# Two theorems on superconductivity in tight-binding metals

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The one-band tight-binding model is used to calculate the effective interaction between electrons in superconductors. Two theorems are proved. One is that the effective interaction is always repulsive when including only electron-electron interactions. The second theorem relates to the electron-phonon interaction. The interaction due to charge fluctuations can become attractive when the effective potential changes sign.

## I. INTRODUCTION

Superconductivity is due to the pairing of electrons at the chemical potential. The mechanism which pairs electrons in high-temperature superconductors is actively debated and still undecided. Most analytical modes of high-$T_c$ superconductors assume a tight-binding model for the electrons in the conduction band. Here we use the tight-binding model to prove two theorems relating to the pairing of electrons. One theorem relates to electron-electron interactions, while the other relates to electron-phonon interactions. These theorems relate to the sign of the effective interaction between quasiparticles: when is it attractive?

There have been many past discussions of the pairing potential between electrons.[1–7] If the effective interaction is written as $V=v_q/\varepsilon(q)$ then this discussion is about the possible sign of the dielectric function $\varepsilon(q)$. References 1–7 provide the inspiration for the present work. Many of these papers also discuss the relation of the sign of the dielectric function to superconductivity. The present theorem should be regarded as an extension of these earlier papers, as well as our earlier paper which argued against a plasmon mechanism for superconductivity.[8]

Electrons in metals are described by several possible basis sets. In the homogeneous electron gas, the eigenstates are plane waves, and the dielectric function depends upon $\varepsilon(q,\omega)$. Previous work[1–7] has related the onset of superconductivity to whether $\varepsilon(q,0)<0$. For a solid with periodic unit cells, the dielectric function depends upon two wave-vector components $\varepsilon(\mathbf{q}+\mathbf{G},\mathbf{q}+\mathbf{G}',\omega)$ where $\mathbf{G}$ are reciprocal-lattice vectors. This function has also been discussed with relation to superconductivity.[2,4]

The other common basis set for discussing electrons is the tight-binding model. Here the electrons are in orbitals on atoms, and motion occurs by weak bonding between neighboring orbitals. This basis has not been previously discussed in relation to the sign of the dielectric function and superconductivity. In prior work, using other methods, the authors have concluded that it is quite important to include an accurate description of local electron correlation. The tight-bonding model does this in a natural way. An advantage of this basis is that, for a single band, the dielectric function again only depends upon a single spatial or wave-vector variable[5–7] $\varepsilon(\mathbf{q},\omega)$.

Our system is a solid, in either two or three dimensions, with a single conduction band given by the overlap of $s$-wave orbitals. We include the hopping term between neighboring atoms. Electron-electron interactions are included between electrons on distant sites $V_{jl}$ as well as on the same site $U=V_{jj}$. Mattis and co-workers[5–7] have shown that the effective potential for charge fluctuations is given by

$$\bar{V}(q)=\frac{U}{2}+\sum_{j\neq 0} V_{j0}e^{i\mathbf{q}\cdot\mathbf{R}_{j0}} . \tag{1}$$

This interaction is strongly repulsive at small wave vector. However, it may change sign and become negative for wave vectors near the edge of the Brillouin zone. We find that the effective interaction between electrons depends upon the sign of $\bar{V}(q)$. The first theorem states that the interaction is repulsive, regardless of the sign of $\bar{V}(q)$, if one includes only electron-electron interactions. The second theorem states that, when including phonons, the pairing due to charge fluctuations is attractive whenever $\bar{V}(q)$ is negative. These theorems are quite general: they apply to any lattice, to any kind of phonon force constants, and to dielectric functions with any kind of local-field corrections. Their only restriction is to a one-hand tight-binding model.

The properties of the superconductor are usually well described by the Eliashberg equations[9–11] for the superconducting correlation function $W(p)$

$$W(p)=-\sum_q V_{\rm eff}(q) \times\frac{W(p+q)}{(p_n+q_m)^2Z(p+q)^2+\xi^2_{p+q}+W(p+q)^2} , \tag{2}$$

$$Z(p)=1-\frac{\Sigma(p)}{ip_n} . \tag{3}$$

We use a four vector notation $p=(\mathbf{p},ip_n)$ in terms of the

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wave vector $\mathbf{p}$ and the complex frequency $ip_n = 2\pi i k_B T(n+1/2)$. The symbol $\xi_{p+q}$ denotes the quasiparticle dispersion in the tight-binding model, while $\Sigma(p)$ is the electron self-energy from the effective interaction $V_{\text{eff}}$. These equations simplify at the transition temperature $T_c$ of the superconductor. There the gap vanishes ($W \to 0$) and one obtains a linear equation for $W$. One also uses the normal-state expression for $\Sigma(p)$. Owen and Scalpino[9] showed that the easiest way to solve the above equations is by staying with imaginary frequencies, rather than continuing the equations to the space of real frequency. One reason is that most of the quantities are real when using imaginary frequency. We find that our discussion of superconductivity is also much easier in this case.

Here we extend this discussion to the case of tight-binding models. We must write down a Hamiltonian, derive the form for the effective interaction $V_{\text{eff}}$, and to examine whether it can be negative. The first theorem is that $V_{\text{eff}}$ is always positive for any value of four vector $q$.

The problem is the minus sign in (2). A solution to the equation requires that one or more of the terms be negative. If $V_{\text{eff}}$ is positive for all values of four vector $q$, then a solution is only found if the negative sign comes from $W(p)$. That is possible, as is discussed in the next section.

## II. EXTENDED HUBBARD MODEL

Here we consider only electronic contributions to the effective interaction, and discuss phonons in the following section. The model will be an extended Hubbard model for a single band

$$H = \sum_{j\delta\sigma} W(\delta) C^{\dagger}_{j+\delta,\sigma} C_{j\sigma} + U \sum_j n_{j\uparrow} n_{j\downarrow} + \sum_{j\neq l} n_j n_l V_{nl} , \tag{4}$$

$$n_{j\sigma} = C^{\dagger}_{j\sigma} C_{j\sigma} , \tag{5}$$

$$n_j = \sum_{\sigma=\pm} n_{j\sigma} , \tag{6}$$

$$V_{jl} = e^2 \int dr_1 dr_2 \frac{\rho(\mathbf{r}_1)\rho(\mathbf{r}_2)}{|\mathbf{r}_1 - \mathbf{r}_2 + \mathbf{R}_{jl}|} . \tag{7}$$

The onsite Coulomb repulsion is $U$ while the Coulomb interaction at different sites is labeled $V_{jl}$. Both depend upon the charge distribution $\rho(\mathbf{r})$ from the orbitals at one site. In the one-band model we assume there is only one site per unit cell of the crystal. We convert the operators to collective coordinates of wave vector, and write the Hamiltonian as

$$H = \sum_{k\sigma} \xi_k C^{\dagger}_{k\sigma} C_{k\sigma} + \frac{1}{2N} \sum_q \left\{ \bar{V}(q) \rho_c(q) \rho_c(-q) - \frac{U}{2} \rho_s(q) \rho_s(-q) \right\} , \tag{8}$$

$$\rho_c(q) = \sum_{k\sigma} C^{\dagger}_{k+q,\sigma} C_{k\sigma} , \tag{9}$$

$$\rho_s(q) = \sum_{k\sigma} \sigma C^{\dagger}_{k+q,\sigma} C_{k\sigma} . \tag{10}$$

The electron-electron interaction has been separated into charge fluctuations and spin fluctuations. We assume that these contributions are independent and do not mix. This assumption underlies most theories of electron correlation. In the present model it is true for random-phase approximation (RPA)-type theories, as well as those including Hubbard corrections. In writing expressions such as $\rho_c \rho_c$ we omit the contribution of a particle interacting with itself. With this form for the interaction, we give the expressions for the change in ground-state energy, the self-energy $\Sigma(p)$ in the normal state, and for the effective interaction in the gap equations. We follow Mattis and employ the screened-exchange approximation[5-7]

$$\delta E_g = -\frac{1}{2} \sum_q \left\{ \ln[1 - \bar{V}(q)P(q)] + \ln\left[1 + \frac{U}{2} P(q)\right] \right\} , \tag{11}$$

$$\Sigma(p) = -\sum_q G(p+q) \left\{ \frac{\bar{V}(q)}{1 - \bar{V}(q)P(q)} - \frac{U/2}{1 + (U/2)P(q)} \right\} , \tag{12}$$

$$V_{\text{eff}} = \frac{\bar{V}(q)}{1 - \bar{V}(q)P(q)} + \frac{U/2}{1 + (U/2)P(q)} \tag{13}$$

$$= \frac{\bar{V}(q) + U/2}{[1 - \bar{V}(q)P(q)][1 + (U/2)P(q)]} . \tag{14}$$

Note that the spin fluctuations have different signs in the contribution for the electron self-energy and for the effective interaction in superconductivity.

The electron polarization operator $P(q)$ is defined and discussed below. In a simple model it could be RPA, but it could also include Hubbard-type local-field corrections. Our theorem includes both cases.

Now we show that $V_{\text{eff}} > 0$ for this form of the interaction. This proof relies on three assumptions:

$$\bar{V}(q) + \frac{U}{2} > 0 , \tag{15}$$

$$P(\mathbf{q}, iq_n) < 0 , \tag{16}$$

$$1 + \frac{U}{2} P(q) > 0 . \tag{17}$$

The first assertion (15) was proved by Mattis.[5] Starting from the definitions of $U$ and $V_{jl}$ one can show that in three dimensions

$$\bar{V}(q) + \frac{U}{2} = \sum_{\mathbf{G}} \frac{4\pi e^2 |\Lambda(\mathbf{G}+\mathbf{q})|^2}{V_0 |\mathbf{G}+\mathbf{q}|^2} , \tag{18}$$

$$\Lambda(\mathbf{G}+\mathbf{q}) = \int dr e^{i\mathbf{r}\cdot(\mathbf{G}+\mathbf{q})} \rho(\mathbf{r}) , \tag{19}$$

where $\mathbf{G}$ are the reciprocal-lattice vectors of the solid. The right-hand side of (18) is positive, which proves (15). A similar proof applies to two dimensions for any distribution of charge $\rho(r)$. A simple result is obtained when the distribution is a three-dimensional Gaussian $\rho(r) = \exp(-r^2/b^2)/(\sqrt{\pi} b)^3$

$$\bar{V}(q)+\frac{U}{2}=\sum_{\mathbf{G}}\frac{2\pi e^2\,\mathrm{erfc}(|\mathbf{G}+\mathbf{q}|b/\sqrt{2})}{A_0|\mathbf{G}+\mathbf{q}|}\ . \tag{20}$$

The interesting aspect is that $\bar{V}(q)$ can be negative for large values of wave vector. However, the combination of $\bar{V}(q)+U/2$ must always be positive. The symbols $V_0$ in (18), and $A_0$ in (20), are the volume and areas of the crystal unit cell.

The second assertion (16) we discuss below. The third assumption (17) is that the system of electrons is nonmagnetic. Reversing the inequality in (17) is an indication that the system prefers the electrons to be magnetically ordered. We assume that this is not the case.

If we assume the validity of (15)–(17) then we can write

$$\left[\bar{V}(q)+\frac{U}{2}\right]P<0\ , \tag{21}$$

$$1+\frac{U}{2}P<1-\bar{V}(q)P\ . \tag{22}$$

The second equation follows immediately from the first. Since we assume that the system is not antiferromagnetic then we combine the inequalities

$$0<1+\frac{U}{2}P<1-\bar{V}(q)P\ . \tag{23}$$

We have proved that both factors in the denominator of $V_{\text{eff}}$ in (14) are positive. The numerator is positive. So we have proved that $V_{\text{eff}}$ is positive, which is the theorem.

This proof does not rely on the specific form for the band dispersion. The theorem is valid in two and three dimensions, and also for layered solids. Neither do we assume any specific approximation for the electron polarizability $P(q)$. The theorem is valid even if one includes contributions such as Hubbard-type local-field corrections.

Now we prove (16). Start with the definition and inset various exact eigenstates $|n\rangle$ and $|m\rangle$ of the Hamiltonian[11]

$$\bar{P}(q,iq_m)=-\frac{1}{V}\int_0^\beta d\tau e^{i\tau q_m}\langle T_\tau\rho_c(\mathbf{q},\tau)\rho_c(-\mathbf{q},0)\rangle \tag{24}$$

$$=-\frac{1}{V}\sum_{nm}e^{-\beta E_n}|\langle n|\rho_c(\mathbf{q})|m\rangle|^2\frac{e^{\beta(E_n-E_m)}-1}{iq_m+E_n-E_m} \tag{25}$$

$$=2\int_{-\infty}^{\infty}d\omega\frac{R(\mathbf{q},\omega)\sinh(\beta\omega/2)}{iq_m-\omega}\ , \tag{26}$$

$$R(\mathbf{q},\omega)=\frac{1}{V}\sum_{nm}e^{-\beta(E_n+\omega/2)}|\langle n|\rho_c(\mathbf{q})|m\rangle|^2\times\delta(\omega+E_n-E_m). \tag{27}$$

We have used the fact that $\rho_c(\mathbf{q})=\rho_c^\dagger(-\mathbf{q})$. It is obvious that the kernal $R(\mathbf{q},\omega)$ is positive or zero for all values of frequency $\omega$. Next, it is easy to prove that

$$R(\mathbf{q},\omega)=R(-\mathbf{q},-\omega)\ . \tag{28}$$

The proof just involves interchanging dummy variables $n$ and $m$ in the definition of $R(\mathbf{q},\omega)$. We assume the lattice has sufficient symmetry that $P(-\mathbf{q},iq_m)=P(\mathbf{q},iq_m)$ which means that $R(-\mathbf{q},\omega)=R(\mathbf{q},\omega)=R(\mathbf{q},-\omega)$. So we have proved that $R(\mathbf{q},\omega)$ is symmetric in frequency if the lattice has a center of symmetry. In this case we can write

$$\bar{P}(\mathbf{q},iq_m)=-4\int_0^\infty d\omega\sinh(\beta\omega/2)R(\mathbf{q},\omega)\frac{\omega}{\omega^2+q_m^2}\ . \tag{29}$$

This proves $\bar{P}(q)<0$ since all factors in the integrand are positive. In the screened-exchange approximation, we have that

$$\bar{P}=\frac{P}{1-\bar{V}(q)P}<0\ . \tag{30}$$

This has two possible solutions. The first is $P<0$ and $1-\bar{V}(q)P>0$. This is in accord with (23), since we assumed that $P<0$ in proving that $1-\bar{V}(q)P>0$. So $P<0$ and $1-\bar{V}(q)P>0$ are consistent statements.

The other case has $P>0$ and $1-\bar{V}(q)P<0$. We believe it is inconsistent, since if $P$ changes sign then $1-\bar{V}(q)P$ does not change sign at the same place. Since $P<0$ at the origin ($iq_n=0,\mathbf{q}\to0$) and it cannot diverge, then it gets to positive values by going through the origin. For infinitesimal positive values one would have that $P>0$ and $1-\bar{V}(q)P>0$ which contradicts the above requirement.

Note that Hubbard-type corrections to the dielectric function do not change this result. They serve to modify the value of $P(q)$, but do not change its sign.

We have shown that $V_{\text{eff}}$ is always positive for all values of $(\mathbf{q},iq_m)$ for any one-band tight-binding model of electron-electron interactions. In deriving this result we make several assumptions: (i) The metal is paramagnetic, so that $1+UP/2>0$; (ii) There is inversion symmetry so that $P(-\mathbf{q},iq_m)=P(\mathbf{q},iq_m)$. Then the result is true for any tight-binding model which involves only one band.

We have shown that tight-binding models require that the effective electron-electron interaction in the Eliashberg equation is always positive. In order to have a superconductor, one must have a solution to (2), which means one must find a minus sign someplace. Three ways have been suggested for finding this sign.

(1) The gap function $W(\mathbf{p},ip_n)$ could vary in sign as the direction of the wave vector $\mathbf{p}$ changes around the Fermi surface. For the cuprate superconductors, where the conduction is largely two dimensional, it has been suggested that the gaps have $d$-wave symmetry. Another way is to have a very anisotropic $s$ wave, with nodes, as we suggested before. Many experiments have been done to test this hypothesis.[12–14]

(2) There has been continuous development[15–21] of the idea that plasmons could be the intermediate boson which pairs the electrons in the superconductor. Most of these theories have used an effective interaction $V_{\text{eff}}$ which is strictly positive, and assumed an isotropic gap. Sham and co-workers[16,17] have suggested that the sign change occurs because $W(\mathbf{p},ip_n)$ changes sign as a function of $ip_n$. Recent work[18,19,21] on plasmon mechanisms includes local-field corrections, which considerably reduce $T_c$ or even eliminate superconductivity.

(3) The third possibility is that phonons could change the sign of the dielectric function. The spin fluctuation is a single site term, and is unaffected by phonons. The effective screening for charge fluctuations is changed

$$\frac{\bar{V}(q)}{1-\bar{V}(q)P}\rightarrow\frac{\bar{V}(q)}{1-\bar{V}(q)P+\varepsilon_{\rm ph}}\ , \tag{31}$$

$$\varepsilon_{\rm ph}=\frac{1}{\bar{V}(q)}\sum_j\frac{g_j(\mathbf{q})}{\omega_j(q)^2+q_m^2}\ , \tag{32}$$

$$g_j(\mathbf{q})=2\omega_j(q)|M_j(\mathbf{q})|^2\ . \tag{33}$$

At first sight this change appears to makes the dielectric function for charge fluctuations more positive since the phonon term $\varepsilon_{\rm ph}$ appears positive. However, the phonon frequencies $\omega_j(q)$ which appear in this expression are not the physical ones measured by neutron scattering or x rays. Instead, they are the phonons calculated without the benefit of electron-electron interactions. They are unscreened. Since they are not the physical frequencies, they may have unphysical properties. Reference 3 discusses the possibility that $\omega_j(q)^2<0$ which could make the phonon term attractive at imaginary frequencies. This contribution, if large enough, could make $V_{\rm eff}<0$ at zero frequency. This is the basis of the phonon theories of superconductivity. They work if the unscreened phonons have $\omega_j(q)^2<0$.

In the cuprate superconductors, the phonons are measured in the antiferromagnetic state, which is an insulator, where there is no screening from charge fluctuations. Here all of the phonons have positive frequencies, as required by crystal stability. The superconductivity state is achieved by doping the sample to make it conducting. According to the phonon scenario, this doping must cause a lattice instability for the unscreened phonons.

## III. PHONONS

The function $g(\mathbf{q})$ does not contain the frequency and it must be positive. However, the factor $\bar{V}(q)$ could be negative at large $\mathbf{q}$, which would make the phonon term negative even for $\omega_j(q)^2>0$. Here we wish to develop this idea further. We prove our second theorem, which is that the denominator in (31) is negative at zero frequency when $\bar{V}(q)<0$.

We adopt the notation of Ref. 22 for the phonons. Let $u_\alpha(l,\kappa)$ be the displacement of the ion in cell $l$ at site $\kappa$ in the direction $\alpha$. Similarly, $e_\alpha(\kappa|\mathbf{q}j)$ is the unit vector which gives the displacement of ion $\kappa$ in the direction $\alpha$ for the mode $(\mathbf{q},j)$ where $j$ denotes polarization. These unit vectors are an orthonormal set. The eigenvalue equation for the phonon modes are given in terms of a symmetric force matrix $\mathcal{D}_{\alpha\beta}$ as

$$\omega_j^2 e_\alpha(\kappa|\mathbf{q}j)=\sum_{\beta\kappa'}\mathcal{D}_{\alpha\beta}(\mathbf{q}|\kappa\kappa')e_\beta(\kappa'|\mathbf{q}j)\ . \tag{34}$$

Divide this expression by $\omega_j^2$, multiply by $e_\mu^*$, and sum over all phonon modes $j$. One then produces the identity

$$\delta_{\alpha\beta}\delta_{\kappa\kappa'}=\sum_{\mu\kappa''}\mathcal{D}_{\alpha\mu}(\mathbf{q}|\kappa\kappa'')\mathcal{H}_{\mu\beta}(\mathbf{q}|\kappa''\kappa')\ , \tag{35}$$

$$\sum_j\frac{e_\alpha(\kappa|\mathbf{q}j)e_\beta^*(\kappa'|\mathbf{q}j)}{\omega_j^2}=\mathcal{H}_{\alpha\beta}(\mathbf{q}|\kappa\kappa')\ . \tag{36}$$

The matrix $\mathcal{H}_{\alpha\beta}$ is the inverse of the phonon force matrix. The usefulness of this result arises when we realize that we can write the numerator in (32) as

$$g_j=|\mathbf{e}\cdot\mathbf{w}|^2\ , \tag{37}$$

$$\varepsilon_{\rm ph}(\mathbf{q},0)=\frac{1}{\bar{V}(q)}\sum_j\frac{g_j}{\omega_j^2} \tag{38}$$

$$=\mathbf{w}\cdot\left[\frac{1}{\bar{V}(q)\mathcal{D}'}\right]\cdot\mathbf{w}^*\ . \tag{39}$$

The vector $\mathbf{w}(\mathbf{q})$ is the force on an electron due to an ion displacement. Vectors are in a space given by $(\alpha,\kappa)$: the spatial direction and ion in the unit cell. The dot product of two vectors is over this space.

We see that we can write the phonon part of the dielectric function, at zero frequency, in terms of simple vectors and matrices. Now we have to decide the proper form for the factor $\mathcal{D}'$ which enters the above expression.

The ion displacements can be expressed in terms of collective coordinates $Q_\alpha(\kappa|\mathbf{q}j)$. Two terms in the Hamiltonian are of interest: the quadratic term in $Q$ for the phonon dispersion, and the linear term in $Q$ for the electron-phonon interaction. They can be written as

$$u_\alpha(l,\kappa)=\frac{1}{\sqrt{N}}\sum_{\mathbf{q}j}Q_\alpha(\kappa|\mathbf{q}j)e^{i\mathbf{q}\cdot\mathbf{r}_j}\ , \tag{40}$$

$$H_{\rm ph}=\sum_{l\kappa}\frac{P_{l\kappa}^2}{2M_\kappa}+\frac{1}{2}\sum_{\alpha\beta\mathbf{q}\kappa\kappa' jj'}Q_\alpha(\kappa|\mathbf{q}j)\mathcal{D}_{\alpha\beta}(\mathbf{q}|\kappa\kappa')Q_\beta^\dagger(\kappa'|\mathbf{q}j')$$
$$+\frac{1}{\sqrt{N}}\sum_{\mathbf{q}}\rho_c(\mathbf{q})\mathbf{Q}\cdot\mathbf{w}(\mathbf{q})\ . \tag{41}$$

Starting from this type of phonon Hamiltonian, Ref. 11 describes several ways of deriving the form for $\varepsilon_{\rm ph}$. The easiest method is just adding the electron-phonon interaction to the electron-electron interaction for charge fluctuations. That is, combine the second term in (8) with the above terms in the following combinations:

$$V=\frac{1}{2}\sum_q\bar{V}(q)\left[\frac{\rho_c}{\sqrt{N}}+\frac{\mathbf{Q}\cdot\mathbf{w}}{\bar{V}(q)}\right]\left[\frac{\rho_c}{\sqrt{N}}+\frac{\mathbf{Q}\cdot\mathbf{w}}{\bar{V}(q)}\right]^\dagger$$
$$+\frac{1}{2}\sum_q\mathbf{Q}\cdot\left[\mathcal{D}-\frac{\mathbf{w}\mathbf{w}^*}{\bar{V}(q)}\right]\cdot\mathbf{Q}^\dagger\ .$$

In this derivation, the expression for $\varepsilon_{\rm ph}$ has precisely the form given in (32), where the phonons have as their effective force tensor the quantity in the last term of the above equation. At zero frequency we derive an expression for the total dielectric function for charge fluctuations

$$\varepsilon=1-\bar{V}(q)P+\mathbf{w}\cdot\left[\frac{1}{\bar{V}(q)\mathcal{D}-\mathbf{w}\mathbf{w}^*}\right]\cdot\mathbf{w}^*\ . \tag{42}$$

The last term is from the phonons, and contains in the denominator the inverse matrix from the effective force tensor. Another method in Ref. 11, of finding the phonon part of the dielectric function, proceeds by treating the electron-phonon and electron-electron interactions as perturbations. This method yields the expression

$$\varepsilon_{\rm ph}=\frac{\mathbf{w}\cdot(1/\mathcal{D})\cdot\mathbf{w}^*}{\bar{V}(q)-\mathbf{w}\cdot(1/\mathcal{D})\cdot\mathbf{w}^*} . \tag{43}$$

The above two expressions for $\varepsilon_{\rm ph}$ are equal.

Equation (42) vanishes when $\bar{V}(q)=0$. In that case the phonon term is minus one, which cancels the first term. This result is the basis for the second theorem. The dielectric screening for charge fluctuations vanishes when $\bar{V}(q)=0$.

The Coulomb part of the effective interaction can be written as

$$V_c=\frac{\bar{V}(q)}{1-\bar{V}(q)P+\varepsilon_{\rm ph}} . \tag{44}$$

When $\bar{V}(q)\to 0$ at zero frequency then both numerator and denominator vanish. Using L'Hôpital's rule, the expression becomes

$$\lim_{\bar{V}=0} V_c=\frac{V_{\rm ph}}{1-V_{\rm ph}P} , \tag{45}$$

$$V_{\rm ph}(\mathbf{q},0)=-\mathbf{w}\cdot\left[\frac{1}{\mathcal{D}}\right]\cdot\mathbf{w}^* , \tag{46}$$

$$V_{\rm ph}(\mathbf{q},iq_m)=-\sum_j \frac{|\mathbf{e}\cdot\mathbf{w}|^2}{\omega_j(q)^2+q_m^2} . \tag{47}$$

Equation (45) is Dyson's equation for the phonon Green's function. The frequencies $\omega_j(q)$ are calculated with the phonon force matrix $\mathcal{D}$. It is the correct interaction, for charge fluctuations, in the absence of electron-electron interactions. In the present example, electron-electron interactions are absent at those values of wave vector where $\bar{V}(q)=0$.

The condition of having $\bar{V}(q)<0$ is easy to achieve. For example, take a square lattice in two dimensions. The largest wave vector is $\mathbf{q}_0=\pi(\pm1,\pm1)/a$ where $a$ is a lattice constant. Assume that the local charge densities are three-dimensional Gaussians. Then using (20) it is easy to show that $\bar{V}(\mathbf{q}_0)<0$ for $b>0.25a$. The numerical factor of 0.25 comes from a summation over reciprocal-lattice vectors in two dimensions.

The interaction $\bar{V}(q)$ is strongly repulsive at small wave vector. If it is negative near the zone edge or corner, then it changes sign by going through zero. In this case there is a surface in the Brillouin zero where $\bar{V}(q)=0$ and there are no electron-electron interactions. On that surface (45) is the correct expression for the phonon Green's function. These phonons are the physical ones which are measured by x rays or by neutron scattering. For physical phonons, the right-hand side of (45) is negative at zero frequency, which requires that $V_{\rm ph}<0$ and $V_{\rm ph}P<1$. Thus we have shown that the charge fluctuations give an attractive interaction whenever $\bar{V}(q)=0$. We assume that the interaction continues to be negative when $\bar{V}(q)<0$, although we have no proof of this latter assumption.

The important question is whether the effective interaction is attractive. When $\bar{V}(q)<0$ does the attractive charge fluctuation overcome the repulsive spin fluctuation? For $\bar{V}(q)=0$ we can write

$$\lim_{\bar{V}(q)=0} V_{\rm eff}=\frac{V_{\rm ph}+U/2}{(1-V_{\rm ph}P)[1+(U/2)P]} . \tag{48}$$

We have shown that both factors in the denominator are positive. However, we have found no theorem relating the two terms in the numerator. The phonon force tensor $\mathcal{D}$ has an inverse factor of the ion mass. We have absorbed into $\mathbf{w}$ an inverse factor of the square root of the ion mass. Thus $V_{\rm ph}(\mathbf{q},0)$ does not have a factor of the ion mass, and contains only electronic energies and forces. Thus this factor should be a similar size to $U$, but of the opposite sign.

## IV. DISCUSSION

Here we have proved two theorems concerning the effective interaction between electrons in superconductors. The theorems apply only to metals which are well described by a one-band tight-binding model. Our model and theorem do not apply to metals such as tin and aluminum, which are described well by the nearly free-electron picture.

One theorem showed that the effective interaction was always repulsive when one considered only electron-electron interactions. In the second theorem, we also included phonons in the interaction term between electrons. The second theorem is that the interaction due to charge fluctuations could be attractive for wave vectors near the edges or corners of the Brillouin zone.

We conclude that the interaction between quasiparticles is attractive for large wave vectors: those near the corners of the Brillouin zone. In this case the interaction is most attractive for electrons on scattering to opposite sides of the Fermi surface, and it is repulsive for scattering by small wave vectors. Earlier[23] we constructed a theory of superconductivity which utilized this behavior. Nonzero solutions to the gap function were found only near to the van Hove singularity in two dimensions.

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