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Phonon-modulated electron-electron interactions

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The phonon modulation of electron-electron interactions are calculated for solids described by tight-binding models. In some cases the interaction can be larger than the usual electron-phonon effects. [S0163-1829(99)00828-0]

I. INTRODUCTION

The traditional derivation of the electron-phonon interaction in solids includes the electron-ion interaction, which is suitably screened by the conduction electrons.[1,2] In tight-binding models, another contribution is the phonon modulation of the hopping term.[3–5] There is another interaction which we introduce here. It arises from the phonon modulation of the electron-electron interactions. We show that this interaction can be sizable in solids whose conduction bands are described by tight-binding models.

There have been numerous papers on electron-electron interactions *mediated* by phonons.[6,7] Those papers calculated the interaction between two electrons by exchanging a phonon. Here the process is different. The electrons interact by the Coulomb interaction e^2/R, but the distance R is *modulated* by the ion vibrations.

The model is a neutral tight-binding system.[3] For this first calculation, the simplest possible model is adopted. There is one atomic site per unit cell, so all sites have identical symmetry. The ion cores are considered closed shell and possess s-wave symmetry. Similarly, the conduction electron orbitals on each ion site also are assumed to possess s-wave symmetry. If the ion cores have a valence of Z, then charge neutrality requires that the average number of conduction electrons on each site is also Z. All of the atoms in the system have conducting electrons. So the average charge on an atom site is zero. Conduction electrons can hop from a site to the neighboring sites. It is assumed the electron orbitals on an ion move with the ion core during the phonon vibration.

This model was conceived to apply to graphite. Considering only the orbitals with p_z symmetry, then $Z=1$. There is an average of one electron per atomic site, and the ion cores also have a charge of one. The present model does not fit graphite, which has two atoms per unit cell.[4] Also, the graphite energy bands have small Fermi surfaces and a linear dispersion. A future paper will discuss this model in relation to graphite, and also to carbon nanotubes.[5] The present paper is intended to derive the general formalism, and to show that the phonon modulated electron-electron interactions can be significant in tight-binding systems.

II. THE HAMILTONIAN

The Hamiltonian is

$$H=H_0+V, \tag{1}$$

$$H_0=-w\sum_{j\delta\sigma} C^{\dagger}_{j+\delta,\sigma}C_{j\sigma}+\sum_{\mathbf{q}} \omega_{\mathbf{q}}a^{\dagger}_{\mathbf{q}}a_{\mathbf{q}}, \tag{2}$$

$$V=\frac{e^2}{2}\sum_{nm}\int\frac{d^3r_1d^3r_2}{|\mathbf{r}_1-\mathbf{r}_2|}[\rho_i(\mathbf{r}_1-\mathbf{R}_n)-C^{\dagger}_nC_n\rho_e(\mathbf{r}_1-\mathbf{R}_n)]\times[\rho_i(\mathbf{r}_2-\mathbf{R}_m)-C^{\dagger}_mC_m\rho_e(\mathbf{r}_2-\mathbf{R}_m)], \tag{3}$$

$$Z=\int d^3r\rho_i(\mathbf{r}), \tag{4}$$

$$1=\int d^3r\rho_e(\mathbf{r}), \tag{5}$$

where $\rho_{i,e}(\mathbf{r})$ are the charge densities due to the ion cores and conduction electrons. The operators $C_{j\sigma}$ refer to electrons and $a_{\mathbf{q}}$ to phonons. The following steps are used to derive an electron-electron interaction. Fourier transform the Coulomb interaction

$$\frac{e^2}{|\mathbf{r}_1-\mathbf{r}_2|}=\frac{1}{\Omega}\sum_{\mathbf{q}} v(q)e^{i\mathbf{q}\cdot(\mathbf{r}_1-\mathbf{r}_2)}, \tag{6}$$

where Ω is the volume of the crystal and $v(q)=4\pi e^2/q^2$. Next perform the integrals over $d^3r_{1,2}$ which brings us to the interaction

$$V=\frac{1}{2\Omega}\sum_{\mathbf{q},nm} v(q)e^{i\mathbf{q}\cdot(\mathbf{R}_n-\mathbf{R}_m)}[\tilde{\rho}_i(\mathbf{q})-C^{\dagger}_nC_n\tilde{\rho}_e(\mathbf{q})]\times[\tilde{\rho}_i(-\mathbf{q})-C^{\dagger}_mC_m\tilde{\rho}_e(-\mathbf{q})], \tag{7}$$

where $\tilde{\rho}_{e,i}(\mathbf{q})$ are the Fourier transforms of the charge densities. Let the atomic position $\mathbf{R}_n=\mathbf{R}^{(0)}_n+\mathbf{Q}_n$, where $\mathbf{R}^{(0)}_n$ is the equilibrium position and $\mathbf{Q}_n$ is the atomic displacement due to the phonons. For the moment it is assumed there is only one atom per unit cell. We extend the results to several atoms in a cell in a later paper. Expand the exponent in powers of $\mathbf{Q}$ and retain only the linear term. Express the electron number operators in terms of collective coordinates

$$C^{\dagger}_nC_n=Z+\frac{1}{N}\sum_{\mathbf{q}\neq 0}\rho(\mathbf{q})e^{i\mathbf{q}\cdot\mathbf{R}^{(0)}_n} \tag{8}$$

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

$$V=\frac{1}{2\Omega}\sum_{\mathbf{q},nm} v(q)e^{i\mathbf{q}\cdot(\mathbf{R}_n^{(0)}-\mathbf{R}_m^{(0)})}[1+i\mathbf{q}\cdot(\mathbf{Q}_n-\mathbf{Q}_m)]$$
$$\times\left[\tilde{\rho}_T(\mathbf{q})^2-\frac{2}{N}\tilde{\rho}_T(\mathbf{q})\tilde{\rho}_e(\mathbf{q})\sum_{\mathbf{q}_1\neq 0}\rho(\mathbf{q}_1)e^{i\mathbf{q}_1\cdot\mathbf{R}_n^{(0)}}\right.$$
$$\left.+\frac{1}{N^2}\tilde{\rho}_e(q)^2\sum_{\mathbf{q}_1\mathbf{q}_2}\rho(\mathbf{q}_1)\rho(\mathbf{q}_2)e^{(i\mathbf{q}_1\cdot\mathbf{R}_n^{(0)}+i\mathbf{q}_2\cdot\mathbf{R}_m^{(0)})}\right],$$
$$\tilde{\rho}_T(\mathbf{q})=\tilde{\rho}_i(\mathbf{q})-Z\tilde{\rho}_e(\mathbf{q}). \tag{10}$$

The symbol $\tilde{\rho}_T(\mathbf{q})$ denotes the Fourier transform of the total average charge density on a lattice site. It vanishes at $\mathbf{q}=0$ due to charge neutrality. The above expression for V contains several types of interactions. The most important three are electron-electron (V_{ee}), electron-phonon (V_{ep}), and the phonon-modulated electron-electron (V_{eep}). For the latter two we expand the ion vibration $\mathbf{Q}$ in terms of phonon coordinates,

$$\mathbf{Q}_n=\sum_{\mathbf{Q}} X_{\mathbf{Q}}A_{\mathbf{Q}}\hat{\xi}_{\mathbf{Q}}e^{i\mathbf{Q}\cdot\mathbf{R}_n^{(0)}}, \tag{11}$$

$$X_{\mathbf{Q}}^2=\frac{\hbar}{2M\omega_{\mathbf{Q}}N},\quad A_{\mathbf{Q}}=a_{\mathbf{Q}}+a_{-\mathbf{Q}}^{\dagger}, \tag{12}$$

$$V_{ee}=\frac{1}{2\Omega}\sum_{\mathbf{q}\neq 0} M_{\mathbf{q}}\rho(\mathbf{q})\rho(-\mathbf{q}), \tag{13}$$

$$M_{\mathbf{q}}=\sum_{\mathbf{G}} v(\mathbf{q}+\mathbf{G})\tilde{\rho}_e(\mathbf{q}+\mathbf{G})^2, \tag{14}$$

$$\mathbf{P}_{\mathbf{Q}}=\sum_{\mathbf{G}} (\mathbf{Q}+\mathbf{G})v(\mathbf{Q}+\mathbf{G})\tilde{\rho}_e(\mathbf{Q}+\mathbf{G})\tilde{\rho}_T(\mathbf{Q}+\mathbf{G}), \tag{15}$$

$$V_{ep}=\frac{i}{\Omega}\sum_{\mathbf{Q}} X_{\mathbf{Q}}A_{\mathbf{Q}}\rho(-\mathbf{Q})(\hat{\xi}_{\mathbf{Q}}\cdot\mathbf{P}_{\mathbf{Q}}), \tag{16}$$

$$\mathbf{L}_{\mathbf{q}}=\sum_{\mathbf{G}} (\mathbf{q}+\mathbf{G})v(\mathbf{q}+\mathbf{G})\tilde{\rho}_e(\mathbf{q}+\mathbf{G})^2, \tag{17}$$

$$V_{eep}=\frac{i}{\Omega}\sum_{\mathbf{qQ}} X_{\mathbf{Q}}(\hat{\xi}_{\mathbf{Q}}\cdot\mathbf{L}_{\mathbf{q}})A_{\mathbf{Q}}\rho(\mathbf{q})\rho(-\mathbf{q}-\mathbf{Q}). \tag{18}$$

In the present notation, the vector $\mathbf{q}$ is confined to the first Brillouin zone, and the summation over reciprocal-lattice vectors $\mathbf{G}$ extends the wave vector to larger values. The electron-phonon interacion V_{ep} has the usual form. It is the usual term, which is calculated. The factor of $(\hat{\xi}_{\mathbf{Q}}\cdot\mathbf{Q})$ gives a deformation-type interaction due to two features: (1) The function $\mathbf{P}_{(\mathbf{Q})}$ is a vector which points in the direction $\mathbf{Q}$, (2) since $\tilde{\rho}_T(\mathbf{q})$ vanishes at zero wave vector, the quantity $v(q)\tilde{\rho}_T(\mathbf{Q})$ goes to a constant at zero wave vector. Usually the interaction is nearly constant due to the screening from electron-electron interactions. Here it is also due to Coulomb interactions, although the formal screening has not yet been included. Our major interest is in the last term which describes phonon-modulated electron-electron interactions.

The effective Coulomb interaction is denoted as $M_{\mathbf{q}}$. It can be expressed as the Hubbard U plus the off-site interaction $U_{\mathbf{q}}$,

$$M_{\mathbf{q}}=U+U_{\mathbf{q}}, \tag{19}$$

$$U_{\mathbf{q}}=\sum_{n\neq 0} e^{i\mathbf{q}\cdot\mathbf{R}_n}V(\mathbf{R}_n), \tag{20}$$

where $V(\mathbf{R}_n)$ is the electron-electron interaction between sites separated by $\mathbf{R}_n$. In this case, the electron-electron interactions can be written in the usual form

$$V_{ee}=U\sum_j [n_{j\uparrow}+n_{j\downarrow}+n_{\uparrow}n_{j\downarrow}]+\frac{1}{2N}\sum_{\mathbf{q}} U_{\mathbf{q}}\rho(\mathbf{q})\rho(-\mathbf{q}). \tag{21}$$

The first term is the Hubbard interaction on the same site, while the second term comprises the extended Hubbard model, for interaction between different sites.

The interaction V_{eep} is the new term that provides a contribution to the interaction between electrons and phonons. The remainder of the paper discusses the self-energy of an electron from this interaction.

III. EXCHANGE MATRIX ELEMENTS

One contribution to the phonon modulation of the electron-electron interactions is the exchange terms. This contribution seems to be the largest. The first step is to eliminate an electron interacting with itself to write

$$\rho(\mathbf{q})\rho(-\mathbf{q}-\mathbf{Q})\equiv\sum_{\mathbf{p}_1\mathbf{k}_1s_1s_2} C_{\mathbf{p}_1+\mathbf{q},s_1}^{\dagger}C_{\mathbf{k}_1-\mathbf{q}-\mathbf{Q},s_2}^{\dagger}C_{\mathbf{k}_1,s_2}C_{\mathbf{p}_1,s_1}.$$

Note that $\mathbf{q}\neq 0$, $\mathbf{q}\neq -\mathbf{Q}$. The only available pairing of any operators is to take the exchange terms. The exchange pairing is to write this as

$$\rho(\mathbf{q})\rho(-\mathbf{q}-\mathbf{Q})\rightarrow-\sum_{\mathbf{p}_1s_1} C_{\mathbf{p}_1-\mathbf{Q},s_1}^{\dagger}C_{\mathbf{p}_1,s_1}[n_{\mathbf{p}_1+\mathbf{q}}+n_{\mathbf{p}_1-\mathbf{q}-\mathbf{Q}}].$$

The two terms in brackets come from the two different ways of exchange pairing. The summation over the wave vector $\mathbf{q}$ can now be evaluated, which defines an effective matrix element

$$U(\mathbf{k},\mathbf{Q})=\hat{\xi}_{\mathbf{Q}}\cdot[\mathbf{S}(\mathbf{k}+\mathbf{Q})-\mathbf{S}(\mathbf{k})], \tag{22}$$

$$\mathbf{S}(\mathbf{k})=\int\frac{d^3q}{(2\pi)^3}\mathbf{q}v_q\tilde{\rho}_e(q)^2n_{\mathbf{k}+\mathbf{q}}. \tag{23}$$

Each matrix element has two terms. The square of the matrix element has four terms. They correspond to the four diagrams in Fig. 1. The evaluation of the function $\mathbf{S}(\mathbf{k})$ is discussed in the Appendix. To a good approximation it can be expressed as

$$\mathbf{S}(\mathbf{k})=-\frac{e^2k_F}{2\pi}\mathbf{k}I, \tag{24}$$

$$U(\mathbf{k},\mathbf{Q})=-\frac{e^2k_F}{2\pi}\mathbf{Q}I\equiv\mathbf{Q}D. \tag{25}$$

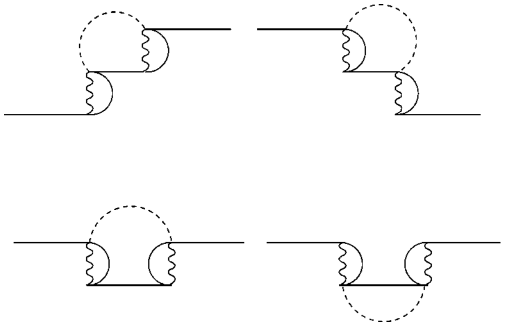

FIG. 1. Four contributions to the exchange part of the phonon-modulated electron-electron interaction.

The constant I depends upon the nature of the electron charge distribution $\tilde{\rho}_e$, and has a value near to unity. This simple approximation for $\mathbf{S}(\mathbf{k})$ makes $U(\mathbf{k},\mathbf{Q})$ independent of $\mathbf{k}$. The resulting interaction now has the form of a deformation potential which is just half of the exchange energy

$$V_{eepx}=\sum_{\mathbf{Q}} M^{(x)}_{\mathbf{Q}} A_{\mathbf{Q}} \rho(-\mathbf{Q}), \tag{26}$$

$$M^{(x)}_{Q}=DX_{Q}\hat{\xi}_{\mathbf{Q}}\cdot\mathbf{Q}, \tag{27}$$

$$D=-\frac{e^2k_F}{2\pi}I. \tag{28}$$

The one-phonon self-energy is now (using a four-vector notation)

$$\begin{aligned}\Sigma_{eepx}(\mathbf{k},ik_n)&=\frac{D^2}{\beta}\sum_{Q} X^2_{\mathbf{Q}}(\hat{\xi}_{\mathbf{Q}}\cdot\mathbf{Q})^2\mathcal{G}(k+Q)\mathcal{D}(Q)\\&=\frac{\hbar D^2}{2\rho}\int\frac{d^3Q}{(2\pi)^3}\frac{(\hat{\xi}_{\mathbf{Q}}\cdot\mathbf{Q})^2}{\omega_{\mathbf{Q}}}\left[\frac{N_{\mathbf{Q}}+1-n_F(\mathbf{k}+\mathbf{Q})}{ik_n-\varepsilon_{\mathbf{k}+\mathbf{Q}}-\omega_{\mathbf{Q}}}\right.\\&\qquad\left.+\frac{N_{\mathbf{Q}}+n_F(\mathbf{k}+\mathbf{Q})}{ik_n-\varepsilon_{\mathbf{k}+\mathbf{Q}}+\omega_{\mathbf{Q}}}\right].\end{aligned}$$

The strength of the electron-phonon interaction is determined by the dimensionless quantity λ defined as

$$\lambda=\frac{D^2}{\rho}\int\frac{d^3Q}{(2\pi)^3}\frac{(\hat{\xi}_{\mathbf{Q}}\cdot\mathbf{Q})^2}{\omega^2_{\mathbf{Q}}}\delta(\varepsilon_{\mathbf{k}}-\varepsilon_{\mathbf{k}+\mathbf{Q}}). \tag{29}$$

The value of this coupling constant is estimated using the Wigner-Seitz model for the unit cell. In the approximation of a spherical unit cell, of radius q_R, the LA (longitudinal acoustical) modes are approximated as

$$\rho\omega^2_{\mathbf{Q}}=\frac{C_{11}}{b^2}\sin^2(Qb), \tag{30}$$

$$b=\frac{\pi}{2q_R}, \tag{31}$$

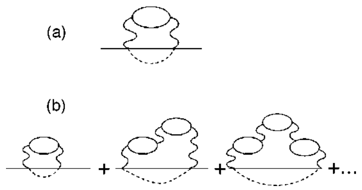

FIG. 2. RPA contributions to the correlation part of the phonon-modulated electron-electron interactions.

$$\lambda=\frac{mb^2D^2}{(2\pi)^2k_F\hbar^2C_{11}}\int_0^{q_R}\frac{Q^3dQ}{\sin^2(Qb)}, \tag{32}$$

$$\lambda=\frac{3E_{ry}(4N_c)^{1/3}}{2\pi^4V_0C_{11}}I_0I^2 \tag{33}$$

$$I_0=\int_0^{\pi/2}\frac{z^3dz}{\sin^2(z)}\approx 1.98, \tag{34}$$

where $N_c=n_0V_0$ is the average number of electrons in the unit cell of volume V_0. The upper limit on the dQ integral is either q_R or $2k_F$, whichever is smallest. For most values of N_c then $2k_F>q_R$ so that q_R is used.

Most insulators have elastic constants on the order of $C_{11}\approx$ 50 GPa. Choosing a lattice constant of $a=0.35$ nm, then the ratio of $E_{ry}/(C_{11}V_0)\approx 4$. If $N_c=1$ then $\lambda=0.20$. This value is increased if C_{11} is reduced. The value of λ is similar to what is often found using the linear electron-phonon interaction V_{ep}.

IV. CORRELATION MATRIX ELEMENTS

Another contribution to the self-energy of the electron is discussed in this section. This self-energy of an electron is also calculated in the one-phonon approximation. It uses the same basic interaction V_{eep} but evaluates another Feynman diagram shown in Fig. 2(a). The dashed line is the phonon, and solid lines are electrons. The closed bubble is a polarization contribution from the electrons. Higher-order diagrams are shown in Fig. 1(b). They utilize the electron-electron interaction to sum a similar set of bubble diagrams. The result of all of these terms gives the self-energy function

$$\begin{aligned}\Sigma(k)&=\frac{\hbar}{2MNA\beta^2}\sum_{qQ}\frac{\mathcal{T}(\mathbf{q},\mathbf{Q})}{\omega_{\mathbf{Q}}}\mathcal{G}(k+q+Q)\mathcal{D}(Q)\\&\quad\times\left[\frac{P(q)}{1-(M_{\mathbf{q}}+U/2)P(q)}\right],\end{aligned} \tag{35}$$

$$\mathcal{T}(\mathbf{q},\mathbf{Q})=[\hat{\xi}_{\mathbf{Q}}\cdot(\mathbf{L}_{\mathbf{q}}+\mathbf{L}_{-\mathbf{q}-\mathbf{Q}})]^2,$$

$$P(q)=\frac{2}{A\beta}\sum_{p}\mathcal{G}(p)\mathcal{G}(p+q)=2\int\frac{d^2p}{(2\pi)^2}\frac{n(\mathbf{p})-n(\mathbf{p}+\mathbf{q})}{iq_n+\varepsilon_{\mathbf{p}}-\varepsilon_{\mathbf{p}+\mathbf{q}}}.$$

The factor of $(M_{\mathbf{q}}+U/2)$ shows that screening is due only to the charge fluctuations. The spin fluctuations do not enter. This result is expected since phonons are a type of charge fluctuation.[8] Our treatment of the Hubbard model is valid only for small and intermediate values of U, where the random-phase approximation (RPA) is still valid. For large values of U then the Hubbard interaction cannot be treated as a perturbation, but is included in H_0.

The angular factor $(\hat{\xi}_{\mathbf{Q}}\cdot\mathbf{L}_{\mathbf{q}})$ in the matrix element has become $\mathcal{T}(\mathbf{q},\mathbf{Q})$ in the self-energy. This change occurs because in the evaluation of the correlation function

$$(\hat{\xi}_{\mathbf{Q}}\cdot\mathbf{L}_{\mathbf{q}})(\hat{\xi}_{\mathbf{Q}}\cdot\mathbf{L}_{\mathbf{q}'})\langle C_{\mathbf{k}}(\tau)\rho(\mathbf{q},\tau_1)\rho(-\mathbf{q}-\mathbf{Q},\tau_1)$$
$$\times\rho(\mathbf{q}',\tau_2)\rho(-\mathbf{q}'+\mathbf{Q},\tau_2)C_{\mathbf{k}}^{\dagger})\rangle. \tag{36}$$

The same self-energy contribution occurs with four combinations of $(\mathbf{q},\mathbf{q}')$: $(\mathbf{q},-\mathbf{q}),(\mathbf{q}+\mathbf{Q},-\mathbf{q}-\mathbf{Q})$, $(\mathbf{q},-\mathbf{q}-\mathbf{Q})$, $(\mathbf{q}+\mathbf{Q},-\mathbf{q})$. Adding them together provides the expression for $\mathcal{T}(\mathbf{q},\mathbf{Q})$.

The self-energy expression (35) has a formal resemblance to the self-energy from the usual electron-phonon interaction V_{ep}. The self-energy has an electron Green's function $\mathcal{G}$, a phonon Green's function $\mathcal{D}$, and a screened interaction $\mathcal{T}P/(1-M'P)$. The important difference is that there is a summation over two independent wave vectors $(\mathbf{q},\mathbf{Q})$. This feature makes the final evaluation very different from the usual expression.

Another interesting feature of this expression is that it is similar to the RPA expression for the correlation energy of the electron gas

$$\Sigma(k)=-\frac{\hbar}{2MN\beta}\sum_{Q}\frac{1}{\omega_{\mathbf{Q}}}\mathcal{D}(Q)\Sigma_c'(k+Q), \tag{37}$$

$$\Sigma_c'(k+Q)=-\frac{1}{A\beta}\sum_{q}\mathcal{T}(\mathbf{q},\mathbf{Q})\mathcal{G}(k+q+Q)$$
$$\times\left[\frac{P(q)}{1-(M_q+U/2)P(q)}\right]. \tag{38}$$

The only difference from the usual correlation energy is the presence of a slightly different matrix element. For this term in the electron self-energy, the phonon modulation of the electron-electron interaction can be considered to be a phonon modulation of the correlation energy.

The next step is to do the summations over the frequency variables. In this step it is useful to employ a Lehmann representation for the correlation energy

$$\Sigma_c'(\mathbf{k}+\mathbf{Q},ik+iQ_n)=\int\frac{d\varepsilon'}{2\pi}\frac{B(\mathbf{k}+\mathbf{Q},\varepsilon')}{ik_n+iQ_n-\varepsilon'}, \tag{39}$$

$$\Sigma(\mathbf{k},ik)=\frac{\hbar}{2MN}\sum_{\mathbf{Q}}\frac{1}{\omega_{\mathbf{Q}}}\int\frac{d\varepsilon'}{2\pi}B(\mathbf{k}+\mathbf{Q},\varepsilon')$$
$$\times\left[\frac{N_Q+n_F(\varepsilon')}{ik+\omega_Q-\varepsilon'}+\frac{N_Q+1-n_F(\varepsilon')}{ik-\omega_Q-\varepsilon'}\right]. \tag{40}$$

At high temperature, where $N_Q\approx k_BT/\hbar\omega_{\mathbf{Q}}$, the largest term in the scattering time is

$$\frac{1}{\tau(\mathbf{k},E)}=-2\,\mathrm{Im}\{\Sigma(\mathbf{k},E)\}$$
$$=\frac{k_BT}{2MN}\sum_{\nu q}\frac{1}{\omega_{\mathbf{Q}}^2}$$
$$\times[B(\mathbf{k}+\mathbf{Q},E+\omega_Q)$$
$$+B(\mathbf{k}+\mathbf{Q},E-\omega_Q)]. \tag{41}$$

At small excitation energies the inverse lifetime from electron-electron interactions goes as $B(k,E)=\Lambda(k)(E-\mu)^2$ so that the above lifetime from the phonon-modulated electron-electron interactions is

$$\frac{1}{\tau(\mathbf{k},E)}=\frac{k_BT}{MN}\sum_{\nu q}\frac{1}{\omega_{\mathbf{Q}}^2}\Lambda(\mathbf{k}+\mathbf{Q})[(E-u)^2+\omega_Q^2]. \tag{42}$$

This expression seems to be small. The factor of ion mass in the denominator ensures that the result is a small contribution. Of the two terms on the right, one has $(E-\mu)^2$ which vanishes at the Fermi surface. The other has the phonon energies ω_Q^2 canceling, so that the ion mass remains and gives a small result. In summary, this term is negligible.

V. TWO DIMENSIONS

The most interesting effects of the phonon-modulated electron-electron interaction come in lower dimension. The primary application is to a single sheet of graphite. Another important application is to single-wall carbon nanotubes (SWNT), which are formed by rolling a graphite sheet into a tube. A graphite sheet is two dimensional, while the SWNT are intermediate between one and two dimensions.[9]

The above derivation needs to be modified for graphite due to the presence of a unit cell with two different atom sites. As shown in Ref. 4 for the electron-phonon interaction in graphite, having two sites per cell introduces various phase factors into the matrix element without changing its basic dependence upon wave vector. Here we shall discuss a model two-dimensional solid with one atom per unit cell.

In two dimensions the wave vectors of the phonon $(\mathbf{Q})$ and electrons $(\mathbf{q}_\perp,\mathbf{q}_\perp+\mathbf{Q})$ are two dimensional. The summation over $\mathbf{q}$ is three dimensional. It is useful to eliminate the dependence upon q_z up front by evaluating

$$F(q_\perp)=\int\frac{dq_z}{2\pi}v(q)\tilde{\rho}_e(q)^2. \tag{43}$$

In order to understand what this integral does, we take a simple example. Assume that $\tilde{\rho}_e=1/(1+q^2/\alpha^2)$ in which case the integral is easy. The symbol q now denotes a two-dimensional (2D) wave vector

$$F(q)=2\pi e^2\left[\frac{1}{q}-\frac{2q^2+3\alpha^2}{2(q^2+\alpha^2)^{3/2}}\right]. \tag{44}$$

The first term in brackets is the usual two-dimensional Fourier transform of the Coulomb interaction. The second term is from $\tilde{\rho}_e^2$ and modulates this interaction at large values of the wave vector. The two interactions of interest are

$$M_{\mathbf{q}}=\sum_{\mathbf{G}} F(\mathbf{q}+\mathbf{G}), \tag{45}$$

$$\mathbf{L}_{\mathbf{q}}=\sum_{\mathbf{G}} (\mathbf{q}+\mathbf{G})F(\mathbf{q}+\mathbf{G}), \tag{46}$$

$$V_{ee}=\frac{1}{2A}\sum_{\mathbf{q}} M_{\mathbf{q}}\rho(\mathbf{q})\rho(-\mathbf{q}), \tag{47}$$

$$V_{eep}=\frac{i}{A}\sum_{\mathbf{qQ}} X_{\mathbf{Q}}(\hat{\xi}_{\mathbf{Q}}\cdot\mathbf{L}_{\mathbf{q}})A_{\mathbf{Q}}\rho(\mathbf{q})\rho(-\mathbf{q}-\mathbf{Q}), \tag{48}$$

where A is the area of the 2D system. The same matrix element $F(\mathbf{q})$ enters both the electron-electron interactions and the phonon-modulated electron-electron interaction. In the above notation, the vectors $\mathbf{q},\mathbf{G},\mathbf{Q}$ are now all two dimensional.

The self-energy of an electron in two dimensions is calculated with this interaction. Again the largest contribution is the exchange interaction. Proceeding as we did in three dimensions, the two-dimensional exchange matrix element is

$$\mathbf{S}(\mathbf{k})=\int\frac{d^q}{(2\pi)^2}\mathbf{q}F(\mathbf{q})n_{\mathbf{k}+\mathbf{q}}\approx D\mathbf{k}, \tag{49}$$

$$D=-\frac{4}{3}\frac{e^2k_F}{\pi}I, \tag{50}$$

where the first factor in D is exact of $\tilde{\rho}_e=1$, and the factor of $I\approx 1$ corrects for the fact that the charge density is not one. The deformation constant D is larger in two dimensions, compared to three dimensions, by the factor of 8/3. Since D is squared in calculating λ, this provides a much larger interaction in two dimensions compared to three. The expression for λ in two dimensions is

$$\lambda=\frac{D^2A_0}{M}\int\frac{d^2Q}{(2\pi)^2}\frac{(\hat{\xi}_{\mathbf{Q}}\cdot\mathbf{Q})^2}{\omega_{\mathbf{Q}}^2}\delta(\varepsilon_{\mathbf{k}}-\varepsilon_{\mathbf{k}+\mathbf{Q}}). \tag{51}$$

It is evaluated using a circular unit cell, with the result

$$\lambda=\frac{32}{9\pi}\frac{E_{ry}}{Mc_s^2}N_c^2I^2I_1, \tag{52}$$

$$I_1=\int_0^{\alpha_0}d\alpha\frac{\sin^2(\alpha)}{\sin^2\left[\dfrac{\pi\sin(\alpha)}{2\sin(\alpha_0)}\right]}, \tag{53}$$

and $\sin(\alpha_0)=1/\sqrt{2N_c}$, where $N_c\approx 1$ is the number of conduction electrons in each unit cell. This value of λ is larger than the corresponding expression in three dimensions. The ratio $E_{ry}/Mc_s^2\approx 1$, where c_s is the speed of sound. The integral I_1 is a function of N_c, and $N_c^2I_1$ is typically in the range of 1/4 to 1/3. Thus in two dimensions we find that $\lambda\sim 0.3-0.4$. The phonon modulation of the electron-electron interaction is a significant process in two dimensions. In a later paper we calculate the value of λ for layered electron gases as found in the superconducting cuprates.

In summary, we have introduced an electron-phonon interaction in conducting solids described by the tight-binding approximation. The interaction comes from the phonon modulation of the electron-electron interactions. In two dimensions the effective coupling constant is estimated to be large.

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APPENDIX

Here we evaluate the function $\mathbf{S}(\mathbf{k})$, which is defined in three dimensions as

$$\mathbf{S}(\mathbf{k})=\int\frac{d^3q}{(2\pi)^3}\mathbf{q}v(q)\tilde{\rho}_e^2(q)n_{\mathbf{k}+\mathbf{q}}. \tag{A1}$$

A vector function of a vector must point in the direction of the vector. So define $\mathbf{S}(\mathbf{k})=\mathbf{k}\mathcal{S}(\mathbf{k})$ where

$$\mathcal{S}(\mathbf{k})=\frac{1}{k^2}\int\frac{d^3q}{(2\pi)^3}\mathbf{k}\cdot\mathbf{q}v(q)\tilde{\rho}_2^2(q)n_{\mathbf{k}+\mathbf{q}}. \tag{A2}$$

The first example is to evaluate setting to one the factors of $\tilde{\rho}_e$. Using $v(q)=4\pi e^2/q^2$ gives that $(x=k/k_F)$

$$\mathcal{S}(k)=-\frac{e^2k_F}{4\pi x^2}\left[1+x^2-\frac{1}{2x}(1-x^2)^2\ln\left|\frac{1+x}{1-x}\right|\right], \tag{A3}$$

$$\mathcal{S}(0)=-\frac{2}{3}\frac{e^2k_F}{\pi}, \tag{A4}$$

$$\mathcal{S}(k_F)=-\frac{1}{2}\frac{e^2k_F}{\pi}. \tag{A5}$$

The result varies from 2/3 of the exchange energy at $k=0$ to 1/2 at $k=k_F$. The electron-phonon interaction is most important for electrons at the Fermi surface, where $k=k_F$, so that we use this value. It is changed somewhat by including the orbital charge densities. They are assumed to have the form

$$\tilde{\rho}_e^2=\frac{1}{(1+q^2/\alpha^2)^{2n}}, \tag{A6}$$

$$\mathcal{S}(k_F)=-\frac{e^2k_F}{2\pi}I, \tag{A7}$$

$$I=\frac{2\beta(1+\beta)}{2n-1}\left[1-\left(\frac{\beta}{1+\beta}\right)^{2n-1}\right]-\frac{2\beta^2}{2n-2}\left[1-\left(\frac{\beta}{1+\beta}\right)^{2n-2}\right], \tag{A8}$$

where $\beta=\alpha^2/4k_F^2$, and β is expected to be a large number. The function is normalized such that $I(\beta)\rightarrow 1$ as $\beta\rightarrow\infty$.

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