Solutions of the magnetic Eliashberg equations for heavy-fermion superconductors

M. R. Norman
Materials Science Division, Argonne National Laboratory, Argonne, Illinois 60439
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Recently, a method was put forth to evaluate quantitatively gap functions and transition temperatures for heavy-fermion superconductors. This formalism involves a modification of the Eliashberg spin-fluctuation equations of Berk and Schrieffer, with the modification being the replacement of the Lindhard susceptibility by the experimentally derived susceptibility. In the case of UPt_3, it was shown that both the mass renormalization and superconducting-transition temperature could be explained by this method. The purpose here is to discuss the results of the solutions to these equations in depth for the cases of UPt_3 and UBe_{13}, as well as some preliminary thoughts on other heavy-fermion metals.

I. INTRODUCTION TO SPIN FLUCTUATIONS

There is a growing body of literature which proposes spin fluctuations, in particular antiferromagnetic (AF) spin fluctuations, as the origin of superconductivity in heavy-fermion metals.[1,2] To test the validity of this proposal, one would need to put such ideas on a more quantitative basis. There are two aspects of this problem which need to be considered: (1) the effect of this interaction on the quasiparticle masses, and (2) whether the proposed interaction will lead to a correct superconducting solution. We have been worried about the former problem for quite some time. The large masses seen in heavy-fermion metals over that given by local-density-approximation (LDA) band calculations could be due to one of two things: (1) The LDA is not valid for these systems, or (2) there are large dynamical corrections to the ground-state LDA results. Certainly, the second point would be the most appealing, but the first cannot be ruled out.[3] It is difficult, though, to understand why the LDA does so well for predicting equilibrium lattice constants and bulk moduli for UPt_3 (Ref. 4) and UBe_{13} (Ref. 15) if point one were so. Recently, de Haas–van Alphen (dHvA) data on UPt_3 have appeared[6] which confirm to a good degree of accuracy the LDA Fermi surface.[7] This point is very significant, as it shows that the most questionable part of the LDA calculations, the ansatz for treating the f electrons as Bloch states obeying single-particle statistics, is valid (at least, for the ground state). Unfortunately, such data are not available on UBe_{13} and $CeCu_2Si_2$, so one cannot rule out that certain pathologies might occur for these metals. For our purpose, though, we will assume that point one is not true and proceed with a discussion of point two.

The mass renormalizations seen in heavy-fermion metals are so large that they limit what dynamical interactions could be involved. For many reasons, spin fluctuations seem to be a likely source. In exchange-enhanced metals like Pd, though, the actual spin-fluctuation enhancement of the mass is small. In that case, it is because of the nearly filled nature of the d band, which drastically reduces the phase space available for virtual spin excitations.[8] Such effects can even be seen in heavy-fermion metals. In the case of USn_3 ($\gamma = 170$ mJ/mol K^2), a mass renormalization factor of about 7.5 is extracted when compared to LDA calculations,[9] yet in the case of the related heavy-fermion magnet $NpSn_3$ ($\gamma = 240$ mJ/mole K^2), a factor of only 2.4 is found.[10] The essential difference between these two metals is that a series of f bands which lie just above the Fermi energy in USn_3 are pulled through the Fermi energy in $NpSn_3$, thus substantially reducing the available states above the Fermi energy for virtual processes in the latter metal. This observation led to an attempt by the author to evaluate the full four-point scattering function due to spin fluctuations[11] for the case of $CeSn_3$, a mixed valent metal whose LDA Fermi surface agrees with dHvA data.[12] This involved program was not successful, which the author feels is due to the nonvariational nature of the expressions used. One important observation, though, came from this work. The Berk-Schrieffer Eliashberg equations for spin fluctuations[13] lead to a mass renormalization proportional to the logarithm of the Stoner factor S. This is a consequence of using a Lindhard susceptibility function. If one replaces the Lindhard static susceptibility in the Berk-Schrieffer equations by a constant, then the mass factor scales with S as opposed to $\log(S)$. Since this is a better representation for heavy fermions because of the weak f-band dispersion, and we know experimentally that γ does indeed scale with χ,[14] the case for spin fluctuations is made stronger. Recently, a method combining density-functional techniques with Green's-function techniques has been used to evaluate spin-fluctuation enhancements in Pd and V.[15] We considered attempting to apply this method to UPt_3, but the evaluation of even the noninteracting susceptibility is complicated because of spin-orbit effects.[16] In fact, there is quite a lively debate at this time about whether the true dynamic susceptibility is even of quasiparticle origin.[2].

The resolution of this depressing state of affairs was to realize that the dynamic-susceptibility function was already given to us by neutron-scattering experiments. Therefore, by using this information in place of the Lindhard function, one could make an attempt to solve the

Berk-Schrieffer equations for heavy-fermion metals, both in the normal and pairing channels (a related approach has been advocated by Lonzarich[17]). This method will be discussed in Sec. III. Before doing this, though, it would be advisable to try to rule out phonons as a mechanism for superconductivity.

II. ELECTRON-PHONON INTERACTION

Since the electron-phonon interaction is responsible for virtually all known superconductors, it would be worth trying to rule it out before proceeding to spin fluctuations. The electron-phonon parameter λ has been evaluated for UPt_3 within the rigid-muffin-tin approximation by Oguchi *et al.*,[18] and comes out to be about 0.3. Plugging this into a McMillan expression gives a transition temperature of about the right value (assuming a very optimistic μ^* value). This paper has been criticized on a number of grounds. First, the λ values for the other heavy-fermion superconductors are much lower than that found for UPt_3.[19] Second, it has been suggested that Migdal's theorem is not valid for heavy-fermion systems because of their low-Fermi temperatures.[3] Recently, the latter point has been extensively addressed by Fenton.[20] If the large mass is due to dynamic effects, then the quoted Fermi temperatures are really just the frequency range over which the mass renormalizations exist. Since the phonons have a low-spectral density in this energy region, then the interaction responsible for the large masses does not affect the electron-phonon interaction to an appreciable extent (we assume that the electron-phonon interaction itself cannot cause mass renormalizations of 20 or more, for obvious reasons). This does not mean, though, that the gap function is not affected by these renormalizations. As Fenton has pointed out, the gap function in the frequency range over which the mass renormalizations exist is reduced by Z, the mass renormalization, thus suggesting that the calculated transition temperature must also be reduced by this factor.

In actuality, the situation is worse than this. This can be seen by doing an analysis similar to what McMillan did for ordinary superconductors,[21] where the frequency dependence of the gap is treated as a step function. In our case, though, an extra step has to be included to represent the fact that the gap is reduced at low frequencies. This frequency limit can be estimated by adding a step of this width on top of the band density of states, and adjusting the width to fit the experimental specific heat. For UPt_3, this turns out to be 15 K (half-width). Using this value and a Z of 20, along with the parameters of Ref. 18, a transition temperature of 10^{-23} K is calculated. To get significant deviations from this result, one requires that the transition temperature calculated without renormalizations is approximately equal to or greater than the renormalization frequency range. In fact, the observed transition temperature could be reproduced if λ was 0.72 and $\mu^*=0.1$. As this λ value is over twice that calculated by Oguchi *et al.*, and the μ^* used is most likely well too small, there would appear to be little hope of a standard electron-phonon solution. In the other heavy-fermion superconductors, the calculated λ's are much smaller than that of UPt_3, so the outlook is even darker for those metals. This does not mean that a more exotic phonon mechanism like that proposed by Razafimandimby, Fulde, and Keller[22] is not conceivable, but it too will have to conform to the guidelines discussed above.

III. THE MAGNETIC ELIASHBERG EQUATIONS

As mentioned in Sec. I some progress can be made in heavy-fermion metals by taking the Berk-Schrieffer magnetic (BSM) Eliashberg equations[13] and replacing the Lindhard function by the experimental susceptibility. The BSM equation in the normal channel is[13,23]

$$\Sigma(p,z)=-\tfrac{3}{2}I^2\sum_q\int_{-B}^{B}d\epsilon\,\delta(\epsilon-\epsilon_{p-q})\int_0^\infty\frac{d\Omega}{2\pi}\mathrm{Im}\chi(q,\Omega)\left[\frac{f(\epsilon)+n(\Omega)}{z-\epsilon+\Omega}+\frac{1-f(\epsilon)+n(\Omega)}{z-\epsilon-\Omega}\right], \tag{1}$$

where I is the contact interaction, and $2B$ the bandwidth. In the case of UPt_3, extensive neutron data by Aeppli *et al.*[24] reveal that to a good approximation

$$\mathrm{Im}\chi=-\chi(q)\Gamma\omega/(\Gamma^2+\omega^2)\,, \tag{2}$$

where $\chi(q)$ is the static susceptibility and Γ is the neutron line width (about 5 meV in the case of UPt_3). This approximate fit turns out to work well for most heavy-fermion and mixed valent metals. The solution of Eq. (1) using Eq. (2) has been derived in Ref. 25. The result for the mass renormalization at the Fermi surface (zero temperature) is

$$m^*/m_b=1+\tfrac{3}{8}I^2N\chi_{\mathrm{av}}=Z \tag{3}$$

with m_b the band mass, and χ_{av} the average of the static susceptibility over the zone. Note that Γ is not present in Eq. (3), but it does set the frequency range over which the mass renormalization exists [see Eq. (3) of Ref. 25]. To solve Eq. (3), we recognize that the ratio of the interacting (experimental) to the noninteracting (band) susceptibility (the Stoner factor, S) is $(1-IN)^{-1}$. Thus I is fixed given the bulk susceptibility and an appropriate LDA calculation (possible ambiguities will be discussed in Sec. V). From the neutron data of Ref. 24, the static susceptibility function at $q=\pi/c\,(0,0,2)$ is approximately twice that at the zone center, thus χ_{av} is about 1.5 times the bulk susceptibility. Given that $\chi(0)$ is about 0.26 states/meV (Ref. 14) and the band density of states N is about 0.0089 states/meV (Ref. 7), we get a Z of 16.5 for UPt_3, which is the value found when comparing either

specific heat or dHvA data to the LDA calculations.[7] In the case of mixed valent $CeSn_3$, one finds a Z of 4.7,[25] which is also consistent with experimental data. Other cases will be discussed in Sec. VI.

One can also evaluate Eq. (1) at finite temperatures, which requires doing the energy integral numerically. From this, one can extract the temperature dependence of γ in the normal state. This has been done for the case of UPt_3 and is plotted in Fig. 1 along with the phonon-corrected experimental data of Renker *et al.*[26] There is rather close agreement between these two curves. Note that this pseudo-$T^2 \ln T$ behavior is a consequence of the frequency dependence of the susceptibility in Eq. (2) and is different from that due to free-electron-like ferromagnetic paramagnons.[13]

This success led to a consideration of the pairing channel. Using a form given by McMillan,[21] it is

$$\Delta_p(z) = -\frac{1}{Z_p(z)}\frac{3}{2}I^2 \times \sum_q \int_{-\omega_c}^{\omega_c} \frac{d\epsilon}{E}\mathrm{Re}[\Delta_{p-q}(\epsilon)]\delta(\epsilon-\epsilon_{p-q})D[\Omega] , \tag{4}$$

where ω_c is a cutoff energy, D is the same frequency integral given in Eq. (1), and E is $(\epsilon^2+\Delta^2)^{1/2}$. The solution of this equation at zero temperature is derived in Ref. 25 and is

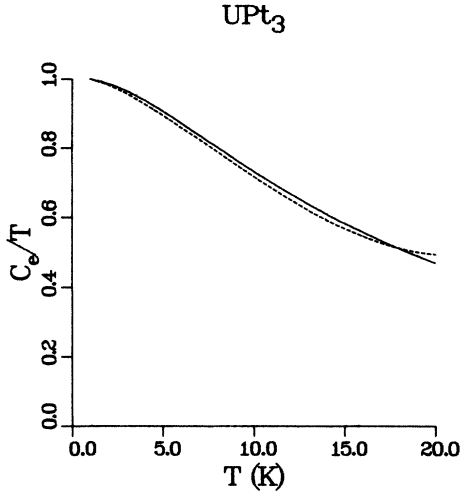


FIG. 1. Calculated dependence of the electronic specific-heat coefficient of UPt_3 in the normal state (solid line) vs temperature (arbitrary units). The dashed line is the phonon-corrected experimental data of Renker *et al.* (Ref. 26).

$$\Delta_p = -\frac{1}{Z_p}\frac{3}{4}I^2\sum_q \Delta_{p-q}\delta(\epsilon-\epsilon_{p-q})\chi(q)\ln\frac{2\Gamma}{\Delta_{p-q}} , \tag{5}$$

where a step function is assumed for the gap $\Delta(\omega)=\Delta$ for $\omega<\omega_c$ and zero otherwise (this approximation will be discussed in Sec. IV). Solving Eq. (4) at the critical temperature and using the results of Eq. (5), we find

$$T_c = \frac{\Gamma}{0.88}\exp\left[\frac{-\sum_q \Delta_{p-q}\delta(\epsilon-\epsilon_{p-q})\chi(q)\ln(2\Gamma/\Delta_{p-q})}{\sum_q \Delta_{p-q}\delta(\epsilon-\epsilon_{p-q})\chi(q)}\right] , \tag{6}$$

where the actual T_c is the maximum value in Eq. (6). In Eq. (6), the Δ's are the zero temperature Δ's given by solving Eq. (5). This assumes that $\Delta_p(T)$ is of the form $\Delta(t)f(p)$, an ansatz which will be justified in Sec. IV. As a final point, Z_p is found from Eq. (3) by replacing $N\chi_{\mathrm{av}}$ by $\sum\delta(\epsilon_{p-q})\chi(q)$. A more extensive discussion of these equations is given in Ref. 25. [Note that if $\chi(x-x')$ can be written in the form $a(x)a(x')$, one can eliminate Δ from Eq. (6) and obtain an expression which only depends on normal state quantities. This has been checked and yields the same results as Eq. (6).]

IV. THE GAP FUNCTION FOR UPt_3

To solve the gap equations of Sec. III one needs to know the Fermi surface and the q dependence of χ. In the case of UPt_3, the former is known since the dHvA data are consistent with the LDA surface; the latter is given approximately from the neutron data of Ref. 24. We model the surface by two ellipsoids at the zone center (Γ) and two disks about the A point $\pi/c(0,0,1)$. $\chi(q)$ is taken to peak at $\pi/c(0,0,2)$ where it has a value twice that at the zone center. The peaking of χ outside the zone boundary is a consequence of the nonsymmorphic nature of the lattice, reflecting antiferromagnetic correlations between the two U atoms in the primitive cell. Thus to solve the problem, we must fold the Kramers-degenerate Fermi surface out into a double zone (the effect this has on the symmetry of the gap function will be discussed below). Since $\chi(q)$ has approximately axial symmetry, we can integrate the ϕ dependence out analytically (where ϕ is the angle in the basal plane) and are left with one-dimensional integrals with respect to k_z to perform. These are done by specifying the gap function at a finite set of k_z values and replacing the integral by a weighted sum with the weights proportional to $dS/|\nabla\epsilon|$ (appropriately normalized to the proper density of states N). Equation (5) is then solved by simple iteration (a mixing factor of 20% is needed for stability) on a minicomputer. Fortunately, the converged solution does not depend on the particular starting values one uses. The inclusion of full hexagonal symmetry was done for one case (which required using Cray computer) but yielded virtually the same results as the axial approximation.

In Ref. 25 the solutions of these equations for various choices of $\chi(q)$ and Fermi surface dimensions were dis-

cussed. Unfortunately, the solutions in that paper were of odd parity.[27] These are not allowed, since by diagram counting, the factor of 3 in Eq. (4) is replaced by a factor of -1 for odd parity, and thus the pairing potential is repulsive. The author has now generated even-parity solutions. The gap functions behave roughly as $\cos(k_z c/2)$ and thus change sign under translation by $\pi/c(0,0,2)$. Because of this, the A-centered surfaces have lines of nodes on their equators. Since one of the zone-centered surfaces extends as far out as $\pi/c(0,0,0.75)$, its gap becomes rather small near the poles. The combination of these two effects leads to a rather small-transition temperature of about 23 mK.

Because the gap function oscillates in sign periodically, the integral over the zone of the gap times the average susceptibility vanishes. This removes the strongly repulsive (isotropic) part of the magnetic-fluctuation interaction, with the superconductivity being due to the oscillatory behavior of χ with q.[1] This is extremely important as it is the fundamental difference between what is being proposed here and a phonon-based mechanism. In the latter, the superconductivity is entirely due to the frequency dependence of the interaction. Another consequence of the change in sign of the gap function under translation by $\pi/c(0,0,2)$ can be seen by Fourier transforming with respect to r, the relative separation of electrons in the Cooper pair. It is trivial to verify that Δ vanishes at $r=0$ and peaks at a value equal to the separation of the hexagonal planes. Thus the gap solution represents pairing between electrons at near-neighbor sites.

We now address the question of whether the calculated transition temperature can be raised. From the form of Eq. (6), we see that T_c scales with Γ, so increasing Γ would raise T_c. As Γ, though, is fairly well fixed by the neutron data, we should seek elsewhere for answers. As will be discussed in Sec. V, there could be some ambiguity associated with the estimation of the contact interaction I. Since the Z function, though, has the same I dependence as the gap function, T_c turns out to be rather insensitive to I. As discussed extensively in Ref. 25, there is some dependence of T_c on Fermi-surface dimensions, but it is not a strong dependence. This leaves two possibilities. The first concerns the frequency dependence of the gap, which has been ignored up to now. This has been checked, though, for the case under consideration[25] and leads to about a 20% reduction in T_c (the procedure will be discussed in depth in Sec. VI for the more relevant case of UBe_{13}). The last possibility is related to the q dependence of χ. There are two aspects to be considered. The first is to realize that the magnitude of the oscillatory behavior of χ with q essentially acts as an effective coupling constant. In fact, if χ is taken to triple at its peak, rather than double, T_c is increased by a factor of 11. On the other side, if χ only increased by 50% at the peak, then T_c would be decreased by a factor of 15. After analyzing the data in Ref. 24, the author feels, though, that the factor-of-2 increase is the most reasonable. This leaves the question of matrix elements. When one calculates the susceptibility from a band structure, one must include matrix elements of the "single-particle" orbitals with the operator $e^{iq\cdot r}$. The effect is to reduce interband terms relative to intraband ones (this is what is responsible for keeping the susceptibility from diverging as one includes more and more bands). To see the importance of these matrix elements for our case, let us look at the Z function again. As shown in the table of Ref. 25, the Z function varies by only about 5% over the zone. If, though, one looks at the comparison of the experimental dHvA masses to the band masses,[7] the implied variation of Z is much greater. Unfortunately, the proper inclusion of these effects would require calculating the full interacting susceptibility from first principles, which would be an extremely involved project. We can, though, include these effects in a crude, phenomenological fashion as will be illustrated next.

To proceed, let us perform a calculation where only the Γ-centered surfaces are treated. In this case, the transition temperature is up to 884 mK. We now realize the importance of matrix-elements effects. By including these, we can start to decouple the two surfaces, leading to a higher-transition temperature. To do this, we simply put in a constant reduction factor for the interband terms in Eq. (5) and solve again. A reduction of the interband terms by 95% relative to the intraband ones is sufficient to boost T_c to 491 mK (the experimental value is about 500 mK). This, to be truthful, is a fudge factor, but there is some physical relevance to this. By analyzing the gap functions, one finds that the polar surfaces have gaps that are substantially smaller than those on the zone-centered surfaces (they are of similar size in the fully coupled case). This means that the polar surfaces will dominate for thermodynamic quantities such as the specific heat, thermal conductivity, and ultrasonic attenuation, as consistent with experimental data.[28] To show this in greater detail, we need to calculate the temperature dependence of the gap for this case. We will not make the ansatz $\Delta(p,T)=\Delta(T)f(p)$ as we wish to test its validity. This requires solving Eq. (4) at each required temperature, with the thermodynamic integrals being done numerically (by use of Gaussian quadratures). Convergence is reasonably fast, except when T gets close to T_c where convergence is extremely slow. The transition temperature is found to be about 0.99 of the value given by Eq. (6), with the 1% discrepancy being due to numerical approximations. Moreover, the above ansatz appears to be true, with $\Delta(T)$ having a BCS temperature dependence. By using these results, the specific heat has been calculated and is compared to the experimental data of Sulpice *et al.*[29] in Fig. 2. The agreement is quite good (the agreement is not as good for the fully coupled case).

V. THE SUSCEPTIBILITY FUNCTION FOR UPt_3

Since the susceptibility function is such a crucial input to this model, an extended discussion of it and how it enters the model is in order. As the reader must have gathered by now, use of the experimental susceptibility has been of great advantage. There is also another advantage not previously discussed. As is well known, there is no Migdal's theorem for spin fluctuations.[30] Fortunately, these effects appear to be important only at in-

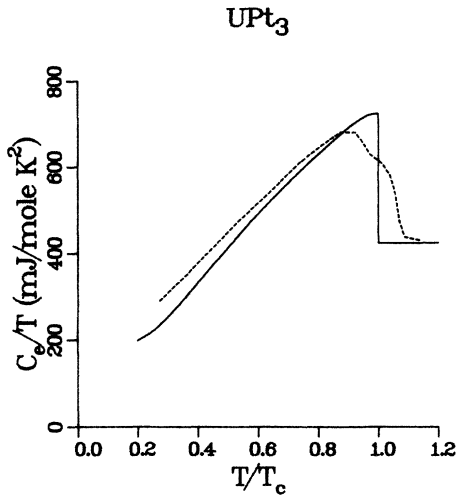


FIG. 2. Calculated dependence of the electronic specific-heat coefficient of UPt_3 in the superconducting phase (solid line) vs temperature for the interband reduction factor equal to 0.05. The dashed line is the experimental data of Sulpice *et al.* (Ref. 29).

termediate to high frequencies,[31] but certainly it would be naive to ignore them. By using the experimental susceptibility, though, certain classes of vertex corrections appear to be included automatically,[32] so there is a hope that further vertex corrections will not severely affect the results discussed above. It must be remembered at this stage that the superconductivity comes from a q dependence as well as an ω dependence, so the applicability of Migdal-type arguments will have to be modified anyway and will be discussed further below. A more severe approximation concerns the proper estimation of the contact interaction I. There are two required inputs: the experimental bulk susceptibility and the (noninteracting) band susceptibility (their ratio is the Stoner factor S) with I being determined from $S=(1-IN)^{-1}$. This can be derived from a variational principle within the context of spin density-functional theory.[33] The validity of this "formula" in the presence of strong spin-orbit coupling is questionable. In particular, a g factor of 2 is assumed when converting the density of states over into susceptibility units. It is comforting to know, though, that the local density estimate for I exceeds that extracted from experiment by only 15% (Ref. 7) in the case of UPt_3, and as the calculated mass renormalization is correct, there appears to be no problem in this case. As will be discussed in the next section, the renormalization factor calculated for UBe_{13} also appears to be correct, so one hopes that the current method for extracting I will stand the test of time. Another problem is that due to the difficulties of obtaining accurate data for the susceptibility function, only a limited region of q space has been sampled. In fact, it is known that Th-doped and Pd-doped UPt_3 actually magnetically order at (1,0,2) as opposed to the (0,0,2) vector considered here.[34] (102) correlations have now been seen in pure UPt_3, but they are weak and occur at a lower frequency scale.[35] The growth of the (102) correlations as one dopes leads to a rapid suppression of the superconductivity.[36] Can this be understood? The (002) correlations correspond to a U atom being antiferromagnetically correlated to its six nearest-U neighbors. (102) correlations, though, cause some of these neighbors to flip their moment directions.[34] Therefore, we would expect this to lead to a substantial pair-breaking effect and thus cause a rapid suppression of superconductivity, as seen experimentally. The point to be garnered here is the more q-dependent data obtained, the better model calculation one can perform.

Ultimately, one would like to be able to calculate the complete dynamical susceptibility from first principles, with full inclusion of matrix-element effects in the BSM equations. The author believes that this will be possible using density-functional techniques, especially given the success of the calculations of Ref. 15 for Pd and V. The author has calculated the noninteracting susceptibility for UPt_3 from bands which reproduce the de Haas–van Alphen Fermi surface. This involves using spin-orbit generalized matrix elements.[16] The calculations indeed show that the susceptibility is strongest at $\pi/c(0,0,2)$, with the peak in the imaginary susceptibility being at about 120 meV. When this is scaled by the Stoner factor of 30, one obtains a value of 4 meV, close to the experimental value of 5 meV. Of course, the experimental susceptibility seems to be well explained from a Kondo-impurity point of view,[2,24] and the fact that the line width does not go to zero at the point (0,0,4) seemed to cast doubt on a quasiparticle description of the susceptibility. In the presence of spin-orbit coupling, though, the latter statement is not valid.[37] This has been verified in the UPt_3 case,[16] where the imaginary susceptibility is substantial at $q=(0,0,0)$ for nonzero frequencies. Thus the author would be most surprised if one could not reproduce the experimental data from a density-functional-based method (an antiferromagnetic tendency for UPt_3 was predicted from LDA calculations before the neutron experiments were performed[4]). A correct density-functional treatment for the interacting susceptibility would require an extension of current spin-density theory to include spin-orbit effects. Although these effects have been included in a passive manner when doing moment-polarized calculations on heavy-fermion metals,[4,10,38] a correct theory is someways off. In particular, no analogous method to that given in Ref. 33 for calculating the susceptibility has been derived in the presence of spin-orbit coupling. Such efforts should be made, though, in an attempt to better understand the physics involved and to find the appropriate connections between density-functional and Kondo-based methods.

Finally, we must consider the validity of the Eliashberg equations themselves. The frequency assumptions implicit in Migdal's theorem seem to be okay. The band calculations on both UPt_3 (Refs. 4 and 7) and UBe_{13} (Refs. 5 and 39) indicate a Fermi temperature of the order of 1000 K. Thus the ratio of Γ (which acts as a Debye temperature) to E_F is a small number. The momentum assumptions are a different matter. The neglect of momentum derivatives in the BSM equations could cause some quantitative problems.[40] Certainly, the implied mass renormalization anisotropies noted in Ref. 7 could be due to

such terms, and/or to the matrix-element effects discussed above (which are themselves taken with respect to a momentum operator). As the superconductivity itself is proposed to be due to a momentum dependence, the inclusion of momentum derivative terms certainly needs to be explored. As this will lead to an enhancement of the anisotropy, one expects that it will also lead to a rise in T_c. To handle these terms, one also needs to calculate the matrix elements, which leads again to the complexity of doing a complete calculation using the band-structure wave functions.

VI. UBe_{13}, URu_2Si_2, AND $CeCu_6$

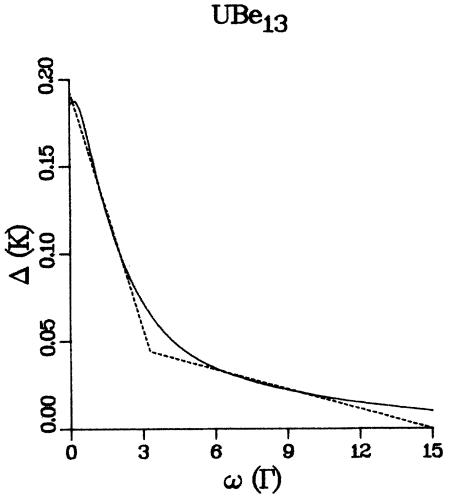
The above success has led to a consideration of other heavy-fermion metals. Preliminary neutron data on UBe_{13} has been reported by Neumann *et al.*,[41] indicating a peak in χ at $\pi/a(2,2,2)$, consistent with antiferromagnetic correlations between the two U atoms in the primitive cell. Note that χ peaking outside the zone is again reflective of the nonsymmorphic nature of the lattice. The data also indicates that χ increases by about a factor of 4 from the zone center to the (2,2,2) point (note, though, that the statistics are poor, and the data was taken at 10 K, above the coherence temperature for UBe_{13}). Other data of Goldman *et al.* at 10 K indicate a line width of about 13 meV.[42] Using the LDA density of states of Ref. 5 and the experimental bulk susceptibility tabulated in Ref. 14, a Stoner factor of about 92 is found. Since χ_{av} should be about 2.5 times the bulk value, a mass renormalization of 89 is found, close to the value of 92 needed. Unfortunately, no dHvA data is available on UBe_{13}, so we must take the LDA Fermi surface on faith. It consists of two nested spheres about Γ which are interconnected along the $\langle 111 \rangle$ lines[5,39] and pillboxes centered at the X points. We thus model the surface as a Γ-centered sphere and an X-centered ellipsoid. Because of the cubic symmetry present, the Fermi surface integrals in Eqs. (5) and (6) have to be treated two-dimensionally, which requires the use of a Cray. As in UPt_3, one must perform a double-zone foldout, this time along the $\langle 111 \rangle$ direction.

At first, no solutions were found. This was remedied by allowing the gap function to have complex phase and allowing the phase to be different on each of the three X ellipsoids. As in UPt_3, the solution appears to be independent of chosen start values for the self-consistency process, but in this case, a bad choice of start values led to divergent solutions, so it is conceivable that the solution space has not been completely searched. The obtained solutions are described in Table I as a function of the interband reduction factor. For the fully coupled case (factor equal to one), the solution is the E_g state of class $O(D_2)$ of Volovik and Gor'kov.[43] The Γ-centered surface has a gap function which vanishes at intersections of the surface with $\langle 111 \rangle$ lines. The X-centered surfaces have gaps which roughly behave as $e^{2\pi i n/3}$, where $n=1,2,3$ for each surface, respectively. There is, though, considerable warping on the surface. For instance, the gap function for the $n=3$ surface has a sizable imaginary component which has zeros when the angle ϕ is equal to odd powers of $\pi/4$. The difference between the Γ- and X-centered surfaces is essentially one of symmetry, with the Γ-centered surface having eightfold symmetry relative to the susceptibility peaks, and the X-centered surfaces only fourfold symmetry. It is encouraging that the Γ-centered gap function has point nodes, as this is expected from transport data[28] (see below). On the other hand, a transition temperature of only 193 mK is calculated. For the uncoupled case (factor equal to zero), the X-centered surfaces have similar gaps as before with a transition temperature of 1665 mK. The Γ-centered surface, however, has a roughly constant gap function with real phase and a transition temperature of 2648 mK. The intermediate case with a factor equal to 0.5 is similar to the fully coupled case, whereas the case with a reduction factor of 0.25 has a Γ-centered gap function with a real part that is larger at the poles than at the equator and an imaginary part which is zero when ϕ is equal to odd multiples of $\pi/4$ (there are no nodes). The transition temperature for this case is equal to the experimental value of 0.9 K.

TABLE I. Superconducting solutions for UBe_{13}. The neutron line width is taken to be 151 K, and the peak value of χ at $\langle 222 \rangle$ is assumed to be four times the bulk value. The solutions are tabulated according to the interband reduction factor (ranging from 1.0 for fully coupled to 0.0 for uncoupled). Listed for each surface is the mass renormalization at the $\theta=0$, $\phi=0$ point for the Γ $\langle 0,0,0 \rangle$ and X $\langle 0,0,2 \rangle$ surfaces, as well as the "transition temperature" for each surface (mK). Only in the uncoupled case, of course, would there be two transitions. The gap functions for the first two cases are of E_g symmetry, whereas those of the last case are of A_{1g} symmetry for Γ and E_g symmetry for X. The third case is a mixture of both symmetries.

Solution	$Z(\Gamma)$	$Z(X)$	$T_c(\Gamma)$	$T_c(X)$
1.0	88.5	88.5	193	186
0.5	81.4	96.8	470	495
0.25	74.7	102.3	821	943
0.0	65.5	111.5	2648	1665

Specific-heat data reveal that there is a sizable strong-coupling correction to the gap jump at T_c.[44] We thus turn to a discussion of the frequency dependence of the gap function as alluded to in Sec. IV. The frequency dependence of Z has already been given by Eq. (3) of Ref. 25 (Z decreases smoothly with frequency). We take as the zero-order gap a step function equal to that of Eq. (5) for $\omega<\omega_c$ and zero otherwise (ω_c is taken to be some reasonable value like 3Γ; the chosen value is not important). As the energy integrals are analytic, we can solve as before to generate the gap as a function of frequency. The resultant $\Delta(\omega)$ is approximated by a two-line segment function so as to keep the energy integrals analytic. After about three iterations, the gap function is reasonably converged. This is shown for one of the UBe_{13} cases in Fig. 3. The gap function drops off rapidly for $\omega>0.25\Gamma$, then begins to even out for $\omega>5\Gamma$. This high-frequency tail is most likely unphysical, since for large enough frequencies, one expects that Coulomb repulsion effects (even in the anisotropic channel) will



FG. 3. Frequency dependence of the gap function for UBe_{13} with the interband reduction factor equal to 0.25. The frequency is in units of the line width (151 K). The straight line segments are approximations used during the iterative process and for calculating the transition temperature. The high-frequency tail would be forced negative by neglected effects, such as that due to the anisotropic Coulomb pseudopotential.

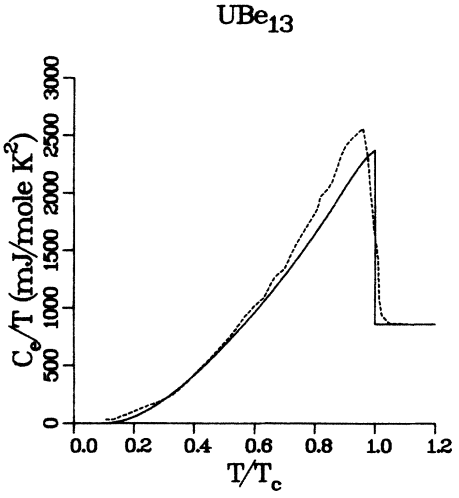


FIG. 4. The electronic specific heat for UBe_{13} in the superconducting phase calculated for the interband reduction factor equal to 0.25. A strong-coupling scaling factor of 0.69 has been included (calculated from Fig. 3). The dashed line is the experimental data of Ott *et al.* (Ref. 44).

come into play, leading to a negative gap function just as in the phonon case. This is equivalent to saying that the attractive nature of the pairing will be lost for high enough frequencies. Given the two-line-segment approximation to $\Delta(\omega)$, Eq. (6) is then solved. For the case of UBe_{13}, a reduction of about 30% for T_c is found, with a weak dependence of this T_c reduction relative to the interband reduction factor. We now solve for the temperature dependence of the gap function. For one case, this was done exactly as done above for UPt_3 (very time consuming), but it was discovered that the temperature dependence is virtually identical to that of BCS theory. We thus assumed a BCS dependence after this, which made the evaluation of the specific heat trivial. Finally, the temperatures were all scaled by the calculated 30% reduction due to strong coupling when calculating the specific heat. In Fig. 4, C/T is shown for the interband reduction factor equal to the 0.25 case, as well as the experimental data of Ref. 44. One sees that the calculated strong-coupling corrections seem to be in good agreement with experiment. The calculated curve, though, is not as broad as the experimental curve in the region $0.5T_c < T < T_c$, perhaps due to fluctuation effects. It is interesting to note that the gap function for the factor equal to 1.0 case has nodes, whereas the factor equal to 0.25 does not, yet their two C/T curves are similar. This illustrates the difficulties of determining gap nodes from experiment in UBe_{13} (in the case of UPt_3, the line of zeros is quite obvious).

At this point, we note the fact that the amount of experimental information on the susceptibility function for UBe_{13} is considerably poorer than that for UPt_3. The published data have large error bars and were taken at a temperature well above the accepted coherence temperature (getting reliable data on UBe_{13} is more difficult than for UPt_3). One wonders, though, what experiments will reveal at lower temperatures. Preliminary data of Mook *et al.*[45] show additional strong structures at lower frequencies (<2 meV) which peak at q vectors different than the $\langle 222 \rangle$ ones considered here. It may take a considerable effort to get as complete information as we have for UPt_3, but the author feels such information is crucial in making improvements over the current set of calculations. Also, several workers have emphasized that quadrupole fluctuations may be important for UBe_{13} (Ref. 46); these effects have not been included in this formalism.

We now turn to a brief discussion of other heavy fermion metals. Experimental data on the susceptibility function are now known for U_2Zn_{17} (Ref. 47), URu_2Si_2 (Ref. 48), and $CeCu_6$ (Ref. 49). The function for U_2Zn_{17} is similar to that of UPt_3, with the difference being that the product IN has exceeded one, leading to a sizable moment for U_2Zn_{17}. Naturally, the system does not superconduct as the energy gain due to magnetic ordering exceeds that for pair condensation. The case for URu_2Si_2 is different, however. The experimental data indicate spin-density-wave (SDW) excitations, and the resulting susceptibility function has a spin-wave gap at low frequencies. The moment of this state is very weak, being of the order of $0.03\mu_b$. One concludes from this that the factor IN is only exceeded in a small neighborhood of the zone about the magnetic ordering vector, and therefore regions away from there can still gain condensation energy via pair formation. Experimentally, URu_2Si_2 superconducts below 1.5 K (Ref. 50) (the SDW transition is at 17.5 K). Although the susceptibility function is now different because of the presence of an SDW gap, the integrals are probably still analytic, and one could proceed in an analogous fashion to what was done before. The major problem is determining a Fermi surface to use for the SDW state. Experimentally, there appears to be a sizable gapping of the Fermi surface in the SDW state.

The author has performed band calculations in the paramagnetic phase for URu_2Si_2 (Ref. 38) which reveal that the product *IN* barely exceeds one. Moreover, nesting is observed with a wave vector equivalent to the experimental ordering vector. This has led to an attempt to treat the AF phase with the same moment-polarized formalism which was applied with success to the heavy-fermion magnet $NpSn_3$ (Ref. 10) (this includes orbital-moment effects). The calculation has only been partially converged, but the preliminary results indicate that the calculated moment far exceeds the $0.03\mu_b$ value, and there appears to be little change in the density of states [sizable gapping was found for $NpSn_3$ (Ref. 10), TmSe (Ref. 51), and UCu_5 (Ref. 38) in agreement with experiment]. This implies that the SDW state may not be treatable by current methods, which means we have no reliable Fermi surface to input until the relevant dHvA data become available.

Local-density studies on the heavy-fermion magnets indicate that the product *IN* greatly exceeds one [$NpSn_3$ (Ref. 10), UCu_5 (Ref. 38), TmSe (Ref. 51)], whereas for the superconducting systems, the product *IN* just exceeds one [UPt_3 (Refs. 4 and 7), UBe_{13} (Ref. 5), URu_2Si_2 (Ref. 38)], with *I* being evaluated via the local spin-density Vosko-Perdew formalism[33] (questionable in the presence of large spin-orbit terms). This interesting correlation brings up the question of the "vegetables," those compounds which are neither magnetic nor superconducting. Band calculations on $CeCu_6$ indicate that *IN* is about 0.64,[52] smaller than that found for (nonmagnetic) mixed-valent $CeSn_3$.[12] Calculations on superconducting $CeCu_2Si_2$ indicate similar factors,[19] but there were certain spherical approximations made in those calculations which were shown to be severe for URu_2Si_2,[38] so the identification of vegetables remains unclear at this time. Experimentally, strong *AF* correlations are seen in $CeCu_6$,[49] so it is not clear why such a metal is not a superconductor. A Fermi surface has been extracted from band calculations,[52] but only a limited amount of dHvA data has been reported,[53] which is insufficient to determine the validity of the LDA surface. The author is being careful at this point, since the Kondo magnet CeB_6 [which has a γ of about 260 mJ/mole K^2 (Ref. 54)] has a Fermi surface consistent with *f* electrons *not* being part of the Fermi surface,[55] as seen in most rare-earth metals. Even accepting the LDA surface, its extreme complexity inhibits any simple modeling as was done in the previous cases. Moreover, the surface was calculated for the high-temperature orthohombic phase, not for the low-temperature monoclinic phase. The low symmetry of this phase, coupled with the possible presence of some ferromagnetic correlations,[49] might be responsible for the absence of superconductivity. Moreover, the neutron line width appears to be of the order of 0.25 meV,[49] a factor of 20 smaller than in UPt_3.

VII. CONCLUSIONS AND SPECULATIONS

This paper and the previous one[25] represent an attempt to put the heavy-fermion superconductivity problem on a more quantitative basis. It is encouraging that mass renormalizations of the correct value and superconducting solutions with the appropriate anisotropy were obtained. The calculated transition temperatures for UPt_3 and for UBe_{13} are about correct. Of course, the history of calculating transition temperatures in superconductivity theory has certainly not been the most illustrious in condensed matter physics, so how much relevance one attaches to numbers at this stage is an open question.

From the theory side, the author feels there are two areas where further work is definitely needed. The first is the validity of the kernel in the integral equations and the correct extraction of *I* in the presence of spin-orbit interactions. The second is the inclusion of momentum derivative terms in the Eliashberg equations, as well as the proper inclusion of matrix elements. The latter is probably the more important, but will substantially increase the computational effort. From the experimental side, more dHvA data and more neutron-scattering data are needed to elucidate the correct Fermi surface and susceptibility function to use in the equations. The former can also be used to check the overall mass renormalization, as well as renormalization anisotropies. Both sets of experiments are extremely difficult, but they are the most important ones to consider at this stage. As of now, relatively complete data are available only in the case of UPt_3.

In conclusion, the author hopes this work will inspire a trend towards more quantitative theories for heavy-fermion systems.

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