

Polarization waves and superconducting instabilities in electron systems

G. S. Atwal

Department of Physics, and the Lewis-Sigler Institute for Integrative Genomics, Princeton University, Princeton, New Jersey 08544, USA

N. W. Ashcroft

Cornell Center for Materials Research, and the Laboratory of Atomic and Solid State Physics, Cornell University, Ithaca, New York 14853-2501, USA

(Received 11 July 2003; revised manuscript received 2 July 2004; published 23 September 2004)

Electron-electron attractions originating with dynamical correlations are considered for inhomogeneous systems where the electrons can be explicitly partitioned into two classes: itinerant (valence) and quasilocalized (core). Dynamical correlations in the near homogeneous itinerant class are well captured by analytical forms of local-field factors when constrained to obey sum rules. For the nonoverlapping quasilocalized electrons a reduced description of their collective dynamical behavior can be given by appealing to bosonic excitations of polarization wave character. It is argued that in addition to the Kohn-Luttinger mechanism of intrinsic superconductivity in the itinerant class, there is another attractive pairing channel (and hence a possible further enhancement of T_c) arising from the exchange of these polarization waves, again of wholly electronic origin. Numerical estimates, via solution of the Eliashberg equation, suggest that the polarization wave channel can be quite significant in mediating electron pairing.

DOI: 10.1103/PhysRevB.70.104513

PACS number(s): 71.45.Gm, 74.20.Mn, 77.22.Ej

I. INTRODUCTION

Electron-based mechanisms of superconductivity are sought in materials where the traditional phonon-based mechanism is known to be insufficient to account for an observed high superconducting transition temperature, T_c (e.g., in the cuprates, MgB_2 , and intercalated fullerenes). Little¹ and Ginzburg² were among the first to suggest the possibility of electron-mediated superconductivity, where the electrons responsible for the pairing physics are spatially separated from those participating in superconductivity. The main appeal of such electron-based mechanisms is that the characteristic energies involved are much higher than the characteristic Debye temperature of the phonon-based mechanism, thereby potentially raising the prefactor in any BCS estimate for T_c .

Kohn and Luttinger³ considered the possibility of superconductivity without phonons or other intermediaries and demonstrated the remarkable result that a homogeneous single-band system of fermions with purely repulsive short-ranged interactions may be unstable against Cooper-pair formation and eventually form a superconductor at sufficiently low temperatures. Thus a homogeneous electron liquid with repulsive Coulombic interactions, sufficiently screened to render them short-ranged, and with no other external interactions can in principle give rise to *intrinsic* superconductivity. The only condition for this new mechanism is that the normal state is a Fermi liquid and thus has a well-defined (sharp) Fermi-surface. An initial estimate³ of the superconducting temperature, for electrons in metals with a Fermi temperature of the order of 10^4 K, using a screened Coulomb potential, suggested possible observations of the transition occurring around 1 mK.

However, homogeneous electron liquids can only be an approximation to real physical systems where, in addition to valence electrons which may participate in the Kohn-

Luttinger instability, there is inhomogeneous electron charge arising from core electrons quasilocalized to the underlying ions and not themselves unstable with respect to Cooper-pair formation. Hitherto, the internal physics of these core electrons has almost always been ignored in the discussion of electron pairing mechanisms, and instead the traditional focus has been on the dynamics of the ions in their entirety (i.e., phonons) as an attractive mediator. However, in metallic systems where the atomic number of the underlying ions is sufficiently large we point out here that the corresponding proliferation of core electrons, treated dynamically, can significantly enhance the polarizability of the system. As with phonons, this new mechanism is not an on-site core effect⁴ but rather due to correlated *coherent* fluctuations in the assembly of ion cores. This provides an additional exciton-like channel for dynamical pairing instability of the valence electrons, so long as there is a clear effective partitioning of the two classes of electrons, i.e., nonoverlap of core and valence bands. It is therefore the purpose of this paper to address this additional pairing instability mechanism, following on from an earlier suggestion of its possible importance.^{5,6} The Kohn-Luttinger question is thus being rephrased, but in the context of inhomogeneous electron systems.

Thus, the viewpoint in what follows is to consider pairing in a valence electron system resulting from separation of the entire electronic charge distribution in a metallic system into formally distinct components. The first, as discussed above, is the assembly of valence electrons themselves whose dynamics, as an interacting system, are typified by the standard plasmon modes. The second originates with the localized charge normally associated with what are termed the ion-cores, each a many-body system in its own right. These clearly present an assembly of long range monopoles, ultimately screened, whose dynamics are embodied in the coherent phonons that emerge from the associated small oscillations problem. But the next term in the multipole sequence

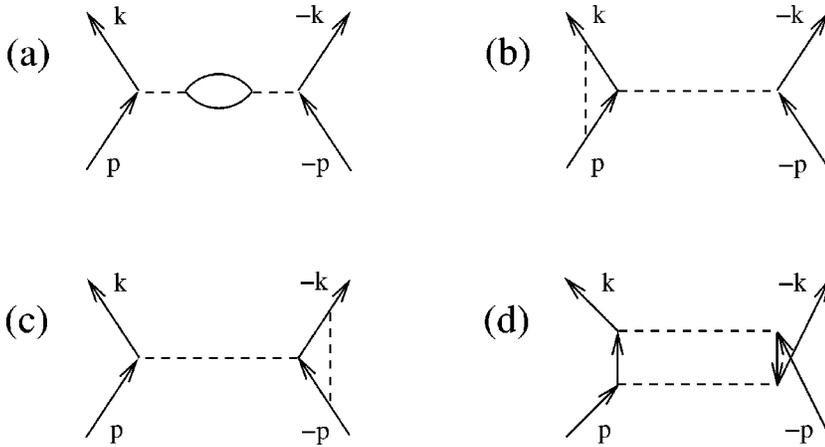


FIG. 1. Second order contribution to the irreducible scattering vertex in the original Kohn-Luttinger argument (Ref. 3): (a) represents the screened direct interaction, (b) and (c) represent vertex corrections due to a wave function modification of the electrons, and (d) represents exchange effects. The full scattering vertex is obtained by a self-consistent summation of all diagrams of these type (see e.g., Ref. 53).

are of dipolar character, and once again these can also lead to coherent collective excitations, in this case quantized waves of polarization. The corresponding dynamics are on time scales different from the phonons and their physical consequences are well known, for they lead to the van der Waals interactions between different cores.⁷ Most importantly for what follows, they are fundamentally nonlocal in an electronic context, and not amenable to standard approximations used in many electronic response problems. In this context it is important to remember that the local density approximation of density functional theory fails to capture the essential algebraic forms of van der Waals interactions,⁸ and their proper treatment is crucial to what follows.

The division of electronic charge implies two distinct linear response problems in quite different limits. For the valence electrons, the unperturbed system can be taken as the standard translationally invariant interacting electron gas problem. But, for the localized charge, periodically arranged, the relation between microscopic \mathbf{D} and \mathbf{E} fields must be through a dielectric matrix.⁹ However, as is well known, if the length scale of interest of a calculated or measured quantity notably exceeds the microscopic scale, the dielectric matrix can be averaged to give a scalar relation between \mathbf{D} and \mathbf{E} in systems with sufficient symmetry. Here we shall take the length scale to be the emergent coherence length in a superconducting state, which significantly exceeds the microscopic scale. The approximation amounts to the neglect of certain Umklapp contributions, and might well require revision in systems with small Cooper pairs. The use of a scalar dielectric function below for both valence and core electrons is therefore directly tied to the essential length scale of superconducting states.

As suggested above, the two different classes of electrons can give rise to two distinct coexistent superconducting channels, above and beyond that arising from phonons, and below we discuss each electronic channel in more detail.

A. Kohn-Luttinger instability

A simplistic explanation for the Kohn-Luttinger instability, hereafter also denoted as intrinsic superconductivity, draws upon the fact that the potential from a test charge immersed in a homogeneous sea of fermions becomes

screened and exhibits a long-ranged oscillatory part (Friedel oscillations) in real space attributable to the presence of a singularity in the slope of the dielectric constant at $q=2k_F$. Thus, similarly, there are regions where the effective electron-electron potential could become attractive, albeit weakly, suggesting the possible intervention of a Cooper instability.

The argument for the Kohn-Luttinger mechanism can be made more rigorous by considering the contributions to the irreducible scattering vertex up to second order in a single-band case. The second order interaction diagrams are shown in Fig. 1 and the essential point to note is that in three dimensions they are all singular when the momentum transfer equals $2k_F$, and as a consequence give rise to an attractive interaction in real space. Kohn and Luttinger presented simple arguments to suggest that, for large angular momentum l of the scattering vertex Λ , the first order contribution must fall off exponentially ($\Lambda_l \approx e^{-l}$) and the second order contribution must fall off algebraically ($\Lambda_l \approx 1/l^4$) so that eventually, for large enough l , the attractive second order diagrams exceed the repulsive first order (bare) Coulombic interaction. Later it was shown¹⁰ that the effective attraction also persists down to very low l , though more accurate recent calculations rule out the possibility of intrinsic s -wave ($l=0$) pairing in a single-band system.¹¹ Relatively recently,¹² the Kohn-Luttinger effect has been reexamined via the many-body renormalization group (RG) approach,¹³ demonstrating that the Kohn-Luttinger effect is robust and ought to be a generic property of Fermi liquids. In this language, the singular second-order diagrams, although acting as irrelevant terms, drive the couplings of the theory away from Landau-Fermi liquid fixed point towards the BCS instability.

The magnitude of the Kohn-Luttinger effect depends on the sharpness of the singularity at $2k_F$ and there is evidence that the inclusion of higher order diagrams, capturing higher order exchange and correlation, and going beyond the static approximation,¹⁴ can also significantly enhance the singularity. Thus any estimation of T_c clearly rests on an accurate assessment and calculation of the dynamical correlation between electrons. To determine the effective electron-electron interaction we shall employ a modified Kukkonen-Overhauser¹⁵ formalism, and the required local-field factors are parametrized using a combination of both perturbation theory and exact sum-rules. This will be the

essential input into the numerical solution of the Eliashberg equation to determine T_c .

B. Core polarization

In both insulators and metals the polarization stemming from the core electrons can significantly screen external charge and, for our purposes, valence electrons. The finite mass associated with the dynamical polarization cloud results in its delayed response to a nearby valence electron. Just as in the conventional phonon mechanism, this delayed charge imbalance may then lead to overscreening and hence attraction of another valence electron (and thence to Cooper pairing). The possibility of superconductivity arising from the dynamic effective electron-electron interaction in the vicinity of a polarizable medium was first remarked upon by Little and Gutfreund.¹⁶ There they discussed the interaction in the vicinity of a single dye molecule and suggested that in principle the effective interaction could indeed be attractive.

A periodic array of polarizable ions can give rise to quantized long-lived coherent excitations, namely polarization waves,^{7,17} which we then take to be the analog of phonons in conventional BCS theory of superconductivity.⁶ To determine the dispersion relation of polarization waves we use the linear response formalism developed by Lundqvist and Sjölander⁷ who analyzed an idealized model of a van der Waals crystal where the neutral constituents, be they atoms or molecules, are assumed to interact via static dipolar couplings (i.e., dipole approximation to the general multipole expansion of the inherent charge density fluctuations). The theoretical justification for such a collective effect was obtained by showing that the correct interaction energy of an atomic lattice is obtained by summing over all coherent polarization wave contributions.⁷ Indeed, the familiar r^{-6} London contribution to the cohesion of atomic crystals requires that the van der Waals fluctuations be coherent across the system. An archetypal van der Waals solid is the highly polarizable C_{60} fullerite which has provided several pieces of spectroscopic evidence of polarization waves.¹⁸

An important difference in the case of metals is that the polarization waves are now screened by valence electrons.^{19,20} Both the core and valence electrons then contribute to the dielectric response, the core response becoming more important at higher energies.²¹ The charge fluctuations arising from both classes of electrons must be treated on a completely equal footing. The characteristic energy of the core electron response is in general much greater than the valence electron plasma frequency but can be comparable in some metallic systems, for example, Cd and In, which possess relatively shallow d states. In addition, technologically important semiconductors such as Ge and GaAs possess shallow cores,²² and thus an accurate determination of band structure must necessitate a correspondingly accurate treatment of the effect of core polarization on valence states. The inclusion of polarization waves has been shown to yield significant improvement between the theoretical and experimental equations of state of potassium^{20,23} whose ions have quite high polarizability. Long wavelength collective descriptions of the core response have also been used to calcu-

late the modified valence plasmon frequencies in simple metals with excellent experimental agreement.^{24,25}

C. Plan of paper

In Sec. II the dynamical effective electron-electron interaction is determined for three-dimensional systems by summing up both the itinerant and core contributions within the framework of linear response theory. Greater attention is paid to the novel introduction of the core electron contribution in Sec. II B following the seminal work of Ref. 7, and in particular, we emphasize the multipole character of the core response in analogy with the usual monopole phonon contribution. In Sec. III the possibility of an attractive interaction is discussed and, as an initial assessment of the possible importance of polarization waves, the strong-coupling Eliashberg equation is numerically solved to determine their effect on superconducting transition, and we end with a summary in Sec. IV.

II. DYNAMICAL EFFECTIVE VALENCE ELECTRON-ELECTRON INTERACTION

The inhomogeneous model consists of N fixed ions at positions $\{\mathbf{R}\}$ and NZ itinerant valence electrons of mass m all in a volume Ω and in a single band. The ions are composites of nuclei, of charge $Z_A e$ and $Z_i = Z_A - Z$ quasilocalized core electrons (charge $Z_i e$) with relative positions $\{\mathbf{r}_l^c(\mathbf{R}), l = 1, \dots, Z_i\}$. In the following determination of the effective valence electron-electron interaction the ions are regarded as compact objects meaning that there is insignificant wave function overlap of core electrons between differing ions, so that a formal multipole expansion can be established.

A. Itinerant contribution

The Kukkonen-Overhauser (KO) form of the effective electron-electron interaction^{15,26} conveniently expresses the renormalization of the direct Coulomb potential in a local approximation via the use of local-field factors which encapsulate exchange and correlation effects. We use a modified form of the KO expression which includes the self-energy of the electrons consistently;²⁷ for a single-band system,

$$V_{\text{eff}}(\mathbf{q}, \omega) = v_q + \frac{v_q^2(1 - G_s(\mathbf{q}, \omega))^2 \bar{\Pi}_0(\mathbf{q}, \omega)}{1 - v_q(1 - G_s(\mathbf{q}, \omega)) \bar{\Pi}_0(\mathbf{q}, \omega)} - \zeta \frac{v_q^2(G_a(\mathbf{q}, \omega))^2 \bar{\Pi}_0(\mathbf{q}, \omega)}{1 + v_q G_a(\mathbf{q}, \omega) \bar{\Pi}_0(\mathbf{q}, \omega)}, \quad (1)$$

where $v_q = 4\pi e / q^2$ the Fourier-transformed (bare) Coulombic potential, $G(\mathbf{q}, \omega)_{s,a}$ are the spin-symmetric and spin-antisymmetric dynamical local-field factors, and $\zeta = 3$ or -1 for singlet or triplet pairing, respectively. The second term in Eq. (1) arises from charge density fluctuations of the correlation hole surrounding each electron and the third term is the interaction mediated by spin fluctuations. The overbar over the Lindhard response, $\bar{\Pi}_0$, denotes we must use the modified form, constructed using an additional local-field

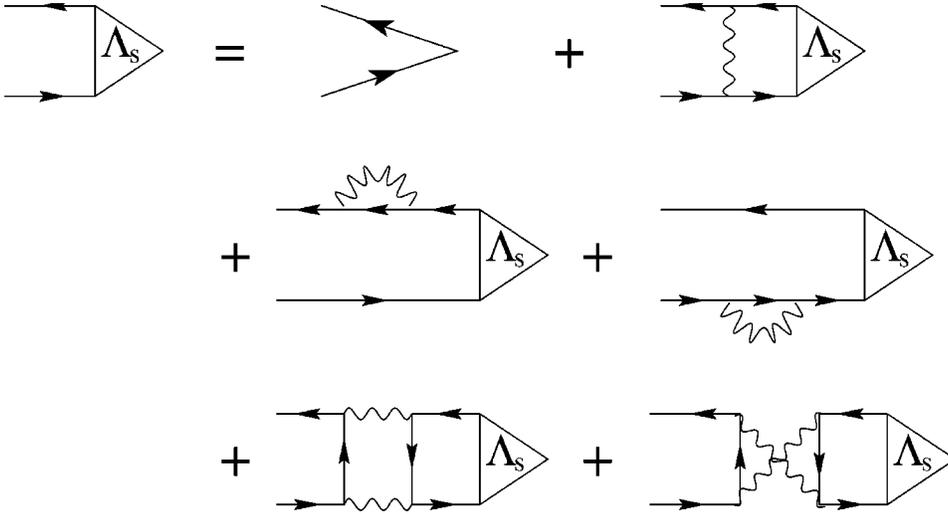


FIG. 2. Diagrammatic equation of the electron-electron scattering vertex corrections for the *spin-symmetric case*. The interaction lines are screened in the RPA. As in Ref. 27 these diagrams contribute to the parameterized form of the local-field factors, G_s and G_n , employed in Eq. (1).

factor $G_n(\mathbf{q}, \omega)$, which corrects for the self-energy renormalization of the electron occupation factors, namely,

$$\bar{\Pi}_0(\mathbf{q}, \omega) = \frac{\Pi_0(\mathbf{q}, \omega)}{1 + v_q G_n(\mathbf{q}, \omega) \Pi_0(\mathbf{q}, \omega)}. \quad (2)$$

The utility of the KO expression lies in that it only requires the local-field factors as input which represent the deviation of the full effective interaction away from the standard random-phase approximation (RPA), i.e.

$$\lim_{G_{s,a,n} \rightarrow 0} V_{\text{eff}}(\mathbf{q}, \omega) = V_{\text{RPA}} = \frac{v_q}{1 - v_q \bar{\Pi}_0(\mathbf{q}, \omega)}. \quad (3)$$

Although the local-field factors must in principle be determined by a seemingly uncontrolled inclusion of scattering diagrams to all orders, accurate approximations can nevertheless be obtained by utilising exact constraints²⁸ (sum-rules) on the asymptotic forms of the local-field factors. In this vein parameterized forms of the local-field factors have been determined^{27,29} with input from both diagrammatic perturbation theory and sum-rule constraints. The higher-order electron-electron scattering vertex diagrams used to fix the behavior of the parameterized local-field factors at $q=2k_F$ are shown in Figs. 2 and 3, in contrast to the diagrams used in the original Kohn-Luttinger argument. The parameterized expressions have so far been shown^{29,30} to compare well with Quantum Monte Carlo simulations,^{31–33} currently available only in the static regime ($\omega=0$).

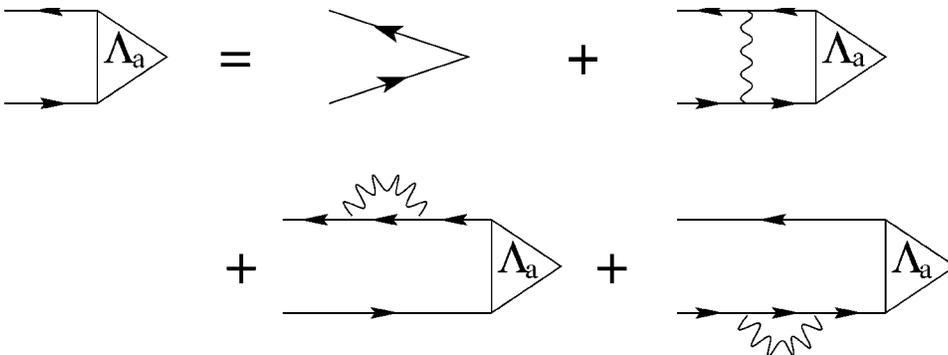


FIG. 3. Diagrammatic equation of the electron-electron scattering vertex corrections for the *spin-antisymmetric case*. The interaction lines are screened in the RPA. As in Ref. 27 these diagrams contribute to the parameterized form of the local-field factors, G_a and G_n , employed in Eq. (1).

B. Core contribution

To determine the coupling between different ions we introduce a density operator $\rho_{\mathbf{R}}^i(\mathbf{r})$ for the ion at \mathbf{R}

$$\hat{\rho}_{\mathbf{R}}^i(\mathbf{r}) = Z_A \delta(\mathbf{r} - \mathbf{R}) - \sum_{i=1}^{Z_i} \delta(\mathbf{r} - \mathbf{R} - \mathbf{r}_i^c(\mathbf{R})) \quad (4)$$

or, in Fourier coordinates,

$$\hat{\rho}_{\mathbf{R}}^i(\mathbf{q}) = e^{i\mathbf{q}\cdot\mathbf{R}} \left[Z + \sum_{i=1}^{Z_i} (1 - e^{i\mathbf{q}\cdot\mathbf{r}_i^c(\mathbf{R})}) \right]. \quad (5)$$

Thus in the thermodynamic limit the interaction operator for a system of ions, ignoring conduction electrons for now, in a volume Ω is given by

$$\hat{V}_{ii} = \frac{1}{2\Omega} \sum_{\mathbf{q}} v(\mathbf{q}) \sum_{\mathbf{R}, \mathbf{R}'} \hat{\rho}_{\mathbf{R}}^i(\mathbf{q}) \hat{\rho}_{\mathbf{R}'}^i(-\mathbf{q}). \quad (6)$$

This term represents the entire sum of multipole-multipole charge interactions between different ions.

At this juncture it is useful to make a further analytical link to the introductory remarks made above on excitations of a general multipole character. To do so, suppose that the picture is now augmented by inclusion of phonon dynamics. The polarizable cores, originally assigned to fixed sites \mathbf{R} , are now displaced by $\mathbf{u}_{\mathbf{R}}$, i.e., $\mathbf{R} \rightarrow \mathbf{R} + \mathbf{u}_{\mathbf{R}}$, the $\mathbf{u}_{\mathbf{R}}$ being syn-

thesized from the normal modes of an initially harmonic problem. An elementary expansion now gives

$$e^{\hat{\rho}_{\mathbf{R}}^i} = e^{i\mathbf{q}\cdot\mathbf{R}}(Ze + iZe\mathbf{q}\cdot\mathbf{u}_{\mathbf{R}} + i\mathbf{q}\cdot\hat{\mathbf{d}}_{\mathbf{R}} + \dots), \quad (7)$$

where $\hat{\mathbf{d}}_{\mathbf{R}} \equiv -e\sum_{i=1}^Z \mathbf{r}_i^c(\mathbf{R})$ is the point-dipole operator at site \mathbf{R} . In Eq. (7) it is clear that $iZe\mathbf{q}\cdot\mathbf{u}_{\mathbf{R}}$ is physically manifesting terms of long range monopole character, the displacements $\mathbf{u}_{\mathbf{R}}$ being coherent and derived from harmonic travelling waves (i.e., the phonons). It has been argued above that the $\hat{\mathbf{d}}_{\mathbf{R}}$, stemming from the next term in the multipole expansion, are linked to an underlying problem whose Hamiltonian has quadratic character, and again are coherent as will be demonstrated below; the travelling waves in this case are the polarization waves whose time scales may differ markedly from those of the phonons. Obviously the expansion in Eq. (7) can be continued to the quadrupolar terms and beyond.

To set an approximate scale for the relative importance of the monopole and dipole excitations embodied in Eq. (7) we first let m_n be the mass of a nucleus, and ω_{pho} a typical phonon energy. Then we have

$$u_{\mathbf{R}}^{2/2}/a_0 \approx \left(\frac{\hbar\omega_{\text{pho}}}{e^2/2a_0}\right)^{1/2} \left(\frac{m}{m_n}\right)^{1/2}, \quad (8)$$

confirming that typical root-mean-square displacements in the phonon problem can be a fraction of Bohr. Next, let α be a static dipole polarizability associated with the localized electrons, and also let ω_0 be a typical excitation energy, also to be associated with these electrons. Then,

$$(\hat{\mathbf{d}}_{\mathbf{R}}/e)^{2/2}/a_0 \approx \left(\frac{\hbar\omega_0}{e^2/\alpha^{1/3}}\right)^{1/2} \left(\frac{\alpha}{a_0^3}\right)^{1/3}. \quad (9)$$

Typical values of ω_0 may be an appreciable fraction of an atomic unit, and for ions with significant core spaces the polarizability, α , can also be substantial on the scale of a_0^3 . Thus depending on the system, the phonon and dipole terms in Eq. (7) can be comparable; it is immediately clear that there can be interference between these terms and, again depending on system, this will not always be constructive. It is also important to note that the phonon approximation neglects anharmonic effects these, as well as disorder etc., leading to finite mean paths. However, as noted by Bergmann and Rainer³⁴ the phonons with the largest influence on T_c are those whose frequencies approximately satisfy $\omega \equiv 2\pi k_B T_c$ and for these the mean free paths can be quite long. In a similar way it is suggested that the frequencies critical to polarization wave induced superconductivity are also those of a longer wave character, and therefore also less prone to damping.

Returning to the nonphonon case, we proceed from the following expansion of the core charge-density operator Eq. (4), i.e.

$$e^{\hat{\rho}_{\mathbf{R}}^i(\mathbf{q})} = e^{i\mathbf{q}\cdot\mathbf{R}}(Ze + i\mathbf{q}\cdot\hat{\mathbf{d}}_{\mathbf{R}} + \dots). \quad (10)$$

Neglect of higher order multipole terms results in the dipole approximation for which

$$\hat{V}_{ii} = \frac{1}{2e^2\Omega} \sum_{\mathbf{q}} v_{\mathbf{q}} \sum_{\mathbf{R},\mathbf{R}'} e^{i\mathbf{q}\cdot(\mathbf{R}-\mathbf{R}')} \times (Ze + i\mathbf{q}\cdot\hat{\mathbf{d}}_{\mathbf{R}})(Ze - i\mathbf{q}\cdot\hat{\mathbf{d}}_{\mathbf{R}'}). \quad (11)$$

Collective and coherent excitations (polarization waves) of the system of core electrons can now occur, and are most readily described at the level of dipole-dipole interactions. To determine the dispersion of the polarization waves we need only consider the dipole-dipole part of the potential operator, which in real space can be written as

$$\hat{V}_{\text{di-di}} = \frac{1}{2} \sum_{\mathbf{R},\mathbf{R}'} \hat{\mathbf{d}}_{\mathbf{R}} \bar{T}(\mathbf{R}-\mathbf{R}') \hat{\mathbf{d}}_{\mathbf{R}'}, \quad (12)$$

where \bar{T} is the $d \otimes d$ dipolar coupling matrix,

$$\bar{T}(\mathbf{R}-\mathbf{R}') = \frac{\delta^2}{\delta\mathbf{R}\delta\mathbf{R}'} \left(\frac{1}{|\mathbf{R}-\mathbf{R}'|} \right). \quad (13)$$

In Fourier space, the coupling matrix $\bar{T}(\mathbf{q}) = \sum_{\mathbf{R}} e^{i\mathbf{q}\cdot\mathbf{R}} \bar{T}(\mathbf{R})$ simplifies for a cubic solid in the long wavelength limit to^{7,17}

$$\lim_{q \rightarrow 0} \bar{T}(\mathbf{q}) = 4\pi \frac{N}{\Omega} \left(\hat{\mathbf{q}}\hat{\mathbf{q}} - \frac{1}{3}\mathbf{1} \right), \quad (14)$$

where $\hat{\mathbf{q}}$ is the unit vector in the \mathbf{q} -direction. Note that Eq. (12) is an approximation of the full dipole-dipole interaction,

$$\hat{V}_{\text{di-di}} = \frac{1}{2} \sum_{\mathbf{R},\mathbf{R}'} \int d\mathbf{r} \int d\mathbf{r}' [\hat{\mathbf{d}}_{\mathbf{R}}(\mathbf{r}) \cdot \nabla_{\mathbf{r}}] [\hat{\mathbf{d}}_{\mathbf{R}'}(\mathbf{r}') \cdot \nabla_{\mathbf{r}'}] \frac{e^2}{|\mathbf{r}-\mathbf{r}'|}, \quad (15)$$

but invokes the same assumption used in Eq. (10), i.e., that the lattice constant is large compared to the ionic size and is such that the interionic interaction becomes essentially that expected of point dipoles. Standard linear-response theory then involves evaluation of the many-body polarization function, $\alpha(\mathbf{q},\omega)$, the linear dipole-dipole response to a frequency-dependent external field $\mathbf{E}(\mathbf{q},\omega)$, and is given by

$$\alpha(\mathbf{q},\omega) = \frac{\sum_{\mathbf{R}} e^{i\mathbf{q}\cdot\mathbf{R}} \langle \hat{\mathbf{d}}_{\mathbf{R}}(\omega) \rangle}{\mathbf{E}(\mathbf{q},\omega)} \quad (16)$$

which can be written as

$$\alpha(\mathbf{q},\omega) = \sum_{\mathbf{R}} \int_{-\infty}^{\infty} dt e^{i(\mathbf{q}\cdot\mathbf{R}-\omega t)} \alpha(\mathbf{R},t), \quad (17)$$

where ($\hbar=1$)

$$\alpha(\mathbf{R}-\mathbf{R}',t-t') = i \langle [\hat{\mathbf{d}}_{\mathbf{R}}(t), \hat{\mathbf{d}}_{\mathbf{R}'}(t')] \rangle \theta(t-t'), \quad (18)$$

with $\theta(t)$ being the Heaviside step function. Solving for the polarizability, in a manner analogous to the application of the RPA in the charge-charge response of an electron liquid, then gives⁷

$$\alpha(\mathbf{q}, \omega) = \frac{\alpha_0(\omega)}{1 - \alpha_0(\omega)\bar{T}(\mathbf{q})} \approx \frac{Z_i e^2}{m(\omega_0^2 - \omega^2)} \quad (19)$$

where $\alpha_0(\omega)$ is the free-ion polarizability,

$$\alpha_0(\omega) = i \int_0^\infty dt e^{i\omega t} \langle [\hat{d}(t), \hat{d}(0)] \rangle. \quad (20)$$

Note that the core electron wave functions are assumed to be sufficiently localized such that exchange and higher order correlation effects between different dipoles can be ignored. The dielectric tensor, stemming from just the polarizability of the core electrons, then takes the familiar form,

$$\epsilon_{\text{core}}(\mathbf{q}, \omega) = 1 + \frac{4\pi n_a \alpha(\mathbf{q}, \omega)}{1 - 4\pi n_a \hat{\mathbf{q}}^T \alpha(\mathbf{q}, \omega) \hat{\mathbf{q}}}, \quad (21)$$

where n_a is the number density of ions. In the long wavelength limit, the longitudinal and transverse dielectric functions both become identical to the familiar Lorenz-Lorentz expression,

$$\lim_{q \rightarrow 0} \epsilon_{\text{core}}(\mathbf{q}, \omega) = 1 + \frac{4\pi n_a \alpha_0(\omega)}{1 - \frac{4\pi n_a \alpha_0(\omega)}{3}} \quad (22)$$

where we have used the limiting expression in Eq. (14). The dispersion, $\omega(\mathbf{q})$, of the collective harmonic modes are then given by the poles of $\alpha(\mathbf{q}, \omega)$, or equivalently, by solutions to

$$\det[\mathbf{1} - \alpha_0(\omega)\bar{T}(\mathbf{q})] = 0. \quad (23)$$

Note that these bosonic collective excitations are quite analogous to the conventional phonon excitations for the corresponding quantized displacement problem in that the dispersion satisfies $\omega(\mathbf{q} + \mathbf{K}) = \omega(\mathbf{q})$, where \mathbf{K} is a reciprocal lattice vector associated with the lattice vectors $\{\mathbf{R}\}$.

The presence of mobile conduction electrons has so far been ignored in the present discussion of the core polarizability; it can be shown²⁰ that inclusion of mobile charge carriers simply screens the polarization waves in such a way that the dispersion of the collective modes are now given by solutions to

$$\det \left[\mathbf{1} - \alpha_0(\omega) \frac{\bar{T}(\mathbf{q})}{\epsilon_v(\mathbf{q}, \omega)} \right] = 0, \quad (24)$$

where $\epsilon_v(\mathbf{q}, \omega)$ is the dielectric function of the valence electrons. To obtain simple order-of-magnitude estimates for the dispersion relationship of the polarization waves we may invoke a number of approximations. First, the frequency dependence of the free-polarizability function $\alpha_0(\omega)$ is taken to be dominated by the largest energy eigenstate spacing, and thus is given by the semiclassical approximation, i.e.,

$$\alpha_0(\omega) = 2 \sum_{\alpha\beta} \frac{\omega_\alpha - \omega_\beta}{(\omega_\alpha - \omega_\beta)^2 - \omega^2} \langle \alpha | \hat{\mathbf{d}} | \beta \rangle \langle \beta | \hat{\mathbf{d}} | \alpha \rangle \quad (25)$$

where ω_α is the exact energy eigenvalue corresponding to eigenstate $|\alpha\rangle$ and ω_0 can be interpreted as the minimum characteristic excitation energy of the ions (typically in the eV range⁶). Another simplification follows by invoking the reasonable limit that the number density of core electrons is greater than the number density of valence electrons (i.e., $Z_i \gg Z$). To satisfy the f -sum rule (i.e., conservation of charge) we know that in the long wavelength limit $\epsilon_v(\mathbf{q}, \omega)$ must take the form

$$\lim_{q \rightarrow 0} \epsilon_v(\mathbf{q}, \omega) = 1 - \frac{\omega_{pv}^2}{\omega^2} \quad (27)$$

where $\omega_{pv} = \sqrt{4\pi n_v e^2 / m}$ is the bare plasmon energy of the valence electrons with density n_v . With these considerations we find the following frequencies of the long wavelength screened polarization waves in a cubic lattice, namely,

$$\lim_{q \rightarrow 0} \omega_{\text{pol}}^2(\mathbf{q}) = \omega_0^2 + \frac{2}{3} \omega_{pc}^2 + \omega_{pv}^2, \text{ longitudinal} \quad (28)$$

$$\lim_{q \rightarrow 0} \omega_{\text{pol}}^2(\mathbf{q}) = \omega_0^2 - \frac{1}{3} \omega_{pc}^2 + \omega_{pv}^2, \text{ transverse} \quad (29)$$

where $\omega_{pc} = \sqrt{4\pi n_c e^2 / m}$, the plasmon energy of a fictitious homogeneous system of electrons with the same averaged density n_c as the core electrons. Correspondingly, the plasmon energy of the valence electrons is also renormalized, this time by the core polarization.³⁵⁻³⁷

C. Combined effective valence electron-electron interaction

The virtual exchange of these polarization waves can lead to an attractive interaction between two scattering valence electrons. This can be seen in the simplest picture in which the effective electron-electron interaction is determined via the total dielectric response

$$V_{\text{eff}} = v_q / \epsilon_{\text{total}} \quad (30)$$

where from addition of polarizabilities

$$\epsilon_{\text{total}} = \epsilon_v + \epsilon_{\text{core}} - 1. \quad (31)$$

Using Eq. (21) the effective longitudinal interaction can then be written as

$$V_{\text{eff}}(\mathbf{q}, \omega) = \frac{v_q}{\epsilon_v} \left(1 - \frac{4\pi n_a \alpha^{\text{sc}}(\mathbf{q}, \omega)}{1 - 4\pi n_a \alpha(\mathbf{q}, \omega) + 4\pi n_a \alpha^{\text{sc}}(\mathbf{q}, \omega)} \right) \quad (32)$$

where $\alpha^{\text{sc}} = \alpha / \epsilon_v$ is the screened polarizability function. The first term in Eq. (32) is the screened Coulomb interaction and the second term is the screened electron-polarization wave interaction which is opposite in sign for small q (polarization wave momentum). Some care is needed in interpreting Eq. (32) within the KO formalism if the polarization waves couple only to the electron charge-density fluctuations [the first term of Eq. (1)] and not to spin-density fluctuations

[third term of Eq. (1)], both of which are present in the electronic dielectric function ϵ_v .

We re-emphasize here that the core contribution to the effective interaction is not an on-site core effect but long wavelength correlated coherent fluctuations in the coupled assembly of cores. The physics of this contribution is quite analogous to the phonon modulation of the effective interaction.

In summary, the full expression of the effective valence electron-electron interaction is then

$$V_{\text{eff}}(\mathbf{q}, i\omega) = \left(v_q + \frac{v_q^2(1 - G_s(\mathbf{q}, i\omega))^2 \bar{\Pi}_0(\mathbf{q}, i\omega)}{1 - v_q(1 - G_s(\mathbf{q}, i\omega)) \bar{\Pi}_0(\mathbf{q}, i\omega)} - \zeta \frac{v_q^2(G_a(\mathbf{q}, i\omega))^2 \bar{\Pi}_0(\mathbf{q}, i\omega)}{1 + v_q G_a(\mathbf{q}, i\omega) \bar{\Pi}_0(\mathbf{q}, i\omega)} \right) \times \left(1 - \frac{4\pi n_a \alpha^{\text{sc}}(\mathbf{q}, i\omega)}{1 - 4\pi n_a \alpha(\mathbf{q}, i\omega) + 4\pi n_a \alpha^{\text{sc}}(\mathbf{q}, i\omega)} \right). \quad (33)$$

Writing the effective interaction in imaginary frequencies simplifies the later numerical work and is also useful, when the Mastubara frequencies $i\omega_n$ are introduced in the next section, for carrying out the calculations for the electron pairing function at finite temperatures. The finite temperature frequency-dependence of any physical quantity is then obtained by analytic continuation $i\omega_n \rightarrow \omega + i\delta$.

The effect of polarization stemming from the coherent motion of the ions may also be implemented by simply adding the traditional electron-phonon coupling term,

$$V_{\text{ph}}(\mathbf{q}, i\omega) = - \frac{a}{1 + (q/2k_F)^2} \left(\frac{\omega_{\text{ph}}^2(\mathbf{q})}{\omega^2 + \omega_{\text{ph}}^2(\mathbf{q})} \right), \quad (34)$$

to Eq. (32), thus treating the valence electrons, polarization waves and phonons all on an equal footing. Note that the screened phonon dispersion $\omega_{\text{ph}}(\mathbf{q})$ in this case is actually softened by both the valence electrons and polarization waves.⁶ The parameter a in Eq. (34) is determined by requiring that the correct electron-phonon coupling parameter λ be reproduced. The phonon contribution will not be discussed further except to say that the lowering of phonon frequencies ought to enhance the coupling to electrons.³⁸

III. ELECTRON PAIRING

The case of intrinsic superconductivity has been discussed in depth,^{11,39-44} where the virtual exchange of correlated charge-density fluctuations (plasmons) and spin-density fluctuations presages an attractive interaction within a homogeneous electron liquid. However, the necessary inclusion of vertex corrections in the effective Cooper-pair interaction, beyond the RPA, can significantly reduce the magnitude of T_c in the plasmon mechanism. As emphasized in Refs. 39 and 43 Migdal's theorem does not hold for the Coulomb interaction and therefore does not support the omission of vertex corrections in the effective Cooper-pair interaction. Hitherto, numerical estimates indicate that this pairing chan-

nel is quite weak, especially for s -wave pairing, in comparison to the traditional phonon channel. In this section we evaluate the consequences of a pairing channel based on the exchange of polarization waves, in addition to the mechanism underlying intrinsic superconductivity, and beyond $l=0$.

The condition for the second term in Eq. (32) to dominate, giving rise to an attractive total potential, is then

$$\alpha(\mathbf{q}, \omega) > \frac{1}{4\pi n_a}. \quad (35)$$

If Eq. (26) is used for the expression of the free-polarizability then the frequency condition that satisfies Eq. (35) is given in the long wavelength limit by

$$\lim_{q \rightarrow 0} \omega^2(\mathbf{q}) > \omega_0^2 - \frac{5}{3} \omega_{\text{pc}}^2 \quad (36)$$

In the weak-coupling regime the effective electron-electron interaction modifies T_c by entering into the pseudopotential,⁴⁵ which in the case of mediation by polarization waves, is expressed as

$$\mu^* = \frac{\mu}{1 + \mu \ln(E_F/\omega_{\text{pol}})}. \quad (37)$$

Thus the high characteristic energy scale of polarization waves ω_{pol} could either raise T_c , as mentioned in Sec. I but could also lower T_c by raising the Coulomb pseudopotential μ^* . To accurately determine whether T_c may be enhanced or lowered we must therefore resort to a numerical solution of the full strong-coupling Eliashberg equation.^{46,47} Previous studies^{27,29,48} have demonstrated the importance in this goal of the frequency-dependence in the intrinsic electron-electron interaction; the BCS superconductivity-formalism which assumes a static interaction becomes unsuitable for determining superconductivity with electron-based pairing mechanisms.

The Eliashberg equation, decomposed into l -wave spherical harmonics, gives a self-consistent equation for the pairing function $\Phi_l(\mathbf{k}, i\omega_n)$ of l -wave superconductivity at temperature $T = T_c$,

$$\Phi_l(\mathbf{k}, i\omega_n) = -T \sum_{\omega_n'} \sum_{\mathbf{k}'} |G(\mathbf{k}', i\omega_{n'})|^2 I_l(\mathbf{k}, i\omega_n; \mathbf{k}', i\omega_{n'}) \times \Phi_l(\mathbf{k}', i\omega_{n'}), \quad (38)$$

where the frequency summation runs over fermionic Matsubara frequencies $\omega_n \equiv \pi T(2n+1)$ with integer n , and $G(k, i\omega_n)$ is the full interacting Green's function. $I_l(k, i\omega_n; k', i\omega_{n'})$ is the l -wave irreducible interaction in the electron-electron channel, i.e.,

$$I_l(\mathbf{k}, i\omega_n; \mathbf{k}', i\omega_{n'}) = \frac{1}{2} \int_0^\pi d\theta \sin \theta P_l(\cos \theta) \times V_{\text{eff}}(\mathbf{q}, i\omega_n - i\omega_{n'}), \quad (39)$$

where $\cos \theta \equiv (\mathbf{k} \cdot \mathbf{k}') / (kk')$, $P_l(\cos \theta)$ are the Legendre polynomials, and $q \equiv |\mathbf{k} - \mathbf{k}'|$. The angular momentum of the Cooper pairs remains a valid quantum number in the crystalline

lattice since the typical size of the pair is much larger than the lattice constant. The same argument holds in the traditional phonon-coupling theory of electron pairing.

Replacing the momentum summation in Eq. (38) by an integral we can then write the gap equation in the form

$$\Phi_l(\mathbf{k}, i\omega_n) = -T \sum_{\omega_n'} \int_0^\infty dk' K_l(\mathbf{k}, i\omega_n; \mathbf{k}', i\omega_n') \times \Phi_l(\mathbf{k}', i\omega_n'), \quad (40)$$

where

$$K_l(\mathbf{k}, i\omega_n; \mathbf{k}', i\omega_n') = \frac{|G(\mathbf{k}', i\omega_n')|^{2k'}}{4\pi k} \int_{|k-k'|}^{k+k'} dq \times P_l\left(\frac{k^2 - k'^2 - q^2}{2kk'}\right) q \times V_{\text{eff}}(\mathbf{q}, i\omega_n - i\omega_n'). \quad (41)$$

The expression for the required full Green's function $G(\mathbf{k}, i\omega_n)$

$$G(\mathbf{k}, i\omega_n) = \frac{1}{G^0(\mathbf{k}, i\omega_n)^{-1} - \Sigma(\mathbf{k}, i\omega_n)}, \quad (42)$$

with

$$G^0(\mathbf{k}, i\omega_n) \equiv \frac{1}{i\omega_n - \epsilon_k - \mu}, \quad (43)$$

can be evaluated self-consistently using the modified KO approximation for the self-energy. Thus, the self energy Σ takes the form

$$\Sigma(\mathbf{k}, i\omega_n) = -T \sum_{\nu_n} \int \frac{d^3q}{(2\pi)^3} V_{\text{se}}(\mathbf{q}, i\nu_n; \mathbf{q} - \mathbf{k}, i\nu_n - i\omega_n) \times G(\mathbf{q}, i\nu_n) \quad (44)$$

where the self-energy potential V_{se} has contributions from both the screened Coulombic interaction¹¹ and the polarization waves, i.e.

$$V_{\text{se}} = \frac{v_q}{1 - v_q \bar{\Pi}_0(\mathbf{q}, i\omega)[1 - G_s(\mathbf{q}, i\omega)]} \times \left(1 - \frac{4\pi n \alpha^{\text{sc}}(\mathbf{q}, i\omega)}{1 - 4\pi n \alpha(\mathbf{q}, i\omega) + 4\pi n \alpha^{\text{sc}}(\mathbf{q}, i\omega)} \right). \quad (45)$$

As described in Ref. 49, the Green's function with full normal-state self-energy effects can be solved by an iterative method. Note that electronic vertex corrections are incorporated in the number-renormalized Lindhard response $\bar{\Pi}_0$.

To solve the Eliashberg equation we utilise a technique pioneered by Rietschel and Sham³⁹ and Takada,⁴⁹ originally developed for intrinsic strongly-coupled superconductivity: the pairing function $\Phi(\mathbf{k}, i\omega_n)$ is first evaluated on a grid of discrete points in momentum and frequency space thereby transforming the Eliashberg equation from an integral equa-

TABLE I. Estimates of T_c evaluated from the effective valence electron-electron interaction for both the homogeneous [Eq. (1)] and inhomogeneous [Eq. (33)] cases. For illustrative purposes the parameters have been chosen to be $r_s=5$, $Z=2$, and $\hbar\omega_0=5$ eV.

l -wave	Z_A	$T_c^{(\text{hom})}$ (K)	$T_c^{(\text{inhom})}$ (K)
s	30	0	0
s	48	0	1.1
d	30	0.3	11.6
d	48	0.3	18.5

tion into a matrix equation with the structure

$$\mathbf{M}_l \Phi_l = \Phi. \quad (46)$$

The solution of the gap equation then consists of converting the matrix equation Eq. (46) into an eigenvalue equation,

$$\mathbf{M}_l \Phi_l = \gamma \Phi, \quad (47)$$

and determining the gap function Φ_l when the largest positive eigenvalue of Eq. (47) equals unity, i.e., $\gamma=1$. At temperatures greater than the transition temperature T_c , the largest positive eigenvalue is always less than unity and at temperatures below T_c the largest positive eigenvalue is always greater than unity.

In Table I we report some numerical estimates of T_c in a three-dimensional electron liquid for both the cases of with or without polarization waves, corresponding to inhomogeneous and homogeneous systems, respectively. As can be seen, the inclusion of polarization-wave coupling leads to an enhancement of T_c , even for $l=0$ (s -wave) pairing, where no solutions were previously found in the case of just intrinsic superconductivity.

IV. DISCUSSION

The calculations summarized above show that dynamical correlation within both classes of electrons (core and valence) can cause the effective valence electron-electron potential to become attractive in an otherwise static lattice. The physics in each class is different. The intrinsic pairing mechanism attributed to the valence electrons arises from the exchange of correlated charge-spin and spin-density fluctuations, and the pairing mechanism due to the core electrons arises from the exchange of polarization waves. Note that these additional pairing channels occur independent of the traditional phonon channel which has been omitted in the present calculations of the superconducting transition. The assumption of independence of the phonon and polarization wave channels rests upon the the disparity of the relevant energy scales, i.e., $\omega_{\text{pol}} \gg \omega_{\text{ph}}$. If, however, there exist systems such that these energies are comparable then interference will occur between the pairing channels and will bear consequences on T_c .

The presence of multiple-band structure, with the ensuing electron-hole interactions, can provide a possible further enhancement of intrinsic pairing. It has been shown¹¹ that an additional attractive term arises in the effective electron in-

teraction in two-band systems because of correlated charge (electron-hole) fluctuations between the bands, these even allowing the possibility of intrinsic s -wave pairing.

An interesting question yet to be investigated is the role of disorder on the polarization wave pairing channel. Generally, weak quenched disorder is expected to soften the dispersion and broaden the spectral peak of collective excitations, especially at higher energies and wave vectors. However, in the numerical solution of the Eliashberg equation, the dominant contribution to the pairing arises at $q=2k_F$ and, so long as the self-energy (in real frequencies) of the polarization waves possess only a small imaginary part, we may expect disorder to have relatively little effect on T_c .

In the pairing analyses presented in this paper it is important to remember that the effective partitioning of the two classes of electrons only becomes possible under the assumption of nonoverlapping core and valence bands. This assumption permits neglect of correlation and exchange between the two classes of electrons, which could otherwise dramatically reduce the pairing amplitude in a manner analogous to the lowering of T_c in plasmon-based models of intrinsic superconductivity when vertex corrections are included.³⁹ Thus although polarization waves may still occur, albeit with a smaller lifetime, in systems of overlapping bands, their contribution to collective electron pairing would be diminished. Indeed, we draw attention to the observation that there is no experimental evidence of superconductivity

in the noble metals where there exists a significant overlap between the d -state core electrons (with considerable polarizability in principle) and the s -state valence electrons.

It is interesting to record that in a limiting sense the polarization wave mechanism developed here and earlier^{5,6} is not unrelated to the bipolaron mechanism of superconductivity, recently suggested as a possible candidate for the high T_c pairing mechanism in the cuprates^{50,51} and metal-ammonia solutions.⁵² The soft limit of polarization waves (i.e., collective static waves at finite wave vectors) can be viewed as reducing the valence electron-electron repulsion in a physically similar manner to the bipolaron mechanism.

Finally, we note that the calculated values of T_c are strongly sensitive to the resolution of the grid on which the pairing function is evaluated and on the form of the local-field factors. In a future publication we hope to present a more comprehensive set of numerical results for both two and three dimensions. Nonetheless, the trend reported so far is quite clear: polarization waves are an additional and viable mechanism to enhance T_c .

ACKNOWLEDGMENTS

This work was supported by the NSF under Grant No. DMR-0302347. We thank P. Allen for helpful comments on the manuscript.

-
- ¹W. A. Little, Phys. Rev. **134**, A1416 (1964).
²V. L. Ginzburg, Zh. Eksp. Teor. Fiz. **47**, 2318 (1964).
³W. Kohn and J. M. Luttinger, Phys. Rev. Lett. **15**, 524 (1965).
⁴A. Zangwill and P. Soven, Phys. Rev. A **21**, 1561 (1980).
⁵N. W. Ashcroft, in *Novel Superconductivity* (Plenum, New York, 1987), p. 301.
⁶N. W. Ashcroft, in *Recent Progress in Many-Body Theories* (Plenum, New York, 1988), Vol. 1, p. 39.
⁷S. Lundqvist and A. Sjölander, Ark. Fys. **26**, 17 (1963).
⁸K. Rapcewicz and N. W. Ashcroft, Phys. Rev. B **44**, 4032 (1991).
⁹H. Ehrenreich, in *The Optical Properties of Solids*, Proceedings of the International School of Physics "Enrico Fermi," Course 34, Varenna, 1965, edited by J. Tauc (Academic Press, New York, 1996), Chap. 13.
¹⁰D. Fay and A. Layzer, Phys. Rev. Lett. **20**, 187 (1968).
¹¹C. F. Richardson and N. W. Ashcroft, Phys. Rev. B **55**, 15130 (1997).
¹²R. Shankar, Rev. Mod. Phys. **66**, 129 (1994).
¹³J. Polchinski, in *Proceedings of the 1992 TASI in Elementary Particle Physics*, edited by J. Harvey and J. Polchinski (World Scientific, Singapore, 1992).
¹⁴V. M. Galitski and S. D. Sarma, Phys. Rev. B **67**, 144520 (2003).
¹⁵C. A. Kukkonen and A. W. Overhauser, Phys. Rev. B **20**, 550 (1979).
¹⁶W. A. Little and H. Gutfreund, Phys. Rev. B **4**, 817 (1971).
¹⁷A. Lucas, Physica (Amsterdam) **35**, 353 (1967).
¹⁸P. Lambin, A. A. Lucas, and J.-P. Vigneron, Phys. Rev. B **46**, 1794 (1992).
¹⁹J. J. Rehr, E. Zaremba, and W. Kohn, Phys. Rev. B **12**, 2062 (1975).
²⁰J. Cheung and N. W. Ashcroft, Phys. Rev. B **23**, 2484 (1981).
²¹C. C. Montanari, J. E. Miraglia, and N. R. Arista, Phys. Rev. A **66**, 042902 (2002).
²²E. L. Shirley, X. Zhu, and S. G. Louie, Phys. Rev. B **56**, 6648 (1997).
²³J. Cheung and N. W. Ashcroft, Phys. Rev. B **24**, 1636 (1981).
²⁴E. Zaremba and K. Sturm, Phys. Rev. Lett. **55**, 750 (1985).
²⁵K. Sturm, E. Zaremba, and K. Nuroh, Phys. Rev. B **42**, 6973 (1990).
²⁶G. Vignale and K. S. Singwi, Phys. Rev. B **32**, 2156 (1985).
²⁷C. F. Richardson and N. W. Ashcroft, Phys. Rev. B **50**, 8170 (1994).
²⁸N. Iwamoto, Phys. Rev. A **30**, 3289 (1984).
²⁹G. S. Atwal, I. G. Khalil, and N. W. Ashcroft, Phys. Rev. B **67**, 115107 (2003).
³⁰M. Lein, E. K. U. Gross and J. P. Perdew, Phys. Rev. B **61**, 13431 (2000).
³¹D. M. Ceperley and B. J. Alder, Phys. Rev. Lett. **45**, 566 (1980).
³²*Quantum Monte Carlo Methods in Physics and Chemistry*, edited by M. P. Nightingale and C. J. Umrigar (Kluwer, Dordrecht, 1999).
³³S. Moroni (private communication, 2002).
³⁴G. Bergmann and D. Rainer, Z. Phys. **263**, 59 (1973).
³⁵A. Fleszar, R. Stumpf, and A. G. Eguiluz, Phys. Rev. B **55**, 2068 (1997).
³⁶K. Widder, M. Knupfer, O. Knauff, and J. Fink, Phys. Rev. B **56**,

- 10154 (1997).
- ³⁷C. L. Bastidas, A. Liebsch, and W. L. Mochán, *Phys. Rev. B* **63**, 165407 (2001).
- ³⁸B. T. Matthias, H. Suhl, and C. S. Ting, *Phys. Rev. Lett.* **27**, 245 (1971).
- ³⁹H. Rietschel and L. J. Sham, *Phys. Rev. B* **28**, 5100 (1983).
- ⁴⁰M. Grabowski and L. J. Sham, *Phys. Rev. B* **29**, 6132 (1984).
- ⁴¹J. Ruvalds, *Phys. Rev. B* **35**, 8869 (1987).
- ⁴²Y. Takada, *Phys. Rev. B* **37**, 155 (1988).
- ⁴³T. Buche and H. Rietschel, *Phys. Rev. B* **41**, 8691 (1990).
- ⁴⁴P. Longe and S. M. Bose, *J. Phys.: Condens. Matter* **4**, 1811 (1992).
- ⁴⁵P. Morel and P. W. Anderson, *Phys. Rev.* **125**, 1263 (1962).
- ⁴⁶G. M. Eliashberg, *Zh. Eksp. Teor. Fiz.* **38**, 966 (1960).
- ⁴⁷P. B. Allen and B. Mitrovic, *Solid State Physics* (Academic, New York, 1982), Vol. 37.
- ⁴⁸D. J. W. Geldart, *Can. J. Phys.* **45**, 3139 (1967).
- ⁴⁹Y. Takada, *Phys. Rev. B* **47**, 5202 (1993).
- ⁵⁰A. S. Alexandrov and N. F. Mott, *Rep. Prog. Phys.* **57**, 1197 (1994).
- ⁵¹A. S. Alexandrov and P. P. Edwards, *Physica C* **331**, 97 (2000).
- ⁵²P. P. Edwards, *J. Supercond.* **13**, 933 (2000).
- ⁵³A. A. Abrikosov, L. P. Gorkov, and I. E. Dzyaloshinski, *Methods of Quantum Field Theory in Statistical Physics* (Dover, New York, 1975).