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Effective electron-electron interactions and the theory of superconductivity

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Electron pairing is examined from a viewpoint which treats electron-electron interactions first (both in a single band and two-band context) and only later adds in electron-phonon coupling. We report solutions to the Eliashberg equation for the one- and two-band interacting electron gas, in the absence of phonons and then with phonons included, using effective electron-electron interactions that are closely constrained by sum rules. No s-wave pairing is found for the one-band case in the absence of phonons but higher angular momentum pairing is possible. In some contrast, intrinsic s-wave pairing is found for the two-band case, and again nonzero angular momentum pairing may arise. With the subsequent inclusion of phonons, but treated on a completely equal footing with electrons, transition temperatures of several simple metals are determined, and found to agree to within 20% of measured values. For low density systems, significant deviations from the predictions of the McMillan expression assuming $\mu^* \approx 0.1$ are found. An important example is Li where we obtain $T_c \approx 0.4$ mK in sharp contrast with previous approximations which give $T_c \sim 1$ K, and are not supported by experiment. [S0163-1829(97)06821-5]

I. INTRODUCTION

In the traditional approach to the theory of superconductivity, the phonon mediated interaction is usually treated first and the direct Coulomb interaction is subsequently introduced in terms of the Morel-Anderson pseudopotential, μ^*. Most calculations of the transition temperature concentrate on treating the phonon mediated interaction, some with great accuracy, while the Coulomb interaction is often incorporated in a fairly approximate way, for example, by simply assuming that $\mu^* \sim 0.1$. However, from a consideration of the energy scales in the initiating problem ($H = H_{e\text{-}e} + H_{e\text{-ph}} + H_{\text{ph}}$, $H_{e\text{-}e} \gg H_{e\text{-ph}} \gg H_{\text{ph}}$), it might appear more reasonable to first take into account the large electron-electron interaction and only then treat the smaller electron-phonon interaction. In the following, we take this viewpoint and first consider the problem of intrinsic superconductivity in the one- and two-band electron liquids. We then reconsider the problem when phonons are present, and added (but with due account taken of their frequency scales) to the electronic problem. As we will show, the phonon mediated interaction and the Coulomb interaction can together be treated on a completely equal footing.

In 1965 Kohn and Luttinger[1] considered the possibility of superconductivity in the three-dimensional homogeneous interacting electron gas without phonons or other intermediaries. A direct consequence of Fermi-Dirac statistics together with an approximate treatment of screening could lead, as they noted, to regions where the effective electron-electron interactions were weakly attractive. Though pairing states with off-diagonal long-range order could then develop in principle, the corresponding critical temperatures were extremely low. Intrinsic superconductivity has since been considered by several authors,[2–4] the most comprehensive exploration in the one-band case being the recent work of Takada[4] where the effective interaction included vertex corrections to all orders made possible by the use of the Kukkonen and Overhauser[5] (KO) approximation. This approach leads to a physically motivated expression for the effective interaction, and it is derived by considering the rearrangement of electrons in the vicinity of a test charge with which other particles interact both through a direct Coulomb term and an exchange and correlation term. The latter is taken to be proportional to the direct interaction contribution where the proportionality term is expressed as a local field factor. In this way, the KO approximation leads to the inclusion of the major many-body effects through the introduction of local field factors. In Takada's work the expression for the effective interaction actually uses Hubbard-like local field factors, and these show quite significant departures from those expected from a more complete description.[6,7] One of the purposes of the present paper, therefore, is to show that the use of more realistic local field factors leads to an absence of intrinsic s-wave superconductivity in the three-dimensional one-band case over a wide range of densities; p- and d-wave pairing are not, however, ruled out.

The two-band case is found to be strikingly different, when again quite realistic forms for the local field factors are used. The possibility that intrinsic superconductivity might occur in a *two-band* electronic system was raised earlier by Geilikman,[8] following on from a suggestion of Little.[9] More recently, Vignale and Singwi[10] and Chakraverty[11] have discussed in some detail the possibility of superconductivity in electron-hole systems, and Ruvalds[12] has examined the possibility that acoustic plasmons in a two-band model could explain the substantial transition temperatures observed in the high-temperature superconductors. In these models, as here, the residual interactions between the two bands lead to physically interesting forms for the effective attractions between electrons. Once again if Hubbard-like forms for the local field factors are used and the Kirzhnits, Maksimov, and Khomskii (KMK) approximation[13] for the calculation of the superconducting transition temperature, T_c, is also used, Vignale and Singwi have found that correlated charge fluctuations (as reflected again in the local-field factors) can mediate a superconducting transition. However, the KMK ap-

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proximation might reasonably be expected to break down for this system since the frequency scale for the attractive interaction is not at all small compared to the Fermi energy.[2,3]

In the following we describe a method which attempts to overcome these difficulties; the key is a complete solution of the frequency and momentum dependent Eliashberg equation using fully self-consistent Green's functions, which incorporate accurate local field factors that satisfy the known sum rules. The principal aims are therefore first to examine the possibility of intrinsic superconductivity in one- and two-band systems, and second to only then reexamine the problem when phonons are included but in a manner in which electrons and phonons are both treated on a *completely equal footing*. In calculations of the superconducting transition temperature in metals, it has become common practice to describe the role of the direct Coulomb interaction through the use of the parameter μ^* (the Coulomb pseudopotential introduced above), which is usually obtained from tunneling data, calculated from the static effective interaction in a square-well approximation, or simply assumed to be about 0.1 (see Ref. 14 for a discussion of the physical origins of μ^*). We shall describe here a technique for calculating the transition temperature where the Coulomb interaction and the phonon mediated interaction are actually treated together, *a priori*. A principal finding is that the role of the Coulomb repulsion in establishing the transition temperature cannot always be treated using the standard approximations for μ^*. In particular, the rather common assumption that $\mu^* \approx 0.1$ appears to significantly overestimate the superconducting transition temperature in low density three-dimensional one-band systems where the Coulomb repulsion is strong. A striking example of this may be found in the element lithium (which, accounting for the band mass has an *effective* $r_s = 5.7$) where the assumption $\mu^* = 0.1$ causes an overestimation of the transition temperature by orders of magnitude. On the other hand, for two-band systems, which we find can be superconducting even without phonons, it will be seen the assumption that $\mu^* \approx 0.1$ can significantly underestimate the superconducting transition temperature.

II. ELIASHBERG EQUATION

The Eliashberg equation[15] for the pairing function, $\Phi_l(k,i\omega_n)$, of l-wave superconductivity can be written as

$$\Phi_l(k,i\omega_n) = -T\sum_{\omega_{n'}} \int_0^\infty dk' K_l(k,i\omega_n;k',i\omega_{n'})\Phi_l(k',i\omega_{n'}), \tag{1}$$

where

$$K_l(k,i\omega_n;k',i\omega_{n'}) = \frac{k'}{4\pi^2 k}|G(k',i\omega_{n'})|^2 \int_{|k-k'|}^{k+k'} dq P_l \times \left(\frac{k^2+k'^2-q^2}{2kk'}\right) qV_{\text{eff}}(q,i\omega_n - i\omega_{n'}), \tag{2}$$

and $V_{\text{eff}}(q,i\omega)$ is the irreducible electron-electron interaction.

Equation (1) can be solved by using a technique similar to that of Rietschel and Sham[2] and Takada.[4] To do so the anomalous self-energy, $\Phi_l(k,i\omega_n)$, is evaluated on a finite grid in k and ω_n with a grid spacing chosen to be small compared to the scale on which $\Phi_l(k,i\omega_n)$ varies. For the evaluation of $\Phi_l(k,i\omega_n)$ at arbitrary k,ω_n we then linearly interpolate between nearest grid points. When we examine the possibility of intrinsic superconductivity, we must select a grid spacing in frequency which is small compared to the Fermi energy at small frequencies and which then increases for large frequencies until it is on the order of the Fermi energy. Later, with phonons included, we must choose instead a grid spacing in frequency which is also small compared to the Debye frequency for small frequencies and which again increases for larger frequencies (until it is again on the order of the Fermi energy). We find, as has Takada,[4] that $\Phi_l(k,i\omega_n)$ possesses considerable structure at the Fermi wave vector; a sharp dip appears in it for frequencies larger than the Fermi energy, and in order to accurately accommodate this structure in our calculations it is essential to use a grid spacing in k that is very small at the Fermi wave vector. For typical transition temperatures, $T_c \sim 10^{-5}\epsilon_f$, this grid spacing at the Fermi wave vector is $\Delta k \approx 0.001 k_f$, but an even smaller spacing is required for systems with smaller transition temperatures. The spacing is also chosen in such a way that it increases as k is moved away from k_f; that it is actually fine enough is ensured by examining the resulting function $\Phi_l(k,i\omega_n)$. If there are regions where $\Phi_l(k,i\omega_n)$ is not slowly varying over the grid, we simply repeat the calculation with additional grid points supplied and repeat this procedure yet again until the determination of the transition temperature is converged.

The method of evaluating $\Phi_l(k,i\omega_n)$ then converts Eq. (1) into a matrix equation with the formal structure

$$\mathbf{M}_l \mathbf{\Phi}_l = \mathbf{\Phi}_l, \tag{3}$$

and it can be straightforwardly converted into an eigenvalue problem by writing

$$\mathbf{M}_l \mathbf{\Phi}_l = \gamma \mathbf{\Phi}_l, \tag{4}$$

showing that Eq. (1) is recovered when one of the eigenvalues, γ, is equal to unity. To calculate the transition temperature, we therefore solve Eq. (4) for the *largest* eigenvalue as a function of T. For high temperatures, this largest eigenvalue is always found to be less than unity; the transition temperature is then determined as that temperature for which the largest eigenvalue eventually equals unity.

Since Eq. (1) involves a sum over Matsubara frequencies, and there are on the order of ϵ_f/T_c such terms in this sum, it would not be feasible to calculate T_c for low temperature systems if we were required to evaluate the integrand at each and every such frequency. However, the integrand is a smooth function of ω_n, and we can therefore easily evaluate the sum using a technique similar to Romberg integration;[16] solutions to Eq. (1) for temperatures at least as low as $T_c \sim 10^{-11}\epsilon_f$ can thereby be obtained. Ultimately, the lowest temperature that can be reached is limited by the sharp structure discussed above in the pairing function, $\Phi_l(k,i\omega)$, namely the dip that occurs near $k = k_f$ for large frequencies. Its origin is traced to the long ranged part of the Coulomb interaction and as noted it was first discovered by Takada[4] in his comprehensive electron gas calculations. For low transition temperature systems, we must use a high density of grid points near $k=k_f$ to resolve this important feature since it grows with decreasing temperature. To see this, we may evaluate Eq. (1) for large frequency by treating $\Phi_l(k',i\omega_{n'})$ inside the integral as a constant and simply replacing the momentum integral by an integral over the density of states, which we also treat as a constant. Ignoring factors and also ignoring terms that do not contribute to the long-wavelength singularity in $P_l[(k^2+k'^2-q^2)/2kk']V_{\mathrm{eff}}(q,i\infty)$, we find

$$\Phi_l(k_f,i\infty)\sim\int_0^{\epsilon_f}d\epsilon\,\frac{1}{\epsilon}\,\tanh\left(\frac{\epsilon}{2T_c}\right)\ln(\epsilon/\epsilon_f)\Phi_l(k_f,i\omega_0), \tag{5}$$

which in turn implies that

$$\Phi_l(k_f,i\infty)\sim-\ln^2(T_c/\epsilon_f)\Phi_l(k_f,i\omega_0), \tag{6}$$

in the limit that $T_c \ll \epsilon_f$. This structure will be evident in all of the pairing functions, $\Phi_l(k,i\omega)$, that we calculate in the following, and as noted it will also be evident that its scale grows with decreasing transition temperature.

III. EFFECTIVE INTERACTIONS

The essential input into the Eliashberg equation (1) is the effective interaction, V_{eff}, which can be defined as the part of the scattering amplitude that is irreducible in the particle-particle channel. For the electron gas, the simplest reasonable approximation to the effective interaction is the random phase approximation (RPA); it includes screening effects but ignores exchange and correlation corrections.[17] Since the RPA leads to the form screened v/ϵ, it might seem that it could be improved by simply using a more accurate dielectric function, ϵ. This is not the case: exchange and correlation effects enter into vertex corrections and electron-hole ladder diagrams, as well as in the dielectric function itself. Kukkonen and Wilkins[18] therefore attempted to improve the RPA by writing the effective interaction as $v\tilde{\Lambda}^2/\epsilon$, where $\tilde{\Lambda}$ is the proper vertex correction evaluated in the local approximation; this means that $\tilde{\Lambda}$ is taken to depend only on the momentum and frequency transfer. This local approximation allows $\tilde{\Lambda}$ to be evaluated in terms of the local field factor, G_s, which is then used to describe the charge response function. However, the Kukkonen-Wilkins interaction is still not sufficient for our purposes since it ignores the electron-hole ladder diagrams. To address this particular omission, Kukkonen and Overhauser[5] derived an expression for the effective interaction that consistently includes exchange and correlation effects to all orders leading to a result which includes the Kukkonen-Wilkins term and the same local approximation to the electron-hole ladder diagrams. The essential inputs into the Kukkonen-Overhauser (KO) approximation[5] are (i) the identical local field factor, G_s, used in the dielectric and the Kukkonen-Wilkins approximation, but additionally (ii) the local field factor, G_a, used to describe the spin response function. Kukkonen and Overhauser derive their result by considering the exchange-correlation hole around an electron and they calculate the interaction of a second electron with this screening cloud. This expression has also been derived by Vignale and Singwi (VS) using a diagrammatic approach.[10,19]

In what follows, we derive the KO expression for a *multiband* electron liquid using the Kukkonen-Overhauser approach. To correctly include self-energy effects we find that the Lindhard function appearing in the effective interaction will have to be modified. This, as we will see, leads to the introduction of a third local field factor, G_r. We will show below that an approximate phonon mediated interaction can also be included, exactly within the same framework.

The Hamiltonian that defines the multiband jellium problem is

$$H=\sum_{\mathbf{k}\alpha}\frac{k^2}{2m_b^\alpha}c^\dagger_{\mathbf{k}\alpha}c_{\mathbf{k}\alpha}+\frac{1}{2V}\sum_{\mathbf{k}\alpha}\sum_{\mathbf{k}'\beta}\sum_{\mathbf{q}\neq0}v_c^{\alpha\beta}c^\dagger_{\mathbf{k}+\mathbf{q}\alpha}c^\dagger_{\mathbf{k}'-\mathbf{q}\beta}c_{\mathbf{k}'\beta}c_{\mathbf{k}\alpha}, \tag{7}$$

where m_b^α are the band masses, V is the volume, and $v_c^{\alpha\beta}=4\pi e^\alpha e^\beta/\epsilon_b q^2$ is the bare Coulomb interaction reduced by the background dielectric constant, ϵ_b. The indices, α and β, indicate both band and spin. We permit the sign of the charge to depend on band index since we wish to consider both electron-electron systems and electron-hole systems. In writing Eq. (7), the assumption at this point is that the ions are static and that the electron-ion interaction corresponds to a periodic situation. In a one electron description it is this periodicity that gives rise to the band structure that is here represented by n separate bands within an effective mass approximation. It leads to a view that there are no further effects of the electron-ion interaction that are not subsumed in the uniform background approximation of the jellium model. Note that the Hamiltonian (7) does *not* lead to interband transitions; this has been shown to be a reasonable approximation if the bands have a small overlap integral such as s and d bands.[20]

In the KO formulation, the effective electron-electron interaction is determined by examining the interactions between a pair of electrons and their accompanying screening clouds. Following this approach, we consider an electron from band i with spin σ; it can induce a change, $\Delta n^{k\nu,i\sigma}$, in the number of electrons in the surrounding electron gas. (For notational simplicity we need not explicitly indicate the momentum and frequency dependence, but it should be remembered that the quantities $\Delta n^{k\nu,i\sigma}$, the local field factors, and the effective interaction all depend both on momentum and frequency transfer.) An electron from band j with spin σ' will interact with both the electron from band i and with $\Delta n^{k\nu,i\sigma}$; the *effective* interaction is therefore given by the interaction between the two electrons augmented by the interaction that the electron from band j feels due to the screening cloud around the electron from band i. The complete effective interaction can therefore be decomposed into a direct part

$$\tilde{V}^{j\sigma',i\sigma}_{\mathrm{direct}}=v_c^{ji}+\sum_{k\nu}v_c^{jk}\Delta n^{k\nu,i\sigma} \tag{8}$$

and an exchange-correlation part

$$\tilde{V}^{j\sigma',i\sigma}_{\mathrm{exc}}=-v_c^{ji}G^{j\sigma',i\sigma}-\sum_{k\nu}v_c^{jk}G^{j\sigma',k\nu}\Delta n^{k\nu,i\sigma}. \tag{9}$$

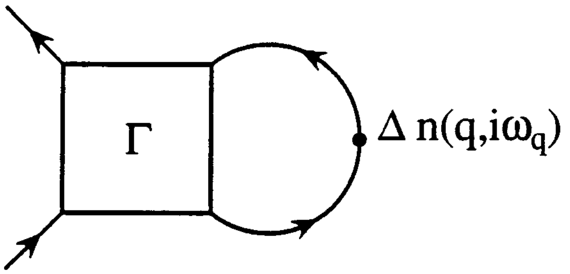

FIG. 1. Feynman diagram for the change in the number of electrons in a screening cloud induced by a charge fluctuation.

The quantities $G^{j\sigma',i\sigma}$ are here defined as proportionality terms in the definition of the exchange-correlation interaction, but as we shall see they are simply related to the standard local field factors used in theories of the electron liquid and they can also be obtained from the response functions. For a static lattice the complete effective interaction is then $\widetilde{V}_{\text{eff}}^{k\nu,i\sigma}=\widetilde{V}_{\text{direct}}^{k\nu,i\sigma}+\widetilde{V}_{\text{exc}}^{k\nu,i\sigma}$, and the effective interaction defined in this way includes interactions that are not included in the irreducible electron-electron interaction since it includes the effects of exchange and correlation between the interacting particles in the first term in Eq. (9). To obtain the irreducible effective interaction we subtract this term, i.e.,

$$V_{\text{eff}}^{j\sigma',i\sigma}=\widetilde{V}_{\text{eff}}^{j\sigma',i\sigma}+v_c^{ji}G^{j\sigma',i\sigma}. \tag{10}$$

The induced change, $\Delta n^{k\nu,i\sigma}$, in the number of electrons in band k surrounding an electron from band i is related to a density-density response function by (this is the local approximation to diagram 1)

$$\Delta n^{k\nu,i\sigma}=\frac{1}{2}\,\overline{\Pi}_0^k\widetilde{V}_{\text{eff}}^{k\nu,i\sigma}, \tag{11}$$

where the factor of $\frac{1}{2}$ is included in Eq. (11) because $\overline{\Pi}_0^k$ includes a summation over spin. This relation can be directly derived from the diagram of Fig. 1 where the scattering amplitude, $\Gamma(\widetilde{k},\widetilde{k}',\widetilde{q})$, is replaced by the effective interaction, $\widetilde{V}_{\text{eff}}^{k\nu,i\sigma}(\widetilde{q})$. Here, we are using a four-vector notation $\widetilde{q}=(i\omega_q,\mathbf{q})$ and $q=|\mathbf{q}|$. Kukkonen and Overhauser originally took the response function, $\overline{\Pi}_0$, to be simply the Lindhard function. All interaction effects *not* included in the Lindhard function are therefore taken to be included in the effective interaction through the introduction of local field factors. However, we adopt a somewhat different physical approach, namely, that the local field factors should describe interactions between *dressed* electrons, not between bare electrons. This viewpoint is quite consistent with the suggestion by Niklasson[21] that self-energy effects should be included in a modified version of the Lindhard function. Accordingly we shall we take $\overline{\Pi}_0$ to be a modified Lindhard function given by the definition

$$\overline{\Pi}_0(\widetilde{q})=-2\int\frac{d^3p}{(2\pi)^3}\int\frac{d\omega_p}{2\pi}\,G(\widetilde{p}+\widetilde{q})G(\widetilde{p}), \tag{12}$$

which is similar to the standard Lindhard function except that the noninteracting Green's function, $G_0(\widetilde{q})$, has now been replaced by the fully interacting Green's function, $G(\widetilde{q})$. Since $\overline{\Pi}_0$ is difficult to evaluate, it is convenient to express it in terms of the Lindhard function by defining the additional local field factor, G_r, referred to above and in such a way that

$$\overline{\Pi}_0^i=\frac{\Pi_0^i}{1+v_c^{ii}G_r^i\Pi_0^i}. \tag{13}$$

By substituting Eq. (11) into Eqs. (8) and (9) we then find that

$$\widetilde{V}_{\text{eff}}^{j\sigma',i\sigma}-\frac{1}{2}\sum_{k\nu}v_c^{jk}(1-G^{j\sigma',k\nu})\overline{\Pi}_0^k\widetilde{V}_{\text{eff}}^{k\nu,i\sigma}=v_c^{ji}(1-G^{j\sigma',i\sigma}), \tag{14}$$

and we can simplify this equation by defining the spin-symmetric interaction

$$\widetilde{V}_s^{ij}=\frac{1}{2}\,(\widetilde{V}_{\text{eff}}^{i\uparrow,j\uparrow}+\widetilde{V}_{\text{eff}}^{i\uparrow,j\downarrow}) \tag{15}$$

and the spin-antisymmetric interaction

$$\widetilde{V}_a^{ij}=\frac{1}{2}\,(\widetilde{V}_{\text{eff}}^{i\uparrow,j\uparrow}-\widetilde{V}_{\text{eff}}^{i\uparrow,j\downarrow}). \tag{16}$$

Equation (14), which can be expressed as a $2n\times 2n$ matrix equation (n is the number of bands), can then be separated into two $n\times n$ matrix equations, and we obtain

$$\widetilde{V}_s^{ij}-\sum_k v_c^{ik}(1-G_s^{ik})\overline{\Pi}_0^k\widetilde{V}_s^{kj}=v_c^{ij}(1-G_s^{ij}) \tag{17}$$

and

$$\widetilde{V}_a^{ij}+\sum_k v_c^{ik}G_a^{ik}\overline{\Pi}_0^k\widetilde{V}_a^{kj}=-v_c^{ij}G_a^{ij}, \tag{18}$$

where the spin-symmetric and spin-antisymmetric local field factors are $G_s^{ij}=\frac{1}{2}(G^{i\uparrow,j\uparrow}+G^{i\uparrow,j\downarrow})$ and $G_a^{ij}=\frac{1}{2}(G^{i\uparrow,j\uparrow}-G^{i\uparrow,j\downarrow})$. By defining the matrices $(\widetilde{\mathbf{V}}_{\mathbf{s}})^{ij}=\widetilde{V}_s^{ij}$, $(\boldsymbol{\Psi}_{\mathbf{s}})^{ij}=v_c^{ij}(1-G_s^{ij})$, $(\overline{\Pi}_0)^{ij}=\overline{\Pi}_0^i\delta_{ij}$, and

$$\boldsymbol{\Pi}_{\mathbf{s}}^{-1}=\overline{\boldsymbol{\Pi}}_{\mathbf{0}}^{-1}-\boldsymbol{\Psi}_{\mathbf{s}}, \tag{19}$$

the solution to Eq. (17) can be compactly given as

$$\widetilde{\mathbf{V}}_{\mathbf{s}}=\overline{\boldsymbol{\Pi}}_{\mathbf{0}}^{-1}\boldsymbol{\Pi}_{\mathbf{s}}\boldsymbol{\Psi}_{\mathbf{s}}. \tag{20}$$

From a consideration of the interaction between test charges[5] it can easily be seen that $\boldsymbol{\Pi}_{\mathbf{s}}$ is the density-density response matrix,[10] and it can also be seen that $G_s^T=G_s+G_r$ is the local field factor normally used to describe the charge-charge response function. Using Eq. (10) and the definition of $\boldsymbol{\Pi}_{\mathbf{s}}$, we find

$$V_s^{ij}=v_c^{ij}+\sum_{km}\Psi_s^{ik}\Pi_s^{km}\Psi_s^{mj}. \tag{21}$$

Similarly, from the definition $\Psi_a^{ij}=-v_c^{ii}G_a^{ii}\delta_{ij}$ and a consideration of the effective potential felt by an electron due to an applied magnetic field, the spin-spin response function can be also shown[5] to be given by

$$\Pi_a^{ij} = \frac{\overline{\Pi}_0^i}{1-\Psi_a^{ii}\overline{\Pi}_0^i}\,\delta_{ij}\,. \tag{22}$$

The spin-spin response function is diagonal in the band index because as noted above we are working within an approximation that neglects interband transitions. The quantity, $G_a^T = G_a + G_r$ is the local field factor normally used to describe the spin-spin response function. For the spin-antisymmetric interaction, we find

$$V_a^{ij} = (\Psi_a^i)^2\Pi_a^i\delta_{ij}\,. \tag{23}$$

Expressing these results in a spin-invariant form, we finally arrive at

$$V^{i\vec{\sigma},j\vec{\sigma}'} = v_c^{ij} + \sum_{km}\Psi_s^{ik}\Pi_s^{km}\Psi_s^{mj} + \vec{\sigma}\cdot\vec{\sigma}'(\Psi_a^i)^2\Pi_a^i\delta_{ij}\,, \tag{24}$$

a result that now has a very compelling physical interpretation: the first term is the bare interaction, the second is the interaction mediated by charge fluctuations, and the third is the interaction mediated by spin fluctuations. The interaction mediated by charge fluctuations is attractive for both the singlet and triplet states, but the interaction mediated by spin fluctuations is only attractive in the triplet state (it is repulsive in the singlet state). Except for the treatment of self-energy effects, Eq. (24) has also been derived using a diagrammatic approach by Vignale and Singwi.[10] Our treatment of self-energy effects can be included within the VS formalism by using the modified Lindhard function instead of the usual Lindhard function. The result of this procedure[22] is then precisely Eq. (24). Since the original KO approximation includes a factor of $z_{k_f}^2$ in the definition of the effective interaction,[10] it should be remembered that the appropriate Green's function to use in calculations involving the original KO approximation is then

$$\hat{G}(q,i\omega) = \left[i\omega - \left(\frac{q^2}{2m^*} - \mu\right)\right]^{-1} \tag{25}$$

and *not* the full quasiparticle Green's function,

$$G(q,i\omega) = z_q\left[i\omega - \left(\frac{q^2}{2m^*} - \mu\right)\right]^{-1}. \tag{26}$$

This point has often been overlooked[4] in calculations of the superconducting transition temperature where the fully interacting Green's function has been used with the original KO approximation; its consequence is an *overestimation* of the transition temperature. To acknowledge this important difference, we have modified the approach by simply avoiding the quasiparticle approximation for the Green's functions. The result is that the effective interaction now depends on the modified Lindhard function as previously discussed. In calculating properties such as the superconducting transition temperature with this modified KO approximation, it is then the fully interacting Green's function that should be invoked.

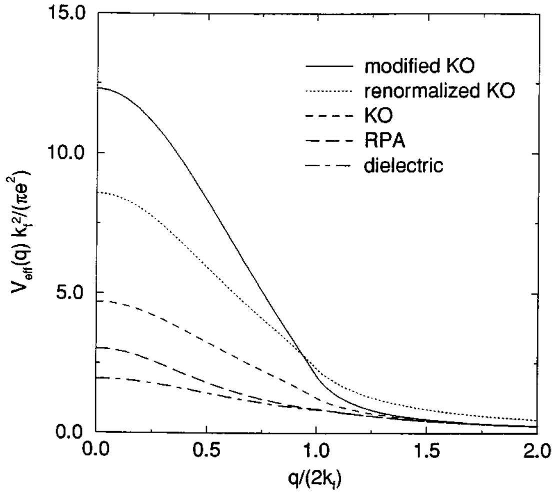

FIG. 2. Effective interaction between electrons in the singlet state in the one-band electron liquid at $r_s = 2$. The renormalized KO approximation is the KO effective interaction multiplied by the quasiparticle renormalization factor $z_{k_f}^{-2}$. The dielectric approximation is given by v_c/ϵ.

For the case of a single band, Eq. (24) simplifies to[5,10]

$$V_{\rm eff} = v_q + \frac{v_q^2(1-G_s)^2\overline{\Pi}_0}{1-v_q(1-G_s)\overline{\Pi}_0} - \alpha\,\frac{v_q^2(G_a)^2\overline{\Pi}_0}{1+v_qG_a\overline{\Pi}_0}. \tag{27}$$

Here v_q is the bare Coulomb interaction and $\overline{\Pi}_0$ is the Lindhard approximation to the density-density response function (but modified to include self-energy effects)[6], and $\alpha = 3$ or -1 for singlet or triplet pairing, respectively. The second term in Eq. (27) is the interaction mediated by charge fluctuations, and in the VS formalism it arises from the screening of the Coulomb interaction, from vertex corrections, and from particle-hole ladder diagrams.[19] The third term is the interaction mediated by spin fluctuations and in the VS formalism it also arises from particle-hole ladder diagrams.[19] In Fig. 2, we plot the effective interaction determined by Eq. (27) along with the results from several other approximations.

For a two-band system, the effective interaction between electrons in band (1) is given from Eq. (24) as[10]

$$V_{\rm eff} = v_q + \frac{v_q^2(1-G_s^{11})^2\overline{\Pi}_0^{(1)}}{1-v_q(1-G_s^{11})\overline{\Pi}_0^{(1)}} - \alpha\,\frac{v_q^2(G_a^{11})^2\overline{\Pi}_0^{(1)}}{1+v_qG_a^{11}\overline{\Pi}_0^{(1)}} + v_{12}^2\Pi^{(2,2)}, \tag{28}$$

where

$$v_{12} = (1-G_s^{12})v_q/[1-v_q(1-G_s^{11})\overline{\Pi}_0^{(1)}]. \tag{29}$$

Here $\Pi^{(2,2)}$ is the density-density response function for carriers in band (2). The additional term in the effective interaction, which is traced to correlated charge (acoustic plasmonlike) fluctuations between the two bands, is crucially different. It is *attractive* and, as we have found, in some circumstances it can overcome the direct Coulomb repulsion. When the lotal field factors are constrained to satisfy the compressibility sum rule and the Ward identities, this attractive term is *exact* in the static, long-wavelength limit for electrons on the Fermi surface. Note the close and important

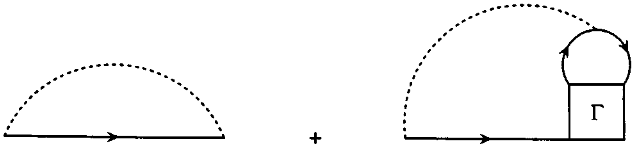

FIG. 3. An exact representation of the self-energy.

formal similarity of the *structure* of this term (the square of an electron-hole matrix element times a ''plasmon propagator'') to that of the conventional phonon-mediated attraction in metals.

The function, $G(k,i\omega_n)$, appearing in Eq. (2), is the fully interacting Green's function whose corresponding self-energy is given by

$$\Sigma(k,i\omega_n)=-T\sum_{\nu_n}\int\frac{d^3q}{(2\pi)^3}V_{\rm se}(\mathbf{q},i\nu_n;\mathbf{q}-\mathbf{k},i\nu_n-i\omega_n)\times G(q,i\nu_n). \tag{30}$$

An approximation for $V^i_{\rm se}$ can be derived from the Kukkonen-Overhauser formalism as the direct interaction and the interaction with the screening cloud produced through exchange and correlation effects, and it is given by

$$V^i_{\rm se}=v^{ii}_c+\sum_{j\sigma}v^{ij}_c\Delta n^{j\sigma,i\sigma'}. \tag{31}$$

No term for the exchange an correlation interaction of the electron with its screening cloud is included here since the exchange-correlation effect is already included in $\Delta n^{j\sigma,i\sigma'}$. This embodies the same physics that leads to a single vertex correction in the exact expression for the self-energy.[23] If an additional exchange-correlation interaction were to be (incorrectly) included, the result would then constitute the Ng-Singwi approximation[24] which has been shown to overcount diagrams.[17,25] [Another way to see that Eq. (31) is correct is to compare Fig. 3, which is an exact representation of the self-energy, to Fig. 1.] If we now substitute from Eq. (11), we find

$$V^i_{\rm se}=v^{ii}_c+\sum_j v^{ij}_c\overline{\Pi}^j_0\left(\Psi^{ij}_s+\sum_{km}\Psi^{ik}_s\Pi^{km}_s\Psi^{mj}_s\right) \tag{32}$$

and by using the definition of Ψ^{ij}_s and Π^{ij}_s [Eq. (19)], this can be reexpressed as

$$V^i_{\rm se}=\frac{1}{\overline{\Pi}^i_0}\sum_j v^{ij}_c\Pi^{ij}_s. \tag{33}$$

Because Eq. (33) is the GWΓ approximation modified to include self-energy effects we will simply refer to this result as the modified GWΓ approximation. In the one-band case, Eq. (32) then becomes

$$V_{\rm se}=\frac{v_c}{1-v_c\overline{\Pi}_0(1-G_s)}, \tag{34}$$

which is similar to the usual GWΓ approximation except that, once again, the Lindhard function has been modified to include self-energy effects. It is worth repeating again that this difference is important since we would be unable to satisfy the Ward identities without it. In contrast to other approximations for $V_{\rm se}(q,iw)$, such as the Ng-Singwi approximation[24] or the usual GWΓ approximation,[24] Eq. (33) is also *exact* in the static, long-wavelength limit for electrons on the Fermi surface. Again, this is a direct consequence of the requirement that the Ward identities and the compressibility sum rule are satisfied. For the one-band case this limit is simply given by

$$\lim_{q\to0}\lim_{\omega\to0}V_{\rm se}(k_f,0;q,i\omega)=\frac{1}{z_{k_f}m^*/m}\frac{\pi^2}{k_fm}. \tag{35}$$

At this point we may finally introduce phonons into the picture. The procedure is completely straightforward and the physical consequences of electron-phonon coupling can be illustrated with sufficient accuracy by adding

$$V_{\rm ph}(q,i\omega)=-\frac{\alpha}{1+(q/2k_f)^2}\frac{\omega^2_q}{\omega^2+\omega^2_q} \tag{36}$$

to the effective interaction. Here the phonon frequencies, ω_q, are given by

$$\omega^2_q=\beta q^2/(1+\gamma q^2). \tag{37}$$

We determine the parameter α by requiring that the correct electron-phonon coupling parameter, λ, is reproduced; the parameter β is determined from the Debye temperature, and γ is determined from the measured values of $\langle\omega\rangle_{\rm ln}$ (Ref. 26) or from the calculated value of $\langle\omega\rangle$.[27] Although this is a very simplified model of the phonon-mediated interaction, it correctly incorporates the major physical features, and so long as the known λ and $\langle\omega\rangle_{\rm ln}$ (or $\langle\omega\rangle$) are reproduced it should result in an accurate value of T_c. It is important to emphasize that from this point onwards electrons and phonons are treated throughout on a *completely equal footing* by a procedure which acknowledges their very different frequency scales.

IV. LOCAL FIELD FACTORS: SUM RULES AND CONSTRAINTS

Exact results for the small and large q limits of the local field factors are known from the compressibility sum rule, the susceptibility sum rule, the virial theorem, and the conditions derived by Niklasson,[21] by Zhu and Overhauser,[28] and by Vignale.[29] These sum rules for the multiband case are the natural generalization of the well-known equivalents for the one-band case.[22] First, the Ward identities can be written as

$$\lim_{k\to0}\lim_{\omega_k\to0}\widetilde{\Lambda}^{ij}_s(k^i_f,0;\widetilde{k})=(z^i_{k_f}m^*_i/m_i)^{-1}\left(\frac{\pi^2}{k^i_fm^i}\right)\left(\frac{\partial^2\epsilon}{\partial n^i\partial n^j}\right)^{-1}, \tag{38}$$

$$\lim_{k\to0}\lim_{\omega_k\to0}\widetilde{\Lambda}^{ij}_a(k^i_f,0;\widetilde{k})=\delta_{ij}(z^i_{k_f}m^*_i/m_i)^{-1}\left(\frac{\pi^2}{k^i_fm^i}\right)\left(\frac{\partial^2\epsilon}{\partial {\xi^i}^2}\right)^{-1}, \tag{39}$$

where ϵ is the energy density, ξ^i is $n^{i\uparrow}-n^{i\downarrow}$, and also

$$\lim_{\omega_k\to 0}\ \lim_{k\to 0}\widetilde{\Lambda}_s^{ij}(k_f^i,0;\widetilde{k})=\lim_{\omega_k\to 0}\ \lim_{k\to 0}\widetilde{\Lambda}_a^{ij}(k_f^i,0;\widetilde{k})=(z_{k_f}^i)^{-1}\delta_{ij}\,. \tag{40}$$

Here, $\widetilde{\Lambda}_s^{ij}(k_f^i,0;\widetilde{k})$ and $\widetilde{\Lambda}_a^{ij}(k_f^i,0;\widetilde{k})$ are spin-symmetric and spin-antisymmetric proper vertex functions, respectively. Next, the compressibility sum rule is given by

$$\lim_{k\to 0}\ \lim_{\omega_k\to 0}\widetilde{\Pi}_s^{ij}(\widetilde{k})=-\left(\frac{\partial^2\epsilon}{\partial n^i\partial n^j}\right)^{-1}. \tag{41}$$

Finally, the susceptibility sum rule is

$$\lim_{k\to 0}\ \lim_{\omega_k\to 0}\widetilde{\Pi}_a^{ij}(\widetilde{k})=-\delta_{ij}\left(\frac{\partial^2\epsilon}{\partial \xi^{i^2}}\right)^{-1}. \tag{42}$$

In Eqs. (41) and (42), $\widetilde{\Pi}_s^{ij}(\widetilde{k})$ and $\widetilde{\Pi}_a^{ij}(\widetilde{k})$ are the proper charge-charge and spin-spin response functions, respectively.

To derive conditions for the large q limits, we approximate the modified Lindhard function by

$$\overline{\Pi}_0^i(\widetilde{q})=2\int\frac{d^3k}{(2\pi)^3}\,\frac{n_{\mathbf{k}}^i-n_{\mathbf{k+q}}^i}{i\omega_q-\epsilon_{\mathbf{k+q}}^i+\epsilon_{\mathbf{k}}^i}, \tag{43}$$

where $\epsilon_{\mathbf{k}}^i=k^2/2m^i$, a form that results in the correct large-wave vector behavior of the effective interaction. It clearly neglects the renormalization of the effective mass but it *does* include the more important effect of particle number renormalization. The local field factors obtained using Eq. (43) give an effective interaction with the correct large q limit; this follows because the divergent part of G_s^T is contained in G_r and this divergence does not affect the large q limit of the effective interaction. If we had used Eq. (12) for $\Pi_0(\widetilde{q})$ both G_s and G_r would diverge for large q and the effective interaction would then fail to approach the bare interaction in this limit. The fact that Eq. (12) does not result in the correct large wave-vector limit of the effective interaction is simply a reflection of the fact that the local approximation is not expected to be accurate when the interacting electrons are taken to have energies far from the Fermi energy. No difficulties are encountered so long as we ensure that the divergent part of G_s^T is entirely contained in G_r.

The large q conditions for the one-band case are

$$\lim_{q\to\infty}G_s(q,i\omega)=\frac{2}{3}[1-g(0)] \tag{44}$$

and

$$\lim_{q\to\infty}G_a(q,i\omega)=\frac{4g(0)-1}{3}. \tag{45}$$

For the two-band case the equivalent is

$$\lim_{q\to\infty}G_s^{(11)}(q,i\omega)=\frac{2}{3}[1-g_{11}(0)]+\frac{1}{3}\frac{n_2}{n_1}[1-g_{12}(0)], \tag{46}$$

with an analogous result for $G_s^{(22)}(q,i\omega)$; we also obtain

$$\lim_{q\to\infty}G_s^{(12)}(q,i\omega)=\frac{1}{3}[1-g_{12}(0)]. \tag{47}$$

In a similar way we find for the spin-antisymmetric local field factor

$$\lim_{q\to\infty}G_a^{(11)}(q,i\omega)=\frac{4g_{11}(0)-1}{3}+\frac{1}{3}\frac{n_2}{n_1}[1-g_{12}(0)], \tag{48}$$

and again an analogous result for $G_a^{(22)}(q,i\omega)$.

At this point we are in a position to construct approximate parametrizations of the local field factors that incorporate these limits. For the one-band case we may use the parametrization of the Monte-Carlo results of Ref. 7 to obtain G_s^T and we obtain G_r as a Padé approximate. In the two-band case Monte Carlo results are not available so we must parametrize *both* G_s^T and G_r as Padé approximates. The correlation energy which is needed in the compressibility sum rule is obtained in the one-band case from the parametrization[30] of Monte Carlo results and in the two-band case we use a self-consistency condition derived from the fluctuation-dissipation theorem in evaluating the correlation energy.

A. The one-band electron liquid

Moroni *et al.*[7] have obtained $G_s^T(q,0)$ from Monte Carlo simulations, and they find that the form

$$G_s^T(q,0)=\{[(A-C)^{-n}+((q/k_f)^2/B)^n]^{-1/n}+C\}(q/k_f)^2 \tag{49}$$

provides a good representation of their Monte Carlo results with $n=8$ for $r_s=2$ or $r_s=5$, and $n=4$ for $r_s=10$. The coefficient A is fixed by the compressibility sum rule, Eq. (41), along with Vosko *et al.*'s[30] parametrization of the correlation energy as determined from Monte Carlo simulations. An expression for C can now be derived from Eq. (43) (Ref. 6) and the result is

$$C=-\frac{\pi}{e^2k_f^3}\,\frac{\partial(r_s\epsilon_c)}{\partial r_s}, \tag{50}$$

where ϵ_c is the correlation energy per electron. The parameter, B, is given by Moroni *et al.*[7] as

$$B=\frac{a+bx+cx^3}{d+ex+fx^3}, \tag{51}$$

where $x=r_s^{1/2}$; specific values for the coefficients are $a=1$, $b=2.15$, $c=0.435$, $d=3$, $e=1.57$, and $f=0.409$.

To obtain the local field factor $G_a^T(q,0)$, we notice that the polarization diagrams contributing to the difference $G_s^T(q,0)-G_a^T(q,0)$ are exclusively of the fluctuation type. Since the result of perturbation theory[6] implies that the contribution of this type of diagram can be reasonably expressed in the Hubbard form, we can therefore use the approximation

$$G_a^T(q,0)=G_s^T(q,0)+\frac{a_aq^2}{1+b_aq^2}. \tag{52}$$

Here, a_a is determined by the susceptibility sum rule, Eq. (42), and b_a is determined from Eq. (45), where Yasuhara's[31] result for the radial distribution function at zero separation, $g(0)$, is used. Although there have been attempts to extract the susceptibility from Monte Carlo simulations, large error bars are generally associated with the results. Takada has calculated the susceptibility and compressibility using the effective potential expansion (EPX) method.[32] Since his results for the compressibility agree very well with the Monte Carlo results and since there are no large statistical errors in his calculated susceptibility, we will use these results to determine $G_a^T(q,0)$.

The final local field factor we require is $G_r(q,0)$, and this is also determined as a Padé approximant, i.e.,

$$G_r(q,0)=\frac{a_r q^2+b_r q^4+c_r q^6}{1+d_r q^4}. \tag{53}$$

The coefficient a_r is fixed by the Ward identity in Eq. (38), $c_r/d_r=C$, b_r/d_r is obtained from Eq. (44), and d_r is obtained by requiring that the dip in $G_r(q,0)$ occur at $q=2k_f$ (we note that the presence of such structure is guaranteed since $a_r<0$ and $c_r>0$).

In the foregoing, all of the local field factors have been treated in the static limit since it is usually argued that they vary slowly on the scale of the Fermi frequency[33] implying therefore that their frequency dependences can be neglected. However, if the frequency dependence of G_r is neglected *entirely*, then it is certainly not possible to satisfy the Ward identity [Eq. (40)]. Accordingly we assume that G_s^T and G_a^T are independent of frequency but incorporate the frequency dependence in G_r, namely

$$G_\omega(i\omega)=\frac{a_\omega \omega^2}{1+b_\omega \omega^4}. \tag{54}$$

Within this approximation, we then write the local field factors as

$$G_s(q,i\omega)=G_s(q,0)-G_\omega(i\omega), \tag{55}$$

$$G_a(q,i\omega)=G_a(q,0)-G_\omega(i\omega), \tag{56}$$

and

$$G_r(q,i\omega)=G_r(q,0)+G_\omega(i\omega). \tag{57}$$

Note that the assumption that G_ω approaches zero for large ω, is in complete conformity with Eq. (43). The coefficient, a_ω, is determined from the Ward identity [Eq. (40)] and the parameter b_ω is fixed by making the reasonable assumption that the characteristic frequency scale for the electronic contribution to G_ω is the plasma frequency, ω_{pl}, i.e., $b_\omega=\omega_{\mathrm{pl}}^{-4}$.

To this point in the discussion of local field factors, the effective interaction has been considered in a complete absence of phonons. When these are included, Migdal's theorem implies that their effect on vertex corrections can be neglected. However, the theorem does not apply[34] in the limit $qk_f/\omega m\rightarrow 0$, and to treat the non-Migdal correction in this limit, we also take

$$G_\omega(i\omega)=\frac{a_\omega \omega^2}{1+b_\omega \omega^4}+\frac{a_{\mathrm{ph}}\omega^2}{1+b_{\mathrm{ph}}\omega^4}. \tag{58}$$

A simple way to see that phonons enter into G_ω but not into $G_r(q,0)$ is to note that the small q limit of $G_r(q,0)$ is related to $(z_{k_f}m^*/m)^{-1}$ which depends only on the momentum derivative of the self-energy, while the small ω limit of G_ω is related to $(z_{k_f})^{-1}$ which depends on the frequency derivative of the self-energy; this is affected by phonon interactions. The coefficient a_{ph} is determined from the Ward identity [Eq. (40)], and b_{ph} is determined by assuming that the contribution to G_ω from phonons varies on the scale of a characteristic phonon frequency, ω_{ph}, i.e., $b_{\mathrm{ph}}=\omega_{\mathrm{ph}}^{-4}$. In our treatment of the phonon mediated interaction, we assume that the phonon frequency approaches a constant for large q, i.e., $q\gg 2k_f$ [see Eq. (37)], and we will take ω_{ph} to be this constant. Because the second term in Eq. (58) only gives a significant contribution to the effective interaction when $\omega<\omega_{\mathrm{ph}}$ and $q/k_f<\omega_{\mathrm{ph}}/\epsilon_f$, it contributes very little to the determination of the superconducting transition temperature. But since it is quite simple to incorporate (and it is certainly present in principle), we nevertheless include it in what follows.

B. The two-band electron liquid

For the two-band case the local field factors will continue to be given by Padé approximates, and we therefore adopt a form

$$G_s^{T(ii)}(q,0)=\frac{a_s^i q^2+b_s^i q^4+c_s^i q^6}{1+d_s^i q^4}, \tag{59}$$

where a_s^i is fixed by the compressibility sum rule, Eq. (41), and c_s^i/d_s^i is given by the large q sum rule, Eq. (50). We also take $d_s^i=(2k_f^i)^{-4}$ since this ensures that the transition region from small q to large q behavior occurs around $q=2k_f$. Finally, b_s^i is given by the condition $G_s^{T(ii)}(2k_f,0)=0.8a_s^i(2k_f)^2$ which is found to give reasonable agreement with the Monte Carlo results for small to intermediate q when Eq. (59) is applied to the one-band case (the coefficient of 0.8 is very close to what is expected from the results of perturbation theory). Motivated by our results from perturbation theory, we write the spin-antisymmetric local field factor as

$$G_a^{T(ii)}(q,0)=G_s^{T(ii)}(q,0)+\frac{a_a^i q^2}{1+d_a^i q^4}, \tag{60}$$

and we determine a_a^i from the susceptibility sum rule [Eq. (42)] and d_a^i from Eq. (48). The same perturbation theory leads to a similar assumption for the form of the off-diagonal local field factor, namely

$$G_s^{12}(q,0)=\frac{a_{12}q^2}{1+b_{12}q^2}. \tag{61}$$

Once again the coefficient a_{12} fixed by the compressibility sum rule and b_{12} is determined from the large q condition [Eq. (47)]. As in the one-band case, we must separate the parts of the local field factors that arise from self-energy effects and we do this by writing G_r^{ii} in the form of Eq. (53) and by determining the coefficients as in the one-band case. Note the absence of G_r^{12}; this is because no part of G_s^{12} arises purely from self-energy effects.

To implement this method of determining the local field factors, we need a procedure for calculating the correlation energy since in turn this is required for the evaluation of the sum rules. Now, the correlation energy can be calculated in terms of response functions through use of the fluctuation-dissipation theorem. This is accomplished by first writing the Hamiltonian as

$$H = H_{11} + H_{22} + H_{12}, \tag{62}$$

where H_{11} and H_{22} are the parts of the Hamiltonian that depend only on electrons from bands (1) and (2), respectively, and H_{12} is the part of the Hamiltonian that describes the interaction between electrons from different bands. We introduce a coupling constant λ into the latter, and provided no ordering ensues as λ proceeds through its values, the Hellmann-Feynman theorem can be used to express the ground state energy per unit volume as

$$E = E_1 + E_2 + \int_0^1 d\lambda \langle \mathcal{H}_{12} \rangle_\lambda, \tag{63}$$

where E_1 and E_2 are the ground state energies of electrons in bands (1) and (2), respectively, when there is no interaction between electrons from different bands; each can be determined from Monte Carlo simulations.[30] The interaction energy per unit volume, $\langle \mathcal{H}_{12} \rangle_\lambda$, can be expressed in terms of the density-density response function as

$$\langle \mathcal{H}_{12} \rangle_\lambda = -\int \frac{dw}{2\pi} \int \frac{d^3q}{(2\pi)^3} v_c^{12} \Pi_s^{12}(q,i\omega;\lambda), \tag{64}$$

where $\Pi_s^{12}(q,i\omega;\lambda)$ is the density-density response function defined in Eq. (19) but with the interaction v_c^{12} scaled by λ. Because, as stated, the correlation energy depends on the local field factors through the response functions, we now arrive at a self-consistent and relatively straightforward procedure for determining the local field factors. Accordingly this now completes our discussion of the determination of effective interactions in the one- and two-band cases, without and with phonons.

V. INTRINSIC PAIRING

With the total effective interaction finally established, we turn to the identification of a possible superconducting transition. Intrinsic superconductivity in both the one- and two-band cases is considered first; we then treat the standard physical case of phonon mediated superconductivity (but in the presence of electron-electron interactions).

A. The one-band case

Proceeding with the method of solution as laid out in Sec. II, we first consider the case where Hubbard-like local field factors are assumed. The findings of Takada, namely that the three-dimensional single-band electron gas can be superconducting at low densities (Takada found solutions for s-wave pairing for $r_s > 5.3$), are confirmed. However, if our sum-rule constrained local field factors are used instead the situation changes considerably; no solutions to Eq. (4) for s-wave superconductivity are found, and from this we conclude that within the present approximations there is no s-wave superconductivity in the homogeneous one-band electron gas, at least for $r_s < 10$. However, the KO approximation is essentially a mean-field theory and is therefore not expected to be accurate in the vicinity of a phase transition to, for example, the Wigner crystal state at much higher values of r_s. Therefore, s-wave pairing in the very low density electron liquid may remain a possibility. Solutions for both p- and d-wave pairing are, however, found, but results for nonzero angular momentum pairing depend *very sensitively* on the assumed form of the local field factors so that at this point definitive conclusions cannot yet be drawn. Our results for s-wave pairing differ from those of Takada primarily because the local field factors we use are quite effectively constrained by additional sum rules and are therefore likely to be more accurate. Takada's effective interaction actually does not satisfy the Ward identities since the quasiparticle renormalization factor, $z_{k_f}^{-2}$, has been omitted. Because of this, the static Coulomb repulsion is significantly underestimated; a further difficulty is that the Hubbard-like local field factors approach an incorrect limit for large q [they should diverge as q^2 (Refs. 6 and 7)]. For this reason, they also substantially underestimate the local field correction at intermediate to large momentum transfers,[7] and this leads to a corresponding additional underestimation of the static Coulomb repulsion.

B. The two-band case

With respect to intrinsic pairing, we find the two-band case to behave in a remarkably different way. As noted already the additional term in the effective interaction in two-band systems (as mediated by correlated charge fluctuations) is *attractive*, and it can be written as

$$V_{\text{ccf}}(q,i\omega) = v_{12}^2(q) \Pi^{(2,2)}(q,i\omega), \tag{65}$$

where v_{12} is an effective coupling between electrons in band (1) and electrons in band (2) as given in Eq. (29). Here $\Pi^{(2,2)}$ is the density-density response function between electrons in band (2), and V_{ccf}, is the effective interaction between electrons in band (1) arising from correlated charge fluctuations between the two bands. Equation (65) represents diagrams that are of the form of a screened interaction which includes at least one bubble diagram from band (2) and also incorporates the appropriate vertex corrections. Our approximation to this interaction is therefore exact in the static long-wavelength limit for electrons on the Fermi surface provided only that the Ward identities and also the compressibility sum rule are together satisfied. Since these local field factors are themselves determined in a self-consistent manner that precisely incorporates the Ward identities and the compressibility sum rule, we expect our results to be accurate in the static long-wavelength limit. And since it is this limit that sets the scale of the effective interaction (see Fig. 4), we expect the results for the transition temperature to be correspondingly accurate. In what follows we will be primarily considering s-wave pairing which as noted is far less sensitive to the shape of the local field factors than is the case for higher angular momentum pairing. As in the one-band case, results for higher angular momentum pairing are expected to be sensitive to the shape of the local field factors and again a more accurate treatment will be required to determine whether higher angular momentum pairing can eventually occur.

Because of the presence of correlated charge fluctuations in the two bands,[10] the effective interaction as outlined above

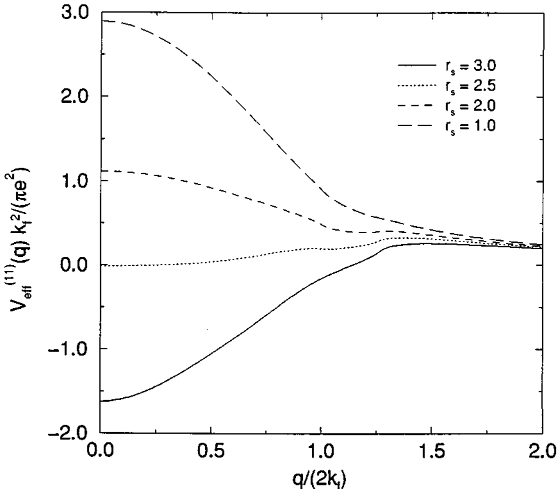

FIG. 4. Effective interaction between electrons from band (1) in the singlet state in the electron-hole liquid with $n_2/n_1=2$ and $m_2/m_1=2$.

is actually negative at small to intermediate momenta in the region where $\lim_{q\rightarrow 0} v_q/\epsilon(q,0)$ is itself small or negative. In this region, a structural phase transition associated with phonon softening can also be expected and this will certainly place an upper limit on the maximum attainable transition temperature achievable in practice with this mechanism.

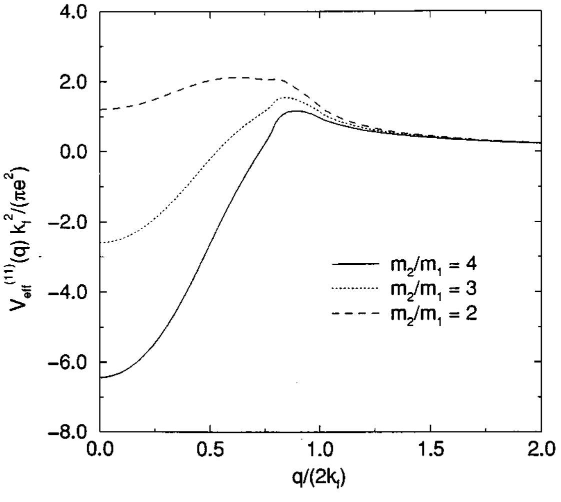

FIG. 5. Effective interactions between electrons in band (1) in the singlet state in the electron-hole liquid with $r_s=2$ and $n_2/n_1=0.5$.

TABLE I. Transition temperatures in the electron-hole liquid.

r_s	n_2/n_1	m_2/m_1	T_c (K)
2.0	0.5	2.0	≈0
2.5	0.5	2.0	1.66
3.0	0.5	2.0	124
2.0	0.5	3.0	10.1
2.0	0.5	4.0	165
2.0	2.0	2.0	0.0066
2.5	2.0	2.0	23.1
3.0	2.0	2.0	312

In Fig. 4 we have shown the static effective interaction in the modified KO approximation. As r_s is increased it becomes progressively more attractive and in consequence the superconducting transition temperature is expected to become correspondingly larger. In Fig. 5, it is seen that increase of the ratio m_2/m_1 of effective masses also makes the interaction more attractive and therefore also increases the transition temperature. Typical results for the transition temperature are presented in Table I and corresponding results for the pairing function $\Phi(k,i\omega)$ are given in Figs. 6 and 7. At the transition temperature, pairing occurs in the band with the most attractive effective interaction (but not in the other). If the effective interaction is attractive in the second band there may yet be another phase transition at a lower temperature were electrons in the second band also to pair. (As a convention we always label the band with the larger transition temperature as band 1.) Note that in this calculation there are no intermediaries (e.g., phonons), an obligatory inclusion for realistic systems. This is the case we turn to next.

VI. PAIRING WITH ELECTRONS AND PHONONS

As stated earlier, the formal inclusion of phonons in this generalized procedure is not difficult, and we have also therefore solved the Eliashberg equation for the one- and two-band electron gas along with a model phonon dispersion. To accommodate the very disparate frequency scales, we follow the prescription described above and choose a grid spacing in frequency which is small compared to the Debye frequency for small frequencies, ω, and which then increases for larger frequencies until it is on the order of the Fermi energy.

A. Superconducting simple metals

From a complete solution of the Eliashberg equation including both electron-electron interactions and electron-phonon interactions (see Sec. II), we have calculated the transition temperature for the five simple polyvalent metals indium, β-gallium, amorphous gallium, thallium, and lead (for these metals tunneling data are available[26]) using the interaction parameters in Eq. (36) extracted from measurement. The resulting transition temperatures are presented in Table II and are seen to agree with the experimental values to within 20%. This level of agreement is quite satisfactory for an *ab initio* treatment of the Coulomb interaction and is actually comparable to the level of agreement obtained using the empirically determined values of μ^* in the McMillan formula.[35] It is important to note that these are all relatively *high* density metals.

In Figs. 8 and 9, are shown the pairing function, $\Phi(k,i\omega)$, at $T=T_c$ for β-gallium and lead, respectively. As discussed above, the sharp structure at $k=k_f$ for large frequencies arises from the singular nature of the long-range Coulomb interaction which is incompletely screened at finite frequencies. In the following it will become apparent that this structure can be far more pronounced in the case of monovalent metal, for example, lithium, a metal of much lower *effective density,* where T_c/ϵ_f is also much smaller than in the metals considered above. The case of metallic

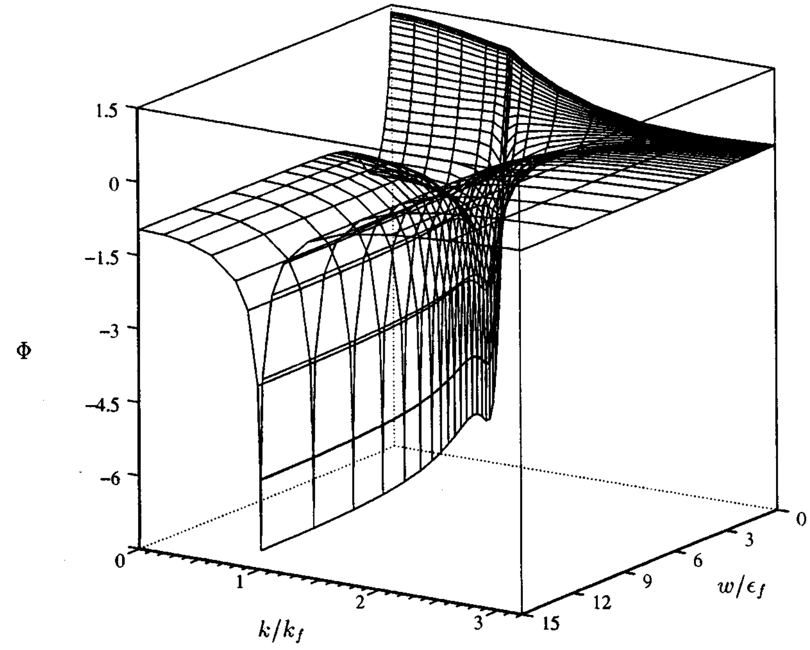

FIG. 6. Pairing function, $\Phi(k,i\omega)$, in the electron-hole liquid at $r_s=2$, $n_2/n_1=0.5$, and $m_2/m_1=3$. Note again the dip (see text) at $k=k_f$.

hydrogen is even more interesting, especially the proton-paired metallic state, and is discussed elsewhere.[36]

Although the results for the simple metals are quite accurate for an *ab initio* treatment of the Coulomb interaction, it is important to discuss possible sources of error that may arise in more complex metallic systems. To begin with, as stated earlier the electron liquid model does not include band structure effects beyond those incorporated in the band mass, m_b. This means that the electron liquid model may correctly give the density of states at the Fermi surface but it will not in general give the correct Fermi energy (since $k_f^2/2m_b$ is the Fermi energy in the electron liquid model and this usually does not agree with the Fermi energy from band structure calculations[37]). The likely importance of this can be gauged by the fact that the Fermi energy enters into the crude square-well approximation for the pseudopotential, i.e.,

$$\mu^*=\frac{\mu}{1+\mu\ \ln(\epsilon_f/\omega_{\mathrm{ph}})}, \tag{66}$$

and we therefore expect an associated error in our calculated transition temperatures; but it is small. Another potential source of error can also be seen from Eq. (66), in this case originating with the phonon frequency, ω_{ph}. A very simplistic form for the phonon dispersion relation has been assumed that gives the correct $\langle\omega\rangle_{\mathrm{ln}}$ but not in general the other average phonon frequencies; for this reason we may not necessarily obtain the correct value of ω_{ph}. Based on the success

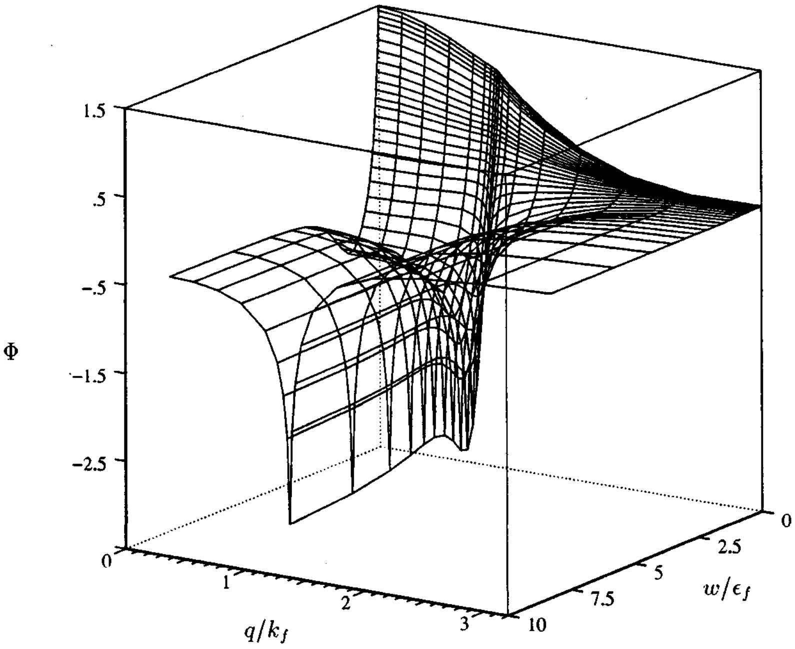

FIG. 7. Pairing function, $\Phi(k,i\omega)$, in the electron-hole liquid at $r_s=2$, $n_2/n_1=0.5$, and $m_2/m_1=4$.

TABLE II. Transition temperatures of the simple metals. The % error is defined as $(T_c^{\mathrm{calc}} - T_c^{\mathrm{expt}})/T_c^{\mathrm{expt}} \times 100\%$.

Metal	λ	$\langle \omega \rangle_{\ln}$ (K)	T_c^{expt} (K)	T_c^{calc} (K)	% error
Indium	0.805	68	3.40	2.98	−12.4
β-gallium	0.97	87	5.90	5.68	−3.7
a-gallium	1.62	55	8.56	7.71	−9.9
Thallium	0.795	52	2.36	2.83	19.9
Lead	1.55	56	7.20	7.69	6.8

we have in calculating the transition temperatures for the metals considered so far, it seems that these effects are actually not very important in the simple metals; but they should certainly be considered in calculating the transition temperature in materials with more complicated band structures and phonon dispersions.

Further, some inaccuracies must also result from our approximate treatment of the effective interaction in the electron liquid itself. Though these can be associated with the assumed forms of the local field factors, we repeat that they are very effectively constrained by the sum rules and from the results of Monte Carlo simulations.[7] We have not investigated *nonlocal* corrections to the pairing interaction since there is at present no reliable technique for calculating them. But because the integrand in the expression for the normal state self-energy is not as sharply peaked at the Fermi surface as the integrand in the Eliashberg equation, nonlocal corrections to the self-energy are expected to be more important than nonlocal corrections to the pairing interaction.[25] Some indication of the error made in our approximation to the self-energy can readily be gained by comparing with the quasiparticle parameters taken from Takada *et al.*'s effective potential expansion[32] (EPX) calculation. The EPX expansion has been shown to give a correlation energy in very good agreement with Monte Carlo simulations and it is therefore reasonable to assume that the EPX also gives good results for the quasiparticle renormalization parameters. We find, in fact, that our estimate of the product, $z^c_{k_f} m^*_c/m_b$, is in good agreement with Takada *et al.*'s results but that we underestimate m^*_c/m_b and overestimate $z^c_{k_f}$. Here, m^*_c, is the electron mass renormalized by the Coulomb interaction but *not* the phonon mediated interaction, and similarly $z^c_{k_f}$ is the quasiparticle renormalization factor arising from the Coulomb interaction. In addition to errors in the local approximation, further uncertainties can arise in principle from the use of local field factors that do not contain the full frequency dependence so that m^*_c/m_b (which depends on the frequency derivative of the effective interaction) may not be obtained accurately; nevertheless, $z^c_{k_f} m^*_c/m_b$, which depends only on the momentum derivative *is* accurately calculated. For the simple metals considered here, $m^*_c/m_b \approx 0.87-0.91$ a range which is reasonably close to the corresponding values from the EPX calculation[32] of $m^*_c/m_b \approx 0.93-0.95$. Accordingly we do not expect significant error from the local approximation to the self-energy. As we will see below, this source of error may be more significant in a lower density (larger r_s) metal, such as lithium.

B. Lithium

Calculations of the superconducting transition temperature in the monovalent and fairly low density metal lithium

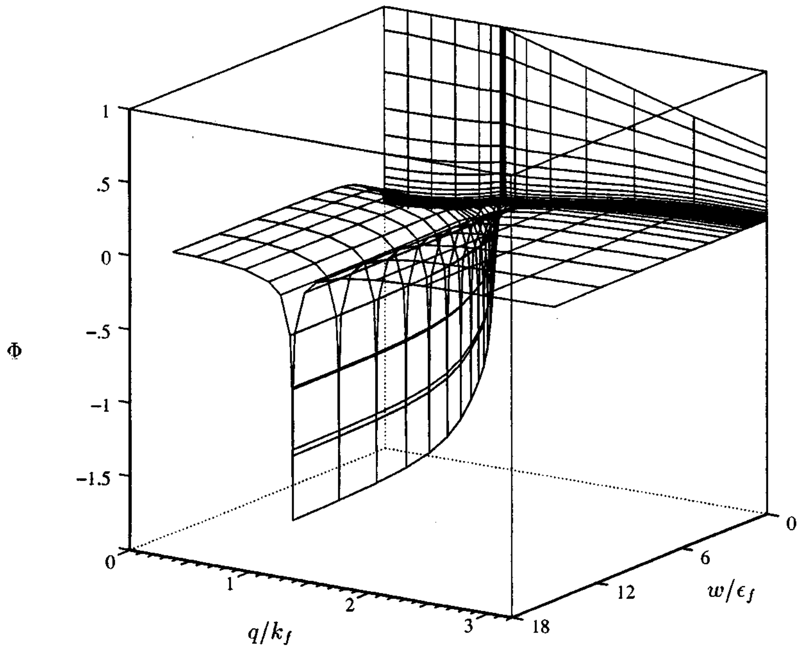

FIG. 8. Pairing function, $\Phi(k,i\omega)$, for β-gallium. Note the sharp dip (see text) at $k = k_f$.

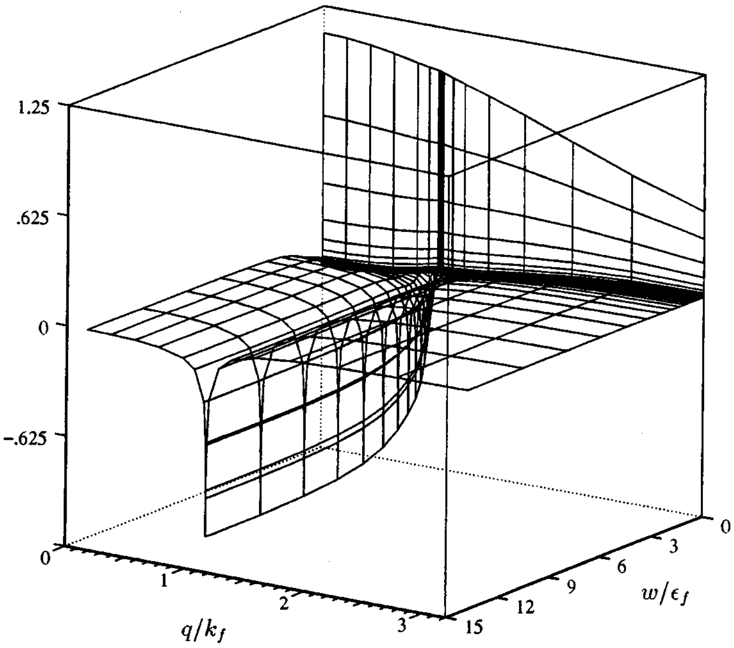

FIG. 9. Pairing function, $\Phi(k,i\omega)$, for lead.

(accounting for the band mass, the *effective* r_s is 5.7) based on *ab initio* electronic structure calculations and the McMillan expression have previously predicted that lithium should be superconducting near $T_c \sim 1$ K. Experimentally, however, there is no sign of superconductivity down to at least 6 mK. Subsequently it has been suggested[38] that the electron-phonon coupling parameter, λ, might be lowered because of a reduction in the density of states at the Fermi surface in the $9R$ phase of lithium, the known low temperature phase. However, band structure calculations[27] indicate that while λ is somewhat smaller in the $9R$ phase than in the bcc phase, it is still sufficiently large that the transition temperature should remain in the vicinity $T_c \sim 1$ K. It has also been suggested[39] that spin fluctuations could be responsible for suppressing T_c, but the corresponding calculations indicate an effective mass inconsistently large compared with specific heat measurements.[27] They also assume, however, that spin fluctuations contribute to the self-energy in the same way that they contribute to the effective pairing interaction; this is also not the case. Spin fluctuations do indeed play an important role in reducing the transition temperature but we find that it is necessary to include the full frequency dependent effective interaction in the calculation of T_c to obtain its correct order of magnitude.

The electron-phonon coupling parameter, λ, and the average phonon frequency, $\langle\omega\rangle$, have been calculated[27] for the $9R$ phase, the values being $\lambda = 0.41$ and $\langle\omega\rangle \equiv 200$ K. An experimental constraint on λ is given by the effective mass determined from specific heat measurements. The thermal mass, which is the effective electron mass, including renormalizations from electron-electron interactions and electron-phonon interactions, is given by[34]

$$\frac{m_{\text{th}}}{m_b} = \left[\frac{1 - \partial\Sigma_{ee}/\partial\omega - \partial\Sigma_{ep}/\partial\omega}{1 + \partial\Sigma_{ee}/\partial\epsilon_k + \partial\Sigma_{ep}/\partial\epsilon_k}\right]_{\omega=0,k=k_f}, \tag{67}$$

where $\Sigma_{ee}(k,\omega)$ and $\Sigma_{ep}(k,\omega)$ are the contributions to the self-energy from electron-electron interactions and from electron-phonon interactions, respectively.[40] Since $\Sigma_{ep}(k,\omega)$ is but a weak function of k, we may neglect the term $\partial\Sigma_{ep}/\partial\epsilon_k$;[34] it then follows that

$$m_{\text{th}} = m_c^*(1+\lambda). \tag{68}$$

Here, as in the McMillan formula, λ includes the Coulomb renormalization factor $(z_{k_f}^c)^2(m_c^*/m_b)$ and if we use $\lambda = 0.41$ with the band mass[27] $m_b = 1.75$ and the effective mass ratio, m_c^*/m_b, (attributable to Coulomb interactions) taken from the EPX calculation of Takada *et al.* ($m_c^*/m_b = 0.90$), we then find a thermal mass $m_{\text{th}} = 2.2$, which is in rather good agreement with the experimental value $m_{\text{th}} = 2.23 \pm 0.05$.[27] This indicates that the value, $\lambda = 0.41$, is a quite satisfactory estimate for lithium in the $9R$ phase. Note that the EPX calculation of Takada *et al.* includes the effects of spin fluctuations, and for this reason the argument[27] that spin fluctuations would cause the thermal mass to be too large if $\lambda = 0.41$ is not sustained. The Coulomb-renormalized mass obtained using the modified $GW\Gamma$ approximation gives $m_c^*/m_b \approx 0.7$; this considerably underestimates the effective mass. By these arguments, we expect that using Takada *et al.*'s values for $z_{k_f}^c$ and m_c^*/m_b in a quasiparticle approximation for the part of the self-energy arising from the Coulomb interaction will give a more accurate treatment of the self-energy than will the modified $GW\Gamma$ approximation.

While the thermal mass provides a useful test of the band-mass corrected jellium model, yet a further test is the spin susceptibility. Experimentally, $\chi_f/\chi = 0.40$ (Ref. 41) for Li at room temperature. To include the band-mass correction, we use Takada's expression[4] for the susceptibility in the electron gas with $r_s = 3.25 \times 1.63$ [the band mass is 1.63 in the room temperature phase of Li (Ref. 27)] and then divide the result by 1.63 to convert χ_f to the free-electron susceptibility as appropriate to electrons with the bare mass. This leads to $\chi_f/\chi = 0.38$ which is also in very good agreement with the experimental value. For the sake of comparison,

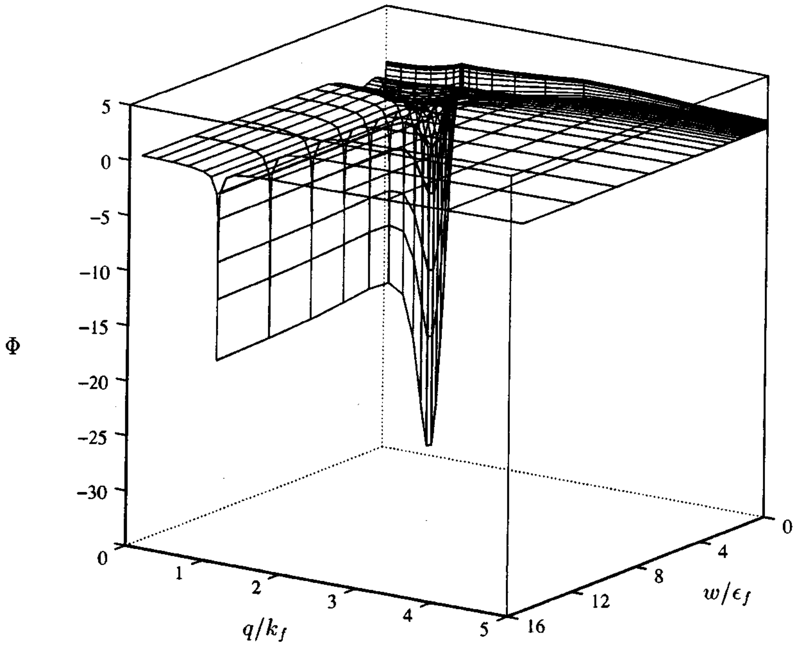

FIG. 10. Pairing function, $\Phi(k,i\omega)$, for lithium. The dip at $k=k_f$ (see text) is very large here because of the small transition temperature.

note that if we had ignored the band-mass correction, we would have obtained $\chi_f/\chi=0.70$; it follows from this that a value obtained using the correct band mass is far more secure than one which ignores the band-mass correction. As expected the band-mass correction is necessary to ensure that the model has the correct density of states at the Fermi energy, $N(0)$. Since the transition temperature depends sensitively on $N(0)$, it is also necessary to include the appropriate band mass in calculations of T_c.

With the modified KO effective interaction and a quasiparticle approximation to the Coulomb part of the self-energy both in hand, we again follow the procedure outlined in Sec. II, the transition temperature we obtain is now 0.40 mK. Though it is clear that the transition temperature arrived at with this approach *must* be low, the calculated value can still only be considered an order of magnitude estimate simply because the net Coulomb repulsion is so closely balanced with the phonon-mediated attraction. Small errors in the net Coulomb repulsion can still yield very large changes in the transition temperature. To see this note that the McMillan formula with $T_c=0.40$ mK implies that $\mu^*=0.237$. If the correct μ^* is just 10% larger than our calculated value, the transition temperature would be 4.1 μK, a reduction in T_c by a further two orders of magnitude. But in the same way, if our calculation should overestimate μ^* by 10%, the transition temperature would be 4.8 mK, which is certainly an order of magnitude larger than the present estimate but still completely consistent with the experimental limit $T_c<6$ mK. The Eliashberg equation has also been solved using the modified $GW\Gamma$ approximation for the self-energy; and in this case we find $T_c\approx 0.2$ μK, again smaller than the result from the quasiparticle approximation primarily because the quasiparticle parameters $z^c_{k_f}$ and m^*_c/m are not accurately obtained in the modified $GW\Gamma$ approximation for low density systems. Because of the errors in the quasiparticle parameters in the $GW\Gamma$ approximation, we regard $T_c\approx 0.4$ mK as the more accurate estimate.

For the purpose of further comparison, we can also find μ^* from the standard square-well approximation, Eq. (66), where we use $\omega_{\mathrm{ph}}=200$ K; the result is $\mu^*=0.174$ which then gives a transition temperature of $T_c=0.08$; this is also inconsistent with the experimental limit. The implication is that for this low density system the approximate formula, Eq. (66), is too crude and that it is therefore necessary to solve the full momentum and frequency dependent Eliashberg if the experimental result $T<6$ mK is to be explained. By ignoring the term in the effective interaction arising from spin fluctuations, Eq. (66) gives $\mu^*=0.108$ leading to a transition temperature of $T_c=0.8$ K. The fact that this is an order of magnitude greater than the estimate including spin fluctuations confirms that spin fluctuations can indeed play an important role in suppressing the transition temperature.

The pairing function $\Phi(k,i\omega)$ for lithium is presented in Fig. 10. As can be seen, the structure at $k=k_f$ is far more dramatic in this case than in the previous calculations since the transition temperature is very small [Eq. (6) shows clearly that the size of the dip grows with decreasing temperature]. Although our main result for lithium, $T_c\approx 0.4$ mK, also cannot be considered a reliable *quantitative* estimate of the transition temperature (because of the extreme sensitivity of T_c to μ^*) it is nevertheless appears to possess sufficient accuracy to resolve the conflict between the standard approximations and the experimental result that lithium is not superconducting down to at least 6 mK. The reason that the standard approximation, $\mu^*\approx 0.1$, fails for this metal is that the effective electron-electron coupling parameter, $r_s=5.7$, is unusually large compared to the superconducting polyvalent simple metals and the ratio $\epsilon_f/\omega_{\mathrm{ph}}$ is unusually small (other metals may share these characteristics). The static Coulomb repulsion grows with increasing r_s, so lithium has a large μ and since $\omega_{\mathrm{ph}}/\epsilon_f$ is unusually small μ^* is also unusually large. Although this qualitative explanation relies on the crude approximation given in Eq. (66), for a more quantitative calculation of the role of the Coulomb repulsion in setting the transition temperature, it is

TABLE III. Transition temperatures of the electron-hole-phonon model.

λ	T_c^{McMillan} $(\mu^*=0)$ (K)	T_c^{McMillan} $(\mu^*=-0.650)$ (K)	T_c (K)
0.0		10.1	10.1
0.4	1.31	15.0	16.8
0.8	4.82	17.4	22.2
1.5	8.83	19.5	31.3

necessary to solve the frequency and momentum dependent Eliashberg equation. Finally, since lithium is reasonably compressible this picture offers a possible test via high pressure studies.

C. The two-band case

Now that it appears established that the modified KO approximation can give a reasonable description of the effective Coulomb interaction in a set of simple metals, we examine the role of the Coulomb interaction in a selected class of two-band metals. In particular, we take the electron-hole models considered above augmented by phonons according to Eq. (36). We choose $\langle\omega\rangle_{\ln}=60$ K as a representative value and calculate the transition temperature for an electron-hole system with $r_s=2$, $n_2/n_1=0.5$, $m_2/m_1=3$ and with various values of λ. The results following from the procedure of Sec. II are summarized in Table III where the value $\mu^*=-0.650$ is chosen to reproduce the result $T_c=10.1$ K in the absence of phonons. For large λ the McMillan formula significantly underestimates the transition temperature, something that also occurs for positive μ^*,[26] although this break-down occurs for smaller λ when μ^* is negative. In cases where the transition temperature is already greater than the phonon frequencies, even with $\lambda=0$, the McMillan formula breaks down entirely.

The discussion has been confined so far to systems with moderate transition temperatures. As seen in Table I, however, there can be cases with very large transition temperatures. For these it must be cautioned that other instabilities (towards charge density waves, or even structural instabilities) will restrict the largest transition temperature that can be obtained for either the correlated charge fluctuation mechanism or the phonon mechanism.

VII. CONCLUSIONS

The solution to the Eliashberg equations involves a numerically intensive procedure even for the isotropic cases considered here; but apart from accommodating the different frequency scales, this fragment of the study is in some sense straightforward and standard. The more important physical issue dealt with here is therefore the nature of the essential input into these equations, namely the manner in which many-body physics is correctly built into the effective interactions, where the essential feature is the inclusion of the effective Coulomb interaction on a completely equal footing with the phonon mediated interaction. It is particularly important to stress again that the effective electron-electron interaction is subject to rather powerful constraints as provided by the sum rules and the Ward identities. For the two-band system, the compressibility sum rule and the Ward identities together guarantee that the attractive term in the effective interaction is exact in the static, long-wavelength limit for electrons on the Fermi surface. Using our best estimate for these effective interactions, the present approximations indicate that no intrinsic s-wave superconductivity occurs in the one-band electron gas at least for $r_s<10$; we cannot rule out the possibility of higher angular momentum pairing. In the two-band electron-hole gas, however, superconductivity can arise if the system is near the region where v_c/ϵ is small or negative. When phonons are included with electrons from the beginning, the transition temperature in high-density one-band systems is adequately described by the McMillan expression with $\mu^*\approx 0.1$, but for lower density systems, which may include many systems of current interest, the role of the Coulomb repulsion is significantly underestimated by assuming $\mu^*\approx 0.1$. For the group of superconducting simple metals that we have considered, the transition temperature is correctly predicted to within 20% by a relatively straightforward procedure. Also calculated is the superconducting transition temperature in lithium and we find that $T_c\approx 0.4$ mK thereby resolving a longstanding discrepancy between previous approximations for the transition temperature and the experimental result that $T_c<6$ mK. If a two-band system happens to be close to the region where $\lim_{q\to 0}v_q/\epsilon(q,0)$ is small or negative, large transition temperatures appear possible (>100 K). However, a charge density wave or structural phase transition should also be anticipated and these will clearly place an upper limit on the maximum obtainable transition temperature.

Finally we note that our technique can in principle be extended to treat *anisotropic* metals by expanding $\Phi(\mathbf{k},i\omega_n)$, $G(\mathbf{k},i\omega_n)$, and $V_{\mathrm{eff}}(\mathbf{k},i\omega_n;\mathbf{k}',i\omega_{n'})$ in Fermi surface harmonics.[42] This will lead to a two-dimensional integral equation, but there are significant practical considerations which might make the solution quite difficult. For example, in the isotropic calculation, most of the computational effort is spent in evaluating the matrix, $\mathbf{M}$, since each matrix element requires a numerical evaluation of a two-dimensional integral. For the anisotropic case, however, we will confront a three-dimensional integral which must be evaluated numerically for each matrix element and this will require significantly more computational effort than is the case for the isotropic examples we have considered above. Furthermore the matrix Eq. (4) will be replaced by one with the structure

$$\sum_{L'} \mathbf{M}_{L,L'}\mathbf{\Phi}_{L'}=\gamma\mathbf{\Phi}_L\,, \tag{69}$$

where L is the index in the Fermi surface harmonics expansion. Since the separate L components do not decouple, the computational effort required to calculate T_c will scale as the square of the number of terms retained in the Fermi surface harmonics expansion. Alternative strategies are therefore being investigated.

ACKNOWLEDGMENTS

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