Spin-fluctuation stabilization of anisotropic superfluid states

W. F. Brinkman
Bell Laboratories, Holmdel, New Jersey 07733

J. W. Serene*†
Cornell University, Ithaca, New York 14850

P. W. Anderson
Bell Laboratories, Murray Hill, New Jersey 07974
and Cavendish Laboratory, Cambridge, England
(Received 28 January 1974)

The role spin fluctuations play in determining the stable superfluid phases of He^3 is investigated. It is shown that the feedback effects of the gap on the spin fluctuations can stabilize the anisotropic Anderson-Morel (AM) state if they are sufficiently strong. The effect is calculated both near T_c and at zero temperature. It is found that the Balian-Werthamer (BW) state is more stable at low temperatures and that the slope of the calculated transition from the AM to BW states qualitatively agrees with the experimental slope of the A to B transition as a function of pressure.

I. INTRODUCTION AND DISCUSSION OF RESULTS

Around 1960 a number of theoretical papers[1-4] suggested that He^3 should become a superfluid of the BCS type in which the pair amplitude is characterized by an angular momentum different from zero. At the time, estimates made either from the effective particle-particle interaction calculated by Brueckner and Gammel[5] or from the Lennard-Jones potential determined phenomenologically by de Poer[3] gave an attractive interaction for d-wave pairing and a very weak p-wave interaction. In 1964 Emery[6] introduced the idea that the interaction should be renormalized by the fluctuations of the medium and showed that this renormalization tends to favor p-state pairing. Somewhat later Berk and Schreiffer[7] pointed out that in a nearly ferromagnetic system the spin fluctuations due to the incipient order tend to suppress normal singlet BCS pairing. Doniach and Engelsberg[8] simultaneously showed that spin fluctuations are important for understanding the specific heat of He^3, and since then their importance in determining a number of other properties of He^3 has been gradually recognized.[9] About this time Layser and Fay[10] pointed out that, although spin fluctuations induced a repulsive interaction for singlet pairing, for triplet pairing, and consequently odd-l pairing, the spin-fluctuation contribution was attractive. This is easily seen since for parallel-spin particles the polarization clouds are aligned and the two particles are attracted to one another. This attractive interaction can easily be calculated in the contact-interaction model to be[10,11]

$$v^{SF}(q,\omega) = -\tfrac{1}{2}I/[1 - I\chi^0(q)] \ , \tag{1.1}$$

where I is the contact interaction and $\chi^0(q)$ is the noninteracting susceptibility defined in Sec. II. It is not difficult to see that the above interaction gives a large attractive contribution to the effective coupling constant for p-wave pairing. Assuming that He^3 should exhibit p-wave pairing, theory also predicts[12] in the weak-coupling approximation that the most stable state is the so-called Balian-Werthamer state and that this state is stable at all temperatures. This prediction was strongly contradicted by the recent experimental observations that He^3 actually exhibits two new phases, the so-called A and B phases of Osheroff *et al.*[13-16] This led two of the present authors[11] to investigate the question of how the spin fluctuations are changed when the superfluid gap is introduced into the quasiparticle spectrum. They showed that the effective interactions for the various components of the triplet pair can be written for the states under consideration as

$$I_{\text{eff}\uparrow\uparrow} = -\tfrac{1}{2}I/[1 - I\chi^0_{zz}(q,\omega)] \ , \tag{1.2}$$

$$I_{\text{eff}\uparrow\downarrow} = \frac{1}{2}\,\frac{I}{1 - I\chi^0_{zz}(q,\omega)} - \frac{2I}{1 - I\chi^0_{xx}(q,\omega)} \ . \tag{1.3}$$

Here we have ignored the density-density fluctuations. The χ^0_{ij} are the various components of the unenhanced susceptibility and are defined in Sec. II and $\uparrow\uparrow$ means $m_s = 1$ along z while $\uparrow\downarrow$ means $m_s = 0$. It was then noted that at q and ω equal to zero in the Balian-Werthamer states all of the susceptibilities χ^0_{ii} are equal and decrease below the transition temperature, thus decreasing the effective interaction. In contrast, for the Anderson-Morel (AM) state only χ^0_{zz} decreases. Since the $m_s = 0$ interaction, i.e., $I_{\text{eff}\,\uparrow\downarrow}$ in Eq. (1.3) is the only one used in forming the pairs for the AM state the effective interaction is *enhanced*. In order to make a quantitative estimate of this effect the changes in the χ^0 for finite q and ω were related to their static values in the same way that the change in conductivity at finite energy and momentum is related to the number of superconducting electrons. An estimate of the change in the fourth-order free energies of the various states was made, and it was shown that the effect was sizable and could explain the presence of the A phase as a stabilization of the AM state at high pressures where spin fluctuations are more important. Various experimental results, the NMR shift,[13] the nondecreasing susceptibility,[13] the pressure dependence of the specific heat,[14] the splitting of T_c into two transitions in a field,[13] and the ultrasonic attenuation[15(b)] appear to be consistent with this interpretation.

In this paper we investigate more carefully the form of $\chi^0_{ij}(q,\omega)$ for finite q and ω and find that the simple relation to the static values used in the original letter is not correct. Although the qualitative result that the feedback effect due to the change in the spin fluctuations favors the AM state remains, the proper evaluation of the susceptibilities makes quantitative differences in the results. We also investigate in this paper the contribution the feedback effect makes to the free energy to sixth order in Δ and its contribution to the zero-temperature energies. In describing this feedback effect we again introduce a dimensionless measure of its importance by defining

$$\delta = \Delta F^{\mathrm{SF}}_{\mathrm{BW}}/(F^0_{\mathrm{BW}} - F^0_{\mathrm{AM}})_{\text{fourth order}}\,; \tag{1.4}$$

i.e., δ is the ratio of change in the contribution the spin fluctuations make to the free energy of the BW state divided by the difference in the weak-coupling free energies of the BW and AM states. In this definition the free energies are evaluated to fourth order in Δ. We find the following results:

(i) Both the BW and AM states decrease in free energy relative to their weak-coupling values. The AM state decreases by 3 times as much as the BW state, so that their free energies cross at $\delta \simeq 0.5$. (See Fig. 1.) This result appears to be more in line with the measured specific-heat data,[16] where it is found that the specific-heat discontinuity is always larger than the weak coupling value attained for the BW state. This implies that the fourth-order terms are smaller than their weak-coupling values, which is what we find.

(ii) From the calculated slope of the A to B transition as a function of δ we find the phase diagram shown in Fig. 2, where the experimental values of the temperature of the first-order transition[17] T_{AB}/T_c are roughly given by the dashed curve in Fig. 2. The shape of this curve is determined by adjusting δ to fit the specific heat discontinuity versus pressure. It was previously shown[18] that the change in the theoretical values of δ with pressure correlates closely with the change in the discontinuity of the specific heat. It is seen that the BW phase is more stable at low temperatures and that the calculated slope of the T_{AB} transition is in qualitative agreement with

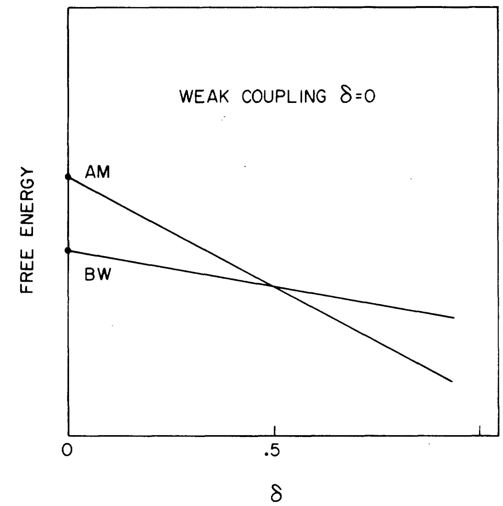

FIG. 1. Crossover of the fourth-order free energies as a function of δ, the measure of the importance of the spin fluctuations. $\delta = 0.5$ is the critical value for stabilization of the AM state.

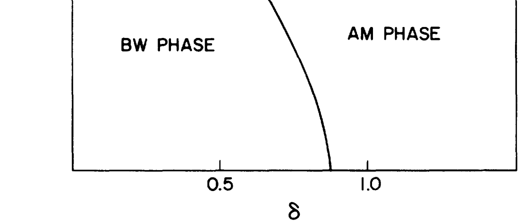

FIG. 2. Calculated phase diagram as a function of δ. Experimental data (dashed line) were deduced from the specific-heat discontinuity as a function of pressure $\delta \sim 0.6$ on the melting curve. Only the slope near T_c and the zero-temperature values have been calculated. Solid curve is a rough interpolation between these results.

experiment.

(iii) The introduction of the correct formulas for the susceptibilities also changes the relations between δ and the various coefficients in the general expansion of the free energy in terms of fourth-order invariants.[19,20] These changes, however, mostly affect the BW phase. The calculated results for the AM state[19] in the presence of an external field, namely, specific-heat discontinuities and the slopes of the second transition with respect to field, are changed by at most 10% and will not be recalculated here.

Briefly, the outline of this paper is that the susceptibilities are calculated in the limit $\xi^{-1} < q < 2k_F$ (ξ is the coherence length and k_F the Fermi wavelength) in Sec. II. In Sec. III the change in spin-fluctuation energy is calculated to fourth order in Δ. In Sec. IV we calculate the energy to sixth order in Δ and then extend the calculation to zero temperature. In the last section we make a few comments about the validity of the approach taken here.

Before beginning we establish notation. The gap function will be written $\Delta_{\alpha\beta}(k)$ and for p-wave pairing it is expressed as

$$\Delta_{\alpha\beta}(\hat{k}) = d_{\lambda i}\hat{k}_\lambda(\sigma_i i\sigma_y)_{\alpha\beta} , \qquad (1.5)$$

where σ_i are the Pauli matrices. The matrix $d_{\lambda i}$ represents the 3×3-component order parameter. The Balian-Werthamer (BW) state is written as $d_{\alpha i} = \Delta\delta_{\alpha i}$. The Anderson-Morel state we work with is $d_{xz} = -id_{yz} = \Delta\sqrt{\tfrac{3}{2}}$. This state is obtained from the AM state,[4]

$$\Delta_{\alpha\beta}(k) = \sqrt{\tfrac{3}{2}}\,\Delta(k_x + ik_y)\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} , \qquad (1.6)$$

by a 90° spin rotation. It differs from the state used by Balian-Werthamer,[12]

$$\Delta_{\alpha\beta}(k) = \sqrt{\tfrac{3}{2}}\,\Delta\begin{pmatrix} k_x + ik_y & 0 \\ 0 & -k_x + ik_y \end{pmatrix} , \qquad (1.7)$$

as the "AM state" in that all pairs have an orbital angular momentum of +1 about the z axis. In weak-coupling theory the phase relation between the up and down spin pairs was unimportant but the spin-fluctuation results act very differently on the two states. The state (1.7) has been shown never to be a minimum energy state.[19,20]

II. CALCULATION OF SUSCEPTIBILITIES

In order to calculate the change in the free energy due to spin fluctuations it is necessary to calculate the changes in the unenhanced susceptibilities due to the introduction of the anisotropic order parameters. The static susceptibilities were previously calculated by BW,[12] but they do not suffice for our purposes here. Let

$$\chi^0_{ij}(q, i\omega_m) \equiv 2\int_0^\beta e^{i\omega_m\tau}\langle T_\tau[M_i(q,\tau)M_j(-q,0)]\rangle d\tau , \qquad (2.1)$$

where

$$M_i(q,\tau) = \frac{\sigma^i_{\alpha\beta}}{2}\sum_p e^{(H_0-\mu N)\tau} \times a^\dagger_{p+q/2,\alpha}a_{p-q/2,\beta}e^{-(H_0-\mu N)\tau} . \qquad (2.2)$$

T_τ designates the usual time-ordering operator and H_0 is the reduced Hamiltonian[12] about which we do perturbation theory. The $\sigma^i_{\alpha\beta}$ are the Pauli matrices and the a's are the usual Fermion-creation and annihilation operators. As will be justified later we need to calculate χ^0_{ij} in the region where $\xi^{-1} \ll q \ll 2k_F$ (ξ is the coherence length proportional to v_F/T_c). In doing this we follow the treatment of the current-response function in superconductivity as developed by Abrikosov, Gorkov, and Dzyaloshinski[21] (AGD). Introducing the single-particle Green's function

$$G_{\alpha\beta}(p,\tau) \equiv \langle T_\tau[a_{p\alpha}(\tau)a^\dagger_{p\beta}(0)]\rangle \qquad (2.3)$$

and

$$F^\dagger_{\alpha\beta}(\tau) = \langle T_\tau[a^\dagger_{-p\alpha}(\tau)a^\dagger_{p\beta}]\rangle , \qquad (2.4)$$

the expression for χ^0_{ij} can be reduced to

$$\chi^0_{ij}(q, i\omega_m) = -\tfrac{1}{2}\sigma^i_{\alpha\beta}\sigma^j_{\gamma\delta}T\sum_{p,n}[G_{\beta\gamma}(p_-)G_{\delta\alpha}(p_+) - F^\dagger_{\alpha\gamma}(p_+)F_{\beta\delta}(p_-)] , \qquad (2.5)$$

where $p_\pm = \{p \pm \tfrac{1}{2}q, \omega_n \pm \omega_{m/2}\}$. If only *unitary* states[12] are considered we find that

$$G_{\beta\gamma}(p) = \delta_{\beta\gamma}(i\omega_n + \epsilon_p)/(\omega_n^2 + \epsilon_p^2 + |\Delta_p|^2) , \qquad (2.6)$$

$$F_{\alpha\beta}(p) = \Delta_{\alpha\beta}(p)/(\omega_n^2 + \epsilon_p^2 + |\Delta_p|^2) . \qquad (2.7)$$

Substituting these expressions into χ^0_{ij} leaves one with a complicated expression which must be summed over ω_n and integrated over p. As discussed by AGD[21] if one is interested only in $\delta\chi^0_{ij} = (\chi^0_{ij})_N - (\chi^0_{ij})_S$, where S and N indicate the superfluid state and the normal state, respectively, one can do the momentum integration first. The integration over the magnitude of p is done first by making the approximation that $\epsilon_{p\pm q/2} = \epsilon_p \pm \tfrac{1}{2}\vec{v}_F\cdot\vec{q}$ where the magnitude of $\vec{v}_F$ is taken to be the Fermi velocity. It is also assumed that $\Delta_{p\pm q/2}$ does not depend appreciably on $|\vec{p}|$ and its q dependence is ignored. Having performed this integral one is left with the integrals over the direction of $\vec{p}$.

This integral is handled by noting that the integrand is dominated by the region where $\vec{v}_F\cdot\vec{q}\sim 0$ because under those circumstances various denominators are small. Therefore one sets $\vec{p}$ perpendicular to $\vec{q}$ in the nonsingular parts of the integrand and performs the integral over the direction of $\vec{p}$ relative to $\vec{q}$. After some simplification one finds that

$$\delta\chi^0_{ij}(q,i\omega_m)=N(0)\frac{\pi^2}{2v_Fq}T\sum_n\int\frac{d\phi_\perp}{2\pi}\left[\delta_{ij}\left(\mathrm{Sgn}(\omega_n)\mathrm{Sgn}(\omega_n-\omega_m)-\frac{\omega_n(\omega_n-\omega_m)}{(\omega_n^2+|\Delta_p|^2)^{1/2}[(\omega_n-\omega_m)^2+|\Delta_p|^2]^{1/2}}\right)\right.$$
$$\left.-\frac{1}{2}\frac{\mathrm{Tr}(\sigma^i\Delta_p\bar{\sigma}^j\Delta_p^\dagger)}{(\omega_n^2+|\Delta_p|^2)^{1/2}[(\omega_n-\omega_m)^2+|\Delta_p|^2]^{1/2}}\right]. \tag{2.8}$$

In this expression $\vec{p}$ is to be taken perpendicular to $\vec{q}$ and the $\phi_\perp$ integration averages over the direction of $\vec{p}$ in the plane. If one takes Δ_p to be of the BCS type, $\Delta_p=i\sigma_y\Delta$, the above expression is identical except for overall coefficients to Eq. (37.26) of AGD.

To obtain an expression for $\delta\chi$ to order Δ^2 we will keep the sums discrete and expand in powers of Δ. The lowest order terms are

$$\delta\chi^0_{ij}(q,i\omega_m)=\frac{N(0)}{2v_FqT}\int\frac{d\phi_\perp}{2\pi}[\delta_{ij}|\Delta_p|^2D_2(m)-\tfrac{1}{2}\mathrm{Tr}(\sigma^i\Delta_p\bar{\sigma}^j\Delta_p^\dagger)D_1(m)], \tag{2.9}$$

where

$$D_1(m)=D_1(-m),\quad m<0;\; D_1(m)=\tfrac{1}{4}\pi^2,\quad m=0;\; D_1(m)=(1/m)[\psi(m+\tfrac{1}{2})-\psi(\tfrac{1}{2})],\quad m>0,$$

and

$$D_2(m)=D_2(-m),\quad m<0;\; D_2(m)=\tfrac{1}{2}\psi'(m+\tfrac{1}{2}),\quad m\geq 0.$$

Here ψ is the digamma function and ψ' its derivative. For triplet spin pairing the expression in square brackets reduces to

$$\delta_{ij}|\vec{d}(p)|^2[D_2(m)-D_1(m)]+[d_i(p)d_j^*(p)+d_j(p)d_i^*(p)]D_1(m),$$

and if we assume p-wave pairing, $\delta\chi^0$ is further reduced to

$$\delta\chi^0(q,i\omega_m)=[N(0)/2v_FqT](\tfrac{1}{2}(\delta_{\alpha\beta}-\hat{q}_\alpha\hat{q}_\beta)\{\delta_{ij}d_{\alpha l}d^*_{\beta l}[D_2(m)-D_1(m)]+(d_{\alpha i}d^*_{\beta j}+d^*_{\alpha i}d_{\beta j})D_1(m)\}).$$

To obtain the zero-temperature expressions we must convert the sum over n to an integral and analytically continue (2.8) with respect to ω_m onto the real axis. Again we simply follow AGD in doing this and find that

$$\mathrm{Re}\,\delta\chi^0_{ij}(q,\omega)=\frac{\pi N(0)}{2v_Fq}\int\frac{d\phi_\perp}{2\pi}\int_{\omega_1}^{\omega_2}d\omega'\left(\frac{\delta_{ij}\omega'(\omega'-\omega)-\frac{1}{2}\mathrm{Tr}(\sigma^i\Delta_p\bar{\sigma}^j\Delta_p^*)}{(\omega'^2-|\Delta_p|^2)^{1/2}[|\Delta_p|^2-(\omega'-\omega)^2]^{1/2}}\right). \tag{2.10}$$

Here $(\omega_1,\omega_2)=(|\Delta_p|,|\Delta_p|+\omega)$ if $\omega<2|\Delta_p|$, and $(\omega_1,\omega_2)=(\omega-|\Delta_p|,\omega+|\Delta_p|)$ if $\omega>2|\Delta_p|$. The ω' integral can be written in terms of complete elliptic integrals in the same way that the corresponding expressions for the conductivity were written for s wave pairing in Refs. 22 and 23.

$$\mathrm{Re}\,\delta\chi^0_{ij}(q,\omega)=\frac{\pi N(0)}{2v_Fq}\int\frac{d\phi_\perp}{2\pi}|\Delta_p|\left[\delta_{ij}\left((1+y)E(z)-\frac{y^2}{(1+y)}K(z)\right)-\frac{1}{2}\frac{\mathrm{Tr}(\sigma_i\Delta_p\bar{\sigma}_j\Delta_p^\dagger)}{|\Delta_p|^2}\frac{K(z)}{(1+y)}\right]. \tag{2.11}$$

Here $y=\omega/2|\Delta_p|$ and $z^2=4y/(1+y)^2$. The K and E are the usual complete elliptic integrals. For the imaginary part we obtain

$$\mathrm{Im}\,\delta\chi^0_{ij}(q,\omega)=\frac{-\pi N(0)}{2v_Fq}\int\frac{d\phi_\perp}{2\pi}\left(\delta_{ij}\omega+\int_{|\Delta_p|}^{\omega-|\Delta_p|}d\omega'\,\theta(\omega-2|\Delta_p|)\frac{\delta_{ij}\omega'(\omega'-\omega)-\frac{1}{2}\mathrm{Tr}(\sigma^i\Delta_p\bar{\sigma}^j\Delta_p^\dagger)}{(\omega'^2-|\Delta_p|^2)^{1/2}[(\omega'-\omega)^2-|\Delta_p|^2]^{1/2}}\right). \tag{2.12}$$

Here $\theta(x)=1$ if $x>0$ and is 0 otherwise. The first term simply subtracts off the normal-state susceptibility. Again, this expression can be written in terms of elliptic integrals.

$$\mathrm{Im}\,\delta\chi^0_{ij}(q,\omega) = -\frac{\pi N(0)}{v_F q}\int \frac{d\phi_\perp}{2\pi}\,|\Delta_p|\left\{\delta_{ij}\left[y+\theta(y-1)\left(\frac{1+2y}{1+y}K(k)-(1+y)E(k)\right)\right]-\frac{1}{2}\,\frac{\mathrm{Tr}(\sigma^i\Delta_p\bar{\sigma}^j\Delta_p)}{|\Delta_1|^2}\,\theta(y-1)\frac{K(k)}{1+y}\right\}. \tag{2.13}$$

In this final expression $k^2=(1-y)^2/(1+y)^2=1-z^2$. The functions of y multiplying the δ_{ij} term and the trace term in Eqs. (2.11) and (2.13) are plotted in Figs. 3(a) and 3(b).

III. CALCULATION OF FREE ENERGIES: FOURTH ORDER

The approach we take in this section is to calculate the effect of spin fluctuations on the free energy of the superfluid state in the same way that the spin fluctuations were previously treated for the normal state.[8,24] We therefore assume that the zero-order Hamiltonian has a weak attractive p-wave interaction and its free energy is simply that of a weakly coupled superfluid. We then add to the free energy the standard spin-fluctuation expression.

$$\Delta F^s = \tfrac{1}{2}T\mathrm{Tr}\sum_m \int \frac{d^3p}{(2\pi)^3}\{\ln[1-I\chi^0_{ij}(q,i\omega_m)] + I\chi^0_{ij}(q,i\omega_m)\}\ . \tag{3.1}$$

This expression is obtained by summing diagrams of the type shown in Fig. 4. The trace here is over the variables i and j. The only anomalous diagrams that are included are those shown in Fig. 4. This approximation has been justified previously.[18] The $\chi^0_{ij}(q,i\omega_m)$ is the susceptibility as calculated for the unperturbed weak-coupling state and as such includes both the normal and anomalous diagrams, as can be seen from expression (2.5). We now expand the free energy in powers of $\delta\chi^0_{ij}$, defined in Sec. II as

$$\delta\chi^0 = (\chi^0)_N - (\chi^0)_S\ , \tag{3.2}$$

where $\chi^0_N(q,i\omega_m)$ is the normal-state noninteracting susceptibility. The first-order term in $\delta\chi^0$ is

$$\Delta F^1 = -\frac{T}{2}\sum_i\sum_m\int\frac{d^3q}{(2\pi)^3}\times\left(\frac{I}{1-I\chi^0_N(q,i\omega_m)}-I\right)\delta\chi^0_{ii}(q,i\omega_m) \tag{3.3}$$

$$= -\frac{T}{2}\sum_i\sum_m\int\frac{d^3q}{(2\pi)^3}\,\frac{I^2\chi^0_N(q,i\omega_m)}{1-I\chi^0_N(q,i\omega_m)}\,\delta\chi^0_{ii}(q,i\omega_m). \tag{3.4}$$

The physical interpretation of ΔF^1 is that it represents the change in free energy between the superfluid and normal states when the effective interaction is taken to be that obtained by virtual exchange of *normal*-state spin fluctuations. We will assume that the effect of this term can be incorporated into the attractive interaction of the unperturbed weak-coupling calculation. This assumption is the major approximation in the calculations presented here. We discuss it further in Sec. IV. The second-order term in ΔF is

$$\Delta F^s = -\frac{T}{4}\sum_{ij}\sum_m\int\frac{d^3q}{(2\pi)^3}\left(\frac{I\,\delta\chi^0_{ij}(q,i\omega_m)}{1-I\chi^0_N(q,i\omega_m)}\right)^2. \tag{3.5}$$

If we write

$$\delta\bar{\chi}_{ij}(q,i\omega_m) \equiv \delta\chi^0_{ij}qv_F/N(0)\ , \tag{3.6}$$

then according to (2.8) $\delta\bar{\chi}$ does not depend on the

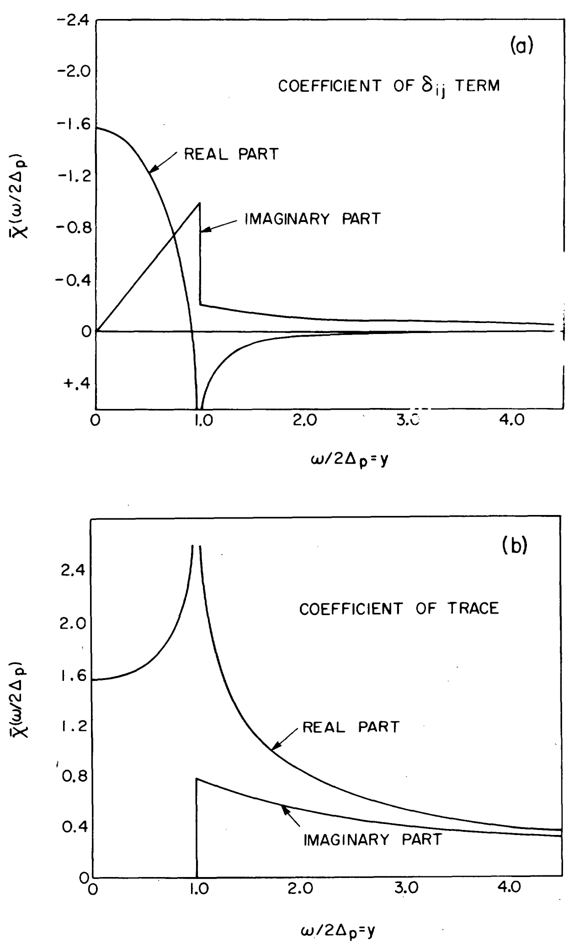

FIG. 3. Plot of the expressions multiplying the δ function and the trace terms in the integrand in Eqs. (2.11) and (2.13).

magnitude of q, and

$$\Delta F^s = -\frac{T}{4}\frac{1}{2\pi^2}\int \frac{dq}{v_F^2}\left(\frac{\bar{I}}{1-\bar{I}+\alpha\bar{I}(q/2k_F)^2}\right)^2 \sum_{ij}\sum_m \int \frac{d\Omega_q}{4\pi}[\delta\bar{\chi}_{ij}(\hat{q}, i\omega_m)]^2 \tag{3.7}$$

$$= -\frac{N(0)}{4\epsilon_F}\int_0^1 dx\left(\frac{\bar{I}}{1-\bar{I}+\alpha\bar{I}x^2}\right)^2 \sum_{ij}\sum_m \int \frac{d\Omega_q}{4\pi}[\delta\bar{\chi}_{ij}(q, i\omega_m)]^2 . \tag{3.8}$$

Using the expressions derived in the previous section for $\delta\bar{\chi}_{ij}$ to second order in Δ we can evaluate the sum over i, j and the average over Ω_q.

One is then left with the sums over m of the D functions. Doing these sums numerically we find

$$\Delta F^s = -\frac{N(0)}{16\epsilon_F T}\int_0^1 dx\left(\frac{\bar{I}}{1-\bar{I}+\alpha\bar{I}x^2}\right)^2 [|d_{\alpha i}^2|^2 + 0.5 d_{\alpha i}^* d_{\alpha j}^* d_{\beta i} d_{\beta j} + 7.0 d_{\alpha i}^* d_{\beta i}^* d_{\alpha j} d_{\beta j} - 2.0(|d_{\alpha i}|^2)^2 + 5.5(d_{\alpha i}^* d_{\beta j}^* d_{\alpha j} d_{\beta i})] . \tag{3.9}$$

The coefficients in this expression are accurate to within a few percent. The difference between the above expression and that obtained previously[19] is that the earlier expression had the absolute value of the coefficients of the last three terms equal and the coefficients of the first two terms zero. For the AM state the bracketed expression becomes $10.5\times 9\Delta^4$ while for the BW state it is $\frac{10}{3}\times 9\Delta^4$. We have normalized the order parameter so that the second-order terms in the free energy are equal. Therefore we see that the free energy of the AM state is decreased by approximately three times more than that of the BW state. Using the weak-coupling free-energy difference, fourth order in Δ,

$$\Delta F_{\rm AM} - \Delta F_{\rm BW} = \tfrac{1}{5}N(0)\tfrac{7}{16}\zeta(3)\Delta^4/(\pi T)^2 ,$$

we define a dimensionless measure of the importance of the spin-fluctuation free energy as

$$\delta = \Delta F^s_{\rm BW}/(F_{\rm AM} - F_{\rm BW})$$

$$= \frac{150\pi^2}{7\zeta(3)}\left(\frac{T_c}{\epsilon_F}\right)\int_0^1 dx \frac{\bar{I}^2}{(1-\bar{I}+\alpha\bar{I}x^2)^2}$$

$$= 140\left(\frac{T_c}{\omega_s}\right)\left(\frac{\bar{I}^3}{\alpha(1-\bar{I})}\right)^{1/2} . \tag{3.10}$$

Substituting the experimental values of these parameters[11] near the melting curve we obtain $\delta = 3$ if we take $\alpha = \frac{1}{3}$. This number is clearly too large. One can understand why by examining the integral in (3.10). Since $(1-\bar{I})\sim 0.25$ using $\alpha = \frac{1}{3}$, the integrand does not drop off appreciably as a function of q. We therefore consider it appropriate to introduce a cutoff of the q integration. A cutoff $q_m \sim 0.2(2k_F)$ would give a value for $\delta \sim 0.6$, which is reasonably close to the values needed experimentally. Because of this cutoff problem we regard δ as the parameter of the theory. Finally it is amusing to note that the so-called polar state[25] $d_{\alpha i} = \sqrt{3}\,\delta_{\alpha x}\delta_{\alpha x}\Delta$ has a lower energy than the AM state at very large δ.

IV. HIGHER-ORDER FREE ENERGIES

In order to attempt to explain the entire phase diagram we calculate here the terms in the spin-fluctuation free energy (3.5) that are sixth order in Δ. We also calculate the spin-fluctuation contributions to the ground-state energies. Only the energies for the AM state and the BW state will be calculated. Consider first the sixth-order terms. Expression (2.3) for the susceptibility must now be expanded to order Δ^4 and inserted into Eq. (3.5), and the averages over angle and the sum over m must be performed. The algebra is somewhat tedious and will be omitted. We find that

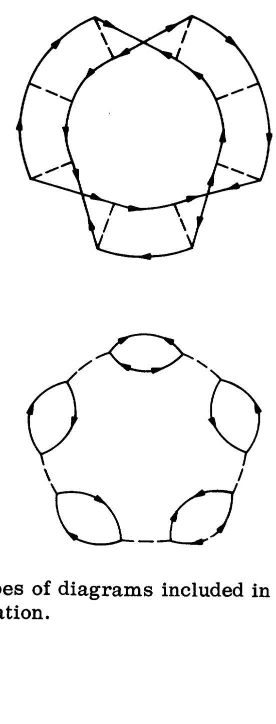

FIG. 4. Types of diagrams included in the free-energy calculation.

$$\Delta F^6_{S\,\mathrm{BW}} = \frac{3.27}{2\pi^2}\frac{N(0)}{\epsilon_F}\frac{\Delta^6}{T^3}\int_0^1 dx\left(\frac{\bar{I}}{1-\bar{I}+\alpha\bar{I}x^2}\right)^2, \tag{4.1}$$

$$\Delta F^6_{S\,\mathrm{AM}} = +2.98\Delta F^6_{S\,\mathrm{BW}} . \tag{4.2}$$

Therefore the terms sixth order in Δ arising from spin fluctuations favor the BW state more than the AM state. To obtain the total free energy the weak-coupling terms must be added. For the BW state they are

$$F_{\mathrm{BW}} = a\Delta^2 + \tfrac{1}{2}b\Delta^4 - \tfrac{1}{3}c\Delta^6 , \tag{4.3}$$

where

$$a = N(0)\ln(T/T_c),$$

$$b = N(0)\tfrac{7}{8}\zeta(3)/(\pi T)^2,$$

$$c = \tfrac{93}{128}\zeta(5)N(0)/(\pi T)^4 .$$

For the AM state we obtain

$$F_{\mathrm{AM}} = a\Delta^2 + \tfrac{6}{5}\tfrac{1}{2}b\Delta^4 - \tfrac{54}{35}\tfrac{1}{3}c\Delta^6 . \tag{4.4}$$

The fourth-order spin-fluctuation terms must also be added to these expressions and the temperature dependences of the two free energies compared. The spin-fluctuation terms are parametrized with the temperature-independent expression (3.10). We can then calculate $dT_{AB}/d\delta$, where T_{AB} is the temperature of the first-order transition between the BW and AM states. We find that the main effect is that the fourth-order weak-coupling terms go as T^{-2}, while the fourth-order spin-fluctuation terms go as $[T(1-\bar{I})\epsilon_F]^{-1}$, so that the weak-coupling terms become larger as the temperature decreases. The final result is that $(T_c - T_{AB})/T_c = 3.5(\delta-\delta_0)$. To compare our result with experiment the pressure dependence of δ is needed. We crudely estimate this by comparing the experimental variation of the discontinuity in the specific heat,[16] which is proportional to the inverse of the coefficient of the fourth-order term, with the result we obtain from our expression involving δ. Since the experimental number at $T_{AB}=T_c$ of $C_</C_>$, the ratio of the heat capacities just below to just above T_c, is 2.70 and our value is 2.60, we assume the 0.1 difference is a pressure-independent contribution and that all pressure dependences come from variations of δ. The theoretical expression (3.10) varies with pressure in essentially the same manner as the $\delta(P)$ determined from the heat capacity.[19]

The experimental slope near T_c is $(T_c - T_{AB})/T_c \simeq (\delta-\delta_0)$, so that there is qualitative agreement between theory and experiment.

To extend the results to lower temperatures we calculate the ground-state energy differences. To do so the summation over m in (3.5) must be converted to an integral

$$\Delta F_s = -\tfrac{1}{2}\sum_{ij}\int_0^\infty \frac{d\omega}{\pi}\int\frac{d^3\alpha}{(2\pi)^3}\,\mathrm{Im}\,\delta\chi^0_{ij}(\mathrm{Re}\,\delta\chi^0_{ij})\times\left(\frac{I}{1-I\chi^0_N(q)}\right)^2 . \tag{4.5}$$

Again factoring out the $N(0)/v_F q$ as in (3.6) we obtain

$$\Delta F_S = -\tfrac{1}{2}N(0)\int_0^1 dx\left(\frac{\bar{I}}{1-\bar{I}+\alpha\bar{I}x^2}\right)^2\times\sum_{ij}\int\frac{d\Omega_q}{4\pi}\int_0^\infty\frac{d\omega}{\pi}\,\mathrm{Im}\,\delta\bar{\chi}^0_{ij}\mathrm{Re}\,\delta\bar{\chi}^0_{ij} . \tag{4.6}$$

Finally the expressions (2.11) and (2.13) for the susceptibilities must be inserted and the integrals over ω and Ω_q performed. For the BW state the Ω_q integral can be done explicitly so that only the ω integral must be done numerically. This is most easily accomplished by subtracting off the form for $\delta\chi$ for large ω and integrating the asymptotic expressions analytically. The numerical integration is then rapidly convergent. For the AM state one has a nontrivial three-dimensional integral since $\delta\chi^0$ itself contains an integral over φ and the Ω_q integral reduces to an integral over the direction of q relative to the unique axis $\bar{l}$. We again have separated the asymptotic form for $\delta\chi^0$ out and performed the integrals involved analytically. Judging from tests with different integration meshes, the numerical part of the three-dimensional integral converged to within 1%. The final answers we obtained are

$$\Delta F_{S\,\mathrm{BW}} = -2.84\frac{N(0)\Delta^3}{\epsilon_F}\int_0^1 dx\left(\frac{\bar{I}}{1-\bar{I}+\alpha\bar{I}x^2}\right)^2, \tag{4.7}$$

and

$$\Delta F_{S\,\mathrm{AM}} = -9.55\frac{N(0)\Delta^3}{\epsilon_F}\int_0^1 dx\left(\frac{\bar{I}}{1-\bar{I}+\alpha\bar{I}x^2}\right)^2 . \tag{4.8}$$

Note that there is again approximately a factor of 3 difference between the two expressions. These results must again be added to the weak-coupling free energies and the total free energy minimized with respect to Δ. The weak-coupling free energy can be written[26]

$$F_0 = N(0)\int\frac{d\Omega_p}{4\pi}\left[-\Delta_p^2\ln\frac{2\omega_S}{\Delta_p} - \Delta_p^2\left(\frac{1}{2}-\frac{1}{\lambda}\right)\right] . \tag{4.9}$$

Here ω_S is the weak-coupling cutoff and λ is the effective coupling constant. If we write the spin-fluctuation energies as $\Delta F_s = N(0)\alpha\Delta^3$ then the minimum gap is, to first order in α,

$$\Delta = \Delta_0(1+\tfrac{3}{2}\alpha\Delta_0)\ , \tag{4.10}$$

where Δ_0 is the weak-coupling zero-temperature gap parameter

$$F_{\min} = N(0)(-\tfrac{1}{2}\Delta_0^2 - \alpha\Delta_0^3 - \tfrac{9}{4}\alpha^2\Delta_0^4)\ . \tag{4.11}$$

Equating the results for the two states and using the fact that $\Delta_0(\mathrm{AM}) = 0.94\Delta_0(\mathrm{BW})$ we find the critical condition to be

$$0.025 = 2.84\ \frac{\Delta_0(\mathrm{BW})}{\epsilon_F}\int_0^1 dx\left(\frac{\bar{I}}{1-\bar{I}+\alpha\bar{I}x^2}\right)^2 . \tag{4.12}$$

Writing $\Delta_0(\mathrm{BW}) = 1.76\ T_c$ and using the definition (3.10) for δ we find the zero-temperature critical value for δ to be $\delta = 0.87$. The theoretical phase diagram given by this calculation is therefore something like the solid line in Fig. 2. As already discussed, the best interpretation of the experimental data is the dashed line. We feel that, considering the crudity of the calculations, the qualitative agreement between experiment and theory is remarkable.

V. REMARKS ON CALCULATIONS

In Sec. IV we simply presented the calculations, leaving a number of steps unjustified. We will now briefly discuss these approximations. The most serious approximation made is the assumption that the interaction via normal-state spin fluctuations (3.4) can be treated with the weak-coupling approximation. In the usual strong-coupling theory of superconductivity,[27] one finds that the free energy is reduced relative to what one would obtain from the weak-coupling estimate because the mass renormalization is reduced owing to the introduction of a gap. This effect is apparently important in lead, where the specific-heat discontinuity is large, 3.71. We do not believe it should be as important here because the specific-heat discontinuity is considerably smaller and a good fraction of the deviation from BCS is presumably due to the feedback effect. It is important to note that any change in mass due to the change in the spin-fluctuation spectrum itself in the normal self-energy is included in the above calculations. This contribution is related to the normal part of $\delta\chi^0$, i.e., the product of the G's in (2.5). These terms have essentially no effect on the relative energies between the AM and BW states. Therefore we conclude that it is not likely that a complete strong-coupling calculation will change appreciably the results of the present calculation.

The next approximation is that of stopping at second order in $\delta\chi^0$. It is not difficult to convince oneself that the higher-order terms in $\delta\chi^0$ always introduce a factor of $(k_F\xi)^{-1}$, where ξ is the coherence length. Therefore all such terms are quite small compared with the expression retained. This remark is also true for those terms of higher order in q^{-1} in δ. As for the self-consistency procedure, it can be shown that the free energy can be written as a functional of the full 4×4 self-energy, just as was done for the normal state by Luttinger and Ward.[28,29] The free energy properly expressed is stationary with respect to variations of Δ. In our calculations we have simply imposed a form for Δ and minimized the free energy with respect to this form. More-detailed frequency-dependent forms should not make a large difference in the results. The free-energy form used here is, of course, not exact, nor has it been shown to be a rigorous upper bound of the exact free energy. We, however, believe it gives a correct description of the changes in the contribution of the spin fluctuations to the free energy in the superfluid states. Since these fluctuations are known to be important in the normal state, we feel that concentration on these changes is justified. Finally we do not believe that working at a constant chemical potential or regarding δ as a function of pressure instead of volume makes any difference because of the very small volume changes involved.

In conclusion then, it appears that the feedback effect does act to stabilize the Anderson-Morel state and also predicts a phase diagram that at least qualitatively agrees with experiment.

ACKNOWLEDGMENTS

The authors have benefitted from a number of useful conversations with E. I. Blount, V. Ambegaokar, D. D. Osheroff, J. C. Wheatley, and D. Rainer.

---

*Present address: Institute of Theoretical Physics, Department of Physics, Stanford University, Stanford, Calif. 94305.

†Supported in part by the U. S. Office of Naval Research under contract N00014-67-A-0077-0010.

[1]L. P. Pitaevskii, Zh. Eksp. Teor. Fiz. 37, 1794 (1959) [Sov. Phys.—JETP 10, 1267 (1960)].

[2]K. A. Brueckner, T. Soda, P. W. Anderson, and P. Morel, Phys. Rev. 118, 1442 (1960).

[3]V. J. Emery and A. M. Sessler, Phys. Rev. 119, 413 (1960).

[4]P. W. Anderson and P. Morel, Phys. Rev. 123, 1911 (1961).

[5]K. A. Brueckner and J. L. Gammel, Phys. Rev. 109,

1040 (1958).
[6]V. J. Emery, Ann. Phys. (N.Y.) 28, 1 (1964).
[7]N. F. Berk and J. R. Schrieffer, Phys. Rev. Lett. 17, 433 (1966).
[8]S. Doniach and S. Engelsberg, Phys. Rev. Lett. 17, 750 (1966).
[9]For a review see C. J. Pethick, in *Lectures in Theoretical Physics*, edited by K. T. Mahanthappa (Gordon and Breach, New York, 1969), Vol. 11.
[10]A. Layzer and D. Fay, Int. J. Magn. 1, 135 (1971); see also H. Bookbinder, Phys. Rev. A 3, 372 (1971).
[11]P. W. Anderson and W. F. Brinkman, Phys. Rev. Lett. 30, 1108 (1973).
[12]R. Balian and N. R. Werthamer, Phys. Rev. 131, 1553 (1963).
[13]D. D. Osheroff, R. C. Richardson, and D. M. Lee, Phys. Rev. Lett. 28, 885 (1972).
[14]R. A. Webb, T. J. Greytak, R. T. Johnson, and J. C. Wheatley, Phys. Rev. Lett. 30, 210 (1973).
[15](a) T. A. Alvesalo, Yu. D. Anufriyev, H. K. Callan, O. V. Lounosmaa, and P. Wennerstrom, Phys. Rev. Lett. 30, 962 (1973). (b) D. T. Lawson, W. J. Gully, S. Goldstein, R. C. Richardson, and D. M. Lee, Phys. Rev. Lett. 30, 541 (1973); D. N. Paulson, R. T. Johnson, and J. C. Wheatley, *ibid.* 30, 829 (1973).
[16]J. C. Wheatley *et al*. (unpublished).
[17]T. J. Greytak, R. T. Johnson, D. N. Paulson, and J. C. Wheatley, Phys. Rev. Lett. 31, 452 (1973).
[18]W. F. Brinkman, in *Proceedings of the Twenty-Fourth Nobel Symposium* (Academic, New York, 1974), p. 116.
[19]W. F. Brinkman and P. W. Anderson, Phys. Rev. A 8, 2732 (1973).
[20]N. D. Mermin and G. Starre, Phys. Rev. Lett. 30, 1135 (1973).
[21]A. A. Abrikosov, L. P. Gorkov, and I. E. Dzyaloshinski, *Methods of Quantum Field Theory in Statistical Physics* (Prentice-Hall, Englewood Cliffs, N. J., 1963), p. 315.
[22]D. C. Mattis and J. Bardeen, Phys. Rev. 111, 412 (1958).
[23]A. A. Abrikosov, L. P. Gorkov, and M. Khalatnikov, Zh. Eksp. Teor. Fiz. 37, 187 (1959) [Sov. Phys.—JETP 10, 132 (1960)].
[24]W. F. Brinkman and S. Engelsberg, Phys. Rev. 169, 427 (1968).
[25]C. M. Varma and N. R. Werthamer, Phys. Rev. A 9, 1465 (1974).
[26]G. Eilenberger, Z. Phys. 182, 427 (1965).
[27]See, for example, D. J. Scalapino, in *Superconductivity*, edited by R. D. Parks (Marcel Dekker, New York, 1969), Vol. 1, p. 449.
[28]The authors would like to thank E. I. Blount for discussions regarding this point.
[29]J. M. Luttinger and J. C. Ward, Phys. Rev. 118, 1417 (1960).