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Phonon-mediated electron-electron interaction in real space

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We have calculated the phonon-mediated interaction between two s-band electrons as a function of their relative separation in real space. We consider the two cases of acoustic phonons in a nonpolar crystal and of optic phonons in an ionic crystal, and present specific results for electrons at the bottom of the band, using parameters of aluminum and lithium chloride, respectively. In the acoustic-phonon case, even when the Coulomb repulsion between the two electrons is not included, the interaction has a wide repulsive core, which extends to a separation of about 200 Å and afterwards oscillates between attractive and repulsive regions as the distance between the electrons increases. Classically, i.e., when the electrons are infinitely heavy, this potential is attractive when the electrons are less than a few angstroms apart and oscillates at greater distances. For ionic crystals one anticipates that the phonon-mediated interaction causes merely the optic-phonon screening of the Coulomb repulsion; i.e., $e^2/\epsilon_\infty r$ is converted to $e^2/\epsilon_0 r$. However, we find that this mechanism produces a striking oscillation (versus r) about the expected result. Consequently, in LiCl, for example, the total potential—the direct Coulomb repulsion plus the phonon-mediated interaction—has deep, attractive potential wells, the first and largest of which has a depth of 28 meV, with its minimum occurring when the electrons are 33 Å apart.

I. INTRODUCTION

An electron in a lattice interacts with the ions about it through the electron-phonon interaction to produce a distortion of the lattice. This distortion, or virtual-phonon cloud, follows the electron during its motion in the lattice. In an ionic crystal, this clothed electron is known as a polaron. When two clothed electrons are in the lattice, an effective electron-electron interaction develops through phonon mediation. Each electron experiences the polarization field produced by the other electron. This happens even in the classical limit, i.e., when the electrons are considered to be infinitely heavy. Quantum mechanically, each electron develops a virtual recoil kinetic energy by interacting with phonons, and this effect modifies dramatically the electron-electron interaction. The resulting interaction has been studied extensively and provides a basis for the Bardeen-Cooper-Schrieffer (BCS) theory of superconductivity. The important feature of this interaction for superconductivity is that it provides an attractive potential between two electrons, so that bound states, or Cooper pairs, may form. Usually this electron-electron potential is studied in reciprocal space, as a function of the wave vector $\vec{q}$ of a phonon that is exchanged between the two electrons. However, no investigation has been made of this potential in real space, i.e., as a function of the relative separation between the two electrons. Such a study is the purpose of this paper.

We begin our discussion here by calculating in Sec. II the distortion created in a lattice by one electron as a function of distance from that electron. This provides physical background for following discussions and illustrates the method to be used in Sec. III to derive the electron-electron potential. In Sec. III A, we produce a general derivation of the effective electron-electron potential for s-band electrons in real space, and apply it in Sec. III B to the case of acoustic phonons in a nonpolar crystal, and in Sec. III C to optic phonons in a polar crystal. We evaluate resulting expressions explicitly for electrons at the bottom of the s band, which yield spherically symmetric potentials. Plots are shown of these potentials for aluminum in Sec. III B and for LiCl in Sec. III C. Finally, in Sec. IV we present the conclusions.

II. LATTICE DISTORTION PRODUCED BY ONE ELECTRON INTERACTING WITH ACOUSTIC PHONONS

Suppose we have one free s-band electron in a harmonic lattice. The Hamiltonian of the system can be written as

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{ep}, \tag{1}$$

where

$$\mathcal{H}_0 = \frac{p^2}{2m} + \sum_{\vec{q}} \hbar\,\omega_{\vec{q}}\,(a_{\vec{q}}^* a_{\vec{q}} + \tfrac{1}{2}), \tag{2}$$

is the Hamiltonian for the noninteracting system and

$$\mathcal{H}_{ep} = \sum_{\vec{q}} A_{\vec{q}}\,(a_{\vec{q}}\, e^{i\vec{q}\cdot\vec{r}_1} - a_q^* e^{-i\vec{q}\cdot\vec{r}_1}), \tag{3}$$

is the electron-phonon interaction at some position $\vec{r}_1$. For longitudinal acoustic phonons, within the Debye model,

$$A_{\vec{q}} = \tfrac{2}{3} i C \left(\frac{\hbar q}{2\rho u}\right)^{1/2} . \tag{4}$$

Here, $\omega_{\vec{q}} = uq$ is the acoustic-phonon frequency, with u and $\vec{q}$ the phonon velocity and wave vector, respectively. $C \approx E_F$ is the electron-phonon coupling constant, where E_F is the Fermi energy. m and p are the mass and momentum of the electron, a^* and a are the phonon creation and annihilation operators, and ρ is the mass density of the crystal.

As the electron moves through the crystal, it produces a distortion of the lattice by polarizing the ions around it, and this virtual-phonon cloud or phonon clothing accompanies the electron in its travels. $B^*_{\vec{k}}$ is the operator that creates this clothed electron, or polaron, where

$$B^*_{\vec{k}} = b^*_{\vec{k}} + \sum_{\vec{q}} A_{\vec{q}} \left(\frac{b^*_{\vec{k}+\vec{q}}\, a_{\vec{q}}}{\Delta^+_{\vec{q}}(\vec{k})} - \frac{b^*_{\vec{k}-\vec{q}}\, a^*_{\vec{q}}}{\Delta^-_{\vec{q}}(\vec{k})} \right), \tag{5a}$$

which corresponds to first-order perturbation theory. $B_{\vec{k}}$ is the corresponding annihilation operator. Here,

$$\Delta^{\pm}_{\vec{q}}(\vec{k}) = \frac{\hbar^2 k^2}{2m} - \left(\frac{\hbar^2 (\vec{k} \pm \vec{q})^2}{2m} \mp \hbar\, \omega_{\vec{q}} \right), \tag{5b}$$

and $b^*_{\vec{k}}$ and $b_{\vec{k}}$ are the creation and annihilation operators for a bare (plane-wave) electron of wave vector $\vec{k}$. The second of the terms within the summation over $\vec{q}$ in Eq. (5a) creates the electron's clothing by emitting virtual phonons, while the first term absorbs phonons that are already present. At zero temperature, the absorption term has no effect if only one electron is present in the lattice.

We wish to ask now what the detailed nature of the phonon cloud about the electron is. Suppose the electron is located at $\vec{r}_1$, i.e., that the bare-electron wave function is $e^{i\vec{k}\cdot\vec{r}_1}$. Consider then the lattice-displacement operator for longitudinal acoustic phonons at some position $\vec{r}_2$:

$$\vec{u}(\vec{r}_2) = \sum_{\vec{q}} \left(\frac{\hbar}{2\rho u q}\right)^{1/2} \left(a_{\vec{q}} e^{i\vec{q}\cdot\vec{r}_2} + a^*_{\vec{q}} e^{-i\vec{q}\cdot\vec{r}_2}\right) \frac{\vec{q}}{q} . \tag{6}$$

Since we want to know the nature of the lattice distortion about the electron, we might ask what the expectation value of this displacement is between clothed electron states. But this yields only zero because, when one averages over all the electron and phonon coordinates, all contributions cancel. That is, on the average, for all positions of the electron in the lattice, there is no net lattice displacment. The mean-square displacement, or the square root of the expectation value of $\vec{u}^2(\vec{r}_2)$ taken between clothed-electron states, gives one only a measure of the average distortion caused by the electron.

In order to calculate the magnitude and shape of this distortion in exact microscopic detail, one must employ a somewhat different approach. We ask what the instantaneous distortion of the lattice is at a position $\vec{s}$ relative to the electron's position $\vec{r}_1$, whatever that may be. Thus we may write

$$\vec{u}(\vec{r}_2) = \vec{u}(\vec{r}_1, \vec{s})$$

$$= \sum_{\vec{q}} \left(\frac{\hbar}{2\rho u q}\right)^{1/2} \left(a_{\vec{q}} e^{i\vec{q}\cdot(\vec{r}_1+\vec{s})} + a^*_{\vec{q}} e^{-\vec{q}\cdot(\vec{r}_1+\vec{s})}\right) \frac{\vec{q}}{q} \tag{7}$$

for the lattice displacement operator, where

$$\vec{s} = \vec{r}_2 - \vec{r}_1 . \tag{8}$$

This operator in Eq. (7) is now perfectly correlated with the position of the electron, so that one could imagine that if $\vec{s}$ is fixed, the distortion would follow the electron around the lattice. For this reason, we calculate a restricted expectation value of this lattice-displacement operator, between clothed electron states, in which we keep the vector $\vec{s}$ fixed, i.e., we integrate over all coordinates except $\vec{s}$.

For simplicity, we will assume here that the system is at zero temperature. A similar analysis follows at finite temperature, with slightly more complicated results, for the restricted expectation value of the lattice displacement, but the identical result emerges at finite temperature for the effective electron-electron interaction, which will be derived in Sec. III. Thus we write the restricted expectation value $\langle \vec{u}(\vec{s}) \rangle_{\vec{s}}$ as

$$\langle \vec{u}(\vec{s}) \rangle_{\vec{s}} = \langle \psi_{\vec{k}} | \vec{u}(\vec{r}_1, \vec{s}) | \psi_{\vec{k}} \rangle_{\vec{s}} , \tag{9}$$

where

$$| \psi_{\vec{k}} \rangle = B^*_{\vec{k}} | 0 \rangle , \tag{10}$$

is the clothed-electron state, $|0\rangle$ is the vacuum state, and $B^*_{\vec{k}}$ is defined in Eq. (5). The notation $\langle\;\rangle_{\vec{s}}$ indicates that all integrations except those over $\vec{s}$ are to be carried out. Explicitly, we have

$$\langle \vec{u}(\vec{s}) \rangle_{\vec{s}} = \langle 0 | B_{\vec{k}}\, \vec{u}(\vec{r}_1, \vec{s}) B^*_{\vec{k}} | 0 \rangle_{\vec{s}}$$

$$= \frac{2}{i} \sum_{\vec{q}} A_{\vec{q}} \left(\frac{\hbar}{2\rho u q}\right)^{1/2} \frac{\sin(\vec{q}\cdot\vec{s})}{\Delta^-_{\vec{q}}(\vec{k})} \frac{\vec{q}}{q} , \tag{11}$$

where $\Delta^-_{\vec{q}}(\vec{k})$ is defined in Eq. (5b) and $A_{\vec{q}}$ in Eq. (4). We now assume that the electron is at the bottom of the s band, or that its initial velocity before interacting with phonons is nearly zero, so that $k \sim 0$. Converting the sum over $\vec{q}$ to an integral and imposing the Debye cutoff q_D yield

$$\langle \vec{u}(\vec{s}) \rangle_{\vec{s}} = -\tfrac{2}{3} C \frac{1}{\rho u^2} \int_{q<q_D} \frac{d^3 q}{8\pi^3} \frac{\sin \vec{q}\cdot\vec{s}}{q[(\hbar q/2mu)+1]} \frac{\vec{q}}{q}$$

$$= -\hat{s} \frac{C}{3\pi^2 \rho u^2 s} \int_0^{q_D} \frac{[\sin(qs) - (qs)\cos(qs)]\,dq}{q[a(q/q_D)+1]}, \tag{12}$$

where $\hat{s}$ is a unit vector in the direction of $\vec{s}$ and

$$a = \hbar q_D / 2mu, \tag{13}$$

is the "phonon" Compton wavelength in units of $4\pi/q_D$ that results when an electron scatters from a phonon of velocity u. The integral in Eq. (12) may be written in closed form in terms of the sine and cosine integral functions $\mathrm{Si}(z)$ and $\mathrm{Ci}(z)$ as

$$\begin{aligned}\langle \vec{u}(\vec{s}) \rangle_{\vec{s}} = -\hat{s} \frac{C q_D^2}{3\pi^2 \rho u^2} \left(\frac{1}{q_D s}\right)^2 \Bigg\{ \mathrm{Si}(q_D s) - \cos\left(\frac{q_D s}{a}\right) \Bigg[& \{\mathrm{Si}[q_D s(1+1/a)] - \mathrm{Si}(q_D s/a)\} \\ & + \left(\frac{q_D s}{a}\right) \{\mathrm{Ci}[q_D s(1+1/a)] - \mathrm{Ci}(q_D s/a)\} \Bigg] \\ + \sin\left(\frac{q_D s}{a}\right) \Bigg[& \{\mathrm{Ci}[q_D s(1+1/a)] - \mathrm{Ci}(q_D s/a)\} \\ & - \left(\frac{q_D s}{a}\right) \{\mathrm{Si}[q_D s(1+1/a)] - \mathrm{Si}(q_D s/a)\} \Bigg] \Bigg\},\end{aligned} \tag{14}$$

where

$$\mathrm{Si}(z) \equiv \int_0^z \frac{\sin t}{t}\, dt, \tag{15a}$$

$$\mathrm{Ci}(z) \equiv \gamma + \ln z + \int_0^z \frac{\cos t - 1}{t}\, dt, \tag{15b}$$

and γ is Euler's constant.[1] $\langle \vec{u}(\vec{s}) \rangle_{\vec{s}}$ is in the radial direction and varies as $(-\vec{s})$ for small s and as $-\hat{s}/s^2$ for large s, with weak oscillations about these dependences. In the classical limit, where the electron is considered to be infinitely massive, i.e., $m \to \infty$ so that $a \to 0$, this expression simplifies considerably and may be written as

$$\langle \vec{u}_{\text{class}}(\vec{s}) \rangle_{\vec{s}} = -\hat{s} \frac{C}{3\pi^2 \rho u^2 s^2} [\mathrm{Si}(q_D s) - \sin(q_D s)]. \tag{16}$$

When an electron deforms the lattice, one often thinks of the analogy of an electron producing a depression in a mattress. Extending this analogy, one expects that if a second electron were in the lattice, it would feel the strain field produced by the first electron. As the two electrons would approach one another, they would both fall into the same depression in the mattress and would thus attract one another at short distances. Indeed, for acoustic phonons, the electron-phonon interaction at a position $\vec{r}_2$ may be written simply as the strain field at that point,

$$\mathcal{H}_{ep} = \tfrac{2}{3} C \operatorname{div} \vec{u}(\vec{r}_2), \tag{17}$$

as can be seen from Eqs. (3), (4), and (6). Then the restricted expectation value of this operator between the clothed electron states of an electron at $\vec{r}_1$ may be considered to be the magnitude of the strain produced at $\vec{r}_2$ by an electron located at $\vec{r}_1$. This can be expressed as

$$\langle \psi_{\vec{k}} | \mathcal{H}_{ep} | \psi_{\vec{k}} \rangle_{\vec{s}} = \tfrac{2}{3} C \operatorname{div} \langle \vec{u}(\vec{s}) \rangle_{\vec{s}} = -\frac{V_0}{(q_D s)^2} \left(\frac{1}{q_D}\right)^2 \int_0^{q_D} \frac{q \sin(qs)\,dq}{a(q/q_D)+1}$$

$$\begin{aligned}= -\frac{V_0}{a q_D s} \Bigg\{ [1 - \cos(q_D s)] - \frac{q_D s}{a} \Bigg[& \cos\left(\frac{q_D s}{a}\right) \{\mathrm{Si}[q_D s(1+1/a)] - \mathrm{Si}(q_D s/a)\} \\ & - \sin\left(\frac{q_D s}{a}\right) \{\mathrm{Ci}[q_D s(1+1/a)] - \mathrm{Ci}(q_D s/a)\} \Bigg] \Bigg\},\end{aligned} \tag{18}$$

where

$$V_0 = (\tfrac{2}{3} C)^2 \frac{q_D^3}{2\pi^2 \rho u^2}. \tag{19}$$

This function is negative (attractive) for small s and achieves its maximum magnitude as $s \to 0$, and thus describes well the picture of two electrons falling into the same depression of a phonon "mattress" as they approach one another. In the classical limit, i.e., when $m \to \infty$ and $a \to 0$, this becomes

$$\langle \psi_{\vec{k}} | \mathcal{H}_{ep} | \psi_{\vec{k}} \rangle_{\vec{s}} = \tfrac{2}{3} C \operatorname{div} \langle \vec{u}(\vec{s}) \rangle_{\vec{s}} \xrightarrow[a \to 0]{} -V_0 j_1(q_D s)/q_D s, \tag{20}$$

where $j_1(z) = (\sin z - z\cos z)/z^2$ is the first-order spherical Bessel function.

As we will see in Sec. III B, the electron-electron potential is given exactly by the expression in Eq. (20) in the classical limit. However, in the quantum case, the virtual recoil kinetic energies of the two electrons play a major role in determining the interaction, which is qualitatively and quantitatively different from that given by Eq. (18). This will be discussed in detail in Sec. III B.

III. PHONON-MEDIATED ELECTRON-ELECTRON INTERACTION

A. General derivation in real space

In this section, we consider two electrons in the lattice together. We will assume that the first electron, located at $\vec{r}_1$, has its spin up and that its momentum and wave vector are $\vec{p}_\uparrow$ and $\vec{k}_\uparrow$. Similarly, we assume that the second electron, located at $\vec{r}_2$, has spin down and that its momentum and wave vector are $\vec{p}_\downarrow$ and $\vec{k}_\downarrow$. We treat the case of opposite spins in order to avoid antisymmetrizing the wave functions and separating the effects of exchange from the pure phonon-mediated electron-electron interaction. With these restrictions we write the Hamiltonian

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{ep}, \tag{21}$$

where

$$\mathcal{H}_0 = \frac{p_\uparrow^2}{2m} + \frac{p_\downarrow^2}{2m} + \sum_{\vec{q}} \hbar\,\omega_{\vec{q}}(a_{\vec{q}}^* a_{\vec{q}} + \tfrac{1}{2}), \tag{22}$$

is the Hamiltonian for the system with no interactions and

$$\mathcal{H}_{ep} = \sum_{\vec{q}} A_{\vec{q}}[a_{\vec{q}}(e^{i\vec{q}\cdot\vec{r}_1} + e^{i\vec{q}\cdot\vec{r}_2}) - a_{\vec{q}}^*(e^{-i\vec{q}\cdot\vec{r}_1} + e^{-i\vec{q}\cdot\vec{r}_2})], \tag{23}$$

is the electron-phonon interaction. We note that the only difference in the Hamiltonian between the case of acoustic phonons in a nonpolar crystal and of optic phonons in a polar crystal is in the definition of $A_{\vec{q}}$, the coefficient in the electron-phonon interaction, Eq. (23). Therefore, in this section, we will derive a general form for the electron-electron interaction in terms of $A_{\vec{q}}$ and later, in Secs. III B and III C, apply the appropriate specific forms for the cases of interest.

The derivation that we will present here of the electron-electron interaction follows the same philosophy as the calculation of the shape of the lattice distortion about the electron calculated in Sec. II. Suppose that $\vec{s} = \vec{r}_2 - \vec{r}_1$, as in Eq. (8), with the two electrons at $\vec{r}_1$ and $\vec{r}_2$. If we keep the relative positions $\vec{s}$ of the two electrons fixed, then we can determine an expression for the effective electron-electron potential $V(\vec{s})$. We accomplish this by first taking the restricted expectation value of the Hamiltonian [Eqs. (21)–(23)], keeping $\vec{s}$ fixed, between states of a pair of clothed electrons. That is, in the expectation value, we integrate over all coordinates except $\vec{s}$. Then we subtract all terms that would be present if the two electrons had been in the lattice one at a time and not together. The remainder is the effective electron-electron interaction $V(\vec{s})$ in real space. As we will see, it is also the only term in the restricted expectation value of the Hamiltonian that depends on $\vec{s}$.

The creation operator $\mathcal{B}_{\vec{k}_\uparrow,\vec{k}_\downarrow}^*$ for the pair of electrons with wave vectors $\vec{k}_\uparrow$ and $\vec{k}_\downarrow$ is given by

$$\mathcal{B}_{\vec{k}_\uparrow,\vec{k}_\downarrow}^* = \frac{N}{2}(B_{\vec{k}_\uparrow}^* B_{\vec{k}_\downarrow}^* - B_{\vec{k}_\uparrow}^* B_{\vec{k}_\downarrow}^*), \tag{24}$$

with the annihilation operator for the pair given by $\mathcal{B}_{\vec{k}_\uparrow,\vec{k}_\downarrow}$. Here $B_{\vec{k}}^*$ is defined in Eq. (5) and N is the normalization defined below. We take the (anti) symmetrized product of the two single-electron operators, since there is no preference as to which electron is created first. This operator creates the state for a pair of electrons, which we will denote as

$$|\Psi_{\vec{k}_\uparrow,\vec{k}_\downarrow}\rangle = \mathcal{B}_{\vec{k}_\uparrow,\vec{k}_\downarrow}^*|0\rangle, \tag{25}$$

where $|0\rangle$ is the vacuum state. These states are orthogonal in the restricted inner product where we integrate over all variables except $\vec{s}$, and the normalization is determined with the same type of product. Thus,

$$\begin{aligned}\langle\Psi_{\vec{k}'_\uparrow,\vec{k}'_\downarrow}|\Psi_{\vec{k}_\uparrow,\vec{k}_\downarrow}\rangle_{\vec{s}} &= \langle 0|\mathcal{B}_{\vec{k}'_\uparrow,\vec{k}'_\downarrow}\mathcal{B}_{\vec{k}_\uparrow,\vec{k}_\downarrow}^*|0\rangle_{\vec{s}} \\ &= \delta_{\vec{k}'_\uparrow,\vec{k}_\uparrow}\delta_{\vec{k}'_\downarrow,\vec{k}_\downarrow}.\end{aligned} \tag{26}$$

The integrations that are performed here are the integrations over the center-of-mass coordinate $\vec{R} = \frac{1}{2}(\vec{r}_1 + \vec{r}_2)$, while the relative coordinate $\vec{s}$ remains fixed. Equation (26) now determines N, which is a function of $\vec{s}$, because N appears in Eq. (24). N is of the form $N \doteq 1 - O(|A_{\vec{q}}|^2)$. Since we retain only terms of order $|A_{\vec{q}}|^2$ or lower, we need not write an explicit expression for N since, in the calculation of the restricted expectation value of $\mathcal{H}$, it either cancels exactly in some terms or multiplies terms already proportional to $|A_{\vec{q}}|^2$.

We can see from Eqs. (5) and (24) that each electron is clothed to first order (in perturbation theory) in the electron-phonon interaction and, in addition, each electron has a first-order term that permits it to strip clothing from the other electron. In the product in Eq. (24), some terms appear that are second order in the electron-phonon coupling $A_{\vec{q}}$, but these are precisely the terms that are needed to assure the proper orthonormalization in Eq. (26).

We now calculate the restricted expectation value of the Hamiltonian with the electrons fixed at some separation $\vec{s}$. As in Sec. II, we will consider the system to be at zero temperature. We have also calculated the phonon-mediated electron-electron interaction for finite temperature and have obtained the same result. Since at finite temperature the intermediate steps are much more complicated, with many cancellations, one can understand better the origin of various contributions to the potential if we display only the zero-temperature calculation.

The restricted expectation value of the electrons' kinetic energies $\mathcal{H}_{\mathrm{KE}}$ is given by

$$\begin{aligned}\langle\Psi_{\vec{k}_\uparrow,\vec{k}_\downarrow}|\mathcal{H}_{\mathrm{KE}}|\Psi_{\vec{k}_\uparrow,\vec{k}_\downarrow}\rangle_{\vec{s}} &= \left\langle 0\left|\mathcal{B}_{\vec{k}_\uparrow,\vec{k}_\downarrow}\left(\frac{p_\uparrow^2}{2m}+\frac{p_\downarrow^2}{2m}\right)\mathcal{B}^*_{\vec{k}_\uparrow,\vec{k}_\downarrow}\right|0\right\rangle_{\vec{s}}\\ &= \frac{\hbar^2}{2m}(k_\uparrow^2+k_\downarrow^2)-\sum_{\vec{q}}|A_{\vec{q}}|^2\Bigg[\frac{\Delta^-_{\vec{q}}(\vec{k}_\uparrow)+\hbar\omega_{\vec{q}}}{[\Delta^-_{\vec{q}}(\vec{k}_\uparrow)]^2}+\frac{\Delta^-_{\vec{q}}(\vec{k}_\downarrow)+\hbar\omega_{\vec{q}}}{[\Delta^-_{\vec{q}}(\vec{k}_\downarrow)]^2}\\ &\qquad -e^{i\vec{q}\cdot\vec{s}}\left(\frac{\Delta^-_{\vec{q}}(\vec{k}_\downarrow)+\hbar\omega_{\vec{q}}}{\Delta^-_{\vec{q}}(\vec{k}_\uparrow)\Delta^-_{\vec{q}}(\vec{k}_\downarrow)}+\frac{\frac{1}{2}[\Delta^-_{\vec{q}}(\vec{k}_\downarrow)+\Delta^+_{\vec{q}}(\vec{k}_\uparrow)]}{\Delta^\pm_{\vec{q}}(\vec{k}_\uparrow)\Delta^-_{\vec{q}}(\vec{k}_\downarrow)}\right)\\ &\qquad -e^{-i\vec{q}\cdot\vec{s}}\left(\frac{\Delta^-_{\vec{q}}(\vec{k}_\uparrow)+\hbar\omega_{\vec{q}}}{\Delta^-_{\vec{q}}(\vec{k}_\uparrow)\Delta^-_{\vec{q}}(\vec{k}_\downarrow)}+\frac{\frac{1}{2}[\Delta^-_{\vec{q}}(\vec{k}_\uparrow)+\Delta^+_{\vec{q}}(\vec{k}_\downarrow)]}{\Delta^-_{\vec{q}}(\vec{k}_\uparrow)\Delta^\pm_{\vec{q}}(\vec{k}_\downarrow)}\right)\Bigg]. \end{aligned} \tag{27}$$

The terms multiplying both $e^{i\vec{q}\cdot\vec{s}}$ and $e^{-\vec{q}\cdot\vec{s}}$ that contain $\Delta^+_{\vec{q}}(\vec{k}_\uparrow)$ and $\Delta^+_{\vec{q}}(\vec{k}_\downarrow)$ in their denominators are the only terms in the entire restricted expectation value of the Hamiltonian that result from having the stripping operator, i.e., the term in Eq. (5a) with $a_{\vec{q}}$, included in the clothed-electron operator. This means that these are also the only terms that contain the type of denominator $\Delta^+_{\vec{q}}(\vec{k})$. It is these terms that produce a dramatic modification from what one would expect from the "mattress" picture discussed in Sec. II.

The restricted expectation value of the harmonic oscillator part of the Hamiltonian $\mathcal{H}_{\mathrm{HO}}$ is

$$\begin{aligned}\langle\Psi_{\vec{k}_\uparrow,\vec{k}_\downarrow}|\mathcal{H}_{\mathrm{HO}}|\Psi_{\vec{k}_\uparrow,\vec{k}_\downarrow}\rangle_{\vec{s}} &= \left\langle 0\left|\mathcal{B}_{\vec{k}_\uparrow,\vec{k}_\downarrow}\sum_{\vec{q}}\hbar\omega_{\vec{q}}(a^*_{\vec{q}}a_{\vec{q}}+\tfrac{1}{2})\mathcal{B}^*_{\vec{k}_\uparrow,\vec{k}_\downarrow}\right|0\right\rangle_{\vec{s}}\\ &= \sum_{\vec{q}}\hbar\omega_{\vec{q}}\left[\tfrac{1}{2}+|A_{\vec{q}}|^2\left(\frac{1}{[\Delta^-_{\vec{q}}(\vec{k}_\uparrow)]^2}+\frac{1}{[\Delta^-_{\vec{q}}(\vec{k}_\downarrow)]^2}+\frac{2\cos(\vec{q}\cdot\vec{s})}{\Delta^-_{\vec{q}}(\vec{k}_\uparrow)\Delta^-_{\vec{q}}(\vec{k}_\downarrow)}\right)\right]. \end{aligned} \tag{28}$$

Combining Eqs. (27) and (28), we obtain the restricted expectation value for $\mathcal{H}_0$ [Eq. (22)]:

$$\begin{aligned}\langle\Psi_{\vec{k}_\uparrow,\vec{k}_\downarrow}|\mathcal{H}_0|\Psi_{\vec{k}_\uparrow,\vec{k}_\downarrow}\rangle_{\vec{s}} &= \frac{\hbar^2}{2m}(k_\uparrow^2+k_\downarrow^2)+\sum_{\vec{q}}\tfrac{1}{2}\hbar\omega_{\vec{q}}\\ &\quad -\sum_{\vec{q}}|A_{\vec{q}}|^2\Bigg\{\frac{1}{\Delta^-_{\vec{q}}(\vec{k}_\uparrow)}+\frac{1}{\Delta^-_{\vec{q}}(\vec{k}_\downarrow)}+e^{i\vec{q}\cdot\vec{s}}\left[\frac{1}{\Delta^-_{\vec{q}}(\vec{k}_\uparrow)}+\frac{1}{2}\left(\frac{1}{\Delta^\pm_{\vec{q}}(\vec{k}_\uparrow)}+\frac{1}{\Delta^-_{\vec{q}}(\vec{k}_\downarrow)}\right)\right]\\ &\qquad +e^{-i\vec{q}\cdot\vec{s}}\left[\frac{1}{\Delta^-_{\vec{q}}(\vec{k}_\downarrow)}+\frac{1}{2}\left(\frac{1}{\Delta^\pm_{\vec{q}}(\vec{k}_\downarrow)}+\frac{1}{\Delta^-_{\vec{q}}(\vec{k}_\uparrow)}\right)\right]\Bigg\}. \end{aligned} \tag{29}$$

Finally, the restricted expectation value of the electron-phonon interaction, $\mathcal{H}_{ep}$ [Eq (23)] is

$$\langle\Psi_{\vec{k}_\uparrow,\vec{k}_\downarrow}|\mathcal{H}_{ep}|\Psi_{\vec{k}_\uparrow,\vec{k}_\downarrow}\rangle_{\vec{s}} = \sum_{\vec{q}}|A_{\vec{q}}|^2\left[\frac{-2}{\Delta^-_{\vec{q}}(\vec{k}_\uparrow)}+\frac{2}{\Delta^-_{\vec{q}}(\vec{k}_\downarrow)}+e^{i\vec{q}\cdot\vec{s}}\left(\frac{1}{\Delta^-_{\vec{q}}(\vec{k}_\uparrow)}+\frac{1}{\Delta^-_{\vec{q}}(\vec{k}_\downarrow)}\right)+e^{-\vec{q}\cdot\vec{s}}\left(\frac{1}{\Delta^-_{\vec{q}}(\vec{k}_\uparrow)}+\frac{1}{\Delta^-_{\vec{q}}(\vec{k}_\downarrow)}\right)\right]. \tag{30}$$

Note that the contributions to the restricted expectation value of $\mathcal{H}_{ep}$ do not contain any terms resulting from the stripping operator in Eq. (5a), i.e., the term containing $a_{\vec{q}}$. Only denominators of the type $\Delta^-_{\vec{q}}(\vec{k})$ from Eq. (5b) appear here.

By combining Eqs. (29) and (30), we can now write the restricted expectation value of the total Hamiltonian $\mathcal{H}$ [Eq. (21)]:

$$\langle \Psi_{\vec{k}_\uparrow,\vec{k}_\downarrow} | \mathcal{H} | \Psi_{\vec{k}_\uparrow,\vec{k}_\downarrow} \rangle_{\vec{s}} = \frac{\hbar^2}{2m}(k_\uparrow^2 + k_\downarrow^2) + \sum_{\vec{q}} \tfrac{1}{2}\hbar\omega_{\vec{q}} + \sum_{\vec{q}} |A_{\vec{q}}|^2 \left[\frac{1}{\Delta_{\vec{q}}^-(\vec{k}_\uparrow)} + \frac{1}{\Delta_{\vec{q}}^-(\vec{k}_\downarrow)} + \tfrac{1}{2} e^{i\vec{q}\cdot\vec{s}} \left(\frac{1}{\Delta_{\vec{q}}^-(\vec{k}_\downarrow)} - \frac{1}{\Delta_{\vec{q}}^+(\vec{k}_\uparrow)} \right) + \tfrac{1}{2} e^{-i\vec{q}\cdot\vec{s}} \left(\frac{1}{\Delta_{\vec{q}}^-(\vec{k}_\uparrow)} - \frac{1}{\Delta_{\vec{q}}^+(\vec{k}_\downarrow)} \right) \right] . \tag{31}$$

The first two terms in Eq. (31) represent the kinetic energies of the two electrons and the energy of the phonons in the absence of the electron-phonon interaction. The third and fourth terms (the first two terms in the summation over $\vec{q}$) are the self-energies of the first and second electrons, respectively. These are the energies that would result if the two electrons were present in the crystal one at a time and not together. In fact, these terms appear if one takes the restricted expectation value of the Hamiltonian with one electron present between the states of each clothed electron separately. The remaining terms are then the electron-electron interaction. These are also the only terms that depend on $\vec{s}$, the relative separation between the two electrons. Thus, the electron-electron potential is

$$V(\vec{s}) = \tfrac{1}{2} \sum_{\vec{q}} |A_{\vec{q}}|^2 e^{i\vec{q}\cdot\vec{s}} \left[\left(\frac{1}{\Delta_{\vec{q}}^-(\vec{k}_\downarrow)} - \frac{1}{\Delta_{\vec{q}}^+(\vec{k}_\uparrow)} \right) + \left(\frac{1}{\Delta_{-\vec{q}}^-(\vec{k}_\uparrow)} - \frac{1}{\Delta_{-\vec{q}}^+(\vec{k}_\downarrow)} \right) \right] , \tag{32}$$

where we have replaced $\vec{q}$ by $-\vec{q}$ in the third and fourth terms in the sum over $\vec{q}$, and where $\Delta_{\vec{q}}^\pm(\vec{k})$ are defined in Eq. (5b). [Although $V(\vec{s})$ in Eq. (32) is complex for finite values of $\vec{k}_\uparrow$ and $\vec{k}_\downarrow$, it can be shown that the actual phonon-mediated electron-electron interaction is just the real part of this expression.]

We note that, although this calculation was done for the case of zero temperature, the same result, Eq. (32), obtains for $V(\vec{s})$ at finite temperature. Indeed, it is well known that the phonon-mediated electron-electron potential can be thought to result from the exchange of virtual phonons between two electrons and is therefore independent of the number of phonons present initially in the system. In fact, this result, Eq. (32), with $A_{\vec{q}}$ defined by Eq. (4), is just the Fourier transform of the usual phonon-mediated inteaction that is derived by other techniques en route to the BCS theory of superconductivity.[2,3] One could have derived the electron-electron potential in $\vec{q}$ space $\hat{V}(\vec{q})$ and then Fourier-transformed it to obtain Eq. (32). For example, one can derive $\hat{V}(\vec{q})$ by calculating the off-diagonal or scattering matrix elements of the Hamiltonian, i.e.,

$$\hat{V}(\vec{q}) = \langle \Psi_{\vec{k}'_\uparrow,\vec{k}'_\downarrow} | \mathcal{H} | \Psi_{\vec{k}_\uparrow,\vec{k}_\downarrow} \rangle ,$$

where one integrates over all coordinates. Then $V(\vec{s})$ is the Fourier transform of $\hat{V}(\vec{q})$. In other words, the scattering matrix element of two clothed electrons of the potential $V(\vec{s})$ is just $\hat{V}(\vec{q})$, the Fourier transform of that potential. We feel, however, that one gains more insight with the method presented in this section.

B. Acoustic phonons in a nonpolar crystal

For the case of two electrons that interact with one another in a nonpolar crystal via acoustic phonons, the phonon-mediated electron-electron interaction becomes

$$V(\vec{s}) = (\tfrac{2}{3}C)^2 \sum_{\vec{q}} \frac{\hbar q}{2\rho u} \hbar\omega_{\vec{q}} e^{i\vec{q}\cdot\vec{s}} \left\{ 1 \Big/ \left[\left(-\frac{\hbar^2}{m} \vec{k}_\downarrow \cdot \vec{q} + \frac{\hbar^2 q^2}{2m} \right)^2 - (\hbar\omega_{\vec{q}})^2 \right] + 1 \Big/ \left[\left(\frac{\hbar^2}{m} \vec{k}_\uparrow \cdot \vec{q} + \frac{\hbar^2 q^2}{2m} \right)^2 - (\hbar\omega_{\vec{q}})^2 \right] \right\} . \tag{33}$$

At this point, for simplicity, and in the spirit of Sec. II, we assume that the initial velocities of the two electrons are very small, i.e., that $k_\uparrow, k_\downarrow \sim 0$. In this way, the potential only depends on the magnitude of $\vec{s}$ and not its direction and is thus spherically symmetric. In general, $V(\vec{s})$ will depend on the direction of $\vec{s}$ relative to $\vec{k}_\uparrow$ and $\vec{k}_\downarrow$. As in Sec. II, we convert the summation over $\vec{q}$ to an integral and perform the angular integrations to obtain

$$V(s) = \frac{V_0}{q_D s} \left(\frac{1}{q_D} \right)^2 \int_0^{q_D} \frac{q \sin(qs) dq}{a^2 (q/q_D)^2 - 1} , \tag{34}$$

where a is defined in Eq. (13) and V_0 in Eq. (19).

Consider first the classical limit of Eq. (34), i.e., $m \to \infty$ and $a \to 0$. This constitutes neglecting the virtual recoil kinetic energies of the two electrons. The potential thus becomes

$$V(s) = -V_0 j_1(q_D s)/q_D s \quad (a \to 0) , \tag{35}$$

which is identical to Eq. (20). That is, in the classical limit, the picture of two electrons on a "mattress" attracting one another at short distances works quite well. This can be seen explicitly from the plot of Eq. (35) in Fig. 1. The parameters used here, except for a, are those appropriate to aluminum. With a lattice constant $a_0 = 4.04$ Å, the Debye wave vector is $q_D = 1.53 \times 10^8\ \mathrm{cm}^{-1}$. With the elastic constant $C_{11} = 1.14 \times 10^{12}\ \mathrm{dyn/cm}^2$ and the mass density of Al, $\rho = 2.73\ \mathrm{g/cm}^3$, the longitudinal acoustic velocity is $u_l = 6.47 \times 10^5$ cm/sec. Thus, the coefficient in front of the interaction in Eq. (35), and defined in Eq. (19), is $V_0 = 15.4$ eV. The inset of Fig. 1 shows the depth of the attractive potential well for $s = 0$, that is $V(s=0) = -V_0/3 = -5$ eV. As shown in the large drawing, the potential becomes repulsive within the length of one lattice spacing and then oscillates with a period of $2\pi/q_D$, the envelope falling off as $1/s^2$.

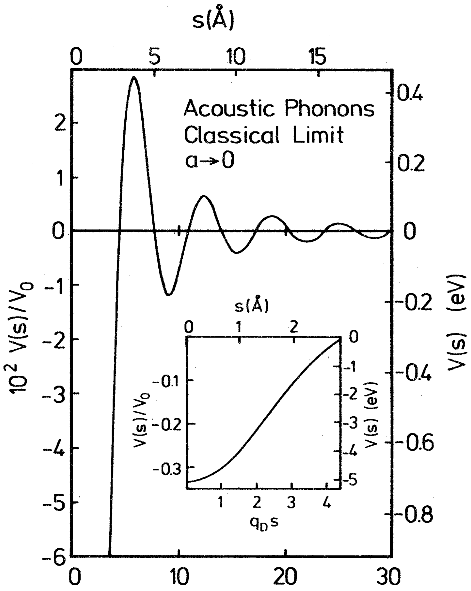

FIG. 1. Plot of the classical limit of the acoustic-phonon-mediated electron-electron interaction $V(s)$ from Eq. (35). Here, $m \to \infty$, so that $a \to 0$, where a is given by Eq. (13). $V_0 = 15.4$ eV is defined by Eq. (19). The inset shows the attractive core of the interaction. Parameters are given in the text.

When the phonon Compton wavelength $a = \hbar q_D/2mu$ [Eq. (13)] is finite, we see that the integral in Eq. (34) is qualitatively different for $a < 1$ compared with $a > 1$. (a is always positive.) For $a > 1$, a pole appears in the integrand that is not present for $a < 1$. For realistic materials, a is usually much larger than 1, e.g., for Al, $a = 137$. At this point, since the case $a < 1$ is qualitatively similar to the classical limit, we will concentrate our attention on the more realistic case here. For $a > 1$, we evaluate the integral in Eq. (34) in the principal-value sense, and then it is expressible in closed form in terms of the sine and cosine integral functions Si(z) and Ci(z) defined in Eq. (15):

$$V(s) = \frac{V_0}{a^2 q_D s}\left[\cos\left(\frac{q_D s}{a}\right)\{\mathrm{Si}[q_D s(1+1/a)] + \mathrm{Si}[q_D s(1-1/a)]\}\right.$$
$$\left. -\sin\left(\frac{q_D s}{a}\right)\{\mathrm{Ci}[q_D s(1+1/a)] - \mathrm{Ci}[q_D s(1-1/a)]\}\right] \quad (a>1)\,. \tag{36}$$

One obtains the $a < 1$ result by taking the absolute values of all the arguments of Si(z) and Ci(z) and changing the + sign in front of $\mathrm{Si}[q_D s(1-1/a)]$ to a − sign.

The function in Eq. (36) is, for realistic parameters, strikingly different from what one would expect for a model of two electrons on a "mattress" attracting one another at short distance. We have plotted this potential in Fig. 2 for Al with $a = 137$. Other parameters are the same as for Fig. 1. The remarkable feature of this curve is the repulsive core. One must remember that the Coulomb repulsion between the two electrons has not been included here, and this is only the phonon-mediated electron-electron interaction. The repulsive core consists of two parts. The first, a short-range part, is only a few angstroms wide, so that it is about the same width as the attractive core in the classical case (Fig. 1). The second is very long ranged, such that $V(s)$ first becomes attractive only for $q_D s \sim a$, or for $s \sim 130$ Å. In addition, the asymptotic behavior for large s is qualitatively different than in the classical case. The period of oscillation is much longer here, since it is determined by the phonon Compton wavelength a, and the envelope falls off as $1/s$ rather than as $1/s^2$ as in the classical case. For $a < 1$, one finds a behavior similar to the classical case, with the asymptotic dependence of the envelope of oscillations falling off as $1/s^2$.

The repulsive core of the interaction in Fig. 2 and Eq. (36) results from the virtual recoil kinetic energies of the two electrons. In the classical case, where these kinetic energies are neglected, the core is attractive, corresponding to the picture of two electrons on a mattress falling into a common depression as they approach one another. Quantum mechanically, this simple picture does not work and, indeed, the first attractive potential well has its minimum only when the two electrons are a few hundred angstroms apart. The origin of this repulsive core comes from the kinetic energy

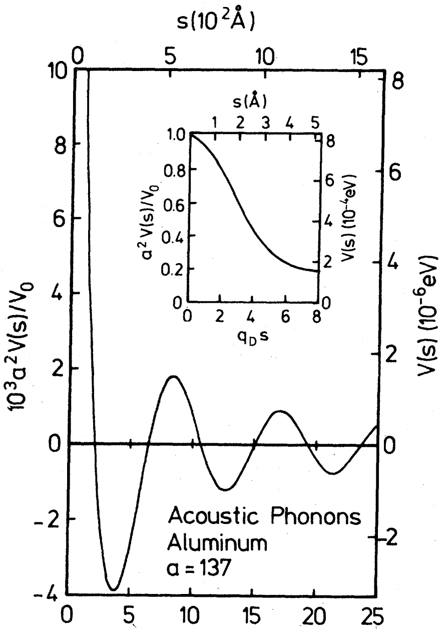

FIG. 2. Plot of the acoustic-phonon-mediated electron-electron interaction $V(s)$ from Eq. (36) for aluminum, with $a=\hbar q_D/2mu=137$ [Eq. (13)]. $V_0=15.4$ eV is defined by Eq. (19). Other parameters are the same as in Fig. 1. The inset shows the repulsive core of the interaction, the remarkable feature of this quantum case.

terms, Eq. (27). The terms that produce this repulsive core are those that contain the denominators $\Delta_{\vec{q}}^{+}(\vec{k}_\uparrow)$ and $\Delta_{\vec{q}}^{+}(\vec{k}_\downarrow)$. These terms remain unaltered in the final expression for $V(s)$, Eq. (32), and thus arise solely from the kinetic energies. It is the neglect of this contribution that causes the mattress model, discussed in Sec. II, to fail.

C. Optic phonons in a polar crystal

Consider the longitudinal optic phonon in a crystal with the rocksalt structure. The displacement operators $\vec{u}_+(\vec{R})$ and $\vec{u}_-(\vec{R})$ of the positive and negative ions, respectively, are[4]

$$\vec{u}_+(\vec{R})=\sum_{\vec{q}}\left(\frac{\hbar}{2\rho\omega_{\vec{q}}}\right)^{1/2}\left(a_{\vec{q}}e^{i\vec{q}\cdot\vec{R}}+a_{\vec{q}}^{*}e^{-i\vec{q}\cdot\vec{R}}\right)\left(\frac{M_-}{M_+}\right)^{1/2}\hat{\epsilon}_{\vec{q}}\,, \tag{37a}$$

$$\vec{u}_-(\vec{R})=\sum_{\vec{q}}\left(\frac{\hbar}{2\rho\omega_{\vec{q}}}\right)^{1/2}\left(a_{\vec{q}}e^{i\vec{q}\cdot\vec{R}}+a_{\vec{q}}^{*}e^{-i\vec{q}\cdot\vec{R}}\right)\left(\frac{M_+}{M_-}\right)^{1/2}(-\hat{\epsilon}_{\vec{q}})\,, \tag{37b}$$

where ρ is the mass density of the crystal, $\omega_{\vec{q}}$ and $\vec{q}$ are the frequency and wave vector of the longitudinal optic phonon, and M_+ and M_- are the masses of the positive and negative ions, respectively. For simplicity, we will assume an Einstein model for the optic phonons, so that $\omega_{\vec{q}}\simeq\omega_{\rm LO}$, the longitudinal-optic frequency at $\vec{q}=0$. Also, we will cut off the phonon spectrum at $\vec{q}_D$, the Debye wave vector. With these assumptions, the electron-phonon interaction at a position $\vec{r}$ becomes (for one electron)

$$\mathcal{H}_{ep}=i\beta\sum_{\vec{q}}\frac{1}{q}\left(a_{\vec{q}}e^{i\vec{q}\cdot\vec{r}}-a_{q}^{*}e^{-\vec{q}\cdot\vec{r}}\right), \tag{38}$$

where

$$\beta=\frac{16\pi e^2}{\epsilon_\infty a_0^3}\left[\left(\frac{M_-}{M_+}\right)^{1/2}+\left(\frac{M_+}{M_-}\right)^{1/2}\right]\left(\frac{\hbar}{2\rho\omega_{\rm LO}}\right)^{1/2}, \tag{39}$$

where ϵ_∞ is the high-frequency, optical dielectric constant and a_0 is the lattice constant of the rocksalt structure.

Thus, in order to use the results of Sec. III A directly, i.e., Eq. (32), we set

$$A_{\vec{q}}=\frac{i\beta}{q}\,. \tag{40}$$

From Eq. (32), we then obtain the phonon-mediated electron-electron interaction in the form

$$V(s)=\frac{2V_0}{\pi q_D s}\int_0^{q_D}\frac{1}{q}\,\frac{\sin(qs)dq}{b^4(q/q_D)^4-1}\,, \tag{41}$$

where

$$V_0=\frac{\beta^2 q_D}{2\pi\hbar\omega_{\rm LO}}\,, \tag{42}$$

and

$$b\equiv\left(\frac{\hbar q_D^2}{2m\omega_{\rm LO}}\right)^{1/2}. \tag{43}$$

In achieving the form of Eq. (41), we have made the same assumptions as for Eq. (34) in Sec. III B. In particular, we have assumed that $k_\uparrow, k_\downarrow\sim 0$, which makes $V(\vec{s})$ spherically symmetric and only dependent on the magnitude s of the separation between the two electrons.

Consider for a moment the classical limit, i.e., $m\rightarrow\infty$, so that $b\rightarrow 0$. In this case, the electron-electron interaction mediated by optic phonons becomes simply

$$V(s)=-\frac{V_0}{q_D s}\left(\frac{2}{\pi}\,\mathrm{Si}(q_D s)\right)\quad(b\rightarrow 0)\,, \tag{44}$$

where Si(z) is the sine integral function defined in Eq. (15a). In the limit as $s\rightarrow\infty$, the electrostatic potential $\phi_{\rm LO}(s)$ due to the optic phonons would then become

$$\phi_{\rm LO}(s\rightarrow\infty)=\frac{V(s)}{-e}=\frac{V_0}{eq_D s}\,. \tag{45}$$

This is the same result that one would obtain by taking the expectation value of $\mathcal{H}_{ep}/(-e)$, $\mathcal{H}_{ep}$ given by Eq. (38), between the clothed-electron states of one electron. The total electrostatic potential of the two-electron system $\phi_{\text{tot}}(s)$ is obtained by adding to Eq. (45) the electrostatic repulsion between the two electrons in the absence of the phonons:

$$\phi_{\text{tot}}(s\to\infty)=\frac{-e}{\epsilon_\infty s}+\phi_{\text{LO}}(s)\equiv\frac{-e}{\epsilon_0 s}\,, \tag{46}$$

where ϵ_0 is the low-frequency static dielectric constant. This means that the coefficient V_0 in front of the interaction in Eqs. (41) and (44) may be written in a simple form in terms of ϵ_0 and ϵ_∞:

$$V_0=-q_De^2\left(\frac{1}{\epsilon_0}-\frac{1}{\epsilon_\infty}\right). \tag{47}$$

The actual function for finite s, Eq. (44), contains mild oscillations about the curve V_0/q_Ds, which are due to the sharp q_D cutoff. This illustrates the well known idea that the virtual optic-phonon clothing of an electron, at least in the classical limit, is nothing more than the ionic distortion that modifies the electron screening from that of the optical dielectric constant to that of the static dielectric constant.[5]

In the case of finite b [Eq. (43)], there are two alternatives ($b<1$ or $b>1$). as in the discussion for acoustic phonons discussed in Sec. III B. We consider only the case with $b>1$ and evaluate the principal part of the integral in closed form in terms of sine and cosine integral functions $\text{Si}(z)$ and $\text{Ci}(z)$, defined in Eq. (15), and in terms of the exponential integral function $E_1(z)$:

$$\begin{aligned}V(s)=\frac{-V_0}{q_Ds}\;\frac{2}{\pi}\Big[&\text{Si}(q_Ds)-\tfrac{1}{4}\cos\left(\frac{q_Ds}{b}\right)\{\text{Si}[q_Ds(1+1/b)]+\text{Si}[q_Ds(1-1/b)]\}\\&+\tfrac{1}{4}\sin\left(\frac{q_Ds}{b}\right)\{\text{Ci}[q_Ds(1+1/b)]-\text{Ci}[q_Ds(1-1/b)]\}\\&-\tfrac{1}{4}\,\text{Im}\{e^{q_Ds/b}E_1(q_Ds(1/b+i))+e^{q_Ds/b}E_1(q_Ds(-1/b+i))\}\Big]\quad(b>1)\,,\end{aligned} \tag{48a}$$

where

$$E_1(z)=\int_z^\infty\frac{e^{-t}dt}{t}\,, \tag{48b}$$

and Im indicates that the imaginary part of the function must be taken.

In studying the nature of this interaction, Eq. (48), we will apply it to the case of LiCl, an ionic crystal that has the rocksalt structure. For this case, we neglect the effects of acoustic phonons on the phonon-mediated electron-electron interaction, since they are very small compared with the optic-phonon effects. In LiCl, the lattice constant is $a_0=5.14$ Å, which gives $q_D=1.20\times10^8\ \text{cm}^{-1}$. $\omega_{\text{LO}}=7.5\times10^{13}\ \text{sec}^{-1}$, so that $b=(\hbar q_D^2/2m\omega_{\text{LO}})^{1/2}=10.6$. Since $\epsilon_0=12.0$ and $\epsilon_\infty=2.7$, we have that $V_0=4.98$ eV. With these parameters, we then plot with a solid curve the phonon-mediated electron-electron interaction $V(s)$ in Fig. 3. As can be seen, large quantum oscillations appear about the expected $(e^2/s)(1/\epsilon_0-1/\epsilon_\infty)$ behavior that is shown by the dashed curve. These oscillations have the same origin as did the repulsive core of the interaction of Sec. III B, shown in Fig. 2 and given by Eq. (36). That is, the virtual-recoil kinetic energies of the two electrons are responsible for this effect.

Now suppose that we add the Coulomb repulsion between the two electrons to the phonon-mediated

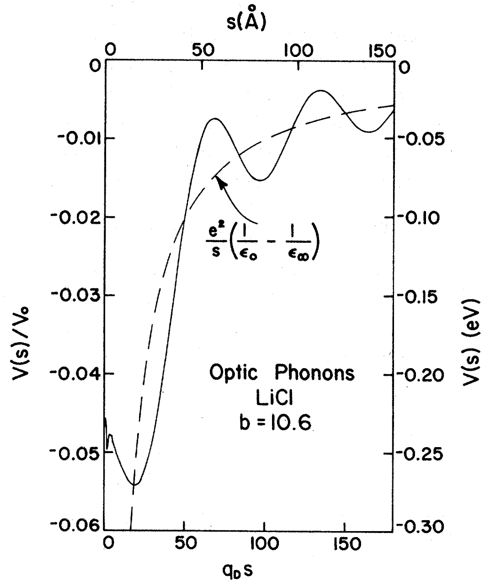

FIG. 3. The solid curve is a plot of the optic-phonon-mediated electron-electron interaction $V(s)$ from Eq. (48) for LiCl with $b=(\hbar q_D^2/2m\omega_{\text{LO}})^{1/2}=10.6$. $V_0=4.98$ eV and is given in Eq. (47). The dashed curve gives the expected, classical, behavior of the screening by optic phonons, $(e^2/s)(1/\epsilon_0-1/\epsilon_\infty)$.

electron-electron interaction, Eq. (48), shown in Fig. 3. That is, we plot $(e^2/\epsilon_\infty s) + V(s)$ in Fig. 4. The dashed curve shows the expected, classical result, while the smooth curve is the quantum result for LiCl. Note that this potential has strong oscillations that produce deep potential wells. The first such well occurs when the electrons are about 33 Å apart, and its depth is about 28 meV. This provides the possibility of having bound states of two electrons in an ionic crystal.

In order to understand better the results presented in Eq. (48) and in Figs. 3 and 4, it is useful to write the leading terms for large s of Eq. (48):

$$V(s) \underset{s\to\infty}{\sim} -\frac{V_0}{q_D s}\left[1 - \tfrac{1}{2}\cos\left(\frac{q_D s}{b}\right)\right]. \tag{49}$$

Actually, even by the time the electrons are sufficiently separated to be in the first attractive well in Fig. 4, this function is fairly well satisfied. [The depth of the first minimum is about 31 meV for Eq. (49) and 28 meV for Eq. (48).] This means that this expression can be used to determine the approximate values of ϵ_0 and ϵ_∞ that are necessary to produce an attractive potential in Fig. 4. The total potential in this limit is then:

$$\left(\frac{e^2}{\epsilon_\infty s} + V(s)\right) \underset{s\to\infty}{\sim} \frac{e^2}{\epsilon_\infty s}\left\{1 + \left(\frac{\epsilon_\infty}{\epsilon_0} - 1\right)\left[1 - \tfrac{1}{2}\cos\left(\frac{q_D s}{b}\right)\right]\right\}. \tag{50}$$

It is easy to see now that the requirement for this to become negative is that $\epsilon_0 > 3\epsilon_\infty$.

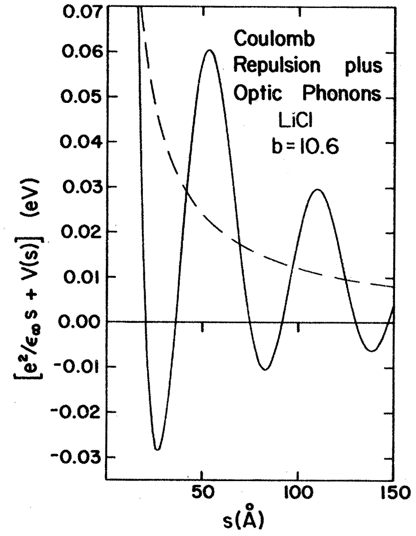

FIG. 4. The solid curve gives the total interaction between two electrons in LiCl, including the contributions from Coulomb repulsion and optic phonons, $(e^2/\epsilon_\infty s) + V(s)$, with $V(s)$ shown in Fig. 3. Classically, the two electrons should repel one another as $e^2/\epsilon_0 s$, as shown by the dashed curve. The potential well of 28 meV in depth for $s \sim 33$ Å opens the possibility of bound states, or electron-pair bubbles.

IV. CONCLUSIONS

In our calculation of the phonon-mediated electron-electron interaction we have found interesting and surprising results. For the case of acoustic phonons in a nonpolar material, we have found that the interaction (excluding e^2/s) has a repulsive core. In other words, when the electrons are close together, they repel rather than attract one another. This core is very wide, extending more than 100 Å. The repulsive core has been found to be due to the virtual-recoil kinetic energies of the two electrons. In the optic-phonon case, we find large quantum oscillations in the phonon-mediated interaction about the expected smooth $1/s$ behavior, where s is the distance between the two electrons. When the usual Coulomb repulsion between the two electrons is added, we find that deep potential wells remain in the total potential, the first of which is about 28 meV deep for LiCl and occurs when the electrons are separated by about 33 Å. This could lead to bound states, or electron-pair bubbles. We have not yet investigated this possibility in detail. The consequences of such bubbles on the properties of ionic crystals could be of considerable interest, especially if these pairs were to undergo a Bose condensation into a common center of mass momentum state.

A subject for future study is an analysis of the potentials presented here when the velocities of the electrons are large. Specifically it is important to see if the potential wells that we have found here for ionic crystals still persist at higher velocities. If that were true, a small concentration of electrons, injected into some ionic crystals, might become superconducting. Finally, it would be useful to know the effects of higher-order corrections of the electron-phonon coupling on our results, especially for optic phonons. Here, our discussion has been limited to the lowest order in perturbation theory required to derive an electron-electron potential.

ACKNOWLEDGMENTS

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[3] See also O. Madelung, *Introduction to Solid State Theory* (Springer, Berlin, 1978), p. 229.

[4] For simplicity we shall neglect the q dependence of the polarization vectors and use their values near $q=0$ throughout the Brillouin zone.

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