Band-Structure Effects in Superconductivity. I. Formalism*

J. W. GARLAND*†
Department of Physics, University of California, Berkeley, California
and
Cavendish Laboratory, University of Cambridge, Cambridge, England
(Received 29 December 1965)

Dyson equations are derived for the interacting electrons and phonons of a perfect crystal. A separation of the electron and phonon fields which is exact within either the Hartree or the Migdal approximation is effected. All umklapp processes and local-field corrections are included, but the hybridization of electronic bands and of phonon modes is given only implicitly. Our equations reduce to previously obtained forms in the jellium approximation and to lowest order in r_s. The Nambu-Gor'kov formalism is used to derive equations for the superconducting energy gap. Since the Migdal approximation is not applicable to the treatment of the Coulomb interaction, we develop other approximations which yield either three-dimensional integral equations for an anistropic energy gap $\mathbf{\Delta}(\mathbf{k},k_0)$ or one-dimensional integral equations for an isotropic energy gap $\Delta(k_0)$. An easy method for the calculation of the anisotropy of the energy gap $\mathbf{\Delta}(\mathbf{k},k_0)$ in the simple metals is presented. The validity of these approximations is discussed and our equations are compared with those of previous authors. The strongly nonlinear homogeneous integral equation for $\Delta(k_0)$ is transformed into a quasilinear, inhomogeneous integral equation. This transformation immediately displays several interesting properties of the solution $\Delta(k_0)$ and yields a method for the rapid numerical calculation of $\Delta(k_0)$.

I. INTRODUCTION

ALTHOUGH the Bardeen-Cooper-Schrieffer theory of superconductivity[1] (hereafter referred to as the BCS theory) has been found to be amazingly successful in explaining and predicting the properties of the superconducting state, in investigating superconductivity, most authors have used apparently oversimplified models in which all band-structure effects are neglected. In particular, most theoretical work in superconductivity has been so strongly focused upon the proper treatment of the attractive electron-electron interaction $\mathbf{V}_{\rm ph}$ arising from the exchange of virtual phonons, that the screened Coulomb interaction $\mathbf{V}_e$ has been treated only within greatly oversimplified models.[1–6] Our primary purpose in this series of papers is (1) to treat some of those superconducting properties of materials which are dependent in any important way upon the band structure of the materials and which thus are not susceptible to calculations based on previous, simpler models,[7–9] and (2) to explain why the previous, apparently oversimplified models have been adequate for most purposes. In this paper, we confine ourselves primarily to the task of finding an easily solvable integral equation for the superconducting energy gap of any material, while including umklapp effects and local-field corrections and retaining the frequency and wave-number dependence of both $\mathbf{V}_{\rm ph}$ and $\mathbf{V}_e$. Also, a new method is presented for the solution of one-dimensional nonlinear integral equations such as usually occur in the theory of superconductivity.

In Sec. II we present a Hamiltonian for the interacting electrons and phonons of a perfect crystal and the resulting Dyson equations. Only two approximations are embodied in our Hamiltonian: (1) the harmonic approximation for lattice vibrations which allows us to neglect phonon-phonon interactions, and (2) the approximation of the bare[10] ionic pseudopoten-

* Supported in part by the National Science Foundation, the Alfred P. Sloan Foundation, and the Science Research Council of Great Britain.

† Permanent address: Department of Physics, University of California, Berkeley, California.

‡ Alfred P. Sloan Foundation Fellow.

[1] J. Bardeen, L. N. Cooper, and J. R. Schrieffer, Phys. Rev. **108**, 1175 (1957).

[2] G. M. Eliashberg, Zh. Eksperim. i Teor. Fiz. **38**, 966 (1960) [English transl: Soviet Phys.—JETP **11**, 696 (1960)].

[3] P. Morel and P. W. Anderson, Phys. Rev. **125**, 1263 (1962).

[4] J. R. Schrieffer, D. J. Scalapino, and J. W. Wilkins, Phys. Rev. Letters **10**, 336 (1963).

[5] References 1–4 are intended only as a representative sample of some of the more important papers on superconductivity which have been concerned almost exclusively with the calculation of the effects of the interaction $\mathbf{V}_{\rm ph}$. The reader is referred to J. R. Schrieffer, *Theory of Superconductivity* (Ref. 6) for a bibliography as well as an excellent historical introduction to the subject of superconductivity and a more detailed treatment for simpler models of some of the formalism presented in this paper.

[6] J. R. Schrieffer, *Theory of Superconductivity* (W. A. Benjamin, Inc., New York, 1964).

[7] Examples of such properties are (1) the isotope effect, (2) the pressure dependence of the transition temperature T_c, (3) the properties of superconducting degenerate semiconductors and semimetals (Ref. 8), (4) the properties of such metals as lanthanum and uranium which have very narrow bands near the Fermi surface (Ref. 9), (5) the anomalous superconducting properties of many alloys, (6) the effects of anisotropy, and (7) the anomalous superconducting properties possibly to be expected in clean transition metals. Even the dependence of T_c upon band structure could be listed as such a property.

[8] M. L. Cohen, Rev. Mod. Phys. **36**, 240 (1964); Phys. Rev. **134**, A511 (1964); J. F. Schooley, W. R. Hosler, and M. L. Cohen, Phys. Rev. Letters **12**, 474 (1964); R. A. Hein, J. W. Gibson, R. Mazelsky, R. C. Miller, and J. K. Hulm, *ibid.* **12**, 320 (1964); L. Finegold, *ibid.* **13**, 233 (1964).

[9] The superconductivity of lanthanum and uranium has been discussed from one point of view by Kuper, Jensen, and Hamilton. See, e.g., D. C. Hamilton and M. A. Jensen, Phys. Rev. Letters **11**, 205 (1963); C. G. Kuper, M. A. Jensen, and D. C. Hamilton, Phys. Rev. **134**, 15 (1964).

[10] By "bare" we mean unscreened by the conduction electrons or, more precisely, screened only by those electronic states over which we do not sum in evaluating the Hamiltonian (1).

tial $\alpha^0(\mathbf{k},\mathbf{q}+\mathbf{g})$ by a local operator $\alpha^0(\mathbf{q}+\mathbf{g})$.[11,12] In particular, umklapp processes and local-field corrections are treated exactly in all calculations. The resultant Dyson equations follow exactly from our Hamiltonian and constitute simply a proper tensor generalization of the usual scalar equations obtained previously within the jellium[13] approximation. The electron- and phonon-fields are separated exactly within the Migdal approximation.

In Sec. III, we develop a new approximation technique for the derivation of an integral equation for the superconducting energy gap $\mathbf{\Delta}(k)$.[14] Even within the jellium model, some approximation technique is necessary in order to reduce the dimensionality of the four-dimensional Dyson equations, which represent coupled equations for the unrenormalized energy gap $\phi(k)$ and the renormalization functions $\mathbf{Z}(k)$ and $\chi(k)$. Previous authors[2–6] have employed the Migdal approximation[15] to simplify the equations for the contribution to superconductivity of the phonon-induced interaction $\mathbf{V}_{\rm ph}$ and have treated the Coulomb contribution only within a very rough approximation. However, this technique is inadequate here, as is shown in Sec. III, because it essentially corresponds to the neglect of all band-structure effects; i.e., to the neglect of that which we wish to calculate.

In Sec. IV we consider those cases in which our integral equations for $\mathbf{\Delta}(k)$ can be reduced to one-dimensional form, and compare our results in these cases with those of previous authors.[1–6,16,17] We find that in the neglect of Coulomb-induced lifetime effects, our equations for $\Delta(\pm k_0,k_0)$ are identical in form to the quasiparticle equation for $\Delta(\pm k_0)$ except for a factor of $Z^{-1}(\pm k_0,k_0)$. We consider both the case of superconductors which are "dirty"[18] in the Anderson[19] sense and that of superconductors which are "clean" but nearly isotropic, and present an easy method for calculating the anisotropy of the energy gap in the simple metals.

In Sec. V a method is presented for reducing to quasi-linear form any one-dimensional, nonlinear integral equation for a single scalar function, provided that the nonlinearity is important only in the neighborhood of some fixed point. The application of this method to numerical calculations is outlined; it is also used to analyze the qualitative form of the solution $\Delta(k_0)$ and its dependence upon the kernel $\mathfrak{K}$ of the integral equation.

II. HAMILTONIAN AND RESULTANT DYSON EQUATIONS

We employ Green's-function techniques here both in order to simplify the comparison of our approximations with those of previous authors[1–6] and to simplify any desired extension of our results to include exchange or other higher order terms. In this section we present and discuss briefly both a Hamiltonian for a crystal with interacting electrons and phonons and the resulting set of Dyson equations. The results presented in this section are not essentially new; they are merely generalizations of results derived formerly only within the jellium[15] approximation. However, we believe our derivation of the hydridization of different phonon branches and polarizations and the general matrix or tensor form of all our results to be new. We express the total electron-electron interaction tensor as the sum of a screened Coulomb interaction $\mathbf{V}_{\rm e}$ and a phonon-induced interaction $\mathbf{V}_{\rm ph}$ and explicitly derive the screening of both. All approximations except those which appear in our Hamiltonian occur in the determination of a dielectric tensor $\boldsymbol{\kappa}(q)$ and a vertex function $\mathbf{\Gamma}(k,q)$; given $\boldsymbol{\kappa}$ and $\mathbf{\Gamma}$, our Dyson equations follow exactly from our Hamiltonian. As an illustrative exercise, we derive the random-phase-approximation (RPA) microscopic, longitudinal dielectric tensor from our electronic Dyson equations. If our results are to be applicable to all superconductors not containing magnetic impurities (simple metals, transition metals, semiconductors, and semimetals), we must not choose a simplified model such as the jellium model. In particular, all umklapp effects must be included correctly. However, while allowing for the existence of core-polarization effects, we do neglect phonon-phonon interactions and approximate the bare ionic pseudopotential[10,11] seen by the conduction electrons by a local operator.[20] Furthermore, for simplicity we neglect all spin-orbit, spin-spin, and magnetic interactions. Although spin-orbit and spin-spin interactions are important in determining such electromagnetic properties

[11] By a "local operator" we mean an operator $\mathcal{O}$ whose matrix elements $\langle\mathbf{k}'|\mathcal{O}|\mathbf{k}\rangle$ depend only upon $\mathbf{q}=\mathbf{k}'-\mathbf{k}$.

[12] For a discussion of the ionic pseudopotential see the following references: M. H. Cohen and V. Heine, *Advances in Physics* (Taylor & Francis, Ltd., London, 1958), Vol. 7, p. 395; Phys. Rev. **122**, 1821 (1961); W. A. Harrison, *ibid.* **118**, 1190 (1960); in *The Fermi Surface*, edited by W. A. Harrison and M. B. Webb (John Wiley & Sons, Inc., New York, 1960); V. Heine and I. Abarenkov, Phil. Mag. **9**, 451 (1964); I. Abarenkov and V. Heine, *ibid.* **11**, 379 (1965); and A. Animalu and V. Heine (to be published). Further references are given in a review article by V. Heine, in *Proceedings of the Ninth International Conference on Low Temperature Physics*, edited by J. G. Daunt, D. V. Edwards, F. J. Milford, and M. Yaqub (Plenum Press, Inc., New York, 1965).

[13] By "jellium" we refer to the model in which the ion lattice of a crystal is replaced by a uniform, positively charged jelly as described by Ziman. J. Ziman, *Electrons and Phonons* (Oxford University Press, New York, 1960), p. 163.

[14] We write k and q for four-momenta, $\mathbf{k}$ and $\mathbf{q}$ for the corresponding wave vectors, and $\hat{k}$ and $\hat{q}$ for the unit vectors $\mathbf{k}/|\mathbf{k}|$ and $\mathbf{q}/|\mathbf{q}|$.

[15] A. B. Migdal, Zh. Eksperim. i Teor. Fiz. **34**, 1438 (1958) [English transl.: Soviet Phys.—JETP **7**, 996 (1958)].

[16] J. W. Garland, Phys. Rev. Letters **11**, 114 (1963).

[17] J. W. Garland (unpublished).

[18] We define "clean" or "dirty" in this paper in accordance with the Anderson theory of dirty superconductors (Ref. 19); see Sec. IVA.

[19] P. W. Anderson, J. Phys. Chem. Solids **11**, 26 (1959).

[20] This approximation of the bare ionic pseudopotential by a local operator is our most important approximation, and is essential to our analysis.

as the Knight shift[21] and nuclear-spin relaxation rate[22] in superconductors, these interactions are unimportant in the determination of such basic thermodynamic quantities as the superconducting transition temperature T_c and consequently are omitted.[23] Also, even though the magnetic interaction between conduction electrons due to their orbital motion leads to the Meissner effect and is thus very important, in the absence of external fields, the small magnetic forces between electrons are almost completely quenched by crystal fields and therefore lead to weak effects. Finally, upon setting $\hbar=1$, assuming crystalline inversion symmetry and neglecting multiphonon processes, we find the Hamiltonian

$$\begin{aligned}H&=H_e+H_{ph}+H_{e-e}+H_{e-ph}\\&=\sum_{\mathbf{k}}\mathbf{c}_{\mathbf{k}}^{\dagger}\cdot\boldsymbol{\varepsilon}(\mathbf{k})\cdot\mathbf{c}_{\mathbf{k}}+\sum_{\mathbf{q}}\mathbf{a}_{\mathbf{q}}^{\dagger}\cdot\boldsymbol{\omega}^0(\mathbf{q})\cdot\mathbf{a}_{\mathbf{q}}\\&\quad+\tfrac{1}{2}\sum_{\mathbf{q}}\sum_{\mathbf{k}}\sum_{\mathbf{k}'}\sum_{\mathbf{g}}\mathbf{c}_{\mathbf{k}+\mathbf{q}}^{\dagger}\mathbf{c}_{\mathbf{k}'-\mathbf{q}}^{\dagger}:\mathbf{V}_e(\mathbf{q}+\mathbf{g};\mathbf{k},\mathbf{k}'):\mathbf{c}_{\mathbf{k}'}\mathbf{c}_{\mathbf{k}}\\&\quad+\sum_{\mathbf{q}}\sum_{\mathbf{k}}\sum_{\mathbf{g}}[\mathbf{c}_{\mathbf{k}+\mathbf{q}}^{\dagger}\cdot\mathbf{M}^T(\mathbf{q}+\mathbf{g};\mathbf{k})\cdot\mathbf{c}_{\mathbf{k}}]\\&\qquad\times[\boldsymbol{\alpha}^0(\mathbf{q}+\mathbf{g})\cdot\boldsymbol{\psi}_q].\end{aligned}\quad(1)$$

Here the wave vectors $\mathbf{k}$, $\mathbf{k}'$, and $\mathbf{q}$ are restricted to the first Brillouin zone, and the $\mathbf{g}$'s are any reciprocal lattice vectors (including the zero vector). All sums over $\mathbf{k}$ and $\mathbf{k}'$ (but not sums over $\mathbf{q}$) implicitly include sums over the suppressed spin indices σ and σ'. The $\mathbf{c}_{\mathbf{k}}^{\dagger}(\mathbf{c}_{\mathbf{k}})$ and $\mathbf{a}_{\mathbf{q}}^{\dagger}(\mathbf{a}_{\mathbf{q}})$ are row (column) vectors whose components are creation (destruction) operators for electrons in Bloch states $|l;\mathbf{k},\sigma\rangle$ and for phonons of wave vector $\mathbf{q}$ and branch-plus-polarization index n. The matrices $\boldsymbol{\varepsilon}(\mathbf{k})$ and $\boldsymbol{\omega}^0(\mathbf{q})$ are diagonal; thus, the terms H_e and H_{ph} contain simply sums over the band indices l and over the phonon indices n, respectively.

We can assume all sums over electronic states to be taken only over valence or conduction states and not sum over core states; were we to sum over all core states as well, the bare pseudopotential $\boldsymbol{\alpha}^0$ would reduce in form to a simple Coulomb interaction. The diagonal elements $\epsilon_l(\mathbf{k})$ of $\boldsymbol{\varepsilon}(\mathbf{k})$ are the eigenvalues for the Bloch states $|l;\mathbf{k},\sigma\rangle$ of a crystal Hamiltonian containing only the electronic kinetic energy and the unscreened pseudopotentials of the bare ion core. The frequencies $\omega_n^0(\mathbf{q})$ which form the diagonal elements of $\boldsymbol{\omega}^0(\mathbf{q})$ are "bare"[10] phonon frequencies, not the observed frequencies of the interacting system of phonons and electrons. The tensor $\mathbf{V}_e(\mathbf{q}+\mathbf{g};\mathbf{k},\mathbf{k}')$, which gives the unscreened Coulomb interaction between electrons in Bloch states, can be written as a direct product

$$\mathbf{V}_e(\mathbf{q}+\mathbf{g};\mathbf{k},\mathbf{k}')=v(\mathbf{q}+\mathbf{g})\mathbf{M}(\mathbf{q}+\mathbf{g};k)\otimes\mathbf{M}(-\mathbf{q}-\mathbf{g};\mathbf{k}').\quad(2)$$

Here, the element $v(\mathbf{q}+\mathbf{g})$ of the column vector $\mathbf{v}(\mathbf{q})$ is the matrix element of the "bare" Coulomb interaction between plane-wave states $|\mathbf{k},\sigma\rangle$ and $|\mathbf{k}+\mathbf{q}+\mathbf{g},\sigma\rangle$. Without loss of generality we can choose wave functions $|l;\mathbf{k},\sigma\rangle$ so that the matrices $\mathbf{M}(\mathbf{q}+\mathbf{g};\mathbf{k})$, which have elements

$$M_{ll'}(\mathbf{q}+\mathbf{g};\mathbf{k})\equiv\langle\mathbf{k}+\mathbf{q},l',\sigma|\exp\{i(\mathbf{q}+\mathbf{g})\cdot\mathbf{r}\}|\mathbf{k},l,\sigma\rangle,\quad(3)$$

will satisfy the equations

$$\mathbf{M}(\mathbf{q}+\mathbf{g};\mathbf{k})=\mathbf{M}^*(\mathbf{q}+\mathbf{g};\mathbf{k})=\mathbf{M}^T(-\mathbf{q}-\mathbf{g};\mathbf{k}+\mathbf{q}),\quad(4)$$

where M^* is the complex conjugate of $\mathbf{M}$, $\mathbf{M}^T$ is the transpose of $\mathbf{M}^*$ and vectors of the form $\mathbf{k}+\mathbf{q}$ or $\mathbf{k}_1\pm\mathbf{k}_2$ are defined to lie in the first Brillouin zone.

The row and column vectors $\boldsymbol{\alpha}^0(\mathbf{q}+\mathbf{g})$ and $\boldsymbol{\psi}_{\mathbf{q}}$ have elements which correspond to different values of the phonon index n. The elements $\alpha_n^0(\mathbf{q}+\mathbf{g})$ are given by the equation

$$\alpha_n^0(\mathbf{q}+\mathbf{g})=(\mathbf{q}+\mathbf{g})\cdot\mathbf{e}_n(\mathbf{q})V_p^0(\mathbf{q}+\mathbf{g})\sum_{\alpha}\exp(i\mathbf{g}\cdot\mathbf{R}_{\alpha}),$$

where $\mathbf{e}_n(\mathbf{q})$ is a phonon-polarization vector, $V_p^0(\mathbf{q}+\mathbf{g})$ is a bare ionic pseudopotential, and where the $\mathbf{R}_{\alpha}$ give the positions of different atoms within a unit cell; the $\psi_{n,\mathbf{q}}$ are ion displacement operators given by the formula

$$\psi_{n,\mathbf{q}}=[2M_{n,\mathbf{q}}\omega_n^0(\mathbf{q})]^{-1/2}[a_{n,-\mathbf{q}}^{\dagger}].\quad(5)$$

Here, $M_{n,\mathbf{q}}$ is equal to the isotropic average M of the ionic masses for any element, but is some weighted average mass depending on both n and $\mathbf{q}$ for alloys and compounds.

We have made only one major approximation: the assumption that the unscreened pseudopotential is a local operator. We must show that this approximation is well justified. First, for a given momentum transfer, changes of the order of the Debye energy $k_B\Theta_D$ in electronic energies produce only slight changes in the corresponding electronic momenta, hence only slight changes in the unscreened pseudopotential for scattering near the Fermi surface, provided that the Debye energy is much less than the Fermi energy E_F. Second, the electron-phonon interaction is important only for electrons not much farther than $k_B\Theta_D$ from the Fermi level. Thus, for a material having a spherical Fermi surface or for a material sufficiently "dirty"[18] that we must average over all anisotropies, this approximation is well justified. Furthermore, the nonlocality of a pseudopotential should introduce only a relatively small error in treating the effects of small anisotropies in the Fermi surface of a metal.

From the Hamiltonian (1) we are now able to generate, without further approximations, a set of Dyson

[21] W. D. Knight, *in Solid State Physics*, edited by F. Seitz and D. Turnbull (Academic Press Inc., New York, 1966), Vol. 2. See Ref. 6 for a discussion of the Knight shift in the superconducting state and for further references.

[22] L. C. Hebel and C. P. Slichter, Phys. Rev. **113**, 1504 (1959). For further references and a brief discussion see Ref. 6.

[23] Spin-orbit interactions are unimportant here because, with the time-reversal pairing characteristic of superconductivity, there is no exchange interaction between paired states. They are important in studying magnetism, where they reduce the exchange interaction.

equations. In 1961, Baym [24] derived equations for the phonon and electron thermodynamic Green's functions and the electron-electron interaction propagator for a monatomic nonsuperconducting metal described by an infinite Bravais lattice. However, Baym wrote these equations in a space-time representation and did not use the property of invariance under translation through a lattice vector to simplify his equation for the electron-electron interaction propagator (except to derive the Lindhard dielectric function for a simple jellium model). For the convenience of the reader, we therefore use the simple variational-derivative technique developed by Schwinger[25] (and used by Baym[24]) to derive *zero-temperature* Dyson equations directly from the Hamiltonian (1). In Appendix A we generalize an unpublished calculation by A. Suna of the zero-temperature Dyson equations for a nonsuperconductor. We allow umklapp processes and introduce the Nambu-Gor'kov[26,27] formalism in order to derive Dyson equations applicable to the superconducting state as well as to the normal state.

With no further approximations we find a Dyson equation of the usual form for the generalized (in the Nambu-Gor'kov sense) single-particle electronic Green's function[14]

$$\mathbf{G}(k)=[\mathbf{G}_0^{-1}(k)-\mathbf{\Sigma}(k)]^{-1}. \tag{6}$$

Both the Green's function and the electronic self-energy

$$\mathbf{\Sigma}(k)=i\sum_{\mathbf{q}}\sum_{\mathbf{g}}\sum_{\mathbf{g}'} v(\mathbf{q}+\mathbf{g})\int_{-\infty}^{\infty}\frac{dq_0}{2\pi}\mathbf{M}(\mathbf{q}+\mathbf{g};\mathbf{k})\tau_3\mathbf{G}(k+q)\times\tau_3\mathbf{\Gamma}(k,q;\mathbf{g}')K_{\mathbf{g}'\mathbf{g}}(q)\exp(iq_0 0^{\pm}) \tag{7}$$

can be expressed as a sum of direct products of the matrices

$$\tau_1=\begin{pmatrix}0&1\\1&0\end{pmatrix},\quad \tau_2=\begin{pmatrix}0&i\\-i&0\end{pmatrix},\quad \tau_3=\begin{pmatrix}1&0\\0&-1\end{pmatrix},$$

and $$\tau_4=\begin{pmatrix}1&0\\0&1\end{pmatrix}$$

in Nambu spin space with matrices whose row and column indices l and l' denote different electronic bands. The infinitesimal time $0^{\pm}$ is 0^+ for the 1, 1 and 1, 2 elements of any matrix in τ space and is 0^- for the 2, 1 and 2, 2 elements. The noninteracting single-particle Green's function

$$\mathbf{G}_0(k)=\{[k_0(1+i0^+)]\mathbf{1}\tau_4-\mathbf{\varepsilon}(\mathbf{k})\tau_3\}^{-1} \tag{8}$$

is diagonal in both τ space and l space.

The equation for the total electron-electron interaction propagator also assumes the usual form

$$\mathbf{K}(q)=[\mathbf{1}-\mathbf{P}_e(q)-\mathbf{P}_{ph}(q)]^{-1} \tag{9}$$

upon defining the polarizabilities

$$[\mathbf{P}_e(q)]_{\mathbf{g}\mathbf{g}'}=-iv(\mathbf{q}+\mathbf{g})\sum_{\mathbf{k}}\int_{-\infty}^{\infty}\frac{dk_0}{2\pi}\mathrm{Tr}\{\mathbf{M}(\mathbf{q}+\mathbf{g};\mathbf{k})\times\mathbf{G}^{11}(k+q)\mathbf{\Gamma}^{11}(k,q;\mathbf{g}')\mathbf{G}^{11}(k)\}\exp(ik_0 0^+)$$
$$\equiv[\mathbf{1}-\boldsymbol{\kappa}(q)]_{\mathbf{g}\mathbf{g}'}, \tag{10}$$

and

$$\mathbf{P}_{ph}(q)=\mathbf{1}-\mathbf{A}_0^{-1}(q), \tag{11}$$

where the tensor $\mathbf{A}_0(q)$ has matrix elements

$$[\mathbf{A}_0(q)]_{\mathbf{g}\mathbf{g}'}=\delta_{\mathbf{g}\mathbf{g}'}+\sum_n\frac{\alpha_n^0(\mathbf{q}+\mathbf{g})\alpha_n^0(\mathbf{q}+\mathbf{g}')}{M_{n,q}v(\mathbf{q}+\mathbf{g}')[q_0^2-(\omega_n^0(\mathbf{q}))^2+i0^+]}. \tag{12}$$

Here the symbol "Tr" denotes "the trace of" and the superscripts 1, 1 denote matrix elements in τ space. The vertex function $\mathbf{\Gamma}$ is defined in the appendix; it reduces to the simple form

$$\mathbf{\Gamma}_0(k,q;\mathbf{g})=\tau_4\mathbf{M}^T(\mathbf{q}+\mathbf{g};\mathbf{k}) \tag{13}$$

in the Hartree approximation. Note that the term $\mathbf{P}_e$ does not represent a completely electronic contribution to the total polarizability, since Eq. (10) for $\mathbf{P}_e$ contains the vertex function $\mathbf{\Gamma}$ which in turn contains both Coulomb and phonon-induced corrections. However, ionic response is taken into account in $\mathbf{P}_e$ only insofar as it contributes to the response of the average electronic density $\langle\rho_q\rangle$ to the effective field $\mathbf{U}$ present in a crystal. Since the phonon contribution to $\mathbf{\Gamma}$ vanishes exactly in the Hartree approximation and is of order Θ_D/E_F or smaller to all orders of perturbation theory, the polarization $\mathbf{P}_e$ may be regarded as purely electronic in origin for the case of metals or, within the Hartree approximation, even for the case of semiconductors and semimetals.

In order to discuss the physical nature of the interaction propagator $\mathbf{K}(q)$ and to compare our Dyson equations (6)–(12) with those of other authors,[2–6] we write $\mathbf{K}(q)$ as the sum

$$\mathbf{K}(q)=\mathbf{K}_e(q)+\mathbf{K}_{ph}(q) \tag{14}$$

of an electronic contribution

$$\mathbf{K}_e(q)=\boldsymbol{\kappa}^{-1}(q) \tag{15}$$

and a phonon induced contribution

$$\mathbf{K}_{ph}(q)=\boldsymbol{\kappa}^{-1}(q)[\mathbf{A}_0(q)-\mathbf{1}][\mathbf{1}-\mathbf{P}_e(q)\mathbf{A}_0(q)]^{-1}. \tag{16}$$

Since the tensor $\mathbf{P}_e(q)\mathbf{A}_0(q)$ is separable in the sense that its matrix elements can be expressed in the form

$$[\mathbf{P}_e(q)\mathbf{A}_0(q)]_{\mathbf{g}\mathbf{g}'}=f_{\mathbf{g}}(q)f'_{\mathbf{g}'}(q), \tag{17}$$

[24] G. Baym, Ann. Phys. (N. Y.) **14**, 1 (1961).
[25] J. Schwinger, Proc. Natl. Acad. Sci. (U. S.) **37**, 452 (1951).
[26] Y. Nambu, Phys. Rev. **117**, 648 (1960).
[27] L. P. Gor'kov, Zh. Eksperim. i Teor. Fiz. **34**, 735 (1958) [English transl.: Soviet Phys.—JETP **7**, 505 (1958)].

Eq. (16) for $\mathbf{K}_{\rm ph}$ can be rewritten in the form

$$\mathbf{K}_{\rm ph}(q)=\boldsymbol{\kappa}^{-1}(q)[\mathbf{A}_0(q)-1]\times\left\{1+\frac{\mathbf{P}_e(q)[\mathbf{A}_0(q)-1]}{1-\mathrm{Tr}[\mathbf{P}_e(q)\mathbf{A}_0(q)]}\right\}\boldsymbol{\kappa}^{-1}(q)$$
$$=\sum_\nu \mathfrak{A}_\nu(\mathbf{q})\{M_{\nu,q}[q_0^2-\omega_\nu^2(\mathbf{q})]\}^{-1}, \quad (18)$$

where the interaction matrix $\mathfrak{A}_\nu(\mathbf{q})$ has elements

$$[\mathfrak{A}_\nu(\mathbf{q})]_{\mathbf{g}\mathbf{g}'}=\alpha_\nu(\mathbf{q}+\mathbf{g})\alpha_\nu(\mathbf{q}+\mathbf{g}')/v(\mathbf{q}+\mathbf{g}'). \quad (19)$$

Here the $\alpha_\nu(\mathbf{q}+\mathbf{g})$ are screened pseudopotentials of the form

$$\sum_{\mathbf{g}'}[\boldsymbol{\kappa}^{-1}(q)]_{\mathbf{g}\mathbf{g}'}\alpha_\nu{}^0(\mathbf{q}+\mathbf{g}'),$$

where the phonon indices ν refer to the hybridized modes of the properly renormalized phonons; the $\omega_\nu(\mathbf{q})$ are renormalized, experimentally observable phonon frequencies.

Note that neither the poles of the diagonal elements of the phonon Green's function $\mathbf{D}(q)$ found in the appendix nor the zeroes of the diagonal elements of $\mathbf{D}^{-1}(q)$ give the proper renormalized phonon frequencies $\omega_\nu(\mathbf{q})$. Just as the electron-electron interaction introduces nonzero off-diagonal matrix elements into the electronic self-energy $\xi(\mathbf{k})$ and thus causes hybridization between electronic bands, the electron-phonon interaction introduces nonzero off-diagonal elements into the phonon self-energy matrix $\boldsymbol{\pi}(q)$, and thus causes hydridization between different phonon modes. This hydridization has two principal effects: (1) it splits the phonon frequencies apart, in simple crystals increasing the longitudinal frequencies and decreasing the transverse frequencies, and (2), in general, it decreases the value of the pseudopotential $\alpha_\nu(\mathbf{q}+\mathbf{g})$ for longitudinal phonons and increases its value for transverse phonons in such a way that the sum

$$\sum_\nu[\alpha_\nu{}^0(\mathbf{q}+\mathbf{g})]^2=\sum_n[\alpha_n{}^0(\mathbf{q}+\mathbf{g})]^2$$

is invariant. The renormalized phonon frequencies $\omega_\nu(\mathbf{q})$ are most easily found from the equation

$$\mathrm{Tr}[\mathbf{P}_e(\mathbf{q},\omega_\nu(\mathbf{q}))\mathbf{A}_0(\mathbf{q},\omega_\nu(\mathbf{q}))]=1, \quad (20)$$

which determines the poles of $\mathbf{K}_{\rm ph}(q)$ in Eq. (18), but may also be found by calculating the eigenvalues of $\mathbf{D}(q)$ from the Appendix.[28,29] The pseudopotentials $\alpha_\nu(\mathbf{q}+\mathbf{g})$ can be obtained either from Eq. (18) or from Eqs. (A43)–(A48) for $\mathbf{D}(q)$, but only with difficulty.

So far we have made no approximations other than those embodied in our Hamiltonian (1); we have found a set of Dyson equations for the interacting electrons and phonons of a crystal which is exact within the harmonic approximation for our crystal lattice and within the approximation of a local pseudopotential. However, our Dyson equations contain two unknowns other than the electronic Green's functions $\mathbf{G}(k)$: (1) the dielectric tensor $\boldsymbol{\kappa}(q)$ and (2) the vertex function $\boldsymbol{\Gamma}(k,q;g)$. In order to determine $\mathbf{G}(k)$ one must adopt some approximation scheme for the evaluation of $\boldsymbol{\kappa}$ and $\boldsymbol{\Gamma}$. Considering first the vertex function $\boldsymbol{\Gamma}$, one finds

$$\boldsymbol{\Gamma}(k,q;\mathbf{g})=-\tau_3(\delta/\delta U(\mathbf{q}+\mathbf{g};q_0))\mathbf{G}^{-1}(\mathbf{k}+\mathbf{q},\mathbf{k};k_0)$$
$$=\mathbf{M}^T(\mathbf{q}+\mathbf{g};\mathbf{k})+\tau_3(\delta/\delta U(\mathbf{q}+\mathbf{g};q_0))\boldsymbol{\Sigma}(\mathbf{k}+\mathbf{q},\mathbf{k};k_0), \quad (21)$$

where $U(\mathbf{q}+\mathbf{g};q_0)$ and $\mathbf{G}(\mathbf{k}',\mathbf{k};k_0)$ are the Fourier transform of $U(\mathbf{q}+\mathbf{g},t)$ and $\mathbf{G}(\mathbf{k}',\mathbf{k};t,0)$ with sources present, and where the self-energy $\boldsymbol{\Sigma}$ is an integral over dk_0' of products of the form $GK\Gamma$. It is then obvious that the term $K\Gamma(\delta G/\delta U)$ provides the only contribution of order less than e^4 to

$$\delta\Sigma/\delta U\sim K\Gamma(\delta G/\delta U)+G\Gamma(\delta K/\delta U)+GK(\delta\Gamma/\delta U). \quad (22)$$

Thus, it is not difficult to find an approximate expression for $\boldsymbol{\Gamma}$ which is simple in form, is valid up to order e^4, and includes exchange effects. However, one can determine the Green's function $\mathbf{G}(k)$ easily only by neglecting all vertex corrections or by including them phenomenologically. Moreover, the expansion of $\boldsymbol{\Gamma}$ as a power series in e^2 or r_s can be formally justified only in a high-density electron gas, and not in most real metals.

Were one actually to expand $\boldsymbol{\Gamma}$ as a power series in e^2 (or r_s) as discussed above, one could then also expand the dielectric tensor $\boldsymbol{\kappa}(q)$ as a power series. However, here we use simply the Hartree approximation $\boldsymbol{\Gamma}_0$ to $\boldsymbol{\Gamma}$ and derive as a simple example the random-phase-approximation (RPA) formula for $\boldsymbol{\kappa}_0\simeq\boldsymbol{\kappa}$. The substitution of Eq. (13) into Eq. (10) yields the expression

$$\kappa_{\mathbf{g}\mathbf{g}'}(\mathbf{q})\simeq 1+iv(\mathbf{q}+\mathbf{g})\sum_{\mathbf{k}}\int_{-\infty}^{\infty}\frac{dk_0}{2\pi}\exp(ik_0 0^+)\times\mathrm{Tr}[\mathbf{M}(\mathbf{q}+\mathbf{g};\mathbf{k})\mathbf{G}^{11}(k+q)\times\mathbf{M}^T(\mathbf{q}+\mathbf{g}';\mathbf{k})\mathbf{G}^{11}(k)]. \quad (23)$$

Approximating $\mathbf{G}^{11}(k)$ and $\mathbf{G}^{11}(k+q)$ by the noninteracting Green's functions $\mathbf{G}_0{}^{11}(k)$ and $\mathbf{G}_0{}^{11}(k+q)$ in Eq. (23) and performing a contour integration around the upper half-plane, we find the RPA or self-consistent-field (SCF) result

$$\boldsymbol{\kappa}_0(\mathbf{q},q_0)=\boldsymbol{\kappa}_0{}^*(\mathbf{q},-q_0)=1+\mathfrak{T}(\mathbf{q},q_0). \quad (24)$$

The susceptibility tensor $\mathfrak{T}$ is equal to the SCF susceptibility $\mathbf{T}$ given by Wiser[30] for energies $q_0<0$ and

[28] Note that the frequencies $\omega_\nu(\mathbf{q})$ are essentially the same in the superconducting state as in the normal state, as was first pointed out [within the context of the Frohlich model (Ref. 29)] by Eliashberg (Ref. 2).

[29] H. Frohlich, Proc. Phys. Soc. (London) **A63**, 778 (1950).

[30] N. Wiser, Phys. Rev. **129**, 62 (1963).

is equal to $\mathbf{T}^*$ for positive energies; its components are

$$\mathfrak{T}_{gg'}(q)=-v(\mathbf{q}+\mathbf{g})\sum_{\mathbf{k}}\sum_{l}\sum_{l'}M_{ll'}(\mathbf{q}+\mathbf{g};\mathbf{k})\times M_{ll'}(\mathbf{q}+\mathbf{g}';\mathbf{k})[f(\epsilon_{l'}(\mathbf{k}+\mathbf{q}))-f(\epsilon_l(\mathbf{k}))]/[\epsilon_{l'}(\mathbf{k}+\mathbf{q})-\epsilon_l(\mathbf{k})-q_0(1+i0^+)], \quad (25)$$

where $f(\epsilon)$ is the Fermi function. Thus, our approximation (24) to the dielectric tensor is equivalent to the SCF microscopic longitudinal dielectric function derived earlier by Adler[31] and by Wiser.[30] For a free-electron gas, our tensor expression (24) for the dielectric function reduces to the simple scalar form

$$\kappa_0(q)=1-v(\mathbf{q})\sum_{\mathbf{k}}[f(\epsilon(\mathbf{k}+\mathbf{q}))-f(\epsilon(\mathbf{k}))]/[\epsilon(\mathbf{k}+\mathbf{q})-\epsilon(\mathbf{k})-q_0(1+i0^+)], \quad (26)$$

which is simply related to the RPA and SCF result derived by Lindhard,[32] Hubbard,[33] Nozieres and Pines[34] and Ehrenreich and Cohen.[35] The reader should consult the literature[32–36] for a discussion of the validity of the RPA dielectric function and to find calculations of higher order corrections to the dielectric function; we have calculated κ_0 merely to illustrate the solution of the Dyson equations (6)–(10) in a simple approximation and to make our discussion of the electron-electron interaction propagator $\mathbf{K}(q)$ more specific.

III. THREE-DIMENSIONAL INTEGRAL EQUATIONS FOR THE ANISOTROPIC SUPERCONDUCTING ENERGY GAP $\mathbf{\Delta}(k)$

In this section we first show that the Dyson equations (6) and (7) of Sec. II represent a set of coupled integral equations from which, in principle, one can determine the superconducting energy gap $\mathbf{\Delta}(k)$.[37] Then, the solution of Eqs. (6) and (7) is discussed, under the assumption that the matrix elements $M_{ll'}(\mathbf{q}+\mathbf{g};\mathbf{k})$, the vertex function $\mathbf{\Gamma}$, and the interaction propagator $\mathbf{K}(q)$ all are known within some approximation. The energy gap $\mathbf{\Delta}(k)$ is defined and Eqs. (6) and (7), which represent a set of four coupled, four-dimensional integral equations for the components of $\mathbf{\Sigma}$ and $\mathbf{G}$, are shown to yield two uncoupled, approximate, three-dimensional integral equations which determine $\mathbf{\Delta}(k)$. All errors introduced by approximations in the derivation of these equations for $\mathbf{\Delta}$ are discussed; where possible, they are also estimated numerically as percentage errors in the determination of $\mathbf{\Delta}$.

Upon following Nambu[26] and Gor'kov[27] (or Schrieffer[6]) and expressing the electronic self-energy

$$\mathbf{\Sigma}(k)=[\mathbf{1}-\mathbf{Z}(k)]k_0\tau_4+\chi(k)\tau_3+\phi(k)\tau_1+\hat{\phi}(k)\tau_2 \quad (27)$$

as a linear combination of the linearly independent τ_i, the interpretation of Eqs. (6) and (7) as energy-gap equations becomes obvious. Then, the substitution of Eqs. (8) and (27) into Dyson's equation (6) immediately yields the result

$$\begin{aligned}\mathbf{G}(k)=&[\mathbf{Z}(k)k_0\tau_4+\xi(k)\tau_3+\phi(k)\tau_1+\hat{\phi}(k)\tau_2]\\&\times\{[\mathbf{Z}^2(k)k_0^2-\mathbf{E}^2(k)+i0^+\mathbf{1}]\tau_4\\&+k_0[\mathbf{Z}(k),\xi(k)\tau_3+\phi(k)\tau_1+\hat{\phi}(k)\tau_2]\\&+i[\xi(k),\hat{\phi}(k)\tau_2-\phi(k)\tau_1]+i[\phi(k),\hat{\phi}(k)]\tau_3\}^{-1}\\=&\{[\mathbf{Z}^2(k)k_0^2-\mathbf{E}^2(k)+i0^+\mathbf{1}]\tau_4\\&-k_0[\mathbf{Z}(k),\xi(k)\tau_3+\phi(k)\tau_1+\hat{\phi}(k)\tau_2]\\&-i[\xi(k),\hat{\phi}(k)\tau_2-\phi(k)\tau_1]-i[\phi(k),\hat{\phi}(k)\tau_3]\}^{-1}\\&\times[\mathbf{Z}(k)k_0\tau_4+\xi(k)\tau_3+\phi(k)\tau_1+\hat{\phi}(k)\tau_2],\end{aligned} \quad (28)$$

where the eigenvalues of the matrices,

$$\xi(k)=\varepsilon(k)+\chi(k) \quad (29)$$

and

$$\mathbf{E}(k)=[\xi^2(k)+\phi^2(k)+\hat{\phi}^2(k)]^{1/2}, \quad (30)$$

give the partially renormalized normal-state energies ξ_l and superconducting-state energies E_l corresponding to the bare electronic energies $\epsilon_l\equiv\epsilon_{ll}$. The substitution of Eqs. (27) and (28) into Eq. (7) now clearly demonstrates that Eqs. (6) and (7) represent a set of four coupled integral equations for ϕ, $\hat{\phi}$, $\mathbf{Z}$, and χ. Furthermore, in the case that the commutators $[\mathbf{Z}(k),\xi(k)]$, $[\mathbf{Z}(k),\phi(k)]$, and $[\mathbf{Z}(k),\hat{\phi}(k)]$ vanish, an examination of the form of Eqs. (28)–(30) readily shows that the fully renormalized normal-state and superconducting-state energy tensors are ξZ^{-1} and EZ^{-1}, so that

$$\mathbf{\Delta}(k)=[\phi^2(k)+\hat{\phi}^2(k)]^{1/2}\mathbf{Z}^{-1}(k) \quad (31)$$

must be the proper renormalized energy-gap tensor. The nonvanishing commutators of $\mathbf{Z}$, ξ, ϕ, and $\hat{\phi}$ in the denominators of Eq. (28) present the first important difficulty, which arises in particular from the replacement of the jellium model by the more realistic model of a periodic lattice of ions with a local electron-ion pseudopotential. Fortunately, the nonvanishing of

---

[31] S. L. Adler, Phys. Rev. **126**, 413 (1962)

[32] J. Lindhard, Kgl. Danske Videnskab. Selskab, Mat. Fys. Medd. **28**, 8 (1954).

[33] J. Hubbard, Proc. Phys. Soc. (London) **A68**, 976 (1955).

[34] P. Nozieres and D. Pines, Nuovo Cimento **9**, 470 (1958).

[35] H. Ehrenreich and M. Cohen, Phys. Rev. **115**, 786 (1959).

[36] J. Hubbard, Proc. Roy. Soc. (London) **A240**, 539 (1957); **A243**, 336 (1957); D. F. Dubois, Ann. Phys. (N.Y.) **7**, 174 (1959); **8**, 24 (1959); A. J. Glick and R. A. Ferrell, *ibid.* **11**, 359 (1960); A. J. Glick *ibid.* **17**, 61 (1962); Phys. Rev. **129**, 1399 (1963); S. Misawa, Progr. Theoret. Phys. (Kyoto) **30**, 780 (1963); D. Pines, *The Many Body Problem* (W. A. Benjamin, Inc., New York, 1961); in *Lectures on the Many-Body Problem, Naples, 1960*, edited by E. Caianiello (Academic Press Inc., New York, 1962). The dielectric function $\kappa(q)$ is also discussed briefly in Ref. 6 and in the following books: D. Pines, *Elementary Excitations in Solids* (W. A. Benjamin, Inc., New York, 1964); P. Nozieres, *Interacting Fermi Systems* (W. A. Benjamin, Inc., New York, 1964); T. D. Schultz, *Quantum Field Theory and the Many-Body Problem* (Gordon and Breach, Science Publishers, Inc., New York, 1964); and C. Kittel, *Quantum Theory of Solids* (John Wiley & Sons, Inc., New York, 1963).

[37] As discussed below, the mathematics involved becomes intractable in the most general case of a clean, anisotropic superconductor. However, we *are* able to treat a very general case which includes all known cases of experimental interest except for the case of superconductivity in clean transition metals, which will be discussed by the author in the third paper of this series.

these commutators may be neglected in most applications. The calculation of superconducting properties in the "dirty" limit in which all anisotropies vanish is particularly simple; in this case the matrices $\mathbf{Z}$, ξ, ϕ, and $\hat{\phi}$ become simply scalar functions of the two variables ϵ and k_0, as is discussed briefly in Sec. IV, and their commutators vanish identically. A second simple case is that of a nearly-free-electron metal whose constant-energy surfaces are very nearly spherical when viewed in an extended-zone scheme, except possibly for small regions in $\mathbf{k}$ space away from the Fermi surface. Here, even when interested in any small anisotropy effects, one may again express $\mathbf{Z}$, ξ, ϕ, and $\hat{\phi}$ as scalar functions of $\epsilon(\mathbf{k})$ and k_0, as is also discussed briefly in Sec. IV. The commutators will also be small in any materials for which the interband matrix elements $M_{ll'}(\mathbf{q}+\mathbf{g};\mathbf{k})$ are small; they contribute only terms of order $[M_{ll'}(\mathbf{q}+\mathbf{g};\mathbf{k})]^2$ to any experimentally significant quantities. In the event that interband scatterings are important, that the nearly-free-electron approximation is not sufficiently good, and that one is concerned with the superconducting properties of a "clean" material, it is necessary to choose a simple two- or three-band model, use this model to determine $\mathbf{G}$ formally as a function $\sum_i \mathbf{G}^{(i)}\tau_i$ of $\mathbf{Z}$, ξ, ϕ, and $\hat{\phi}$, and then solve by iteration the resultant exceedingly complicated set of integral equations.[38]

Since this case is of interest only for a very few problems and has no general formal solution, we assume throughout the remainder of this paper that the commutators of $\mathbf{Z}$, ξ, ϕ, and $\hat{\phi}$ with one another either vanish identically or are negligibly small. Thus, we express the Green's function $\mathbf{G}(k)$ approximately as an anticommutator,

$$\mathbf{G}(k)\cong\tfrac{1}{2}\{[\mathbf{Z}(k)k_0\tau_4+\xi(k)\tau_3+\phi(k)\tau_1+\hat{\phi}(k)\tau_2], [\mathbf{Z}^2(k)k_0^2-\mathbf{E}^2(k)+i0^+\mathbf{1}]^{-1}\}. \quad (28a)$$

This expression is exact in the limit that the commutators vanish, provides a reasonable first approximation to $\mathbf{G}$ for all cases in which the commutators do not vanish, and has the same simple formal structure as the corresponding Nambu-Gor'kov[26,27] Green's function for the jellium model.

The second important new difficulty arises from our inability to use the Migdal approximation[15] to eliminate the ϵ' dependence of the self-energy $\mathbf{\Sigma}(k')$ on the right-hand side of Eq. (7); it follows directly from our interest in band-structure effects. Were one to consider only interactions between states having energies ξ such that $N(\xi)$ is essentially constant,[39] no deviation from the law of corresponding states which arise from band-structure effects (as distinguished from strong-coupling effects) could possibly be obtained. On the other hand, the Migdal approximation is valid only if one considers solely interactions between states having energies ξ such that $N(\xi)$ is essentially constant.[39]

Thus those interactions in which we are most interested are precisely those which are important for large energy transfers $q_0\sim E_F$ and for the study of which the Migdal approximation is inapplicable, namely, the Coulomb interaction in metals and both the Coulomb interaction and the phonon-induced electron-electron interaction in degenerate semiconductors and semimetals.

Previous authors[2–6] have used the Migdal approximation to reduce the dimensionality of the integral equation (7); fortunately, we have found an alternative way to reduce its dimensionality which is valid even when the Migdal approximation breaks down. First, as have previous authors,[2–6] one notes that the wave vector $\mathbf{k}$ can be expressed as a function $\mathbf{k}(\hat{k},\epsilon_l)$ of the unit vector $\hat{k}$ and the bare electronic energy $\epsilon_l(\mathbf{k})$. Then, by approximating the renormalization energy $\chi_{ll}(\mathbf{k},k_0)$ by the function

$$\chi_{ll}^{(0)}(\mathbf{k})=\tfrac{1}{2}[\chi_{ll}(k,\xi_{ll}(\mathbf{k}))+\chi_{ll}(k,-\xi_{ll}(k))], \quad (32)$$

one may express $\mathbf{k}$ approximately as a function $\mathbf{k}(\hat{k},\xi_{ll})\equiv\mathbf{k}(\hat{k},\epsilon_{ll}+\chi_{ll}^{(0)})$ of the unit vector $\hat{k}$ and the renormalized energy $\xi_{ll}(\mathbf{k})$. This approximation, which allows one to eliminate the function χ from the equations for $\mathbf{Z}$, ϕ, and $\hat{\phi}$, is justified (1) by the weak dependence of $\chi(\mathbf{k},k_0)$ upon k_0, (2) by the fact that the dominant contributions to $\mathbf{Z}$, ϕ, and $\hat{\phi}$ come from poles in the complex ξ plane at (or very near) the points

$$\xi_{ll}=\pm(Z_{ll}^2(\mathbf{k},k_0)k_0^2-\phi_{ll}^2(\mathbf{k},k_0)-\hat{\phi}_{ll}^2(\mathbf{k},k_0), \cong\pm Z_{ll}(\mathbf{k},k_0)k_0\simeq\pm k_0,$$

and (3) by the weak dependence of $\mathbf{Z}$, ϕ, and $\hat{\phi}$ upon the argument ξ_{ll} of $\mathbf{k}(k,\xi_{ll})$.[40]

Next, one should go to a representation in which the renormalized normal-state energy tensor $\xi(k)$ is diagonal with eigenvalues $\xi_l\equiv\xi_{ll}$, define $\mathbf{k}'\equiv\mathbf{k}+\mathbf{q}$, replace the sum over $\mathbf{q}$ in Eq. (7) by an integral over angles $\int_\Omega d\hat{k}'$ and an integral over energy

$$\int_{-\infty}^{\infty} d\xi',$$

formally evaluate the integral over $d\xi'$ by contour integration, and then evaluate the integral over dk_0'. This procedure leads to the conclusion that all contributions to either $\mathbf{Z}$, ϕ, or $\hat{\phi}$ which arise from the

[38] This problem should arise only in the calculation of such complicated anisotropy effects as should undoubtedly exist in a clean superconducting transition metal. It should not arise in the calculation of anisotropy effects in the simple metals, which possess a nearly spherical Fermi surface.

[39] The condition that $N(\xi)$ be essentially constant for all values of ξ to be considered is obviously not the rigorously proper condition to use here. However, except in extremely pathological cases, it is equivalent to the proper condition that variations of the position in $\mathbf{k}$ space of the constant-energy surfaces $\xi(k)$ be negligible as ξ takes on all values to be considered. It is chosen here because of its simplicity and ease of physical interpretation.

[40] These justifications are discussed below.

nonvanishing of the off-diagonal elements of $\mathbf{E}^2$ in the denominator of Eq. (28a) are of order

$$[\phi^2(k')+\hat{\phi}^2(k')]/[\xi_{l'}(\mathbf{k}')-\xi_l(\mathbf{k}')]^2\lesssim 10^{-5},$$

and may thus be neglected. To be consistent with our neglect of the commutators which appear in Eq. (7), we also neglect the small off-diagonal elements[41] of $\mathbf{Z}$ and rewrite Eq. (7) in the form

$$\begin{aligned}\boldsymbol{\Sigma}_{ll'}(k)&\equiv\boldsymbol{\Sigma}_{ll'}(l,\hat{k},\xi_l;k_0)=\boldsymbol{\Sigma}_{ll'}(l',\hat{k},\xi_{l'};k_0)\\&\simeq\frac{i}{2}\sum_{l''}\sum_{l'''}\sum_{l_1=l'',l'''}\int_{-\infty}^{\infty}\frac{dk_0}{(2\pi)^4}\int_{\Omega}d^2\hat{k}'\int_{-\infty}^{\infty}d\xi'\\&\times[\mathbf{Z}'k_0'\boldsymbol{\tau}_4-\boldsymbol{\xi}'\boldsymbol{\tau}_3-\boldsymbol{\phi}'\boldsymbol{\tau}_1-\hat{\boldsymbol{\phi}}'\boldsymbol{\tau}_2]_{l''l'''}\\&\times\mathfrak{K}(\xi')/[\mathbf{Z}'^2k_0'^2-\mathbf{E}'^2+i0^+\mathbf{1}]_{l_1l_1}.\end{aligned}\tag{33}$$

Here, for notational simplicity, we have defined $\mathbf{Z}'\equiv\mathbf{Z}(l_1,\hat{k}',\xi';k_0')$, $\boldsymbol{\phi}'\equiv\boldsymbol{\phi}(l_1,\hat{k}',\xi';k_0')$, $\hat{\boldsymbol{\phi}}'\equiv\hat{\boldsymbol{\phi}}(l_1,\hat{k}',\xi'\ k_0')$, and $\mathbf{E}'\equiv\mathbf{E}(l_1,\hat{k}',\xi';k_0')$ and have introduced the kernel

$$\begin{aligned}\mathfrak{K}(\xi')&\equiv\mathfrak{K}(l,l';\hat{k},\xi_l;l'',l''';l_1,\hat{k}',\xi';q_0)\\&=[|\mathbf{k}'|^2(d\xi'/d|\mathbf{k}'|)^{-1}]_{\mathbf{k}'=\mathbf{k}(l_1,\hat{k},\xi')}\\&\times\sum_{\mathbf{g}}\sum_{\mathbf{g}'}v(\mathbf{q}+\mathbf{g}')M_{ll'}(\mathbf{q}+\mathbf{g}';\mathbf{k})\\&\times\boldsymbol{\Gamma}_{l''l'''}(k,q;\mathbf{g})K_{\mathbf{g}\mathbf{g}'}(q).\end{aligned}\tag{34}$$

Since both the ξ' path of integration and the dependence upon ξ' of the kernel $\mathfrak{K}(\xi')$ can be sufficiently well determined independently of any knowledge of the energy $\mathrm{Re}\{\chi(k)\}$, as is discussed in Ref. 42, it is never necessary in practice to solve Eq. (33) for $\mathrm{Re}\chi$.

Now, noting that the kernel

$$\mathfrak{K}(\xi)\equiv\sum_i\mathfrak{K}^{(i)}(\xi)\boldsymbol{\tau}_i\tag{35}$$

is a matrix in τ space owing to the matrix character of the vertex function

$$\boldsymbol{\Gamma}\equiv\sum_i\boldsymbol{\Gamma}^{(i)}\boldsymbol{\tau}_i,\tag{36}$$

it is obvious that one can obtain energy-gap equations of the usual form[6] only by neglecting the terms $\boldsymbol{\Gamma}^{(1)}$, $\boldsymbol{\Gamma}^{(2)}$, and $\boldsymbol{\Gamma}^{(3)}$ and approximating $\boldsymbol{\Gamma}$ by the single term $\boldsymbol{\Gamma}^{(4)}\boldsymbol{\tau}_4$. Although any detailed discussion or justification of this approximation is beyond the scope of this paper, it is at least necessary to discuss it briefly. The first term in the expansion of $\boldsymbol{\Gamma}=\sum_n\boldsymbol{\Gamma}_n$ as a power series in e^2 or r_s (the Hartree approximation $\boldsymbol{\Gamma}_0$) is given by Eq. (13); the second term $\boldsymbol{\Gamma}_1$ is given by Eqs. (7), (21), and (22):

$$\begin{aligned}\boldsymbol{\Gamma}_1(k,q;\mathbf{g})&=i\sum_{\mathbf{q}'}\sum_{\mathbf{g}'}\sum_{\mathbf{g}''}\int_{-\infty}^{\infty}\frac{dq_0'}{2\pi}\mathbf{M}(\mathbf{q}'+\mathbf{g}'';\mathbf{k}+\mathbf{q})\\&\times\mathbf{G}(k+q+q')\boldsymbol{\tau}_3\boldsymbol{\Gamma}_0(k+q',q;\mathbf{g})\mathbf{G}(k+q')\\&\times\boldsymbol{\tau}_3\boldsymbol{\Gamma}_0(k,q';\mathbf{g}')v(\mathbf{q}'+\mathbf{g}'')K_{\mathbf{g}'\mathbf{g}''}(q')\exp(iq_00^{\pm}).\end{aligned}\tag{37}$$

The first term has the desired simple form $\boldsymbol{\Gamma}_0=\boldsymbol{\Gamma}_0^{(4)}\boldsymbol{\tau}_4$, and, by the Migdal theorem, the phonon contribution to the second term and all subsequent terms must be of order $(m/M)^{1/2}$ for metals. One can argue from these two observations alone that $\boldsymbol{\Gamma}^{(1)}$, $\boldsymbol{\Gamma}^{(2)}$, and $\boldsymbol{\Gamma}^{(3)}$ must be small in the superconducting simple metals such as aluminium, lead, or tin. Since these metals are fairly well described within the high-density limit, the corrections to the Hartree approximation $\boldsymbol{\Gamma}_0$ should be small. Moreover, both theoretical calculations[16,42,43] and experimental evidence[44–46] suggest that the Coulomb contributions to $\mathbf{Z}$, $\boldsymbol{\phi}$, and $\hat{\boldsymbol{\phi}}$ should be small.

A study of the form of Eq. (37) suggests that $\boldsymbol{\Gamma}^{(1)}$, $\boldsymbol{\Gamma}^{(2)}$, and $\boldsymbol{\Gamma}^{(3)}$ should be small even for the cases of degenerate semiconductors or semimetals and of transition metals, and reinforces the rather naive arguments mentioned above. Let us substitute Eq. (37) for $\boldsymbol{\Gamma}_1$ into Eqs. (33) and (34) and observe the relative magnitude of the four contributions to $\boldsymbol{\Sigma}$ arising from the four $\boldsymbol{\Gamma}_1^{(i)}$, respectively. In calculating the contribution of $\boldsymbol{\Gamma}_1^{(4)}$ to $\boldsymbol{\Sigma}$, one finds only a very small degree of cancellation upon integrating over dq_0', except for large values of q_0 [q_0^2 greater than some typical important value of $(k_0+q_0')^2$]. However, when calculating the contribution of $\boldsymbol{\Gamma}_1^{(1)}$, $\boldsymbol{\Gamma}_1^{(2)}$, or $\boldsymbol{\Gamma}_1^{(3)}$ to $\boldsymbol{\Sigma}$, one finds a high degree of cancellation for all values of q_0 upon integrating over dq_0'.[47] Therefore, the terms $\boldsymbol{\Gamma}_1^{(1)}$, $\boldsymbol{\Gamma}_1^{(2)}$, and $\boldsymbol{\Gamma}_1^{(3)}$ should be less important for the calculation of $\boldsymbol{\Sigma}$ than is the ordinary exchange term $\boldsymbol{\Gamma}_1^{(4)}$ which is in turn smaller than the Hartree term $\boldsymbol{\Gamma}_0$. Similar arguments will show that the terms $\boldsymbol{\Gamma}_n^{(i)}$ are small for $i=1$, 2, or 3 for any value of n. Thus, although

[41] Remember that $\mathbf{Z}$ is equal to the unit matrix $\mathbf{1}$ in the weak-coupling high-density limit, so that the off-diagonal elements of $\mathbf{Z}$ are small for two different reasons.

[42] J. W. Garland, Phys. Rev. (to be published).

[43] S. D. Silverstein, Phys. Rev. **128**, 631 (1963); **130**, 912 (1963); T. M. Rice, Ann. Phys. (N.Y.) **31**, 100 (1965).

[44] Since the Coulomb and phonon contributions to $\mathbf{Z}$ can be differentiated experimentally only through the determination of the Pauli paramagnetic spin susceptibility χ (see Ref. 45) which is difficult to measure, there is almost no direct experimental evidence of the size of the Coulomb contribution to $\mathbf{Z}$. However, the experimentally observed coefficients $\mathfrak{z}=0.5$ $(1-\zeta)$ of the isotope effect in superconductivity do show that the Coulomb contribution to the gap function $\boldsymbol{\phi}$ is small, particularly in the simple metals, as does the electron-tunneling data for lead (Ref. 46). See Ref. 42 for a discussion of this point and for references to the experimental determination of $\mathfrak{z}$.

[45] R. T. Schumacher and C. P. Slichter, Phys. Rev. **101**, 58 (1956); R. T. Schumacher and W. E. Vehse, Bull. Am. Phys. Soc. 4, 296 (1960); J. Phys. Soc. Japan Suppl. **B1**, 460 (1962).

[46] W. L. McMillan and J. M. Rowell, Phys. Rev. Letters **14**, 108 (1965).

[47] This cancellation is most effective in the case of the simple metals, for which the kernel $\mathfrak{K}(\xi')$ has only a very weak dependence on the energy ξ'. It arises from the integration over dq_0' of terms proportional to $\mathbf{G}^{(i)}(k+q+q')\mathbf{G}^{(4)}(k+q')\mathfrak{K}(q')$ or to $\mathbf{G}^{(4)}(k+q+q')\mathbf{G}^{(i)}(k+q')\mathfrak{K}(q')$, where $i\neq4$.

one cannot estimate the contributions to $\mathbf{\Sigma}$ of $\mathbf{\Gamma}^{(1)}$, $\mathbf{\Gamma}^{(2)}$, or $\mathbf{\Gamma}^{(3)}$ without extensive numerical calculations, one may state that their contributions are small and approximate the kernel $\mathfrak{K}(\xi')$ in Eq. (33) by its principal component $\mathfrak{K}(\xi')\tau_4 \equiv \mathfrak{K}^{(4)}(\xi')\tau_4$. This, in turn, allows us to set $\hat{\boldsymbol{\phi}} \equiv \mathbf{0}$ without any further loss of generality, simply by choosing phases appropriately, and to write

$$\mathbf{\Sigma}_{ll'}(k) = \frac{i}{2}\sum_{l''}\sum_{l'''}\sum_{l_1=l'',l'''}\int_{-\infty}^{\infty}\frac{dk_0'}{(2\pi)^4}\int_{\Omega}d^3\hat{k}'\int_{-\infty}^{\infty}d\xi' \times \mathfrak{K}(\xi')[\mathbf{Z}'k_0'\tau_4 - \xi'\tau_3 - \boldsymbol{\phi}'\tau_1]_{l''l'''}/ [\mathbf{Z}'^2k_0'^2 - \mathbf{E}'^2 + i0^+\mathbf{1}]_{l_1l_1}. \quad (33a)$$

It is now obvious, assuming particle-hole symmetry about the Fermi surface for small energies, that the only important contributions to χ are from interactions which involve large energy transfers. Thus, the dependence of χ upon k_0 must be weak, as was asserted above. Also the weak dependence of $\mathbf{\Sigma}$ upon ξ, which was also asserted above, is now apparent from the weak dependence of the kernel $\mathfrak{K}(l,l';\hat{k},\xi;l'',l''';l_1,\hat{k}',\xi';q_0)$ upon ξ.

Having reduced Eq. (7) to the much simpler form (33), which is valid whenever the matrices $\mathbf{Z}$ and $\boldsymbol{\phi}$ either reduce to scalar form or are nearly diagonal, and then having approximated $\mathfrak{K}(\xi)$ by its principal term $\mathfrak{K}(\xi)\tau_4$, we next proceed to simplify Eq. (33a) insofar as is possible without the introduction of further approximations. First, one follows the integration procedure of Eliashberg,[2] defining the kernel $\mathfrak{K}$ as the sum $\mathfrak{K}^u+\mathfrak{K}^l$ of parts analytic in the upper and lower halves, respectively, of the complex k_0' plane. One finds the matrix equation

$$\begin{bmatrix}\phi_{ll'}\\ (\delta_{ll'}-Z_{ll'})k_0\end{bmatrix} = \sum_{l''}\sum_{l'''}\sum_{l_1=l'',l'''}\int_{\Omega}d^2\hat{k}'\int_{-\infty}^{\infty}d\xi' \times\int_0^{\infty}\frac{dk_0'}{(2\pi)^4}\mathrm{Im}\left\{\{[\mathbf{Z}'^2k_0'^2-\mathbf{E}'^2+i0^+\mathbf{1}]_{l_1l_1}\}^{-1} \times\begin{pmatrix}\phi'_{l''l'''} & 0\\ 0 & Z'_{l''l'''}\end{pmatrix}\right\}\cdot\begin{pmatrix}\mathfrak{K}_+(\xi';k_0',k_0\\ \mathfrak{K}_-(\xi';k_0',k_0)\end{pmatrix}, \quad (38)$$

where the kernels $\mathfrak{K}_\pm$ are defined by the equation

$$\mathfrak{K}_\pm(\xi';k_0',k_0) = \mathfrak{K}^u(\xi';-k_0'-k_0) \pm \mathfrak{K}^l(\xi';k_0'-k_0). \quad (39)$$

Then in order to replace the ξ' integration of Eq. (38) by an easily evaluated contour integral, one may replace the functions $\mathfrak{K}$, $Z_{l''l'''}$ and $\phi'_{l''l'''}$ by functions of the form $\sum_j[(2\pi i)(\xi'-u_j-iv_j)]^{-1}\mathfrak{K}^{(j)}$,

$$\sum_j[(2\pi i)(\xi'-x_j(l'',l''')-iy_j(l'',l'''))]^{-1}Z'^{(j)}_{l''l'''},$$

and

$$\sum_j[(2\pi i)(\xi'-\eta_j(l'',l''')-i\gamma_j(l'',l'''))]^{-1}\phi'^{(j)}_{l''l'''},$$

which are analytic throughout the complex ξ' plane except for isolated simple poles at the points u_j+iv_j, x_j+iy_j, and $\eta_j+i\gamma_j$, respectively.[48] These replacements of $\mathfrak{K}$, $\mathbf{Z}$, and $\boldsymbol{\phi}$ by analytic functions of ξ' can be performed to any desired degree of accuracy along any path in the complex ξ' plane on which they are defined, even though $\mathfrak{K}$, $\mathbf{Z}'$, and $\boldsymbol{\phi}'$ themselves are nonanalytic functions of ξ'[49]; thus, these replacements can be considered formally as exact. It is this new technique of replacing $\mathfrak{K}$, $\mathbf{Z}'$, and $\boldsymbol{\phi}'$ by simple analytic functions of ξ' which ultimately allows us to reduce the dimensionality of Eq. (38).

If the ξ' dependence of $\boldsymbol{\phi}'$ and $\mathbf{Z}'$ were known, one could now immediately evaluate the ξ' integral of Eq. (38). However, neither is the ξ' dependence of $\boldsymbol{\phi}'$ and $\mathbf{Z}'$ known *a priori*, nor can it be totally neglected. In order to proceed further it is necessary to classify the different sets of contributions to $\mathbf{\Sigma}$ which one would obtain were one able to perform the ξ' integration. To obtain equations which display insofar as possible a simple relationship to the quasiparticle picture, it is best to evaluate the ξ' integral of Eq. (38) by performing contour integrations around both the upper and lower parts of the complex ξ' plane and then formally averaging the results. One finds contributions from several distinct sets of poles. The residues associated with the poles at

$$\xi' = \xi_s(l_1,\hat{k};k_0') \equiv s[Z_{l_1l_1}{}^2(l_1,\hat{k}',\xi_s;k_0')k_0'^2 - \phi_{l_1l_1}{}^2(l_1,\hat{k}',\xi_s;k_0')]^{1/2} \simeq s[Z_{l_1l_1}{}^2(l_1,\hat{k}',sk_0';k_0')k_0'^2 - \phi_{l_1l_1}{}^2(l_1,\hat{k}',sk_0';k_0')]^{1/2} \quad (40)$$

give the dominant contributions to superconductivity, where $s=\pm1$. Neglecting the ξ' dependence of $\mathbf{Z}'$, these poles very nearly give the standard quasiparticle results.[50] However, both the residues associated with the poles of the kernels $\mathfrak{K}^\pm$ and those associated with the poles of $\mathbf{\Sigma}'$ which arise from the ξ' dependence of $\boldsymbol{\phi}'$ and $\mathbf{Z}'$ contribute additional terms to the self-energy $\mathbf{\Sigma}$. Fortunately, by grouping terms properly[51] one can show that many of these contributions are negligible.

In order to study these contributions in a systematic manner, we label each contribution by a set of three indices i, j, and k, each of which can assume the values

[48] The positions of the points $u_j\pm iv_j$, $x_j\pm iy_j$, and $\eta_j\pm i\gamma_j$ of course depend upon all the arguments (except ξ') of the functions $\mathfrak{K}$, $Z'_{l''l'''}$, and $\phi'_{l''l'''}$, respectively, although they depend only weakly upon q_0 (or k_0').

[49] That these replacements can be performed to any desired degree of accuracy is a purely formal point. Of course, in principle, the path $\xi'=\epsilon'+\chi'$ is not given, since one must solve Eq. (33) for χ in order to find the path. However, since our results are nearly independent of the choice of path for any reasonable choice of path, as is shown in Ref. 42, it is sufficient to determine the path $\xi'=\epsilon'+\chi'$ within the quasiparticle approximation. See, for example, J. J. Quinn and R. A. Ferrell, Phys. Rev. **112**, 812 (1958).

[50] See Sec. IVC for a discussion of this point.

[51] Whenever poles in two different functions which are multiplied by one another become close together in the complex ξ' plane, the residues associated with each of the poles tend to become very large, although the sum of the residues remains approximately constant. Thus, such residues should always be grouped together.

zero or one. For all contributions arising from the poles of $\mathbf{G}$ at ξ_s, i assumes the value unity; for all other contributions, i assumes the value zero. For any contribution calculated under the assumption that $\boldsymbol{\phi}'(\xi')=\boldsymbol{\phi}'(0)$ and/or $\mathbf{Z}'(\xi')=\mathbf{Z}'(0)$, the indices j and/or k assume the value zero. For any contribution arising from the ξ' dependence of $\boldsymbol{\phi}'$ and/or $\mathbf{Z}'$, the indices j and/or k assume the value unity. We also define three characteristic energies for any superconductor: (1) the maximum superconducting energy gap Δ, (2) the maximum phonon frequency $\omega_{\rm ph}$, and (3) the largest energy ω_b such that the density of states $N_l(\xi)$ of any important band[52] remains essentially constant as ξ varies from $-\omega_b$ to $+\omega_b$.[39] If our results are to be sufficiently general to be applicable to the case of superconducting semiconductors and semimetals, we cannot neglect quantities of order $\omega_{\rm ph}/\omega_b$ as is customary.[2–6,53] However, we shall neglect quantities of order $\Delta/\omega_b \lesssim 0.01$ and terms of second and higher order in $\Delta/\omega_{\rm ph}\lesssim 0.1$.

Together, the four contributions to $\boldsymbol{\Sigma}$ denoted by the indices $(1,j,k)$ give a total contribution

$$\begin{pmatrix}\phi_{ll'}{}^{(1)}\\ [\delta_{ll'}-Z_{ll'}{}^{(1)}]k_0\end{pmatrix}=-\sum_{l''}\sum_{l'''}\sum_{l_1=l'',l'''}\sum_{s=\pm1}\int_0^\infty\frac{dk_0'}{4(2\pi)^3}$$
$$\times\int_\Omega d^2\hat{k}'\,\mathrm{Re}\left\{s\xi_s'^{-1}\begin{pmatrix}\phi'_{l''l'''}(\xi_s') & 0\\ 0 & Z'_{l''l'''}(\xi_s')k_0'\end{pmatrix}\right\}$$
$$\times\begin{pmatrix}\Re_+(\xi_s')\\ \Re_-(\xi_s')\end{pmatrix}. \quad (41)$$

The evaluation of the dominant (1,0,0) contribution does not require any knowledge of the ξ' dependence of $\boldsymbol{\phi}'$ or $\mathbf{Z}'$. The (1,1,0) contribution to $\boldsymbol{\phi}$ is a factor of order $\theta\lesssim 0.1$ smaller than the dominant contribution for any superconductor[54–56]; the (1,1,0) contribution to Z is of order 10^{-3} or less, and may be neglected. The sum of the remaining two $i=1$ contributions to $\boldsymbol{\Sigma}$ is even smaller than the (1,1,0) contribution to $\boldsymbol{\phi}$.[57]

The four $i=0$ contributions arising from the poles of $\Re^{\pm}$, $\boldsymbol{\phi}'$, and $\mathbf{Z}'$ in the complex ξ' plane are all very small. Two, the (0,0,0) and (0,1,0) contributions,

$$\begin{pmatrix}\phi_{ll'}{}^{(0,0,0)}\\ [\delta_{ll'}-Z_{ll'}]^{(0,0,0)}\end{pmatrix}=\sum_j\sum_{l''}\sum_{l'''}\sum_{l_1=l'',l'''}\int_0^\infty\frac{dk_0'}{(2\pi)^4}$$
$$\times\int_\Omega d^2\hat{k}'\,\mathrm{Im}\left\{[[\mathbf{Z}'(0)^2k_0'^2-(u_j+iv_j)^2\mathbf{1}-\boldsymbol{\phi}'(0)^2]_{l_1l_1}]^{-1}\right.$$
$$\left.\times\begin{pmatrix}\phi'_{l''l'''}(0) & 0\\ 0 & Z'_{l''l'''}(0)\end{pmatrix}\right\}\begin{pmatrix}\Re_+{}^{(j)}\\ \Re_-{}^{(j)}\end{pmatrix} \quad (42)$$

and

$$\begin{pmatrix}\phi_{ll'}{}^{(0,1,0)}\\ [\delta_{ll'}-Z_{ll'}]^{(0,1,0)}\end{pmatrix}\cong\sum_j\sum_{l''}\sum_{l'''}\sum_{l_1=l'',l'''}\int_0^\infty\frac{dk_0'}{(2\pi)^4}$$
$$\times\int_\Omega d^2\hat{k}'\Re_+(\eta_j+i\gamma_j)$$
$$\times\mathrm{Im}\left\{[[\mathbf{Z}'(0)^2k_0'^2-(\eta_j+i\gamma_j)^2\mathbf{1}]_{l_1l_1}]^{-1}\right.$$
$$\left.\times\begin{pmatrix}\phi'_{l''l'''}{}^{(j)}\\ 0\end{pmatrix}\right\}, \quad (43)$$

reduce to zero in the limit as the imaginary part of the kernel $\Re$ vanishes, since in this limit the contributions arising from the poles of $\Re$ and $\boldsymbol{\phi}'$ in the lower half of the complex ξ' plane cancel those arising from their poles in the upper half of the ξ' plane. They are approximately two orders of magnitude smaller than the dominant (1,0,0) contribution for the case of metals and approximately $1\frac{1}{2}$ orders of magnitude smaller for the case of superconducting semiconductors and semimetals. The sum of the reamining two contributions, which arise from the ξ' dependence of $\mathbf{Z}'$, is equally small; it cannot be expressed in simple form, and shall be neglected here.

In sum, we have found that the self-energy $\boldsymbol{\Sigma}$ of any material can be expressed as a sum of three contributions:

(1) a contribution $\boldsymbol{\Sigma}_0$ which contains both the dominant (1,0,0) contribution and the (1,1,0) contribution and which depends only upon the self-energy at the two points $\xi'=\xi_s'$, $s=\pm1$, for any given energy k_0', and which is equivalent to the quasiparticle contribution in the limit as $\mathbf{Z}-\mathbf{1}\to\mathbf{0}$.

(2) a contribution $\boldsymbol{\Sigma}_\phi$ which arises entirely from lifetime effects and vanishes in the limit as the imaginary parts of the energies ξ' and $\boldsymbol{\phi}'$ both vanish, and which ldepends upon $\boldsymbol{\phi}'(\xi')$ for all ξ', but which is very smal

[52] By "important band" we mean any band or subband whose existence directly influences the superconducting properties of a material to any important extent.

[53] L. P. Kadanoff, Lectures at the 1963 Spring School of Physics, Ravello, Italy (to be published).

[54] For metals θ is given approximately by the formula

$$\theta\sim(\omega_{\rm ph}/8\omega_b)+[8+2\ln(\omega_{\rm pl}/\omega_{\rm ph})]^{-1}\sim 0.05,$$

where $\omega_{\rm pl}$ is the electronic plasma frequency; for semiconductors and semimetals it is given approximately by the formula $\theta\sim[2\ln(\omega_{\rm ph}/\Delta)]^{-1}<0.1$. The factors of two and eight occurring in these expressions are obtained from highly approximate numerical calculations and cannot be explained in detail here. The factor of two arises from the fact that the change in the density of states $N(\xi)$ of hole states as ξ increases in the negative direction and the change in the density of states of electronic states as ξ increases in the positive direction tend to cancel in the calculation of $\boldsymbol{\Sigma}$. The factor of eight comes from this factor of two multiplied by a factor of four which corresponds roughly to the inverse of the kernel $\Re_e$ appropriate to the second step of the Tolmachev two-step-function model (Ref. 55) used by Swihart (Ref. 56), Morel and Anderson (Ref. 3), and the author (Refs. 16 and 42). The dependence of θ upon Δ, $\omega_{\rm ph}$, ω_b, and $\omega_{\rm pl}$ is readily seen.

[55] N. N. Bogoliubov, V. V. Tolmachev, and D. V. Shirkov, *A New Method in the Theory of Superconductivity* (Consultants Bureau Inc., New York, 1959), Sec. 6.3.

[56] J. C. Swihart, IBM J. Res. Develop. **6**, 14 (1962).

[57] For metals it is smaller by a factor of the order of the electronic contribution $[\delta_{ll'}-Z_{ll'}]_e\lesssim 0.3$ to the tensor $\mathbf{1}-\mathbf{Z}$; for semiconductors and semimetals it is smaller by a factor of order $|Z_{ll'}-\delta_{ll'}|$, also $\lesssim 0.3$.

and depends only upon $\mathbf{Z}'(0)$, not upon $\mathbf{Z}'(\xi')$ for all ξ', and

(3) a contribution $\mathbf{\Sigma}_Z$ which depends upon $\mathbf{Z}'(\xi')$ as well as upon $\boldsymbol{\phi}(\xi')$ for all ξ', but which is very small. For metals $\mathbf{\Sigma}_Z$ is nearly two orders of magnitude smaller than $\mathbf{\Sigma}_0$; for superconducting semiconductors or semimetals it is more than a factor of 10 smaller. This suggests that one should calculate the contribution $\mathbf{\Sigma}_0$ and if necessary then calculate the ξ dependence of $\boldsymbol{\phi}_0$ and use it to determine $\mathbf{\Sigma}_\phi$ approximately. One finds

$$[\boldsymbol{\phi}_0(\xi)]_{ll'}{}^{l_0l_0}=-\sum_{l''}\sum_{l'''}\sum_{l_1=l'',l'''}\sum_{s=\pm1}\int_0^\infty\frac{dk_0'}{4(2\pi)^3}\int_\Omega d^2\hat{k};$$
$$\times\left[\Re_+(sk_0'Z'(0))\,\mathrm{Re}\left\{\frac{[\boldsymbol{\phi}_0'(sk_0'Z'(0))]_{l''l'''}{}^{l_1}}{\{Z'(0)^2k_0'^2-[\boldsymbol{\phi}_0'(sk_0'Z'(0))]_{l_1l_1}{}^2\}^{1/2}}\right\}\right], \quad (44)$$

or, including lifetime effects properly,

$$\phi_{ll'}{}^{l_0l_0}(\xi)\cong-\sum_{l''}\sum_{l'''}\sum_{l_1=l'',l'''}\sum_{s=\pm1}\int_0^\infty\frac{dk_0'}{4(2\pi)^3}\int_\Omega d^2\hat{k}'\left[\Re_+(sk_0'Z'(0))\,\mathrm{Re}\left\{\frac{\phi'_{l''l'''}{}^{l_1}(sk_0'Z'(0))}{\{Z'(0)^2k_0'^2-\phi'_{l_1l_1}{}^2(sk_0'Z'(0))\}^{1/2}}\right\}\right.$$
$$\left.+\pi^{-1}\sum_j\Re_+{}^{(j)}\,\mathrm{Im}\left\{\frac{[\boldsymbol{\phi}_0'(u_j+iv_j)]_{l''l'''}{}^{l_1}}{(u_j+iv_j)^2-Z'(0)^2k_0'^2}\right\}+\pi^{-1}\sum_j\Re_+(\eta_j+i\gamma_j)\,\mathrm{Im}\left\{\frac{[\boldsymbol{\phi}_0'^{(j)}]_{l''l'''}{}^{l_1}}{(\eta_j+i\gamma_j)^2-Z'(0)^2k_0'^2}\right\}\right], \quad (45)$$

where we have defined $\phi_{ll'}{}^{l_0l_0}(\xi)\equiv\phi_{ll'}(l_0,\hat{k},\xi;k_0)$, $\phi'_{l''l'''}{}^{l_1}(\xi_1)=\phi_{l''l'''}(l_1\hat{k}',\xi';k_0')$, $\phi'_{l_1l_1}\equiv\phi'_{l_1l_1}{}^{l_1}$ and $\mathbf{Z}'(0)=[\mathbf{Z}'(0)]_{l_1l_1}$ for notational simplicity. For almost any case the difference between Eqs. (44) and (45) is negligible in the sense that uncertainties in the determination of the kernal $\Re_+$ are a more important source of error in Eq. (44) than is the neglect of the final two groups of terms in Eq. (45).

If one neglects the small contribution ϕ_Z, one may now further simplify the calculation of ϕ by eliminating the dependence of ϕ upon the function $Z'(0)$ in Eqs. (44) and (45). In order to do this one must first define the renormalized energy-gap functions

$$\Delta_{ll}(\xi)=\phi_{ll}(\xi)/Z_{ll}(0) \quad (46)$$

and

$$\Delta_{ll'}{}^{l_0l_0}(\xi)=\phi_{ll'}{}^{l_0l_0}(\xi)/Z_{l_0l_0}(0). \quad (47)$$

Then, rewriting Eqs. (44) and (45) in terms of these new functions, one finds

$$[\boldsymbol{\phi}_0(\xi)]_{ll'}{}^{l_0l_0}=Z_{ll}(0)[\boldsymbol{\Delta}_0]_{ll'}{}^{l_0l_0}$$
$$=-\sum_{l''}\sum_{l'''}\sum_{l_1=l'',l'''}\sum_{s=\pm1}\int_0^\infty\frac{dk_0'}{4(2\pi)^3}\int_\Omega d^2\hat{k}'\left[\Re_+(sk_0'Z'(0))\,\mathrm{Re}\left\{\frac{[\boldsymbol{\Delta}_0'(sk_0'Z'(0))]_{l''l'''}{}^{l_1}}{\{k_0'^2-[\boldsymbol{\Delta}_0'(sk_0'Z'(0))]_{l_1l_1}{}^2\}^{1/2}}\right\}\right] \quad (48)$$

and

$$\phi_{ll'}{}^{l_0l_0}(\xi)=-\sum_{l''}\sum_{l'''}\sum_{l_1=l'',l'''}\sum_{s=\pm1}\int_0^\infty\frac{dk_0'}{4(2\pi)^3}\int_\Omega d^2\hat{k}'\left[\Re_+(sk_0'Z'(0))\,\mathrm{Re}\left\{\frac{\Delta'_{l''l'''}{}^{l_1}(sk_0'Z'(0))}{\{k_0'^2-\Delta'_{l_1l_1}{}^2(sk_0'Z'(0))\}^{1/2}}\right\}\right.$$
$$\left.+\pi^{-1}\sum_j\Re_+{}^{(j)}\,\mathrm{Im}\left\{\frac{[\boldsymbol{\Delta}_0'(u_j+iv_j)]_{l''l'''}{}^{l_1}}{Z'^{-2}(0)(u_j+iv_j)^2-k_0'^2}\right\}+\pi^{-1}\sum_j\Re_+(\eta_j+i\gamma_j)\,\mathrm{Im}\left\{\frac{[\boldsymbol{\Delta}_0'^{(j)}]_{l''l'''}{}^{l_1}}{Z'^{-2}(0)(\eta_j+i\gamma_j)^2-k_0'^2}\right\}\right]. \quad (49)$$

Note (1) that the dominant terms in Eqs. (48) and (49) depend upon Z' only through the negligible dependence of $\Re_+(sk_0'Z'(0))\cong\Re_+(sk_0')$ and $\Delta(sk_0'Z'(0))\cong\Delta(sk_0')$ upon[58] $Z'(0)$ and (2) that the very small additional contributions to Δ in Eq. (49) arise from residues at poles far from the origin of the complex ξ' plane and thus depend only slightly on the value of $Z'(0)$, especially in the region of small k_0', where $Z'(0)$ differs most substantially from unity. This means that one may set $Z'(0)$ equal to unity throughout Eqs. (48) and (49) without introducing a total error greater than approximately 3% for the case of metals and 6% for the case of semiconductors and semimetals.[59]

[58] Since $Z'(0)$ is approximately unity for very large k_0', the quantity $|k_0'(Z'(0)-1)|$ is much less than E_F for $k_0'\lesssim E_F$ and much less than k_0' for $k_0'\gtrsim E_F$. Then, since $\Re(\xi')$ is a slowly varying function of ξ' approximately proportional to $(\xi'+E_F)^{1/2}$ for small ξ', $\Re(sk_0'Z'(0))$ is very nearly equal to $\Re(sk_0')$ for all k_0' (except for $sk_0'\simeq-E_F$). Furthermore, the errors introduced by setting $\Re(sk_0'Z'(0))$ equal to $\Re(sk_0')$ tend to cancel as one sums over $s=\pm1$.

[59] Of course the limits of error stated here refer to effective errors in the kernel $\Re$; i.e., to errors in the corresponding quantity $N(0)V=[\ln(2\omega_{\mathrm{ph}}/\Delta)]^{-1}$ for the simple BCS gap equation. Our limits of error do *not* refer to limits of error in the calculation of Δ, which is a nonlinear function of $\Re$. Furthermore, the limits of error quoted here include only those errors which result from the approximations employed in the derivation of Eqs. (47) and (58) from Eq. (33a). In particular, they do not include errors which result from our ignorance of the exact kernel $\Re$, from our approximation of the kernel $\Re$ by its principal component $\tau_4\Re^{(4)}$ or from the possible nonvanishing of the commutators of $\hat{\xi}$, $\mathbf{Z}$, $\boldsymbol{\phi}$, and $\hat{\boldsymbol{\phi}}$ with one another, since these errors vary greatly from case to case and cannot be estimated accurately. Nor do these limits include errors which in principle can be made to vanish, such as possible errors in the evaluation of the poles and residues of $\Re$ and $\boldsymbol{\phi}$ or in the numerical solution of integral equations.

We find the approximate equations

$$[\mathbf{\Delta}_0(\xi)]_{lv}{}^{l_0}\cong -Z^{-1}(0)\sum_{l''}\sum_{l'''}\sum_{l_1=l'',l'''}\sum_{s=\pm 1}\int_0^\infty \frac{dk_0'}{4(2\pi)^3}\int_\Omega d^2\hat{k}'\left[\Re_+(sk_0')\,\mathrm{Re}\left\{\frac{[\mathbf{\Delta}_0(sk_0')]_{l''l'''}{}^{l_1}}{\{k_0'^2-[\mathbf{\Delta}_0'(sk_0')]_{l_1l_1}{}^2\}^{1/2}}\right\}\right] \quad (48a)$$

and

$$\Delta_{lv}{}^{l_0}(\xi)\cong -Z^{-1}(0)\sum_{l''}\sum_{l'''}\sum_{l_1=l'',l'''}\sum_{s=\pm 1}\int_0^\infty \frac{dk_0'}{4(2\pi)^3}\int_\Omega d^2\hat{k}'\left[\Re_+(sk_0')\,\mathrm{Re}\left\{\frac{\Delta'_{l''l'''}{}^{l_1}(sk_0')}{\{k_0'^2-\Delta'_{l_1l_1}{}^2(sk_0')\}^{1/2}}\right\}\right.$$

$$\left.+\pi^{-1}\sum_j \Re_+{}^{(j)}\,\mathrm{Im}\left\{\frac{[\mathbf{\Delta}_0'(u_j+iv_j)]_{l''l'''}{}^{l_1}}{(u_j+iv_j)^2-k_0'^2}\right\}+\pi^{-1}\sum_j \Re_+(\eta_j+i\gamma_j)\,\mathrm{Im}\left\{\frac{[\mathbf{\Delta}_0'^{(j)}]_{l''l'''}}{(\eta_j+i\gamma_j)^2-k_0'^2}\right\}\right]. \quad (49a)$$

Finally, following a procedure similar to that of Kadanoff,[53] one can eliminate the dependence of Δ upon $Z(0)$ given by Eqs. (48a) and (49a), leaving an integral equation for Δ in which enither Z nor Z' appears. In order to do this, it is only necessary to write equations for $1-Z_0$ and $1-Z$ equivalent to Eqs. (48a) and (49a) for Δ_0 and Δ and then to substitute them into Eqs. (48a) and (49a). Since the quantity $Z-1$ arises largely from the exchange of virtual phonons and is small for large arguments k_0, andsince it is small in semiconductors and semimetals, any percentage error in the calculation of Z will be smaller than the corresponding error in the calculation of ϕ. Moreover, it is obvious from the form of Eqs. (48a) and (49a) that corresponding systematic errors in the calculation of Z and of ϕ tend to cancel in the determination of Δ. Thus, by eliminating Z from Eqs. (48a) and (49a) in this manner, we reduce our previously accumulated errors rather than enhancing them. We find

$$[\mathbf{\Delta}_0(\xi)]_{lv}{}^{l_0}\cong -\sum_{l''}\sum_{l'''}\sum_{l_1=l'',l'''}\sum_{s=\pm 1}\int_0^\infty \frac{dk_0'}{4(2\pi)^3}\int_\Omega d^2\hat{k}'$$

$$\times[\Re_+(sk_0')\,\mathrm{Re}\{[\mathbf{\Delta}_0']_{l''l'''}{}^{l_1}[k_0'^2-[\mathbf{\Delta}_0']_{l_1l_1}{}^2]^{-1/2}\}$$

$$-[k_0'/k_0][\mathbf{\Delta}_0(\xi)]_{lv}{}^{l_0}\Re_-(sk_0')\,\mathrm{Re}\{[k_0'^2-[\mathbf{\Delta}_0']_{l_1l_1}{}^2]^{-1/2}\}] \quad (50)$$

and

$$\Delta_{lv}{}^{l_0}(\xi)\cong -\sum_{l''}\sum_{l'''}\sum_{l_1=l'',l'''}\sum_{s=\pm 1}\int_0^\infty \frac{dk_0'}{4(2\pi)^3}\int_\Omega d^2\hat{k}'\{\Re_+(sk_0')\,\mathrm{Re}\{\Delta'_{l''l'''}{}^{l_1}[k_0'^2-\Delta'_{l_1l_1}{}^2]^{-1/2}\}$$

$$+\pi^{-1}\sum_j \Re_+{}^{(j)}\,\mathrm{Im}\{[\mathbf{\Delta}_0'(u_j+iv_j)]_{l''l'''}{}^{l_1}/[(u_j+iv_j)^2-k_0'^2]\}+\pi^{-1}\sum_j \Re_+(\eta_j+i\gamma_j)$$

$$\times\mathrm{Im}\{[\mathbf{\Delta}_0'^{(j)}]_{l''l'''}{}^{l_1}/[(\eta_j+i\gamma_j)^2-k_0'^2]\}-[k_0'/k_0][\Delta_{lv}{}^{l_0}(\xi)\Re_-(sk_0')Re\{[k_0'^2-\Delta'_{l_1l_1}{}^2]^{-1/2}\}$$

$$-2\sum_j u_jv_j\Re_-{}^{(j)}[(u_j{}^2+v_j{}^2)^2-2k_0'^2(u_j{}^2-v_j{}^2)+k_0'^4]^{-1}]\}, \quad (51)$$

where the kernels

$$\Re_+(\xi')\equiv\Re_+(l,l',\hat{k},\xi;l'',l''';l_1,\hat{k}',\xi';k_0',k_0)$$

and

$$\Re_-(\xi')\equiv\Re_-(l_0,l_0,\hat{k},\xi;l'',l''';l_1,\hat{k}',\xi';k_0',k_0)$$

have indices corresponding to the component indices l, l' of $\boldsymbol{\phi}$ and l_0, l_0 of $\mathbf{Z}$, respectively. These two equations are much easier in principle to solve than any of the preceding equations, because they contain no integral over $d\xi'$ and because the integrand of each equation contains only one unknown function, $\mathbf{\Delta}_0$ in Eq. (50) and $\mathbf{\Delta}$ in Eq. (51). Furthermore, these equations determine $\mathbf{\Delta}$ within an accuracy of 2 or 3% for the case of metals and better than 5% for the case of superconducting semiconductors and semimetals.[59]

IV. SOLUTION OF THE GAP EQUATION FOR DIRTY SUPERCONDUCTORS AND NEARLY ISOTROPIC SUPERCONDUCTORS

In this section we consider those cases in which the three-dimensional integral equations (50) and (51) can be reduced to one-dimensional form. Making reference to the simple physical arguments of Anderson,[19] which are supported by the more detailed, quantitative work of Markowitz and Kadanoff,[60] it is first shown that in the important dirty limit, both $\boldsymbol{\phi}$ and $\mathbf{Z}$ become simply scalar functions $\phi(\epsilon,k_0)$ and $Z(\epsilon,k_0)$ of the scalar variables ϵ and k_0. The reduction of Eqs. (50) and (51) to scalar form then becomes obvious. Next, an approximation scheme is presented for reducing Eqs. (50) and (51) to one-dimensional form in the case of clean but nearly isotropic superconductors. Fortunately, these two cases include almost all cases of interest: the case of dirty superconductors is applicable to almost all experimental results pertaining to the superconductivity of transition metals or degenerate semiconductors or semimetals; the case of nearly isotropic superconductors is applicable to all of the simple metals.

Finally, our one-dimensional equations are compared with the corresponding equations of Schrieffer[6] and with

[60] D. Markowitz and L. P. Kadanoff, Phys. Rev. 131, 563 (1963).

those derived previously by the author[16,17] in the random-phase approximation (RPA) using complex Bogoliubov quasiparticle transformations[61] and a generalization of the Englert effective Hamiltonian.[62] In this way, those results of our analysis which differ from previous results are isolated, so that they may be discussed further.

A. Dirty Superconductors

As was pointed out by Anderson,[19] one may divide superconductors into two classes: (1) the class of relatively pure superconductors for which scattering has a rather sharp effect on superconducting transition temperatures, and (2) the class of dirty superconductors for which additional scattering has very little effect.[63] The fundamental assumption of the Anderson theory is that for class (2) superconductors, the wave functions of the superconducting state are best constructed by first diagonalizing the interaction between the normal-state electrons and the impurity and imperfection-scattering centers, and then calculating the interaction between electrons. That is, one must first find a new set of one-electron wave functions $|\mu,\sigma\rangle$ to replace the standard Bloch functions $|l;\mathbf{k},\sigma\rangle$ for the electrons, and then consider the matrix elements of all interactions relative to these new wave functions.

Anderson observes that if $|\mu,\sigma\rangle$ is an exact one-electron wave function, then the time-reversed state $|\mu,\sigma\rangle^*$ is also an exact eigenfunction of the one-electron Hamiltonian in the absence of magnetic scattering. Furthermore, $|\mu,\sigma\rangle$ and $|\mu,\sigma\rangle^*$ have the same energy, $\epsilon(\mu)$. Since the interaction $V_{\mu\mu'}$ between states $|\mu,\sigma\rangle$ and $|\mu',\sigma\rangle$ is simply the average interaction over all states $|l;\mathbf{k},\sigma\rangle$ which make up the scattered state $|\mu,\sigma\rangle$, and since, for strong scattering, the states $|l;\mathbf{k},\sigma\rangle$ are taken more or less at random from the smeared out constant-energy surface $\epsilon_l(\mathbf{k})\cong\epsilon(\mu)$, the interaction $V_{\mu\mu'}$ is a function only of the energies $\epsilon(\mu)$ and $\epsilon(\mu')$.

Following Anderson, we write

$$|\mu,\sigma\rangle=\sum_l\sum_{\mathbf{k}}\sum_{\sigma'}(\mu,\sigma|l;\mathbf{k},\sigma')|l;\mathbf{k},\sigma'\rangle, \tag{52}$$

where the sum over $\mathbf{k}$ extends only over the first Brillouin zone. The assumption of perfectly random scattering yields the result

$$\sum_{\sigma'}|(\mu,\sigma|l;\mathbf{k},\sigma')|^2=\bar{\delta}(\epsilon(\mu)-\epsilon_l(\mathbf{k}))/N(\epsilon(\mu)), \tag{53}$$

which is accurate to order $\tau_s^{-1}(dN(\epsilon)/d\epsilon)_{\epsilon=\epsilon(\mu)}\ll 1$, where τ_s is an average scattering time for an electron of energy $\epsilon(\mu)$ and $\bar{\delta}$ is a spread-out delta function of approximate width τ_s^{-1}. Both this equation and the assumption that the coefficients $(\mu,\sigma|l;\mathbf{k},\sigma')$ have random phase should be valid in the region $\Delta\ll\tau_s^{-1}\ll E_F$, where the assumption of random scattering corresponds only to the assumption of randomness after a large number of successive scatterings.

It is now clear from the above discussion that Eq. (8) for the noninteracting Green's function $\mathbf{G}_0$ assumes the simple form

$$\mathbf{G}_0(\epsilon,k_0)=[k_0(1+i0^+)\tau_4-\epsilon\tau_3]^{-1} \tag{8a}$$

for the case of a dirty superconductor. Then, neglecting the unimportant spread in energy of the spread-out delta function $\bar{\delta}$ of Eq. (53), the form of Eq. (7) for the electronic self-energy $\mathbf{\Sigma}$ is easily simplified. We find the result

$$\mathbf{\Sigma}(\epsilon,k_0)=i\int_{-\infty}^{\infty}\frac{dk_0'}{(2\pi)^4}\int_{-\infty}^{\infty}d\epsilon'\tau_3\mathbf{G}(\epsilon',k_0')\times\tau_3\mathfrak{K}(\epsilon,\epsilon';k_0'-k_0), \tag{7a}$$

where the kernel $\mathfrak{K}$ is defined by the equation

$$\mathfrak{K}(\epsilon,\epsilon';q_0)=[N(\epsilon)]^{-1}\sum_{\mathbf{g}}\sum_{\mathbf{g}'}\int\frac{d^3\mathbf{q}}{(2\pi)^3}v(\mathbf{q}+\mathbf{g}')K_{\mathbf{g}\mathbf{g}'}(q)\times\int d^3\mathbf{k}\sum_l\sum_{l'}M_{ll'}(\mathbf{q}+\mathbf{g}';\mathbf{k})\mathbf{\Gamma}_{l'l}(k,q;\mathbf{g})\times\delta(\epsilon-\epsilon_l(\mathbf{k}))\delta(\epsilon'-\epsilon_{l'}(\mathbf{k}+\mathbf{q})), \tag{54}$$

where $\mathbf{G}$ and $\mathbf{\Sigma}$ are matrices only in τ space and where the integrals over $d^3\mathbf{q}$ and $d^3\mathbf{k}$ are defined as in Secs. II and III; i.e., both integrals extend only over the first Brillouin zone, and the $\mathbf{k}$ integration (but not the q integration) implicitly includes a sum over spin states. Equations (50) and (51) of Sec. III then immediately yield the simplified results

$$\Delta_0(\xi,k_0)\cong-\sum_{s=\pm1}\int_0^{\infty}\frac{dk_0'}{4(2\pi)^3}[\mathfrak{K}_+(\xi,sk_0';k_0'-k_0)\mathrm{Re}\{\Delta_0'(sk_0')[k_0'^2-\Delta_0'^2(sk_0')]^{-1/2}\}-[k_0'\Delta_0(\xi,k_0)/k_0]\mathfrak{K}_-(\xi,sk_0';k_0'-k_0)\,\mathrm{Re}[\{k_0'^2-\Delta_0'^2(sk_0')]^{-1/2}\}] \tag{50a}$$

[61] Reference 55, Secs. 1.2 and 2.1.

[62] F. Englert, J. Phys. Chem. Solids **11**, 23 (1947).

[63] Here we consider only superconductors either so clean that scattering by impurities and lattice defects may be neglected or else so dirty as to belong to class (2); we do not consider the more difficult intermediate case studied by Markowitz and Kadanoff (Ref. 60).

and

$$\Delta(\xi,k_0)\cong-\sum_{s=\pm1}\int_0^\infty\frac{dk_0'}{4(2\pi)^3}\{\Re_+(\xi,sk_0';k_0'-k_0)\,\mathrm{Re}\{\Delta'(sk_0')[k_0'^2-\Delta'^2(sk_0')]^{-1/2}\}$$

$$+\pi^{-1}\sum_j\Re_+^{(j)}(\xi;k_0'-k_0)\,\mathrm{Im}\{\Delta_0'(u_j+iv_j)/[u_j+iv_j)^2-k_0'^2]\}+\pi^{-1}\sum_j\Re_+(\xi,\eta_j+i\gamma_j;k_0'-k_0)$$

$$\times\mathrm{Im}\{\Delta_0'^{(j)}/[(\eta_j+i\gamma_j)^2-k_0'^2]\}-[k_0'/k_0][\Delta(\xi,k_0)\Re_-(\xi,sk_0';k_0'-k_0)\,\mathrm{Re}\{[k_0'^2-\Delta'^2(sk_0')]^{-1/2}\}$$

$$+\pi^{-1}\Delta_0(\xi,k_0)\sum_j\Re_-^{(j)}(\xi;k_0'-k_0)\,\mathrm{Im}\{[(u_j+iv_j)^2-k_0'^2]^{-1}\}]\,,\quad(51a)$$

where the kernel $\Re(\xi,\xi';q_0)$ is defined to within a very good degree of approximation by the equation

$$\Re(\xi,\xi';q_0)=[N(\xi_1)]^{-1}\sum_{\mathbf{g}}\sum_{\mathbf{g}'}\int\frac{d^3\mathbf{q}}{(2\pi)^3}v(\mathbf{q}+\mathbf{g}')K_{\mathbf{g}\mathbf{g}'}(q)$$

$$\times\sum_l\sum_{l'}\int d^3\mathbf{k}[d\xi'/d\xi_1']^{-1}M_{l'l}(\mathbf{q}+\mathbf{g}';\mathbf{k})\boldsymbol{\Gamma}_{l'l}(k,q;\mathbf{g})$$

$$\times\delta(\xi_1-\mathrm{Re}\{\xi_l(k)\})\delta(\xi_1'-\mathrm{Re}\{\xi_{l'}(\mathbf{k}+\mathbf{g})\})\,,\quad(54a)$$

where ξ_1 and ξ_1' are simply the real parts of the energies ξ and ξ', respectively, and the functions $\Re_\pm(\xi,\xi';q_0)$ and $\Re_\pm^{(j)}(\xi;q_0)$ are defined in terms of the τ_4 components of $\Re(\xi,\xi';q_0)$ by precise analogy with the definition in Sec. III of $\Re_\pm(\xi')$ and $\Re_\pm^{(j)}$ in terms of the kernel $\Re(\xi')\equiv\Re(l,l';\hat{k},\xi;l'',l''';l_1,\hat{k}',\xi';q_0)$.

B. Nearly Isotropic Superconductors

Considering for the moment an extended-zone scheme, we see that all matrix elements of the form $\langle\mathbf{k}+\mathbf{q}+\mathbf{g}'|\exp\{i(\mathbf{q}+\mathbf{g}'')\cdot\mathbf{r}\}|\mathbf{k}+\mathbf{g}\rangle$, except those for which $\mathbf{g}''$ is equal to $\mathbf{g}'-\mathbf{g}$, must approach zero in the isotropic or free-electron limit. This immediately implies that the Green's function $\mathbf{G}(\mathbf{k},k_0)$ reduces to the simple scalar form $G(|\mathbf{k}|,k_0)\equiv G(\epsilon(\mathbf{k}),k_0)$ in the free-electron limit. Since it has been demonstrated that the band structure of the simple metals differs from a spherical free-electron band structure only through perturbation by a *small* electron-ion pseudopotential,[11] for the case of the simple metals one should be able to treat as small any correction

$$[\boldsymbol{\delta}\mathbf{G}_0(k)]_{ll'}=[\mathbf{G}_0(k)]_{ll'}-G_0(\epsilon_{ll}(\mathbf{k}),k_0)\delta_{ll'}\quad(55)$$

to the elements of the noninteracting, free-electron Green's function defined by Eq. (8a) above. This immediately suggests that we rewrite Eq. (7) for the self-energy $\boldsymbol{\Sigma}(k)$ in the form

$$\boldsymbol{\Sigma}(k)=i\int_{-\infty}^\infty\frac{dk_0'}{(2\pi)^4}\int_{-\infty}^\infty d\epsilon'\boldsymbol{\tau}_3\mathbf{G}(\epsilon',k_0')$$

$$\times\boldsymbol{\tau}_3\Re(k,\epsilon';k_0'-\mathrm{k}_0)+\boldsymbol{\delta}_2\boldsymbol{\Sigma}(k)\,,\quad(7b)$$

where the kernel $\Re(k,\epsilon';k_0'-k_0)$ has components

$$\Re_{ll'}(k,\epsilon';q_0)=\sum_{\mathbf{q}}\sum_{\mathbf{g}}\sum_{\mathbf{g}'}v(\mathbf{q}+\mathbf{g}')K_{\mathbf{g}\mathbf{g}'}(q)$$

$$\times\exp(iq_00^\pm)\sum_{l''}M_{ll''}(\mathbf{q}+\mathbf{g}';\mathbf{k})$$

$$\times\boldsymbol{\Gamma}_{l''l'}(k,q;\mathbf{g})\delta(\epsilon'-\epsilon_{l''}(\mathbf{k}+\mathbf{q}))\,,\quad(56)$$

and is nearly isotropic.

The definition of the isotropic, average Green's function

$$\mathbf{G}(\epsilon',k_0')\equiv\mathbf{G}(\epsilon_{l'}(\mathbf{k}'),k_0')\equiv\mathbf{G}_{ll}(k')-\boldsymbol{\delta}\mathbf{G}_{ll}(k')$$

$$=[\mathbf{G}_0^{-1}(\epsilon',k_0')-\boldsymbol{\Sigma}(\epsilon',k_0')]^{-1}\quad(57)$$

in terms of the isotropic, average self-energy $\boldsymbol{\Sigma}(\epsilon,k_0)$ given by Eq. (7a) immediately shows that the diagonal elements of the small term

$$\boldsymbol{\delta}_2\boldsymbol{\Sigma}(k)=i\sum_{\mathbf{q}}\sum_{\mathbf{g}}\sum_{\mathbf{g}'}v(\mathbf{q}+\mathbf{g}')\int_{-\infty}^\infty\frac{dq_0}{2\pi}\mathbf{M}(\mathbf{q}+\mathbf{g}';\mathbf{k})$$

$$\times\boldsymbol{\tau}_3\boldsymbol{\delta}\mathbf{G}(k+q)\boldsymbol{\tau}_3\boldsymbol{\Gamma}(k,q;\mathbf{g})K_{\mathbf{g}\mathbf{g}'}(q)\exp(iq_00^\pm)\quad(58)$$

on the right-hand side of Eq. (7b) are second order in the small anisotropy of the self-energy $\boldsymbol{\Sigma}(\epsilon_l(\mathbf{k}),\hat{k},k_0)\equiv\boldsymbol{\Sigma}(k)$, and may be neglected. Since the off-diagonal elements of $\boldsymbol{\Sigma}(k)$ enter into physically meaningful or experimentally observable quantities only in second order, we may also neglect the off-diagonal elements of the small term $\boldsymbol{\delta}_2\boldsymbol{\Sigma}(k)$. Thus, we can construct an easily applied approximation scheme for determining the anisotropic energy gap $\Delta(\xi_{ll}(\mathbf{k}),\hat{k},k_0)$.

As a first approximation to $\Delta(k)$, one finds the isotropic, average energy gap $\Delta_0(\xi,k_0)$ from Eq. (50a).

Then one writes

$$\Delta_{ll}(k)\cong-\sum_{s=\pm1}\int_0^\infty\frac{dk_0'}{4(2\pi)^3}\Bigg[\Re_+(k,sk_0';k_0'-k_0)]_{ll}\,\mathrm{Re}\left\{\frac{\Delta_0(sk_0',k_0')}{[k_0'^2-\Delta_0^2(sk_0',k_0')]^{1/2}}\right\}+\pi^{-1}\sum_j[\Re_+^{(j)}(k;k_0'-k_0)]_{ll}$$
$$\times\mathrm{Im}\left\{\frac{\Delta_0(u_j+iv_j,k_0')}{(u_j+iv_j)^2-k_0'^2}\right\}+\pi^{-1}\sum_j[\Re_+(k,\eta_j+i\gamma_j;k_0'-k_0)]_{ll}\,\mathrm{Im}\left\{\frac{\Delta_0^{(j)}(k_0')}{(\eta_j+i\gamma_j)^2-k_0'^2}\right\}\Bigg]$$
$$\div\left\{1-\sum_{s=\pm1}\int_0^\infty\frac{dk_0'}{4(2\pi)^3}\frac{k_0'}{k_0}[[\Re_-(k,sk_0';k_0'-k_0)]_{ll}\,\mathrm{Re}\{[k_0'^2-\Delta^2(sk_0',k_0')]^{-1/2}\}\right.$$
$$\left.+2\pi^{-1}\sum_j u_jv_j[\Re_-^{(j)}(k;k_0'-k_0)]_{ll}/[(u_j^2+v_j^2)^2-2k_0'^2(u_j^2-v_j^2)+k_0'^4]]\right\},\quad(51b)$$

where $\Re_\pm(k,\xi';q_0)$ and $\Re_\pm^{(j)}(k;q_0)$ are defined in terms of the τ_4 component of the kernel $\Re(k,\xi';q_0)$ by precise analogy with the definitions in Sec. III of $\Re_\pm(\xi')$ and $\Re_\pm^{(j)}$ in terms of the kernel

$$\Re(\xi')\equiv\Re(l,l';\hat{k},\xi;l'',l''';l_1,\hat{k}',\xi';q_0).$$

This equation gives the anisotropy of the energy gap $\Delta(k)$ to first order merely by integration. It is easily possible to perform further iterations and thus, in theory, to find the anisotropy of $\mathbf{\Delta}(k)$ to higher order and to find the off-diagonal elements of $\mathbf{\Delta}(k)$; however, this is impractical for the case of the simple metals (and for any other cases of interest known to the author). If one is concerned primarily with the determination of the anisotropy of the energy gap $\Delta(k)$ in the simple metals, one can simplify its determination even further by neglecting all terms on the right-hand side of Eq. (51b) except those in which ξ' is set equal to sk_0'. The neglected terms all must have a very small effect upon the anisotropy of the energy gap (1) because of the Migdal theorem[15] and (2) because of the unimportance of the Coulomb interaction for the determination of $\Delta(k)$ in the simple metals.[64]

C. Comparison with Earlier Results

We now wish to compare the form of Eqs. (50a) and (51a) with that of the integral equations derived by previous authors.[6,16,17] First, it is important to note that by the Migdal theorem[15] our equations reduce to the much simpler form presented by Schrieffer[6] for the case of a metal with a vanishing Coulomb interaction, although our kernel is of course different from that of Schrieffer.[65] The extra terms included in our equations but not in those of Schrieffer are important only (1) in determining the effect of the Coulomb interaction, (2) for the case of superconducting semiconductors or semimetals, and (3) for the case of those few metals such as lanthanum and uranium for which band-structure effects very near the Fermi level are important. Since Schrieffer has dealt primarily with the superconducting properties of the simple metals and has been especially interested in the strong-coupling superconductors, his equations were not intended for use in calculating the effects of the Coulomb interaction upon superconductivity or for cases (2) or (3).

The only equations previously presented which have been intended for use in calculating the role of the Coulomb interaction in superconductivity are those of Tolmachev,[55] Morel and Anderson,[3] and the author.[16,17] That of the author,

$$\Delta(\xi)=\int_{-\infty}^{\infty}\frac{d\xi'}{(2\pi)^3}\frac{\Delta(\xi')\cos\delta'}{[\xi'^2+\Delta^2(\xi')]^{1/2}}\Re(\xi,\xi';\xi'-\xi),\quad(59)$$

is the most recent and the most general of these. Here, the factor $\cos\delta'=\xi'(\xi_1'^2+\xi_2'^2)^{-1/2}$ is a lifetime effect which results from allowing the energies $\xi'\equiv\xi_1'+i\xi_2'$ to assume complex values and from using generalized complex Bogoliubov quasiparticle transformations.[61,66] This quasiparticle equation for the superconducting energy gap is identical in form to Eq. (50a) in the limit that $\cos\delta'$ approaches unity, that the imaginary part of the gap function Δ vanishes and that the kernel $\Re_-$ vanishes [that $Z(k_0)$ approaches unity]. Thus the Green's-function technique yields an equation for Δ which in the neglect of lifetime effects is no more difficult to solve than the quasiparticle equation[67] (59), provided that one knows $Z(k_0)$. It yields (1) an important correction to the quasiparticle results which arises from wave function renormalization, (2) small corrections arising from lifetime effects, and (3) a method in principle for determining a kernel better than that which

[64] See Ref. 42 for a discussion of this point.

[65] Our equations for $\Re_\pm$ reduce to the form of Eq. (7-70) of Schrieffer (Ref. 6) for $K_\pm$ in the appropriate limit. However, in determining Σ our $\Re_+$ is multiplied by ϕ', whereas the K_+ of Schrieffer is multiplied by $-\phi'$; our equations agree with those of Eliashberg (Ref. 2) in the appropriate limit. We presume that this discrepancy arises from a misprint in Ref. 6. (The same error occurs in Ref. 4.)

[66] The factor $\cos\delta'$ in Eq. (59) corresponds to, but is different from, the factor $(d\xi'/d\xi_1')^{-1}$ which appears implicitly in Eqs. (50a) and (51a) through the factors $\Re_\pm(\xi,\xi';q_0)$ and $\Re_\pm^{(j)}(\xi;q_0)$. Thus, as might be expected, it does not lead to the correct evaluation of lifetime effects.

[67] This remark is of course valid at finite temperatures as well as at the absolute zero.

the author derived previously[17] using a generalization of the Englert effective-Hamiltonian formalism.[62] Even on purely formal grounds, one might well be surprised by the agreement with experiment found by the author in his first calculations of the coefficient of the isotope effect in superconductivity, since they were based on a simple quasiparticle approximation. In fact, the phonon contribution $Z_{\rm ph}$ to the wave-function-renormalization constant substantially reduces the calculated deviation from the BCS value of -0.5 for the coefficient of the isotope effect.

V. QUASILINEARIZATION OF THE GAP EQUATION AND ANALYSIS OF THE FORM OF ITS SOLUTION

In this section we present a technique for the quasilinearization of the energy-gap equations (50a) and (51a) of Sec. IVA. The homogeneous nonlinear integral equation (50a) is transformed into an inhomogeneous integral equation which, since its kernel vanishes at the point $k_0=\Delta_0$, is nearly linear. This technique is applicable to any other one-dimensional nonlinear integral equation whose nonlinearity is important only in the neighborhood of a single point and is applicable both to numerical computations and to the approximation of the energy gap by purely analytic means. Here, its application to numerical computations is outlined only briefly, but it is used to analyze the behavior of the energy gap $\Delta(\xi,k_0)$ as a function of the form of the kernel $\mathfrak{K}(\xi,\xi';k_0,k_0')$.

We first consider Eq. (50a), which can be rewritten in the form

$$\Delta_0(\xi,k_0)=-Z_0^{-1}(\xi,k_0)\sum_{s=\pm1}\int_0^\infty dk_0'\mathcal{K}_+(\xi,sk_0';k_0,k_0')\times\mathrm{Re}\{\Delta_0(sk_0',k_0')\times[k_0'^2-\Delta_0^2(sk_0',k_0')]^{-1/2}\}. \quad (60)$$

Here the renormalization constant Z_0 is given by the equation

$$Z_0(\xi,k_0)=1-\sum_{s=\pm1}\int_0^\infty dk_0'\mathcal{K}(\xi,sk_0';k_0,k_0')\times\mathrm{Re}\{k_0'[k_0'^2-\Delta_0^2(sk_0',k_0')]^{-1/2}\}, \quad (61)$$

and the kernels $\mathcal{K}_\pm$ are defined by the equations

$$\mathcal{K}_\pm(\xi;sk_0';k_0,k_0')=\tfrac{1}{4}[1/(2\pi)^3]k_0^{-\frac{1}{2}(1\mp1)}\times\mathfrak{K}_\pm(\xi,sk_0';k_0,k_0'). \quad (62)$$

Since Eq. (60) is a generalization of the gap equation of Scalapino, Schrieffer, and Wilkins[4,6] (and of other forms of the propagator equations), the quasilinearization technique to be presented here is applicable to many different calculations.

Equation (60) contains two sources of nonlinearity: (1) the factor $\Delta_0(sk_0',k_0')[k_0'^2-\Delta_0^2(sk_0',k_0')]^{-1/2}$, which appears explicitly in Eq. (60), and (2) the factor $\mathrm{Re}\{k_0'[k_0'^2-\Delta_0^2(sk_0',k_0')]^{-1/2}\}$ which appears implicitly through the factor $Z_0^{-1}(\xi,k_0)$. However, the second source introduces only a negligible nonlinearity of order $\Delta^2/\omega_{\rm ph}^2$, so that we may replace $Z_0(\xi,k_0)$ or even $Z(\xi,k_0)$ by its normal state value $Z_{00}(\xi,k_0)$ in all calculations to order $\Delta^2/\omega_{\rm ph}^2<0.01$. In attempting to minimize the effects of the nonlinearity of the first factor, it is convenient first to define the normalized gap function

$$\Xi_0(\xi,k_0)=\Delta_0(\xi,k_0)/\Delta_0, \quad (63)$$

and the normalized kernel

$$I_+(\xi,\xi';k_0,k_0')=\mathcal{K}_+(\xi,\xi';k_0,k_0')/\mathcal{K}_+(0,0;\Delta_0,\Delta_0), \quad (64)$$

in terms of the energy gap Δ_0 which is defined by the self-consistency condition $\Delta_0=\Delta_0(0,\Delta_0)$. Upon substituting Eqs. (63) and (64) into Eq. (60), setting ξ equal to zero and k_0 equal to Δ_0, and multiplying both sides of Eq. (60) by $I_+(\xi,0;k_0,\Delta_0)/\Delta_0$, one finds the result

$$0=\sum_{s=\pm1}\Big[I_+(\xi,0;k_0,\Delta_0)+Z_0^{-1}(0,\Delta_0)\int_0^\infty dk_0'\times I_+(0,sk_0',\Delta_0,k_0')\mathcal{K}_+(\xi,0;k_0,\Delta_0)\times\mathrm{Re}\{\Delta_0(sk_0',k_0')[k_0'^2-\Delta_0^2(sk_0',k_0')]^{-1/2}\}\Big]. \quad (65)$$

Then, upon dividing Eq. (60) by Δ_0, multiplying Eq. (69) by $Z_0(0,\Delta_0)Z_0^{-1}(\xi,k_0)$ and adding the resultant equations, one finds the quasilinear equation

$$\Xi_0(\xi,k_0)=Z_0^{-1}(\xi,k_0)\Big[I_+(\xi,0;k_0,\Delta_0)Z_0(0,\Delta_0)-\sum_{s=\pm1}\int_0^\infty dk_0'[\mathcal{K}_+(\xi,sk_0';k_0,k_0')-I_+(0,sk_0';\Delta_0,k_0')\mathcal{K}_+(\xi,0;k_0,\Delta_0)]\times\mathrm{Re}\{\Xi_0(sk_0',k_0')[k_0'^2-\Delta_0^2\Xi_0^2(sk_0',k_0')]^{-1/2}\}\Big]. \quad (66)$$

In order to see that Eq. (66) is indeed quasilinear, note that although the nonlinear factor $\Delta_0(sk_0',k_0')\times[k_0'^2-\Delta_0^2(sk_0',k_0')]^{-1/2}$ of Eq. (60) remains in Eq. (66), it is now multiplied by the new kernel

$$\mathcal{K}_+(\xi,sk_0';k_0,k_0')-I_+(0,sk_0';\Delta_0,k_0')\mathcal{K}_+(\xi,0;k_0,\Delta_0),$$

which vanishes at the point $k_0'=\Delta_0$ of maximum nonlinearity. Not only does this kernel vanish at the point $k_0'=\Delta_0$, it vanishes linearly at this point, whereas the nonlinear factor has at worst only a square-root singularity at this point. Furthermore, this kernel vanishes for $k_0=\Delta_0$ as well, and is small for small values of k_0. Thus, the most important nonlinearity present in Eq. (60), that arising from the explicit factor $\Delta_0(sk_0',k_0)$

$\times[k_0'^2-\Delta_0^2(sk_0',k_0')]^{-1/2}$ is reduced in Eq. (66) to a small correction factor of order $\Delta_0/\omega_{\rm ph}<0.1$. Thus, Eq. (66) is quasilinear in the sense that the replacement of Δ_0 by zero at all points in Eq. (66) and the evaluation of both Z_0 and the kernels I_+ and K_+ in the normal state lead to the *linear* integral equation

$$\Xi_0(\xi,k_0)\simeq\Xi_{01}(\xi,k_0)$$
$$=Z_{00}^{-1}(\xi,k_0)\Big[I_+(\xi,0;k_0,0)Z_{00}(0,0)$$
$$-\sum_{s=\pm1}\int_0^\infty dk_0'[\mathcal{K}_+(\xi,sk_0';k_0,k_0')-I_+(0,sk_0';0,k_0')$$
$$\times\mathcal{K}_+(\xi,0;k_0,0)]k_0'^{-1}\Xi_{01}(sk_0',k_0')\Big], \quad (66a)$$

which determines $\Xi_0(k_0)$ within a factor of order $\Delta/\omega_{\rm ph}$.

Of course, Eq. (66a) determines only $\Xi_{01}(k_0)$ and hence the approximate ξ and k_0 dependence of $\Delta_0(\xi,k_0)$, not the value of Δ_0. However, given both the k_0 dependence of $\Delta_0(sk_0,k_0)$ and any reasonable zero-order estimate Δ_{00} of Δ_0,[68] one can easily evaluate the expression

$$\Delta_{01}=[\omega_{\rm ph}\Delta_{00}]^{1/2}\,\mathrm{sech}\Big(\mathcal{K}_+(0,0;0,0)^{-1}\Big[Z_{00}(0,0)$$
$$+\sum_{s=\pm1}\int_{(\Delta_{00}\omega_{\rm ph})^{1/2}}^\infty dk_0'\mathcal{K}_+(0,sk_0';0,k_0')$$
$$\times\mathrm{Re}\{\Xi_{01}(sk_0',k_0')\}k_0'^{-1}\Big]\Big), \quad (67)$$

which gives a first approximation to Δ_0 accurate within a factor of the order of $\max(\Delta_{00}/\omega_{\rm ph},\ \Delta_{01}^2/\Delta_{00}\omega_{\rm ph}<0.1$. If greater accuracy is desired, one can solve the equation

$$\Delta_{0,\nu+1}=-\Delta_{0,\nu}Z_{00}^{-1}(0,0)\sum_{s=\pm1}\int_0^\infty dk_0'\mathcal{K}_+(0,sk_0';0,k_0')$$
$$\times\mathrm{Re}\{\Xi_{01}(sk_0',k_0')[k_0'^2-\Delta_{0,\nu}^2\Xi_{01}^2(sk_0',k_0')]^{-1/2}\} \quad (68)$$

iteratively, obtaining values of $\Delta_{0,\nu}$ which bracket the solution $\Delta_{0,\infty}$ and converge toward it with a convergence ratio better than $[1+\ln(\omega_{\rm ph}/\Delta_{0,\infty})]^{-1}$.

In order to determine $\Delta_0(\xi,k_0)$ numerically by our quasilinearization scheme, one should first invert Eq. (66a) to find $\Xi_{01}(\xi,k_0)$ and then determine Δ_{01} by integrating Eq. (67). Equation (66a) is easily inverted numerically, because it has the simple matrix form

$$[\mathbf{1}-\mathbf{M}]\cdot\boldsymbol{\Xi}=\mathbf{I}, \quad (69)$$

where $\mathbf{I}$ and $\boldsymbol{\Xi}$ are vectors in k_0 space and $\mathbf{M}$ is a matrix in k_0 space; but of course it cannot be inverted analytically. If greater accuracy is desired, one may then approximate Ξ_0 on the right-hand side of Eq. (70) by Ξ_{01} and either invert the resultant linear integral equation or solve it by iteration[69] to obtain $\Xi_{02}(\xi,k_0)$. Finally, one may then substitute Ξ_{02} into Eq. (72) for Ξ_{01} and solve this equation iteratively once or twice. The resultant approximation $\Delta_{02}(\xi,k_0)$ to the solution $\Delta_0(\xi,k_0)$ of Eq. (60) will be accurate to order 1%.

In order to find an approximation to $\Delta_0(\xi,k_0)$ by analytic means, we must find a zero-order approximation $\Delta_{00}(\xi,k_0)$ to $\Delta_0(\xi,k_0)$ for use in iterating Eq. (66a). The inhomogenous term of Eq. (66a),

$$I(\xi,k_0)\equiv Z_{00}^{-1}(\xi,k_0)I_+(\xi,0;k_0,0)Z_{00}(0,0),$$

is unfortunately a poor approximation to $\Xi_0(\xi,k_0)$ since it corresponds to the replacement of the factor $\mathrm{Re}\{\Delta_0(sk_0',k_0')[k_0'^2-\Delta_0^2(sk_0',k_0')]^{-1/2}\}$ in the integrand of Eq. (60) by the delta function $\delta(k_0')$. This approximation would (1) yield structure at energies k_0 which should actually occur at energies $k_0+\Delta_0$ and (2) fail to take account of the broadening or damping of the structure of the kernel $K_+(\xi,sk_0';k_0,k_0')$ produced by its convolution with the function $\mathrm{Re}\{\Delta_0(sk_0',k_0')\times[k_0'^2-\Delta_0^2(sk_0',k_0')]^{-1/2}\}$. The first objection to this choice is easily overcome by simply redefining $\Delta_{00}(k_0)$ as $I_0(k_0-\Delta_{0\nu})$ as soon as we find the approximation $\Delta_{0\nu}$ to Δ_0. However, the second objection is serious and cannot be overcome without modifying the form of the function $I(\xi,k_0)$.

The broadening of the structure of the kernel $\mathcal{K}_+(\xi,sk_0';k_0,k_0')$ produced by its convolution with the function $\mathrm{Re}\{\Delta_0(sk_0',k_0')[k_0'^2-\Delta_0^2(sk_0',k_0')]^{-1/2}\}$ yields a normalized gap function $\Xi_0(\xi,k_0)$ which differs from $I(\xi,k_0)$ in two principal respects: (1) any sharp structure in the function $I(\xi,k_0)$ is spread out in $\Xi_0(\xi,k_0)$ over an energy several times as large as the gap energy Δ_0,[70] and (2) the absolute value of $\Xi_0(\xi,k_0)$ is, in general, less than the absolute value of $I(\xi,k_0)$, especially for values of k_0 much greater than the maximum phonon frequency $\omega_{\rm ph}$. Although the first of these differences may be neglected, since any sharp structure in $I(\xi,k_0)$ is already broadened by the integration over phonon frequencies in the determination of $\mathcal{K}_+(\xi,0;k_0,0)$, the second one is important. Taking account of it in an approximate manner, one may define Ξ_{00} in terms of a zero-order estimate Δ_{00} to Δ_0. One finds

$$\Xi_{00}(\xi,k_0+\Delta_{00})=\{I(\xi,k_0)-\alpha I(\xi,\omega_e)+[\ln(\omega_{\rm ph}/\Delta_{00})]^{-1}$$
$$\times[I(\xi,|k_0-\omega_M|)-I(\xi,k_0)]\}\div\{1-\alpha I(\xi,\omega_e)$$
$$+[\ln(\omega_{\rm ph}/\Delta_{00})]^{-1}[I(\xi,\omega_M)-I(\xi,0)]\}, \quad (70)$$

where α is a numerical factor which it is convenient to set equal to 0.6 for simple metals, 0.5 for transition metals, and 0.2 for degenerate semiconductors or semi-

[68] Such a reasonable zero-order estimate can be obtained either from experiment or from any such simple approximation as the two-step-function model of Tolmachev (Ref. 55).

[69] Its solution by iteration will converge very rapidly since the first approximation $\Xi_{01}(\xi,k_0)$ is very good.

[70] For example, a step-function discontinuity in $I(\xi,k_0)$ at the point $k_0=\omega_{\rm ph}$ would produce only a continuous change in $\Xi_0(\xi,k_0)$ centered near the point $k_0=\omega_{\rm ph}+\Delta_0$ with maximum slope less than $K_+(0;0,0)[I(\omega_{\rm ph}+0^+)-I(\omega_{\rm ph}-0^+)]\Delta_0^{-1}<\Delta_0^{-1}$.

conductors,[71] and where $I(\xi,\omega_e)$ is an average value of $I(\xi,k_0)$ for k_0 much greater than the maximum phonon frequency $\omega_{\rm ph}$ but much less than the electronic plasma frequency $\omega_{\rm pl}$ and where $I(\xi,\omega_M)$ is the maximum value of $I(\xi,k_0)$. Note that although Eq. (70) reduces to the simple form

$$\Xi_{00}(\xi,k_0)\simeq[I(\xi,k_0)-\alpha I(\xi,\omega_e)]/[I(\xi,0)-\alpha I(\xi,\omega_e)] \quad (70a)$$

in the weak-coupling limit and thus determines $\Xi_{00}(\xi,k_0)$ independently of Δ_0, Eq. (70) is quite unreliable in extreme weak-coupling cases. This unreliability follows from the fact that $\Xi_0(\xi,k_0)$ approaches plus or minus infinity for all values of k_0 except $k_0=0$ as $\ln(\omega_{\rm ph}/\Delta_0)$ approaches infinity; it is a necessary consequence of the nonlinearity of Eq. (60).

Now, given any reasonable zero-order estimate Δ_{00} of the gap energy Δ_0,[68] one can easily determine first-order approximations to both Ξ_0 and Δ_0 from the equation

$$\Xi_{01}(\xi,k_0+\Delta_{00})\simeq I(\xi,k_0)-Z_{00}^{-1}(\xi,k_0)$$
$$\times\sum_{s=\pm1}\int_0^\infty dk_0'[\mathcal{K}_+(\xi,sk_0';k_0,k_0')-I_+(0,sk_0',\Delta_{00},k_0')$$
$$\times\mathcal{K}_+(\xi,0;k_0,\Delta_{00})]\,{\rm Re}\{\Xi_{00}(sk_0',k_0')$$
$$\times[k_0'^2-\Delta_{00}^2\Xi_{00}^2(sk_0',k_0')]^{-1/2}\}, \quad (71)$$

and from Eq. (67), where the function $\Xi_{00}(\xi,k_0)$ is given by Eq. (70).

One may use the arguments of this section to analyze the effect of changes in the kernel $\mathfrak{K}$ and renormalization constant Z upon the form $\Xi(\xi,k_0)$ and magnitude Δ of the gap function $\Delta(\xi,k_0)$, since the solution $\Delta(\xi,k_0)$ of Eq. (51a) differs only very slightly from that of Eq. (50a). However, we reserve such an analysis for the following paper,[42] where it is useful in discussing the isotope effect, and present here only a simple argument as to why the dynamic interaction arising from the virtual exchange of phonons of frequency $\omega\simeq\omega_{\rm ph}$ is most important in inducing superconductivity. We have seen that $\Xi(\xi,k_0)$ has very approximately the same form as the function $I(k_0)$ or $\mathcal{K}_+(\xi,0;k_0,0)$, but with the structure of the function $I(\xi,k_0)$ spread out and diminished and with the value of the ratio $\Delta(\xi,k_0)/I(\xi,k_0)$ much smaller for $k_0>\omega_{\rm ph}$ than for $k_0<\omega_{\rm ph}$. It follows immediately from this fact that an increase in the absolute value of the kernel $\mathcal{K}_+(\xi,0;k_0,0)$ for almost any value[72] of k_0 must lead to an increase in the gap width Δ, provided only that the kernel $\mathcal{K}_+(0,0;0,0)$ is negative (attractive). It immediately follows that the dynamic interaction arising from the virtual exchange of phonons of frequency $\omega\simeq\omega_{\rm ph}$ must play a much greater role in determining Δ than either (1) any dynamic interaction whose resonance frequency is significantly less than $\omega_{\rm ph}$ or (2) any quasistatic interaction such as the Coulomb interaction.

VI. CONCLUSIONS AND SUMMARY

Since this paper is intended only to give the formalism necessary for applications to physical problems presented elsewhere[42] or to be presented elsewhere,[73] we have few conclusions of physical significance. Those few conclusions which are presented here relate to the validity or interpretation of approximations such as the jellium approximation and the quasiparticle approximation as applied to superconductivity; other conclusions, related to the role of the Coulomb interaction in superconductivity, are presented elsewhere.[42]

First we note that the replacement of the jellium approximation by the assumption of a crystal lattice with a local pseudopotential leads to no physically new results for the case of a dirty superconductor. Even for the case of a clean superconductor, this replacement leads to no new qualitative results other than the introduction of an easily calculated anisotropy in the energy-gap function $\mathbf{\Delta}(k)$, except possibly for the case of clean transition-metal superconductors, which is not discussed here.

Next, we consider the quasiparticle approximation. In the unreal but interesting case of metals with a vanishing Coulomb interaction, the application of the Migdal theorem[15] and the Nambu-Gor'kov[26,27] Green's-function techniques yields an integral equation for the energy gap $\phi(k)$ which can be described within a generalized quasiparticle picture in which the energy of an excitation of wave vector $\mathbf{k}$ is given by the equation

$$k_0=E=Z^{-1}(\xi^2+\phi^2)^{1/2}. \quad (72)$$

In the case of superconducting semiconductors or semimetals, or even in the case of metals with a nonvanishing Coulomb interaction, the inapplicability of the Migdal theorem leads to gap equations which cannot be interpreted exactly within any generalized quasiparticle picture. However, in the neglect of lifetime effects we find an energy-gap equation identical to that which is found for quasiparticles having the properly renormalized energies $Z^{-1}\xi$ in the normal state. Furthermore, those lifetime effects which cannot be treated within a generalized quasiparticle picture are unimportant in determining the superconducting properties of metals. Thus, a generalized quasiparticle picture can be constructed which yields results identical to those of the Green's-function formalism for those cases to which the Migdal theorem is applicable, for

[71] It is possible to determine the factor α self-consistently for any given kernel by comparing $\Xi_{00}(k_0)$ to the next order approximation $\Xi_{01}(k_0)$, which is given later. However, this complicated procedure is not necessary; a simple good approximation to α is given by the formula $\alpha=\beta/(1+\beta)$, where $\beta=Z_{00}^{-1}(0,0)K(0;0,0)\times\int_{2\omega_{\rm ph}}^\infty dk_0'I(k_0')/k_0'$.

[72] By almost any value of k_0 we mean any value of k_0 such that $I(\xi,k_0)\Xi(\xi,k_0)$ is positive; except for a pathological kernel or in the extreme weak-coupling limit, the product $I(\xi,k_0)\Xi(\xi,k_0)$ is positive for all values of k_0.

[73] J. W. Garland (to be published).

either weak or strong coupling,[74] and very nearly equivalent to those of the Green's-function formalism for all metallic superconductors.

In this paper we have performed essentially four calculations. First, in Sec. II the usual scalar Dyson equations appropriate to the jellium model are generalized to a set of tensor equations appropriate to the interacting electrons and phonons of a perfect crystal, and the electron and phonon fields are separated. Second, in Sec. III a set of three-dimensional integral equations for the energy gap $\mathbf{\Delta}(k)$ and the renormalization function $\mathbf{Z}(k)$ is derived; the role of the Coulomb interaction is specifically calculated. This calculation corresponds essentially to the derivation of a method for the calculation of the effective Coulomb pseudopotential U of Schrieffer[4,6] or, alternatively, to the calculation of the corrections to the results of an appropriately generalized quasiparticle calculation of $\mathbf{\Delta}(k)$. The terms calculated are of the order of 2 to 10% corrections to the quantity $\ln(\omega_{\rm ph}/\Delta)$ and are calculated to order 20 or 25% accuracy. Third, in Sec. IV our three-dimensional equations are reduced to one-dimensional form for the case of dirty superconductors and an easy method is presented for the determination of any nearly isotropic energy gap $\Delta(k)$, such as is found in the case of the simple metals. Fourth, in Sec. V a technique is presented for the quasilinearization of any one-dimensional gap equation. This technique is used to analyze both the general form of the gap function $\Delta(\xi,k_0)$ and the influence upon $\Delta(\xi,k_0)$ of the Coulomb interaction.

Although for the ease of the reader all derivations are presented only in the zero-temperature limit, our results are easily generalized to the case of finite temperatures by the technique of Abrikosov, Gor'kov, and Dzyaloshinski.[75] One finds, as expected, that the integrand on the right-hand side of every integral equation for $\boldsymbol{\phi}(k)$ or $\mathbf{\Delta}(k)$ should be multiplied by the factor $\tanh(k_0'/2k_BT)$. At the temperatures of interest here ($T\leqslant T_c\ll\Theta_D$) all other quantities calculated are essentially independent of temperature.

ACKNOWLEDGMENTS

It is a pleasure to thank the Cavendish Laboratory of the University of Cambridge for its gracious hospitality during the spring and summer of 1965 when this work was completed, in particular to thank Professor Sir Nevill Mott and Dr. V. Heine. It is also a pleasure to acknowledge many interesting and instructive discussions with Professor Leo P. Kadanoff, to thank Professor M. H. Cohen for reading the manuscript and for helpful comments, to acknowledge many helpful discussions with Dr. A. Suna and Dr. E. Pytte during the preliminary stage of research on this paper, and to thank Dr. K. Bennemann for reading the final manuscript. Finally, the author wishes to thank Professor J. R. Schrieffer for making available to him sections of his book *Theory of Superconductivity* in advance of publication.

APPENDIX: DERIVATION OF THE DYSON EQUATIONS

Here we derive and discuss briefly a set of Dyson equations for the system of interacting electrons and phonons of a perfect crystal at zero temperature. We restrict ourselves to the zero-temperature case in order to avoid unnecessary complication for the reader; however, our results are easily generalized to the case of finite temperatures by the technique of Abrikosov, Gor'kov and Dzyaloshinski.[75] We include all effects of umklapp processes, calculate the renormalization of phonon frequencies by electron-phonon interactions, and express our results in terms of the renormalized phonon frequencies.

In the Heisenberg picture, the Hamiltonian (1) yields the equation of motion

$$i\dot{\mathbf{c}}_{\mathbf{k}}(t)=[\mathbf{c}_{\mathbf{k}}(t),H(t)]$$
$$=\boldsymbol{\varepsilon}_{\mathbf{k}}\cdot\mathbf{c}_{\mathbf{k}}+\sum_{\mathbf{q}}\sum_{\mathbf{g}}[v(\mathbf{q}+\mathbf{g})\rho_{\mathbf{q}+\mathbf{g}}+\boldsymbol{\alpha}^0(\mathbf{q}+\mathbf{g})\cdot\boldsymbol{\phi}_{-\mathbf{q}}]\times\mathbf{M}^T(\mathbf{q}+\mathbf{g};\mathbf{k})\cdot\mathbf{c}_{\mathbf{k}+\mathbf{q}}, \quad \text{(A1)}$$

where the elements

$$\rho_{\mathbf{q}+\mathbf{g}}=\sum_{\mathbf{k}}\mathbf{c}_{\mathbf{k}+\mathbf{q}}{}^{\dagger}\cdot\mathbf{M}(\mathbf{q}+\mathbf{g};\mathbf{k})\mathbf{c}_{\mathbf{k}} \quad \text{(A2)}$$

of the column vector $\boldsymbol{\rho}_{\mathbf{q}}$ are Fourier components of the electronic-charge density. The form of Eqs. (A1) and (A2) suggests adding to the Hamiltonian (1) the source term

$$H_s=\sum_{\mathbf{q}}[\mathbf{F}_{\mathbf{q}}(t)\cdot\boldsymbol{\phi}_{\mathbf{q}}(t)+\mathbf{J}_{-\mathbf{q}}\cdot\boldsymbol{\rho}_{\mathbf{q}}], \quad \text{(A3)}$$

which adds the term

$$[\mathbf{c}_{\mathbf{k}},H_s]=\sum_{\mathbf{q}}\sum_{\mathbf{g}}J_{\mathbf{q}+\mathbf{g}}\mathbf{M}^T(\mathbf{q}+\mathbf{g};\mathbf{k})\cdot\mathbf{c}_{\mathbf{k}+\mathbf{q}} \quad \text{(A4)}$$

to the commutator (A1). We assume that the external fields $\mathbf{F}_{\mathbf{q}}(t)$ and $\mathbf{J}_{\mathbf{q}}(t)$ vanish at $t=\pm\infty$, introduce the Nambu spinor

$$\mathbf{\Psi}_{\mathbf{k}}=\begin{pmatrix}\mathbf{c}_{\mathbf{k}\uparrow}\\ \mathbf{c}_{-\mathbf{k}\downarrow}{}^{\dagger}\end{pmatrix}, \quad \text{(A5)}$$

and the Pauli spin matrices

$$\boldsymbol{\tau}_1=\begin{pmatrix}0&1\\1&0\end{pmatrix},\quad \boldsymbol{\tau}_2=\begin{pmatrix}0&i\\-i&0\end{pmatrix},\quad \boldsymbol{\tau}_3=\begin{pmatrix}1&0\\0&-1\end{pmatrix}$$
$$\text{and}\quad \boldsymbol{\tau}_4=\begin{pmatrix}1&0\\0&1\end{pmatrix}. \quad \text{(A6)}$$

[74] Of course, as has been shown by Schrieffer (Ref. 6) and others (Ref. 5), the appropriate generalized quasiparticle picture reduces to the standard, simple quasiparticle picture only in the extreme high-density weak-coupling limit.

[75] A. A. Abrikosov, L. P. Gor'kov, and I. E. Dzyaloshinski, *Methods of Quantum Field Theory in Statistical Physics* (Prentice-Hall, Inc., Englewood Cliffs, New Jersey, 1963).

We can then define a generalized electronic Green's function

$$\mathbf{G}(1,2)\equiv\mathbf{G}(\mathbf{k}_1,\mathbf{k}_2;t_1,t_2)=-i\langle T_W\{\Psi_{\mathbf{k}_1}(t_1)\Psi_{\mathbf{k}_2}^{\dagger}(t_2)\}\rangle \quad \text{(A7)}$$

in this τ space, where T_W is the Wick time-ordering operator, and where the elements of Ψ and $\Psi^{\dagger}$ are to be considered as column vectors and row vectors, respectively, in l space.

The symbol $\langle\ \rangle$ is defined by the equation

$$\langle\mathcal{O}_1(t_1)\mathcal{O}_2(t_2)\rangle\equiv\langle 0|U(\infty,t_1)\mathcal{O}_1(0)U(t_1,t_2)\times\mathcal{O}_2(0)U(t_2,-\infty)|0\rangle/\langle 0|U(\infty,-\infty)|0\rangle. \quad \text{(A8)}$$

Here, the $\mathcal{O}(t)$'s are Heisenberg operators for the Hamiltonian $H_t=H+H_s$, $|0\rangle$ is the ground state of our system, and

$$U(t',t'')=T_H\left\{\exp\left[-i\int_{t''}^{t'}dtH_t(t)\right]\right\} \quad \text{(A9)}$$

is the Heisenberg time-development operator, where T_H is the Heisenberg time-ordering operator.

We now use the Hamiltonian source term (A3) to generate the equation of motion of the electronic Green's function (A6) and to obtain Dyson equations. The definitions (A8) and (A9) immediately yield the equations

$$\delta\langle\mathcal{O}(t)\rangle/\delta J_{\mathbf{q}+\mathbf{g}}(t')=i[\langle\mathcal{O}(t)\rangle\langle\rho_{-\mathbf{q}-\mathbf{g}}(t')\rangle-\langle T_H\{\mathcal{O}(t)\rho_{-\mathbf{q}-\mathbf{g}}(t')\}\rangle], \quad \text{(A10)}$$

and

$$\delta\langle\mathcal{O}(t)\rangle/\delta\mathbf{F}_{\mathbf{q}}(t')=i[\langle\mathcal{O}(t)\rangle\langle\boldsymbol{\phi}_{\mathbf{q}}(t')\rangle-\langle T_H\{\mathcal{O}(t)\boldsymbol{\phi}_{\mathbf{q}}(t')\}\rangle]. \quad \text{(A11)}$$

Thus, from Eqs. (A1) and (A4) and the Hermitian-conjugate equations, we find the relationship

$$\sum_{\mathbf{k}_3}\left\{\left[i\frac{\partial}{\partial t_3}-\tau_3\varepsilon(\mathbf{k}_3)\right]\delta_{\mathbf{k}_1\mathbf{k}_3}-\tau_3\sum_{\mathbf{g}}\mathbf{M}(\mathbf{k}_1-\mathbf{k}_3-\mathbf{g};\mathbf{k}_3)\times[U_{\pm(\mathbf{k}_3-\mathbf{k}_1+\mathbf{g})}(t_3)+iv(\mathbf{k}_3-\mathbf{k}_1+\mathbf{g})(\delta/\delta J_{\mp(\mathbf{k}_3-\mathbf{k}_1+\mathbf{g})}(t_3^{\pm}))+i\boldsymbol{\alpha}^0(\mathbf{q}+\mathbf{g})(\delta/\delta\mathbf{F}_{\mp(\mathbf{k}_3-\mathbf{k}_1)}(t_3^{\pm}))]\right\}\mathbf{G}(3,2)=\tau_4\delta_{\mathbf{k}_1\mathbf{k}_2}\delta(t_3-t_2)\mathbf{1}, \quad \text{(A12)}$$

where the element

$$U_{\mathbf{k}_1+\mathbf{g}}(t_1)=v(\mathbf{k}_1+\mathbf{g})\langle\rho_{\mathbf{k}_1+\mathbf{g}}(t_1)\rangle+\boldsymbol{\alpha}^0(\mathbf{k}_1+\mathbf{g})\cdot\langle\boldsymbol{\phi}_{-\mathbf{k}_1}(t_1)\rangle+J_{\mathbf{k}_1+\mathbf{g}}(t_1) \quad \text{(A13)}$$

of the column vector $\mathbf{U}(1)$ is the $\mathbf{k}_1+\mathbf{g}$ component of the effective Hartree field at the time t_1, and where $\mathbf{1}$ is the unit matrix in l space. The sign $\pm$ is defined to be $+$ for the 1,1 and 1,2 elements in τ space and to be $-$ for the 2,1 and 2,2 elements; the $t^{\pm}$ is defined to be $t\pm 0^+$, where 0^+ is a positive infinitesimal. In order to convert Eq. (A12) into a Dyson equation, we note that

$$\delta\mathbf{G}=-\mathbf{G}\cdot\delta(\mathbf{G}^{-1})\cdot\mathbf{G}, \quad \text{(A14)}$$

where the inverse of the Green's function is defined by the equation

$$[\mathbf{G}^{-1}\mathbf{G}]_{12}\equiv\sum_{\mathbf{k}_3}\int_{-\infty}^{\infty}dt_3\mathbf{G}^{-1}(1,3)\mathbf{G}(3,2)=\delta_{\mathbf{k}_1\mathbf{k}_2}\delta(t_1-t_2)\mathbf{1}. \quad \text{(A15)}$$

Next, we note from Eq. (A15) that, even with sources present, Eq. (A12) defines the inverse

$$\mathbf{G}_0^{-1}(1,2)=\{[i\tau_4\mathbf{1}(\partial/\partial t_2)-\tau_3\varepsilon(\mathbf{k}_1)]\delta_{\mathbf{k}_1\mathbf{k}_2}-\tau_3\sum_{\mathbf{g}}U_{\pm(\mathbf{k}_2-\mathbf{k}_1+\mathbf{g})}(t_2)\mathbf{M}(\mathbf{k}_1-\mathbf{k}_2-\mathbf{g};\mathbf{k}_2)\}\times\delta(t_1-t_2) \quad \text{(A16)}$$

of the "noninteracting" Green's function. Now, treating the U's rather than the J's as independent functions, a vertex function

$$\boldsymbol{\Gamma}(1,2;3)\equiv\boldsymbol{\Gamma}(\mathbf{k}_1,\mathbf{k}_2;l_1,l_2;\mathbf{k}_3+\mathbf{g}_3;t_1,t_2;t_3)=-\tau_3[\delta/\delta U_{\pm(\mathbf{k}_3+\mathbf{g}_3)}(t_3)][\mathbf{G}^{-1}(1,2)]_{l_1l_2} \quad \text{(A17)}$$

can be defined in such a way that the lowest order term in $\boldsymbol{\Gamma}$ is particularly simple. Substituting Eq. (A16) for G_0^{-1} into Eq. (A17), we find

$$\boldsymbol{\Gamma}_0(1,2,3)=\tau_4\delta_{\mathbf{k}_3,\mathbf{k}_2-\mathbf{k}_1}\delta(t_1-t_2)\delta(t_1-t_3)M_{l_1l_2}(\mathbf{k}_3+\mathbf{g}_3;\mathbf{k}_1). \quad \text{(A18)}$$

Then, we introduce the transformation matrices

$$\mathbf{R}(1,2)\equiv\delta\mathbf{U}(1)/\delta\mathbf{J}(2) \quad \text{and} \quad \mathfrak{R}(1,2)\equiv\delta\mathbf{U}(1)/\delta\mathbf{F}(2),$$

which have matrix elements

$$R(1,2)=\delta_{\mathbf{k}_1\mathbf{k}_2}\delta_{\mathbf{g}_1\mathbf{g}_2}\delta(t_1-t_2)+v(\mathbf{k}_1+\mathbf{g}_1)\times(\delta\langle\rho_{\mathbf{k}_1+\mathbf{g}_1}(t_1)\rangle/\delta J_{\mathbf{k}_2+\mathbf{g}_2}(t_2))+\boldsymbol{\alpha}^0(\mathbf{k}_1+\mathbf{g}_1)\cdot(\delta\langle\boldsymbol{\phi}_{-\mathbf{k}_1}(t_1)\rangle/\delta J_{\mathbf{k}_2+\mathbf{g}_2}(t_2)), \quad \text{(A19)}$$

and

$$\mathfrak{R}(1,2)=\delta_{\mathbf{k}_1\mathbf{k}_2}\delta(t_1-t_2)+v(\mathbf{k}_1+\mathbf{g}_1)\times(\delta\langle\rho_{\mathbf{k}_1+\mathbf{g}_1}(t_1)\rangle/\delta F_{n_2,\mathbf{k}_2}(t_2))+\boldsymbol{\alpha}^0(\mathbf{k}_1+\mathbf{g}_1)\cdot(\delta\langle\boldsymbol{\phi}_{-\mathbf{k}_1}(t_1)\rangle/\delta F_{n_2,\mathbf{k}_2}(t_2)), \quad \text{(A20)}$$

respectively. Finally, we obtain the Dyson equation

$$[\mathbf{G}_0^{-1}\mathbf{G}]_{12}=\tau_4\delta_{\mathbf{k}_1\mathbf{k}_2}\delta(t_1-t_2)\mathbf{1}+i\sum_{\mathbf{k}_3}\cdots\sum_{\mathbf{k}_7}\sum_{\mathbf{g}_6}\sum_{\mathbf{g}_7}\int_{-\infty}^{\infty}dt_3\times\cdots dt_7\mathbf{M}(\mathbf{k}_7+\mathbf{g}_7;\mathbf{k}_3)\tau_3\mathbf{G}(3,4)\tau_3\boldsymbol{\Gamma}(4,5;6)\times\mathbf{G}(5,2)[v(\mathbf{k}_7+\mathbf{g}_7)R(6,7)+\boldsymbol{\alpha}^0(\mathbf{k}_7+\mathbf{g}_7)\cdot\mathfrak{R}(6,7)]\times\delta_{\mathbf{k}_7,\mathbf{k}_3-\mathbf{k}_1}\delta(t_3-t_1)\delta(t_7-t_1^{\pm}). \quad \text{(A21)}$$

We now remove all sources and make use of the invariance of the Hamiltonian H of Eq. (1) under translations either in time or though any lattice vector $\mathbf{R}_{ij}$ in space. For nonsuperconductors, it is obvious that the generalized single-particle Green's function $\mathbf{G}(1,2)$ is diagonal in spin space. Assuming that the ground state

$|0\rangle$ need not be an eigenstate of the total number operator and assuming Cooper pairing[76] in the superconducting state,[77] one finds that the Green's function $\mathbf{G}(1,2)$ and the interaction propagators $\mathbf{R}(1,2)$ and $\mathfrak{R}(1,2)$ reduce to the simple form

$$\mathbf{G}(1,2)=\delta_{\mathbf{k}_1\mathbf{k}_2}\mathbf{G}(\mathbf{k}_1;t_1-t_2), \tag{A22}$$

$$\mathbf{R}(1,2)=\delta_{\mathbf{k}_1\mathbf{k}_2}\mathbf{R}(k_1;t_1-t_2), \tag{A23}$$

and

$$\mathfrak{R}(1,2)=\delta_{\mathbf{k}_1\mathbf{k}_2}\mathfrak{R}(k_1;t_1-t_2), \tag{A24}$$

in all cases. This simplification of the form of $G(1,2)$, $R(1,2)$, and $\mathfrak{R}(1,2)$ allows us to define the simple Fourier transforms

$$\mathbf{G}(k)\equiv\int_{-\infty}^{\infty}dt\mathbf{G}(\mathbf{k},t)\exp(ik_0t), \tag{A25}$$

$$\mathbf{R}(q)\equiv\int_{-\infty}^{\infty}dt\mathbf{R}(\mathbf{q},t)\exp(iq_0t), \tag{A26}$$

$$\mathfrak{R}(q)\equiv\int_{-\infty}^{\infty}dt\mathfrak{R}(\mathbf{q},t)\exp(iq_0t), \tag{A27}$$

and

$$[\mathbf{\Gamma}(k,q;\mathbf{g})]_{12}\equiv\int_{-\infty}^{\infty}dtdt'\times\mathbf{\Gamma}(\mathbf{k}+\mathbf{q},\mathbf{k};l_1,l_2;\mathbf{q}+\mathbf{g};t,0;t-t')\times\exp[i(k_0t+q_0t')], \tag{A28}$$

where the arguments $k\equiv\mathbf{k},k_0$ and $q\equiv\mathbf{q},q_0$ are four momenta. This, in turn, allows us to rewrite the Dyson equation (A21) in the simplified form

$$\mathbf{G}(k)=[\mathbf{G}_0^{-1}(k)-\mathbf{\Sigma}(k)]^{-1}, \tag{A29}$$

where

$$\mathbf{\Sigma}(k)=i\sum_{\mathbf{q}}\sum_{\mathbf{g}1}\sum_{\mathbf{g}2}\int_{-\infty}^{\infty}\frac{dq_0}{2\pi}\mathbf{M}^T(\mathbf{q}+\mathbf{g}_2;\mathbf{k})\tau_3\mathbf{G}(k+q)\times\tau_3\mathbf{\Gamma}(k,q;\mathbf{g}_1)v(\mathbf{q}+\mathbf{g}_2)K_{12}(q)\exp(iq_00^{\pm}) \tag{A30}$$

is the irreducible self-energy tensor, and where

$$K_{12}(q)=[\mathbf{R}(q)]_{12}+\sum_n\alpha_n(\mathbf{q}+\mathbf{g}_2)\mathfrak{R}_n(\mathbf{q}+\mathbf{g}_1,q_0)/v(\mathbf{q}+\mathbf{g}_2) \tag{A31}$$

is the total interaction propagator.

Finally, in order to evaluate Eq. (A30) for the self-energy $\mathbf{\Sigma}$, we must find a simple expression for the interaction propagator $\mathbf{R}$ and $\mathfrak{R}$. This requires the evaluation of the double commutator $[[\phi_{n,q},(H+H_s)]$, $(H+H_s)]$, which yields the equation

$$M_{n,\mathbf{q}}[-(\partial^2/\partial t^2)-(\omega_n{}^0(\mathbf{q}))^2]\langle\phi_{n,-\mathbf{q}}(t)\rangle=F_{n,\mathbf{q}}(t)-i\sum_{\mathbf{g}}\alpha_n{}^0(\mathbf{q}+\mathbf{g})\sum_{\mathbf{k}}\times\mathrm{Tr}[\mathbf{M}(\mathbf{q}+\mathbf{g};\mathbf{k})\mathbf{G}^{11}(\mathbf{k},\mathbf{k}+\mathbf{q};t,t^+]), \tag{A32}$$

where $\mathbf{G}^{11}$ is the 1,1 component of $\mathbf{G}$ in τ space. Another set of equations for $\langle\phi_{n,\mathbf{q}}(t)\rangle$ arises from the definitions (A2) and (A13) of ϱ and $\mathbf{U}$:

$$\boldsymbol{\alpha}^0(\mathbf{q}+\mathbf{g})\cdot\langle\boldsymbol{\phi}_{-\mathbf{q}}(t)\rangle=U_{\mathbf{q}+\mathbf{g}}(t)-J_{\mathbf{q}+\mathbf{g}}(t)+iv(\mathbf{q}+\mathbf{g})\times\sum_{\mathbf{k}}\mathrm{Tr}[\mathbf{M}(\mathbf{q}+\mathbf{g},\mathbf{k})\mathbf{G}^{11}(\mathbf{k},\mathbf{k}+\mathbf{q};t,t^+)]. \tag{A33}$$

It is now clear that the elimination of $\langle\phi_{n,\mathbf{q}}(t)\rangle$ between Eqs. (A32) and (A33) and the functional differentiation of the resultant equation with respect to $\mathbf{J}_q$ and $\mathbf{F}_q$ should yield equations for $\mathbf{R}(q)$ and $\mathfrak{R}(q)$, respectively. Removing all sources, one finds the equations

$$\mathbf{R}(q)=[\mathbf{1}-\mathbf{A}_0(q)\mathbf{P}_e(q)]^{-1} \tag{A34}$$

and

$$\mathfrak{R}_n(\mathbf{q}+\mathbf{g})=M_{n,\mathbf{q}}{}^{-1}\sum_{\mathbf{g}'}R_{\mathbf{g}\mathbf{g}'}(\mathbf{q})\alpha_n{}^0(\mathbf{q}+\mathbf{g}')/[q_0{}^2-(\omega_n{}^0(\mathbf{q}))^2], \tag{A35}$$

where the tensor $\mathbf{A}_0(q)$ has matrix elements

$$[\mathbf{A}_0(q)]_{\mathbf{g}\mathbf{g}'}=\delta_{\mathbf{g}\mathbf{g}'}+\sum_n\frac{\alpha_n{}^0(\mathbf{q}+\mathbf{g})\alpha_n{}^0(\mathbf{q}+\mathbf{g}')}{M_{n,\mathbf{q}}v(\mathbf{q}+\mathbf{g}')[\mathbf{q}_0{}^2-(\omega_n{}^0(q))^2+i0^+]}, \tag{A36}$$

and where the tensor $\mathbf{P}_e(q)$ has matrix elements

$$[\mathbf{P}_e(q)]_{\mathbf{g}\mathbf{g}'}=-iv(\mathbf{q}+\mathbf{g})\sum_{\mathbf{k}}\int_{-\infty}^{\infty}\frac{dk_0}{2\pi}\exp(ik_00^+)\times\mathrm{Tr}[\mathbf{G}^{11}(k+q)\mathbf{M}(\mathbf{q}+\mathbf{g};\mathbf{k})\times\mathbf{G}^{11}(k)\mathbf{\Gamma}^{11}(k,q;\mathbf{g}')], \tag{A37}$$

which give the electronic contribution to the polarizability of any crystal and define the dielectric tensor

$$\boldsymbol{\kappa}(q)=\mathbf{1}-\mathbf{P}_e(q)=\mathbf{K}_e{}^{-1}(q). \tag{A38}$$

Finally, from Eqs. (A31) and (A34)–(A36) we find the total interaction propagator

$$\mathbf{K}(q)=[\mathbf{A}_0{}^{-1}(q)-\mathbf{P}_e(q)]^{-1}. \tag{A39}$$

Given the definitions (A17), (A28), (A36), (A37), and (A39), of $\mathbf{\Gamma}$ and $\mathbf{K}$, Eqs. (A29) and (A30) constitute a complete set of Dyson equations for the electrons of a perfect crystal, in either the superconducting state or the normal state. However, our equations for the total-interaction propagator $\mathbf{K}(q)$ do not have a

[76] L. N. Cooper, Phys. Rev. **104**, 1189 (1956).

[77] These are essentially the two basic assumptions of the BCS theory.

convenient form. We should express $\mathbf{K}(q)$ as a sum

$$\mathbf{K}(q)=\mathbf{K}_e(q)+\mathbf{K}_{\rm ph}(q) \tag{A40}$$

of Coulomb and phonon-induced contributions, where the phonon-induced contribution is expressed in terms of the renormalized, experimentally observable phonon frequencies $\omega_\nu(\mathbf{q})$, rather than the bare frequencies $\omega_n{}^0(\mathbf{q})$.[78]

In order to determine the renormalized phonon frequencies, we now find the phonon Green's function

$$\mathbf{D}(1,2)\equiv i\langle T_H\{\boldsymbol{\phi}_{\mathbf{q}_1}(t)\boldsymbol{\phi}_{\mathbf{q}_2}{}^\dagger(t_2)\}\rangle. \tag{A41}$$

The functional differentiation of Eq. (A32) with respect to $F_{n',\mathbf{q}'}(t')$ yields the equation

$$M_{n,\mathbf{q}_1}[(\partial^2/\partial t_1{}^2)+(\omega_n{}^0(\mathbf{q}_1))^2]\{D_{nn'}(1,2)-i\langle\phi_{n,\mathbf{q}_1}(t_1)\rangle \times\langle\phi_{n',\mathbf{q}_2}{}^\dagger(t_2)\rangle=\delta_{nn'}\delta_{\mathbf{q}_1\mathbf{q}_2}\delta(t_1-t_2) -i\sum_{\mathbf{g}}\alpha_n{}^0(\mathbf{q}_1+\mathbf{g})\sum_{\mathbf{k}}\frac{\delta}{\delta\mathbf{F}_{n',\mathbf{q}_2}(t_2)} \times\{\mathrm{Tr}[M(\mathbf{q}_1+\mathbf{g};\mathbf{k})\mathbf{G}^{11}(\mathbf{k},\mathbf{k},+\mathbf{q}_1;t_1,t_1{}^+)]\}, \tag{A42}$$

which is analogous to Eq. (A12). This equation yields the simple formula

$$[\mathbf{D}_0{}^{-1}(1,2)]_{n,n'}=M_{n,\mathbf{q}_2}[(\partial^2/\partial t_2{}^2)+(\omega_{n'}{}^0(\mathbf{q}_2))^2] \times\delta_{nn'}\delta_{\mathbf{q}_1\mathbf{q}_2}\delta(t_1-t_2) \tag{A43}$$

for the noninteracting phonon Green's function, even in the presence of source terms. Making use of the invariance properties of the Hamiltonian H of Eq. (1), we see that the phonon Green's function must have the simple form

$$\mathbf{D}(1,2)=\delta_{\mathbf{q}_1\mathbf{q}_2}\mathbf{D}(\mathbf{q}_1;t_1-t_2). \tag{A44}$$

[78] As we shall show, the index ν of $\omega_\nu(\mathbf{q})$ does not have precisely the same meaning as the index n of $\omega_n{}^0(q)$. Renormalized phonon states are hybridized by electron-phonon interactions in the same way that electronic bands are hybridized by electron-electron interactions.

This allows us to define the Fourier transform

$$\mathbf{D}(q)=\int_{-\infty}^{\infty}dt\,\mathbf{D}(\mathbf{q},t)\exp(iq_0t), \tag{A45}$$

and to write the phonon Dyson equation

$$\mathbf{D}(q)=[\mathbf{D}_0{}^{-1}(q)-\boldsymbol{\Pi}(q)]^{-1}, \tag{A46}$$

where from Eqs. (A42) and (A43) the phonon self-energy is given by

$$\boldsymbol{\Pi}(q)=\sum_{\mathbf{g}}[\mathfrak{A}_0(q)[\mathbf{P}_e(q)-\mathbf{1}]]_{\mathbf{g}\mathbf{g}}, \tag{A47}$$

and where the tensor $\mathfrak{A}_0(\mathbf{q})$ has matrix elements

$$[\mathfrak{A}_0(\mathbf{q})]_{nn',\mathbf{g}\mathbf{g}'}=\alpha_n{}^0(\mathbf{q}+\mathbf{g})\alpha_{n'}{}^0(\mathbf{q}+\mathbf{g}')/v(\mathbf{q}+\mathbf{g}'). \tag{A48}$$

Remembering that the quantity $\mathrm{Re}\{[\mathbf{P}_e(q)\mathbf{K}_e(q)]_{\mathbf{g}\mathbf{g}'}\}$ is negative for values of q_0 less than the $\mathbf{g},\mathbf{g}'$ component of the plasma-frequency matrix $\boldsymbol{\omega}_{\rm pl}(\mathbf{q})$ [79] and that it decreases very rapidly from plus infinity at $q_0=[\boldsymbol{\omega}_{pl}(\mathbf{q})]_{\mathbf{g}\mathbf{g}'}$ to a value of order unity for larger values of q_0, we see immediately from Eq. (21) that the eigenvalues $D_\nu(q)$ of the phonon Green's function $\mathbf{D}(\mathbf{q})$ must each have more than one pole in the complex q_0 plane. The first and most important pole occurs at a frequency $\omega_\nu(\mathbf{q})$ which is lower than the unrenormalized frequency $\omega_\nu{}^0(\mathbf{q})$ and which, for acoustic phonons, approaches zero as $\mathbf{q}$ approaches zero. This pole gives the renormalized phonon frequency. The other poles, which are at frequencies slightly higher than the frequencies $[\boldsymbol{\omega}_{pl}(\mathbf{q})]_{\mathbf{g}\mathbf{g}'}$, and which correspond to plasma oscillations, give a total contribution to the integral

$$2M_{\nu,\mathbf{q}}\int_{-\infty}^{\infty}\frac{q_0}{2\pi}D_\nu(q)dq_0=1, \tag{A49}$$

which is only of order $m/M_{\nu,\mathbf{q}}\ll1$ for metals. Even in degenerate semiconductors these poles at higher energies contribute only negligibly to the sum rule (A49).

[79] The 0,0 component of $\boldsymbol{\omega}_{\rm pl}(\mathbf{0})$ is the conventional plasma frequency $\omega_{\rm pl}$; the real part $\mathrm{Re}\{\kappa_{ij}(\mathbf{q},q_0)\}$ of the i,j component of the dielectric tensor vanishes at the frequency $[\boldsymbol{\omega}_{\rm pl}(q)]_{ij}$, which in general is greater than $\omega_{\rm pl}$.