$v(r) = 7250 \left[1200\, e^{-4.82r} - \frac{1.24}{r^6} - \frac{1.89}{r^8} \right] {}^{\circ}K \qquad (40$$

has been used (r is measured in A°). This interaction has not been studied in the quantum-mechanical region although it is known to have too little attraction by at least 10%.[10]

For a form of $\mathcal{L}(k)$, we have used the results of Brueckner and Gammel.[12,13] Their potential does not include rearrangement energies which, on nuclear matter, have an appreciable effect. Consequently, we

have taken their potential for a particle excited from the Fermi surface ($f = 1.0$; see Ref. 12) and kept the same general shape whilst altering the scale so that $\mathcal{e}(k_F)$ is equal to the mean binding energy, and also requiring the effective mass at the Fermi surface to be 2.0 rather than 1.85, which was obtained.[12] A good approximation to the curve was found to be given by the following analytic function:

$$\mathcal{e}(k) = \frac{\hbar^2}{2m} \begin{cases} -0.632 + 0.50\, k^2 & \text{for } 0 < k < 0.9, \\ k^2 - 1.043 + 1.03\,(k - 0.9) & \text{for } 0.9 < k < 1.913, \\ k^2 & \text{for } 1.913 < k. \end{cases} \tag{41}$$

where k is in units of $A^{\circ -1}$ and k_F has been taken as $0.8\ A^{\circ -1}$. Calculations were also performed with no single-particle potential, i.e.

$$\mathcal{e}(k) = \frac{\hbar^2 k^2}{2m}. \tag{42}$$

The value of $L(\beta_c)$ for $\mathcal{e}(k)$ given by Eq. (38) is determined by putting $m^* = m$ in Eq. (33). For $\mathcal{e}(k)$ given by Eq. (37),

$$L(\beta_c) = \frac{2m^*}{\pi \hbar^2 k_F} \ln\left(\frac{1.57\, \hbar^2 k_F^2 \beta_c}{m^*}\right), \tag{43}$$

with $m^* = 2m$. Thus the more complicated potential of Eq. (41) simply

causes a factor $1.57/2.28 = 0.69$ in the expression (34) for T_c.

2. The Transition Temperature

The results of the numerical calculations are summarized in Table I. The Schrödinger equation has also been used to evaluate $\langle \varphi | v | k_F \rangle$ (see Appendix I). It can be seen in Table I that $\langle \varphi | v | k_F \rangle$ is not sensitive to (i) the influence of the exclusion principle (cf. first and second entries for $\langle \varphi | v | k_F \rangle$) or (ii) to the dispersive effect of $\epsilon(k)$ (cf. the second and third entries for $\langle \varphi | v | k_F \rangle$). The dispersive effect would be important, however if $v(r)$ were a hard core plus attraction. At the same time, since kT_c depends exponentially on $\langle \varphi | v | k_F \rangle$, there is an order-of-magnitude difference between the corresponding values of kT_c.

V DISCUSSION

The values of T_c for $m^* = m$ indicate the sensitivity of T_c to the slope of $\epsilon(k)$ at the Fermi surface. A change in the specific-heat curve at low temperatures could change the experimental value of m^* and thus have a large effect on the calculated value of T_c.

The results indicate a considerable sensitivity to the assumed form of $v(r)$, the ~~difference~~ agreement between T_c obtained from the 6-12 potential and the Yntema-Schneider potential being entirely consistent with the ~~different~~ D-state scattering which they predict.[14]

It should be noted that these potentials are primarily obtained from the second virial coefficient which depends on the scattering for all angular momentum states and does not determine the potential accurately for any one angular momentum state. Certainly a small change in the potential could have a large effect on T_c without causing an appreciable change in the calculated value of the second virial coefficient.

Probably the best value of T_c which we can quote at present is $0.11^{\circ}K$ which is obtained using the (adjusted) Brueckner and Gammel potential (Eqs. (41) and (43)) and the 6-12 potential of de Boer (Eq. (39)).

This value for the transition temperature lies in the region where no transition has been observed experimentally. However, this result does not necessarily imply a contradiction beween the theory and experiment, since it has been shown that a small change in the two-body potential or in the low-temperature specific heat (in the normal state) can have a rather large effect on the predicted value of the transition temperature.

At the same time, it is true that the validity of the theory depends on the assumption that the normal fluid can be described as a system of weakly interacting quasiparticles. It is possible that the temperature at which this description becomes good is somewhat lower than our best predicted value of T_c. In this connection it is important to note the linear behaviour of the specific heat[6] and the rapid increase of the self-diffusion coefficient[16] at low temperatures. These experiments lend strong support to the increasing validity of the quasi-particle description of the normal fluid, at decreasing temperatures.

We have not investigated, in this paper, the properties of the highly correlated phase other than to calculate the discontinuity in the specific heat. There are, however, many properties of the state which should be subject to experimental investigation. In particular, there should be

interesting spatially dependent properties associated with orientation of the liquid, as well as striking effects in the magnetic susceptibility.

The excitation energy near the Fermi surface is given by $2|F(\underline{k})|$ for $|\underline{k}| = k_F$. Since $F(\underline{k})$ is a function of the direction of k, it will be zero for some directions unless, when $F(\underline{k})$ is expanded in spherical harmonics, the spherically symmetric part is dominant. (The angular average of the non-spherically-symmetric part is zero.) This is certainly not the case near to β_c, where the D-state solution dominates, and seems to be unlikely for $\beta > \beta_c$ although the essential non-linear character of Eq. (14) makes it difficult to make a precise statement.

In these circumstances the highly correlated phase is expected to exhibit a strongly enhanced fluidity with a viscosity which decreases with fluid velocity. However, perfect superfluidity should not be observed.

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APPENDIX I

Numerical Procedures

To evaluate $\langle \underline{\phi} | v | k_F \rangle$, the coordinate space representative of Eq. (25) was solved numerically using the IBM 704 at the Computer Center of the University of California in Berkeley, and a program written by means of the FORTRAN II system.

For very small transition termperatures, β_c is large and the hyperbolic tangent in Eq. (26) differs from unity only for k very near to k_F. Thus, since the rest of the integrand in Eq. (26) is non-singular near k_F, the exact value of β_c is unimportant in the evaluation of $\langle r | G_0 | r' \rangle$ (provided β_c is large) and $\tanh(1/2)\beta \epsilon(k)$ may be replaced by unity for this purpose.

In coordinate space, Eq. (25) becomes

$$\underline{\varphi}(r) = k_F r j_2(k_F r) - \int_0^\infty dr' \langle r | G_0 | r' \rangle v(r') \underline{\varphi}(r') . \qquad (A1)$$

This equation was solved by replacing the integral by a Gaussian quadrature approximation, the ensuing set of linear inhomogeneous equations being solved by means of a library subroutine.[15]

For the quadrature, the range of integration was broken into three parts bounded by $a < b < c < d$ in each of which an r_1-point Gaussian quadrature formula was used. The best locations of a, b, c, and d were determined by trial. The values used were $a = 1.0$ A° (since $\underline{\phi}(r)$ was essentially zero at this point), $b = 1.997$ A° (since $v(r)\,\underline{\phi}(r)$ had its maximum at this point so that the greatest number of Gauss points fell into the region in which $v(r)\,\phi(r)$ was rapidly varying), $c = 3.5$ A° (results were insensitive to this value) and $d = 7.0$ A° (increasing d beyond this

value caused no change in $\langle \underline{\phi} | v | k_F \rangle$ owing to the short range of $v(r)$).

The difference in $\langle \underline{\phi} | v | k_F \rangle$ for $n_1 = 10$ and $n_1 = 16$ was 1%.

To evaluate $\langle r | G_0 | r' \rangle$ write

$$\langle r | G | r' \rangle = G_1(r, r') + G_2(r, r') \qquad (A2)$$

where

$$G_1(r, r') = -\frac{m}{\hbar^2 k_F} \begin{cases} (k_F r)(k_F r')\, j_2(k_F r)\, n_2(k_F r'), & r < r' \\ (k_F r)(k_F r')\, j_2(k_F r')\, n_2(k_F r), & r > r' \end{cases} \qquad (A3)$$

where $j_2(k_F r)$ and $n_2(k_F r)$ are spherical Bessel functions of order 2),

and

$$G_2(r, r') = \frac{1}{\pi} \int_0^\infty dk\, k^2 r r' \left[j_2(kr) j_2(kr') - j_2(k_F r) j_2(k_F r') \right] \times \left\{ \frac{1}{|c(k) - c(k_F)|} - \frac{1}{\frac{\hbar^2}{2m}(k^2 - k_F^2)} \right\}. \qquad (A4)$$

In this form, the integral over k could be terminated at $k = \underline{K} = 4.5\ A^{o\,-1}$ with good accuracy and the integral evaluated by an n_2-point Gaussian quadrature in each of the ranges $0 \leq k \leq k_F$ and $k_F \leq k \leq \underline{K}$. ($k_F = 0.8\ A^{o-1}$). Changing n_2 from 6 to 10 caused a 1/2% change in $\langle \underline{\phi} | v | k_F \rangle$. The integral $\langle \underline{\phi} | v | k_F \rangle$ was performed by a $3n_1$-point Gauss quadrature formula.

The time required to solve the problem with $n_1 = 16$ and $n_2 = 10$ was approximately 30 minutes. Of course this time could have been reduced considerably by decreasing the number of Gauss points in the regions in which the integrand was varying slowly. However, since so few different values of $\langle \underline{\phi} | v | k_F \rangle$ were required, the total computer time was less than would have been used by economizing trials.

The calculations were expected to be sensitive to the singular regions of $v(r)$ which becomes sharply repulsive near $r = 2.56\ A^{o}$. If $v(r)$ had been a hard core plus outside attraction $v(r)\underline{\psi}(r)$ would have had a $\underline{\delta}$-function behaviour at the core. In fact $v(r)\underline{\phi}(r)$ did not vary too sharply in the core region and the accuracy of the solution in this region was checked (*i*) by changing n_1 from 10 to 16 and (*ii*) by putting $G_2(r,r') = 0$ so that the problem reduced to the Schrödinger equation for which an approximate analytic solution could be obtained in the region in which $v(r)$ was repulsive. The programming accuracy and, to some extent, the numerical accuracy were checked by evaluating the Schrödinger equation phase shifts ($\tan \underline{\delta}_{\ell_F} = - \langle \underline{\phi} | v | k_F \rangle$) and comparing them with the known values.

APPENDIX II

Solutions Below the Transition Temperature

In this paper we have not solved the non-linear equation (14) which describes the correlated state, but have only examined the linear equation (15) for the transition temperature, which is thus independent of the nature of the non-linear solution. However, the predicted properties of the correlated state, such as the specific-heat discontinuity at the transition temperature and the flow properties, depend explicitly upon the solution of the non-linear equation.

There exists a solution $F(\underline{k})$ to the non linear equation which is non-zero for $|\underline{k}| = k_F$, for at least some directions. For this solution the coefficients $\beta_{\underline{k}}$ in the trial function Ψ are discontinuous functions of angle for $|\underline{k}| = k_F$. We know of no reason to impose the requirement that Ψ be continuous, but observe that Ψ would be continuous if $F(\underline{k})$ were identically zero for $|\underline{k}| = k_F$. There appears to be a solution of the non-linear equation of this nature, which would imply a zero energy gap, a consequent reduction in the specific-heat discontinuity at the transition temperature, and an increase in viscosity in the correlated state. We reject this solution, however, in favor of the solution with $F(\underline{k})$ non-zero for $|\underline{k}| = k_F$, since the latter gives a lower value for the free energy at any temperature.

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CAPTION

Table I Values of $\langle \varphi | v | k_F \rangle$ (Eq. 25, 26) and the transition temperature, for various input functions.

TABLE I

Two-Body Potential	Single-Particle Potential	$\frac{-\hbar^2 k_F}{m\langle \varphi \vert v \vert h_F \rangle}$	L(β_c) Evaluation	T_c°
6-12 (Eq. 39)	None (Eq. 42) Schrödinger Equation	3.14	$m^*/m = 2.00$ (Eq. 34)	1.0
	None (Eq. 42)	4.51	$m^*/m = 2.00$ (Eq. 34)	0.35
	B. and G. (Eq. 41)	5.46	$m^*/m = 2.00$ (Eq. 34)	0.16
			$m^*/m = 1.00$ (Eq. 34)	0.0045
			B. and G. (Eq. 43)	0.11
Y-S (Eq. 40)	None (Eq. 42) Schrödinger Equation	3.18 ~~7.83~~	$m^*/m = 2.00$ (Eq. 34)	0.14 ~~0.039~~
	B. and G. (Eq. 41)	~~11.67~~ 5.56	$m^*/m = 2.00$ (Eq. 34)	0.0018 ~~0.00125~~
			B. and G. (Eq. 43)	~~0.0008~~