Electron-phonon mass enhancement in metal multilayers

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A strong electron-phonon interaction in a metal increases the electron density of states in the vicinity of the Fermi energy dramatically. This phenomenon is called electron-phonon mass enhancement. In this paper, the question of whether the mass enhancement can be manipulated in multilayers of two metals with strong and weak electron-phonon interaction is investigated. A rich behavior is observed for different thickness ranges of the layers. For thin layers, one observes a rather homogeneous averaged enhancement. However, for an intermediate thickness range, the mass enhancement is highly anisotropic, i.e., direction dependent as well as position dependent. For large layer thicknesses, one obtains the bulk behavior for each metal.

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I. INTRODUCTION

A strong electron-phonon interaction (EPI) alters the electronic properties of a metal rather dramatically. It enhances the electron density of states in the vicinity of the Fermi energy. This phenomenon has been intensively investigated in the 1960s (see, for example, Refs. 1–3). Since then, it enjoys a strong experimental and theoretical interest.4–11

The overall strength of the EPI is summed up in a parameter \( \lambda \). Lead is a good example for a metal with strong EPI having a \( \lambda \) value of \( \lambda \approx 1.6 \). As a consequence, the electron density of states at the Fermi energy is enhanced by the factor \( Z = 1 + \lambda = 2.6 \). In addition, the Fermi velocity \( v_F = \hbar k_F / m^* \) is reduced by the factor \( Z \) corresponding to an enhancement \( Z \) of the mass. (Therefore, this effect is often called “mass enhancement.”) Since metals with strong EPI are generally superconducting, a number of superconducting properties are also enhanced, for example, the upper critical field \( B_{c2} \).

Although there have been many experiments which investigated the properties of double and multilayers of a metal \( S \) with strong EPI and a metal \( W \) with weak EPI, the author is not aware of any theoretical investigation of how the contact between \( S \) and \( W \) influences the mass enhancement in \( S \) or \( W \). Such an investigation is the goal of this paper.

In a metal with a strong electron-phonon interaction, the Fermi surface is not sharp even at zero temperature. This is shown in Fig. 1. The occupation below the Fermi momentum (we discuss here the case of clean metals) is less than 1 and above the Fermi energy the occupation is not zero but finite.

At the Fermi energy, the occupation drops by the value \( Z^{-1} \). The reason for this distribution is the following. An electron \( \mathbf{k}' \) below the Fermi energy can virtually emit a phonon \( \mathbf{q}, \lambda \) and make a transition into a satellite state \( \mathbf{k}'' \) above the Fermi energy. This process does not fulfill energy conservation since the satellite state [consisting of an electron \( \mathbf{k}'' \) above the Fermi energy and a phonon \( \mathbf{q}, \lambda \)] has an excess energy of \( \Delta E = \hbar \omega_{\mathbf{q}, \lambda} - \epsilon_{\mathbf{k}'} \). The satellite causes a finite electron occupation of the states \( \mathbf{k}'' \) above the Fermi surface and a finite hole occupation of the states \( \mathbf{k}' \) below the Fermi surface.

In Fig. 1, an electron is introduced into a state \( \mathbf{k}_0 \) directly above the Fermi energy. It changes the occupation of the \( \mathbf{k}_0 \) state only by \( Z^{-1} < 1 \) because this state was already partially occupied, and after the introduction into the state \( \mathbf{k}_0 \), part of the electron makes virtual transitions into the other states above the Fermi energy. This reduces the occupation of the state \( \mathbf{k}_0 \). Part of the electron is smeared over an energy range of \( \hbar \omega_D \) in combination with single virtual phonons.

Therefore, mass enhancement in an electron state \( \mathbf{k}_0 \) above the Fermi energy has two contributions.

1. The preoccupation of the state \( \mathbf{k}_0 \) is larger than 0: The state \( \mathbf{k}_0 \) is already partially occupied before an additional electron is introduced.

2. The postoccupation of the state \( \mathbf{k}_0 \) is less than 1: After the introduction of an additional electron, the state is not completely occupied because the electron makes virtual transitions into the other states above the Fermi energy. Both contributions are roughly equal.

Since the occupation of the state \( \mathbf{k}_0 \) changes only by \( Z^{-1} \), the energy (of the quasiparticle in \( \mathbf{k}_0 \)) is only \( \epsilon_{\mathbf{k}_0} / Z \). Therefore, the quasiparticle energies are closer together and their density of states is enhanced by the factor \( Z \).

In Appendix A, a short review of the treatment of the electron-phonon mass enhancement with Green’s functions is given. The discussed physical interpretation of the mass enhancement in terms of pre- and postoccupation is sketched. However, the Green’s function method cannot be easily expanded to multilayers. Therefore, in this paper I use self-consistent perturbation theory.

In Sec. II, the electron-phonon interaction and matrix element in multilayers are derived. In Sec. III, the amplitudes of the electron-phonon satellites are discussed. In a
multilayer, these satellites interfere in real space. This is discussed in Sec. IV. In Appendix B, the ground-state wave function in the presence of electron-phonon interaction is derived in self-consistent perturbation theory. Finally, Appendix C treats the ground state plus an additional electron above the Fermi energy.

Even in a homogeneous strong-coupling metal, the derivation of the relation $Z=1+\lambda$ is a complex and extended calculation. The multilayer system is highly inhomogeneous, and I attempt a more modest goal. I calculate the occupation of the electron states in real space in self-consistent (Brillouin-Wigner) perturbation theory. This yields an expression for the position and momentum dependent mass enhancement. A numerical evaluation is left for future work.

II. ELECTRON-PHONON INTERACTION IN MULTILAYERS

Now the questions are as follows: What happens in a double layer? Does the finite occupation above the Fermi energy leak from the strong-coupling metal into the weak-coupling metal? If this is the case, then one finds an enhanced density of states also in the normal metal (because an additional electron above the Fermi energy does not change the occupation by one). To analyze these questions, we investigate a very simple model of a double layer.

Model

We consider a double layer of a strong-coupling metal S and a weak-coupling or normal metal W. To keep the analysis simple, a primitive cubic lattice is used for both films with the same lattice constant $a$. The films are parallel to the $x$-$y$ plane. The metal S consists of $N^x_s$ layers and lies in the range $0 \leq z \leq d_s=N^x_s a$; and the metal W has $N^x_w$ layers in the regime $d_s \leq z \leq d_s+d_w=L_z=N_z a$, where $d_w=N^x_w a$ and $N_z$ is the total number of layers in the $z$ direction. For normalization reasons, the double layer has a finite but large extension in the $x$ and $y$ directions with the lengths $L_x=N_x a$ and $L_y=N_y a$. Furthermore, we use periodic boundary conditions in all three dimensions. This represents a multilayer of S and W. (We expect that this is equivalent to an isolated double layer with half the thicknesses $d_s/2$ and $d_w/2$.) The total number of atoms is $N=N_s N_w (N^x_s+N^x_w)$.

The electron density in both films is the same and the electrons behave as free electrons. The electron states are given by the wave number $k=(k_x,k_y,k_z)$ with the quantization $k_x=n_x 2 \pi /L_x$, $n_y=i$ (i.e., $x,y,z$). (The quantization in the $z$ direction extends over the total thickness $L_z=d_s+d_w$.)

Furthermore, we assume that the elastic properties of both metals are identical. Therefore, the phonons propagate through both films without scattering. The same quantization as for electrons applies to the wave vector $q=(q_x,q_y,q_z)$ of the lattice oscillations $q_x=\mu_x 2 \pi /L_x$ ($i=x,y,z$). Here, $\mu_x$ lies in the range $-N^x_s/2<\mu_x<N^x_s/2$.

The last assumption is rather artificial since metals with large electron-phonon interaction are generally softer in their elastic properties. However, such a more realistic model would complicate the following considerations dramatically. We make this assumption for the sake of simplicity in this initial treatment of the electron-phonon mass enhancement in multilayers.

Next, we derive the electron-phonon matrix element (EPME) $g_{k_2-k_1,q,\lambda}$ for the transition of an electron from a state $k_1$ into $k_2$ by absorbing a phonon $(q,\lambda)$ or emitting a phonon $(-q,\lambda)$. The EPME is derived in a number of textbooks. Therefore, only the essential results are given here.

The atoms oscillate with the amplitude $u_n$, and their position is given by

$$r_n = R_n + u_n,$$

where $R_n=na$ is the average position of the atom $n$ with $n=(n_x,n_y,n_z)$ being an integer.

In the lower strong-coupling film for $0 \leq z \leq d_s$, the atoms have a potential $V(r)$. The potential change due the lattice oscillations is

$$U(r) = V(r-R_n) - V(r-R_n).$$

We will use the free-electron approximation. This is equivalent to using $U(r)$ as the effective atomic potential.

In the upper weak-coupling film for $d_s \leq z \leq d_s+d_w$, the atoms have zero electron potential. For zero displacement of the atoms, the electron potential vanishes in both films. Therefore, we treat the electrons in both films as free.

The potential due to the lattice oscillations is

$$U(r) = \sum_{n_i} \left( u_{n_i} \cdot \nabla \right) V(r-R_n) = i \sum_{n_i} \sum_p (u_{n_i} \cdot p) V_p e^{i(p-R_n)},$$

where the sum over $n_i$ represents the sum over all atoms in $S$. The displacement $u_n$ of the atom at $R_n$ is expressed in terms of the annihilation and creation operators $a_{q',\lambda}$, $a^*_{-q',\lambda}$ for the phonons $(q',\lambda)$ and $(-q',\lambda)$,

$$u_n = \frac{1}{\sqrt{N}} \sum_{q',\lambda} \left( \frac{\hbar}{2 M \omega_{q',\lambda}} \right)^{1/2} e_{q',\lambda}^* e_{q}^* R_n (a_{q',\lambda} + a^*_{-q',\lambda}),$$

where $e_{q',\lambda}$ is the unit vector of polarization $\lambda$. This yields the electron-phonon interaction Hamiltonian

$$H_{e,p} = \sum_{k_1,k_2,q',\lambda} g_{k_2-k_1,q',\lambda} c^*_{k_1} c_{k_2} (a_{q',\lambda} + a^*_{-q',\lambda}),$$

with the electron-phonon matrix element $g_{k_2-k_1,q',\lambda}$

$$g_{k_2-k_1,q',\lambda} = i N \left( \frac{\hbar}{2 M \omega_{q',\lambda}} \right)^{1/2} \left[ (k_2-k_1) \cdot e_{q',\lambda} \right] V_{k_2-k_1} S_q'(q' - (k_2-k_1)),$$

where the structure factor $S_q(Q)$ [with $Q=q'-(k_2-k_1)$] is given by

$$S_q(Q) = \frac{1}{N} \sum_{k} \left( \frac{\hbar}{2 M \omega_{q',\lambda}} \right)^{1/2} \left[ (k_2-k_1) \cdot e_{q',\lambda} \right] V_{k_2-k_1} \delta_q'(q' - (k_2-k_1)).$$
where $\mathbf{G}$ is a reciprocal-lattice vector.

This means that there is no conservation of the $z$ component of the lattice momentum for the electron-phonon processes. For comparison, we denote the electron-phonon matrix element for the pure metal $S$ as $g_{k_0-k_0,q',\lambda}$. Its structure factor $S_f(Q)=\sum_{\mathbf{G}} \delta(Q,G)$ with $Q=q'-(k_2-k_1)$ fulfills conservation of lattice momentum,

$$S_f^0(Q) = i\sqrt{\frac{\hbar}{2M\omega_{q',\lambda}}} \left[ (k_2 - k_1) \cdot \mathbf{e}_{q',\lambda} \right] V_{k_2-k_1} \delta_{k_2-k_1, q'+G}. \tag{4}$$

For these electron-phonon processes in the multilayer which conserve the lattice momentum, i.e., when $k_2-k_1=q'+G$, one obtains

$$g_{k_2-k_1,q',\lambda} = \frac{N_0}{N_z} g_{k_2-k_1,q',\lambda} = \frac{d_z}{d_z + d_w} g_{k_2-k_1,q',\lambda}. \tag{5}$$

The weight of the EPME which conserves lattice momentum is reduced by the factor $d_z/(d_z + d_w)$.

### III. ELECTRON-PHONON SATELLITES

At $T=0$ in the absence of the electron-phonon interaction, all states within the Fermi sphere with $k \leq k_F$ ($k_F$ is the Fermi wave number) are occupied and all other states are empty. We denote this state as $|\psi_0\rangle = \prod_{k} c_{k,\lambda}^d |\Omega_0\rangle$, where $|\Omega_0\rangle$ is the vacuum. We select from the full Fermi sphere an occupied state $k'$. (In the following, such states $k$ will be sometimes denoted by their creation operators such as $c_{k,\lambda}^c$.) Furthermore, we choose from the phonon spectrum a phonon state $(q,\lambda)$. The state $k'$ can make a transition into a state $k''$ (above the Fermi surface) and create a phonon $(q,\lambda)$. Such a state can be described as a $k''$-electron--$k'$-hole plus one phonon $(q,\lambda)$. We denote its amplitude as $\alpha_{k''k',q,\lambda}$. The resulting ground state $|\psi_0\rangle$ in the presence of EPI is derived in Appendix B in self-consistent perturbation theory. One obtains for the amplitude of the satellites

$$\alpha_{k''k',q,\lambda} = \frac{g_{k''k',q,\lambda}}{(\eta_{k''} - \epsilon_{k''} - \hbar\omega)}, \tag{6}$$

where $\eta_{k''}$ is given in Appendix B by the self-consistent equation (B4).

This means that a state $c_{k''}^+$ with the occupation “1” generates satellites $c_{k''}^* a_{\lambda}^d$ with the (relative) occupation $|\alpha_{k''k'',q,\lambda}|^2$. After normalizing the total electron state, one obtains for the occupation of an electron state $k''_0$ below the Fermi energy and an electron $k''_0$ above the Fermi energy

$$n(k''_0) = \frac{1}{1 + \sum_{k''_0,q,\lambda} |\alpha_{k''_0k'',q,\lambda}|^2}, \tag{7}$$

$$n(k''_0) = \frac{1}{1 + \sum_{k''_0,q,\lambda} |\alpha_{k''_0k'',q,\lambda}|^2}. \tag{8}$$

The step at the Fermi energy is reduced because (i) a state $k''_0$ above the Fermi energy is partially occupied and (ii) a state $k''_0$ below the Fermi energy is partially empty. As we discussed above, both effects contribute to the electron mass enhancement.

### IV. INTERFERENCE OF THE SATELLITE WAVE FUNCTIONS IN A MULTILAYER

In a multilayer, one expects that the occupations $n(k''_0)$ and $n(k''_0)$ in the ground state for energies below and above the Fermi energy are position dependent. For simplicity we ignore umklapp processes with $\mathbf{G} \neq 0$. Then, in a homogeneous metal, one obtains for a given $k'$ state $c_{k'}^c$ within the Fermi sphere and a given phonon state $(q,\lambda)$ just one satellite state $c_{k''}^* c_{k''}^d a_{\lambda}^d |\Omega_0\rangle$ with $k''=k'-q$. This is different for the double layer. Here, $k''$ can take many possible values,

$$k'' = k' - q + \sqrt{\frac{2\pi}{d_z + d_w}} z = k''_0 + \mathbf{g}, \tag{9}$$

where $k''_0 = k' - q$ and $\mathbf{g} = \frac{2\pi}{d_z + d_w} \mathbf{z}$. We call the states $c_{k''_0+\mathbf{g}}^* c_{k''_0+\mathbf{g}}^d a_{\lambda}^d |\Omega_0\rangle$ with the amplitude $g_{k''_0+\mathbf{g},q,\lambda}/(\eta_{k''_0+\mathbf{g}} - \epsilon_{k''_0+\mathbf{g}} - \hbar\omega)$ a family of satellite states to $c_{k''}^d$. Each member of the family has the same hole $k'$ and the same phonon $(q,\lambda)$. The members only differ in the wave number of the state $k''$ by $\mathbf{g}$. The states of a family are coherent and can interfere. Their phases differ by $\exp(i\mathbf{g} \cdot \mathbf{z})$. This yields a modulation of the amplitude of $c_{k''}^* c_{k''}^d a_{\lambda}^d |\Omega_0\rangle$ in real space.

The total amplitude of the family $c_{k''_0+\mathbf{g}}^* c_{k''_0+\mathbf{g}}^d a_{\lambda}^d |\Omega_0\rangle$ of hole-electron-phonon states in real space is

$$A_{k''_0+\mathbf{g},q,\lambda}(r) = \sum_{\nu} a_{k''_0+\mathbf{g},q,\lambda} e^{i\mathbf{g} \cdot \mathbf{r}} = \sum_{\nu} \frac{g_{k''_0+\mathbf{g},q,\lambda}}{(\eta_{k''_0+\mathbf{g}} - \epsilon_{k''_0+\mathbf{g}} - \hbar\omega)} e^{i\mathbf{g} \cdot \mathbf{r}}. \tag{10}$$

With $Q_z = -q_z - (k''_0 - k'_0) = -gv$, we obtain with Eq. (2)
Before we evaluate this result in more detail, we consider two extreme cases.

(1) Only the term with \( \nu=0 \) contributes. Then, we have

\[
A_{k',k',\mathbf{q},\lambda}(\mathbf{r}) = i\sqrt{N} \left( \frac{\hbar}{2M\omega_{q,\lambda}} \right)^{1/2} \frac{(-\mathbf{q} \cdot \mathbf{e}_{q,\lambda})V_{-\mathbf{q}}}{(\eta_{k'} - \epsilon_{k'_0} - \hbar\omega)N_z} \frac{N_z^p}{N_z(\eta_{k'} - \epsilon_{k'_0} - \hbar\omega)},
\]

where \( g_{q,-\mathbf{q},\lambda}^0 \) is the electron-phonon matrix element for the homogeneous metal S. This wave function has constant density in the metals S and W. The electron-phonon matrix element of the metal S is averaged over the total double-layer thickness and reduced by the factor of \( d_s/(d_s+d_w) \). The satellite state is equally distributed over both films and partially blocks the state \( k'_0 \) in both films equally. This means that both films have an identical enhancement factor.

(2) If the contribution of the term \( rg \) can be neglected in the expressions \( \eta_{k'} - \epsilon_{k'_0} - \hbar\omega \) and \( (-\mathbf{q} + \nu \mathbf{g}) \cdot \mathbf{e}_{q,\lambda} \), then we obtain

\[
A_{k'-\mathbf{q},k',\mathbf{q},\lambda}(\mathbf{r}) = \frac{g_{\mathbf{q},-\mathbf{q},\lambda}^0}{(\eta_{k'} - \epsilon_{k'_0} - \hbar\omega)} S(z),
\]

where \( S(z) \) is essentially a step function which is equal to 1 in the strong-coupling metal S and 0 in the normal metal W. In Fig. 2, the function \( S(z/\omega) \) is shown for a multilayer with \( N_z^p=10 \) and \( N_z^w=8 \). If the conditions for case (2) are fulfilled, the state \( k'_s \) has its full amplitude in the metal S and its amplitude is essentially zero in the normal metal W. In this case, we expect the full mass enhancement in S and no mass enhancement in W.

This yields

\[
A_{k'-\mathbf{q},k',\mathbf{q},\lambda}(\mathbf{r}) = g_{\mathbf{q},-\mathbf{q},\lambda}^0 \frac{1}{(\eta_{k'} - \epsilon_{k'_0} - \hbar\omega)\nu} \sum_{n=-N_z/2}^{N_z/2} \frac{1}{N_z} \left[ 1 - \exp \left( -\frac{2\pi i\nu N_z^p}{N_z} \right) \right] \exp \left( \frac{2\pi i\nu}{L_z} z \right),
\]

\[
S(z) = \sum_{n=-N_z/2}^{N_z/2} \frac{1}{N_z} \left[ 1 - \exp \left( -\frac{2\pi i\nu N_z^p}{N_z} \right) \right] \exp \left( \frac{2\pi i\nu}{L_z} z \right).
\]

V. DISCUSSION

For a realistic evaluation, we consider a sandwich of ten atomic layers of S and eight atomic layers of W. For S and W, we use the electronic density and Debye temperature of Pb with \( \epsilon_F=9.5 \) eV, \( k_F=1.6 \times 10^{10} \) m\(^{-1}\) and \( \Theta_D=90 \) K but assume a simple cubic lattice with \( a=3.28 \times 10^{-10} \) m. The vector \( g \) has the value of \( 1.9 \times 10^9 \) m\(^{-1}\).

Figure 3 shows a typical electron-phonon process. The electron in the state \( k' \) below the Fermi surface emits a phonon \( (\mathbf{q},\lambda) \) and makes a transition into a state \( k'' \) above the Fermi surface. The amplitude in the satellite state is proportional to the inverse energy denominator \( (\eta_{k'} - \epsilon_{k''} - \hbar\omega)^{-1} \). Therefore, the main contribution is from the regime where \( |\epsilon_{k''}|, |\epsilon_{k'}| < \epsilon_F \) and the states \( k' \) and \( k'' \) lie close to the Fermi energy.

In one scenario, the main satellite state \( k''_s \) lies close to the \( z \) direction. In this case, the substates \( k''=k''_s + rg \) with negative \( \nu \) are occupied and not available. The substates with positive \( \nu \) lie above the Fermi energy by an energy of \( \delta E(\nu)=\nu \epsilon_F \frac{2\pi}{\nu} = 0.06 \nu \epsilon_F \). Since the Fermi energy corresponds to a temperature of about \( 1.1 \times 10^5 \) K, the next substate \( k''=k''_s + g \) lies above the Fermi level by an energy corresponding to 6600 K. This is very large compared to the Debye temperature of 90 K. Because of the large energy denominator \( (\eta_{k'} - \epsilon_{k''} - \hbar\omega)^{-1} \), the substates with \( k''=k''_s + rg \).
can be neglected. In this direction, only the main state \( k_0^\ast \) contributes, i.e., only the value \( \nu=0 \) contributes as discussed in case (1). It is remarkable that one can increase the film thicknesses by a factor of 100 before the energy \( \delta E(\nu=1) \) is of the order of the Debye energy.

The situation is different when \( k_0^\ast \) lies in the \( x \) direction. This is shown in Fig. 3 on the left side where \( k_0^\ast \) points in the negative \( x \) direction. Here, the states \( k'=k^\ast+q \) are available. Their energy separation from the state \( k_0^\ast \) is given by
\[
\delta E(\nu)=\frac{(h v g)^2}{2m}=\left(\frac{v g}{k_0^\ast}\right)^2 v \approx 0.014 v^2 v \approx 0.1540 \text{ K}
\]
Again, this value lies considerably above the Debye temperature of 90 K. However, when we increase the thicknesses \( d_x \) and \( d_y \) by a factor 10, then \( \delta E \) reduces to 15 K and the subsatellites have to be included in the calculation.

This background occupation (at \( T=0 \)) yields about one-half of the mass enhancement. From the dependence of the energy separation \( \delta E(\nu) \) on \( \nu \) and \( g \), we obtain the following results as a function of the total thickness \( (d_x+d_y)=N_{x+a} \):

1. \( N_x<50 \): The electron-phonon matrix element is reduced by the factor \( p^2=N_x/(N_x+N_{x+a}) \). Both films are equally enhanced but the enhancement factor is reduced by \( p^2 \).

2. \( 50<N_x<300 \): The occupation of a state \( k_0^\ast \) depends critically on the direction of \( k_0^\ast \); for \( k_0^\ast \) parallel to the \( z \) direction, its occupation is the same in \( S \) and \( W \). Here, one still has an averaged EPME. For \( k_0^\ast \) parallel to the film plane, the occupation of \( k_0^\ast \) in \( S \) takes its full value while it approaches zero in \( W \). The enhanced density of states in both films is highly anisotropic.

3. \( N_x>300 \): The occupation of the state \( k_0^\ast \) approaches the individual value for the two metals \( S \) and \( W \).

The second half of the mass enhancement is due to virtual electron-phonon processes which start from the quasiparticle state \( k_0^\ast \) with final states \( k'' \), \( (q, \lambda) \) where the sum goes over all free-electron states \( k'' \) above the Fermi energy. As before, the weight of these processes in \( S \) and \( W \) depends strongly on the final state. However, since now we have to sum over the final states \( k'' \), the resulting anisotropy for the state \( k_0^\ast \) is strongly reduced. One obtains as before the thin-film regime for \( N_x<50 \) where the EPME is averaged over the two metals and the bulk limit for \( N_x>300 \) where the individual bulk mass enhancements are reinstated. In the intermediate thickness range, one has a slow transition between the two extremes.

In the present consideration, we used a strongly simplified model of the electrons, phonons, and their interaction in multilayers. Nevertheless, we obtained a rather rich and complex behavior of their electron-phonon mass enhancement. In real multilayers, one has a number of additional complications: (i) The lattice parameter of the two metals might be noncommensurable. (ii) The two lattices might be not epitaxial. (iii) The Fermi momenta of the two metals are generally different (the metals may possess different bands). (iv) The Debye energy of the two lattice will generally be quite different, because the strong-coupling metal has normally a lower Debye energy. As a consequence, the high-frequency spectrum of the weak-coupling metal (with the higher Debye temperature) will be confined to the weak-coupling metal. (v) In a realistic model, one has also to include umklapp processes in the electron-phonon processes.

As long as the two lattices are well matched, these complications can be included (at least in principle) in an extensive numerical calculation for multilayers. When the Fermi-surfaces of the electrons of the two metals are rather different, then one has a partial confinement of the electrons with the shorter Fermi wavelength. Similarly, the phonon will be partially confined if their Debye frequencies are rather different.

For the case of a double layer, the confinement the electrons and phonons becomes even more important. In the direction perpendicular to the layers, one obtains discrete quantization of the momentum and standing waves.

In addition to the electron-phonon mass enhancement, one has also a contribution from electron-electron interaction in metals. The electron-electron mass enhancement yields generally only an increase of the density of states by 10% and is therefore much smaller than the electron-phonon process. In our simplified model of the multilayer, the electronic properties are assumed to be identical. Therefore, the electron-electron interaction and the resulting electron-electron mass enhancement are the same in both metals. In this model, the multilayer does not alter the electron-electron mass enhancement.

VI. CONCLUSIONS

In this paper, mass enhancement is investigated in double layers and multilayers of two metals with strong- and weak-coupling electron-phonon interaction. The mass enhancement is due to the fact that an electron injected into a state \( k_0^\ast \) above the Fermi energy changes the occupation of this state by less than 1. This is for two reasons: (i) the state \( k_0^\ast \) was even at \( T=0 \) already partially occupied due to electron tran-
sitions from the occupied Fermi sea into the state \( k_0 \), emitting a virtual phonon \((q, \lambda)\), and (ii) the injected electron makes transitions into states \( k'' \) above the Fermi surface, emitting virtual phonons \((q, \lambda)\) and reducing the occupation of the state \( k_0 \). In multilayers, one has modified electron-phonon matrix elements and a finite quantization of electron and phonon states perpendicular to the film planes. As a consequence, one has to consider interference between electron-phonon processes which start from the same initial electron state \( k' \) \((k' < k_F)\), emit the same phonon \((q, \lambda)\), and yield a superposition of different \( c^{\dagger}_{k''} \) for the final electron state. After the emission of the virtual phonon, the electron no longer has a well-defined momentum. This interference yields a spatial dependence of the preoccupation of the electron state \( k_0 \). This results in very interesting properties of the mass enhancement in multilayers of metals with strong- and weak-coupling electron-phonon interaction. In the thin-film limit, the electron-phonon matrix element is averaged over both films. In an intermediate thickness range, 50% of the mass enhancement in each film depends strongly on the direction of the electron momentum \( k_0 \). In both films, the mass enhancement approaches the bulk value in the direction parallel to the film planes, while perpendicular to the films one obtains an averaged mass enhancement. This will cause a rather anisotropic propagation of the conduction electrons parallel and perpendicular to the films. In strong-coupling superconductors in contact with normal films, it will influence the boundary condition between the films and as a consequence the superconducting transition temperature of the double layer or multilayer as well the upper critical field. Even for the simple model which is considered in this paper, an extensive numerical calculation is required to obtain the details of the mass enhancement because it depends on the direction of the electron wave number \( k_0 \) in both metals.

**APPENDIX A: CONNECTION WITH GREEN’S FUNCTION SELF-ENERGY**

In the derivation of the mass enhancement in a pure bulk metal \( S \), one generally starts from the fully occupied free-electron Fermi sphere. A standard treatment uses the Green’s function method. Here, one calculates the self-energy of an additional electron \( k_0 \) just above the Fermi energy (see, for example, Refs. 1–3). This has two contributions. Figure 4 shows the well-known processes involved.

(a) The inserted electron in state \( k_0 \) emits a phonon \((q, \lambda)\) and makes a virtual transition into the state \( k'' \).

(b) An electron in the state \( k_0 \) blocks all electron-phonon processes in which an electron from an occupied state \( k' \) emits a phonon \((q, \lambda)\) and makes a transition into the state \( k_0 \).

The corresponding self-energies of the state \( k'' \) are

\[
\Sigma_a(k_0, E) = \sum_{k', q, \lambda} \frac{|g_{k'' - k_0 - q, \lambda}|^2}{E - \epsilon_{k''} - \hbar \omega + i \delta},
\]

\[
\Sigma_b(k_0, E) = -\sum_{k', q, \lambda} \frac{|g_{k'' - k', -q, \lambda}|^2}{E - \epsilon_{k'} - \hbar \omega + i \delta}.
\]

The inverse dressed Green’s function has then the form

\[
G^{-1} = E - \epsilon_{k_0} + i \delta - \Sigma,
\]

where \( \Sigma = \Sigma_a + \Sigma_b \). The new quasiparticle energy is given by the pole of \( G \), i.e., by solving the implicit equation

\[
E_{k_0} = \epsilon_{k_0} + \text{Re} \left( \Sigma(k_0, E_{k_0}) \right) = \epsilon_{k_0} + \sum_{k', q, \lambda} \frac{|g_{k'' - k_0 - q, \lambda}|^2}{E_{k_0} - \epsilon_{k'} - \hbar \omega + i \delta} + \sum_{k', q, \lambda} \frac{|g_{k'' - k', -q, \lambda}|^2}{E_{k_0} - \epsilon_{k'} - \hbar \omega + i \delta}.
\]

The self-energy depends on the momentum \( k_0 \) only through the matrix element, and this dependence is very weak and can be neglected. If \( k_0 \) lies directly above the Fermi energy, i.e., \( k_0 = k_F^\pm \), then we have the relation

\[
E_{k_F^\pm} = \Sigma(k_F^\pm, E_{k_F^\pm}).
\]

Next, we can expand \( \Sigma(k_0, E) \) in terms of \( E \) about the energy \( E_{k_F^\pm} \),

\[
\Sigma(k_0, E) = \Sigma(k_F^+, E_{k_F^+}) + (E - E_{k_F^+}) \frac{\partial}{\partial E} \Sigma(k_F^+, E_{k_F^+}) = \Sigma(k_F^+, E_{k_F^+}) - E_{k_F^+} \frac{\partial}{\partial E} \Sigma(k_F^+, E_{k_F^+}) + E \frac{\partial}{\partial E} \Sigma(k_F^+, E_{k_F^+}).
\]

This yields for the quasiparticle energy

\[
E_{k_0} = \epsilon_{k_0} + \Sigma(k_F^+, E_{k_F^+}) + (E_{k_0} - E_{k_F^+}) \frac{\partial}{\partial E} \text{Re} \left( \Sigma(k_F^+, E_{k_F^+}) \right),
\]

\[
E_{k_0} = \frac{1}{1 - \frac{\partial}{\partial E} \text{Re} \left( \Sigma(k_F^+, E_{k_F^+}) \right)} \left[ \epsilon_{k_0} + \text{Re} \left( \Sigma(k_F^+, E_{k_F^+}) \right) - E_{k_F^+} \frac{\partial}{\partial E} \Sigma(k_F^+, E_{k_F^+}) \right].
\]

The terms \(-\text{Re} \left( \Sigma(k_F^+, E_{k_F^+}) \right) + E_{k_F^+} \frac{\partial}{\partial E} \text{Re} \Sigma(k_F^+, E_{k_F^+}) \) yield essentially a constant energy shift which will be absorbed in the chemical potential. Then, the Green’s function takes the form
For each \( H_0 \)

\[
G(k_0, E) = \frac{1}{E - e_{k_0} - \frac{\partial}{\partial E} \text{Re} \Sigma(k_F, E_{k_F}) + i\Gamma_{k_0}}
\]

or

\[
G(k_0, E) = \frac{1}{Z} \frac{1}{E - \frac{\partial}{\partial E} \Sigma(k_F, E_{k_F}) + i\Gamma_{k_0}}.
\]

where

\[
Z = 1 - \frac{\partial}{\partial E} \Sigma(k_F, E_{k_F}) > 1
\]

and \( \Gamma_{k_0} \) is an imaginary contribution from the self-energy which we neglected in the discussion.

When one performs the derivative of the self-energy, one realizes that its real part represents the relative occupation of the states \( k'' \). As an example, we take \( \Sigma_0 \) and obtain for

\[
-\frac{\partial}{\partial E} \Sigma_0(k_F, E_{k_F}) \sim 1
\]

For each \( k' \), \( q \) the right sum represents the occupation of the electron state \( k'' \) and a phonon \( q \) due to a virtual transition from a state \( k_F \) just above the Fermi energy. The total sum represents the reduction of the occupation of the state \( k_F \) (before normalization).

**APPENDIX B: SATELLITE STATES IN THE GROUND STATE**

At \( T=0 \) in the absence of the electron-phonon interaction, all states within the Fermi sphere with \( k < k_F \) (\( k_F \) is the Fermi wave number) are occupied and all other states are empty. We denote this ground state of the electron system as \( |\Psi_0\rangle = \Pi c_{k_F}^\dagger |\Phi_0\rangle \). We have virtual electron-phonon emissions \( k'' < k_F \) from the occupied state \( k' \) into the empty states \( k'' \) emitting phonons \( (q, \lambda) \). Now, the state \( k' \) makes a transition into one (or several) states \( k'' \) and creates a phonon \( (q, \lambda) \). The resulting state can be described as

\[
\tilde{c}_{k'} = \left( c_{k''}^\dagger \sum_{k''} a_{k'', k', q, \lambda} c_{k''}^\dagger a_{k''}^\dagger \right) = \left( 1 + \sum_{k''} a_{k'', k', q, \lambda} c_{k''}^\dagger a_{k''}^\dagger \right) c_{k'}^\dagger.
\]

We denote the amplitude of the satellites as \( a_{k'', k', q, \lambda} \). This state is not normalized.

For the new ground state, we make the product ansatz

\[
\tilde{\Psi}_0(t) = \left[ \prod_{k'} \left( 1 + \sum_{k''} a_{k'', k', q, \lambda} c_{k''}^\dagger a_{k''}^\dagger \right) \right] |\Psi_0\rangle e^{-(i\hbar)E_0t}, \tag{B1}
\]

where \( E_0 \) is the new ground-state energy. All products over \( k' \) and summations \( k'' \) are restricted to \( k' < k_F, k'' > k_F \). The Hamiltonian is

\[
H = \sum_{p} \varepsilon_p c_p^\dagger c_p + \sum_{p, p', q, \lambda} g_{p, p', q, \lambda} c_p^\dagger a_{q, \lambda} c_{p', q, \lambda}^\dagger + a_{q, \lambda}^\dagger.
\]

The Schrödinger equation is

\[
H\tilde{\Psi}_0 = E_0\tilde{\Psi}_0.
\]

In order for \( \tilde{\Psi}_0 \) in Eq. (B1) to be an approximate eigenstate of the Hamiltonian to first order in the electron-phonon interaction \( g_{p, p', q, \lambda} \), the states \( c_{k'}^\dagger + \sum_{q, \lambda} g_{k', q, \lambda} c_{k', q, \lambda} \) (\( |\Phi_0\rangle \)) must be (approximate) eigenstates of the Hamiltonian, i.e.,

\[
H\left( c_{k'}^\dagger \sum_{k''} a_{k'', k', q, \lambda} c_{k''}^\dagger a_{k''}^\dagger \right) |\Phi_0\rangle = \eta_{k'}^0 \left( c_{k'}^\dagger \sum_{k''} a_{k'', k', q, \lambda} c_{k''}^\dagger a_{k''}^\dagger \right) |\Phi_0\rangle.
\]

This yields

\[
\eta_{k'}^0 \left( c_{k'}^\dagger \sum_{k''} a_{k'', k', q, \lambda} c_{k''}^\dagger a_{k''}^\dagger \right) |\Phi_0\rangle = \sum_{k''} \left[ \varepsilon_{k''} + \sum_{k''} (\varepsilon_{k'} + \hbar \omega) a_{k'', k', q, \lambda} c_{k''}^\dagger a_{k''}^\dagger + \sum_{k''} g_{k'', k', q, \lambda} c_{k''}^\dagger a_{k''}^\dagger \right] \left( c_{k'}^\dagger \sum_{k''} a_{k'', k', q, \lambda} c_{k''}^\dagger a_{k''}^\dagger \right) |\Phi_0\rangle.
\]

This yields

\[
\eta_{k'}^0 \left( c_{k'}^\dagger \sum_{k''} a_{k'', k', q, \lambda} c_{k''}^\dagger a_{k''}^\dagger \right) |\Phi_0\rangle = \sum_{k''} \left[ \varepsilon_{k''} + \sum_{k''} (\varepsilon_{k'} + \hbar \omega) a_{k'', k', q, \lambda} c_{k''}^\dagger a_{k''}^\dagger + \sum_{k''} g_{k'', k', q, \lambda} c_{k''}^\dagger a_{k''}^\dagger \right] |\Phi_0\rangle.
\]

It follows that

\[
\eta_{k'}^0 = \varepsilon_{k'} + \sum_{k''} g_{k'', k', q, \lambda} a_{k'', k', q, \lambda}, \tag{B2}
\]

with the self-consistency condition

\[
\eta_{k'}^0 = \varepsilon_{k'} + \sum_{k''} \frac{g_{k'', k', q, \lambda}}{\eta_{k'}^0 - \varepsilon_{k''} - \hbar \omega}. \tag{B4}
\]

There are two approximations involved in the product ansatz: (a) The Pauli principle excludes for \( c_{k_1} c_{k_2} = (c_{k_1}^\dagger)^2 + \sum_{k_3} a_{k_3, k_1, q, \lambda} c_{k_3}^\dagger a_{k_3, q, \lambda} \) the double occupancy of the state \( c_{k_1}^\dagger c_{k_2}^\dagger \) for \( k_1 = k_2 \). (b) The electron-phonon interaction can introduce a transition from the state \( c_{k_1}^\dagger \) into the satellite of \( c_{k_1}^\dagger \), yielding a state

\[
c_{k_1}^\dagger a_{q, \lambda} c_{k_1}^\dagger a_{q, \lambda}.
\]

This state is neglected.

The total ground-state energy in this approximation is
The occupation of the satellite states $c^*_k \sigma_q \lambda \rightarrow c^*_k$ is given by

$$|\alpha_{k^* k', q \lambda}|^2 = \left| \frac{g_{k^* k', -q \lambda}}{(\eta_k - \epsilon_{k^*} - \hbar \omega)} \right|^2.$$ 

To normalize each state $\widetilde{c}_k$, it has to be divided by

$$\left[ 1 + \sum_{k'' q \lambda} g_{k'' q \lambda} \right]^{1/2}.$$

It should be emphasized that the energy $\eta_k^0$ is not the energy of a hole at $k'$. It is here only a mathematical abbreviation.

**APPENDIX C: GROUND STATE PLUS ONE ELECTRON**

Now, we perform self-consistent perturbation calculation starting with the unperturbed ground state plus one electron $k_0$. We call this state $\Psi_{0 k_0}$ (with $|k'| < k_F$),

$$\Psi_{0 k_0} = c_{k_0} \prod_{k'} c_{k'} |\Phi_0\rangle.$$

The resulting state in the presence of electron-phonon interaction is

$$\widetilde{\Psi}_{0 k_0} = \widetilde{c}_{k_0} \prod_{k'} \widetilde{c}_{k'} |\Phi_0\rangle,$$

with $\widetilde{c}_{k'} = (c_{k'} + \sum_{k'' q \lambda} \alpha_{k'' k', q \lambda} c_{k''} d_{k', q \lambda})$ where $k'' \neq k_0$.

When we derive the corresponding Schrödinger equations, we obtain for $|k'| < k_F$

$$\alpha_{k^* k', q \lambda} = \frac{g_{k^* k', -q \lambda}}{(\eta_k - \epsilon_{k^*} - \hbar \omega)}.$$

The amplitude $\alpha_{k^* k', q \lambda}$ has a slightly different energy denominator compared with the ground state since $\eta_k^0$ is replaced by $\eta_k$. However, the difference is of third order in the electron-phonon matrix element and will be neglected in our approximation. For the state $c_{k_0} = (c_{k_0} + \sum_{k'' q \lambda} \alpha_{k'' k_0, q \lambda} c_{k''} d_{k_0, q \lambda})$, one obtains in analogy

$$\alpha_{k^* k_0, q \lambda} = \frac{g_{k^* k_0, -q \lambda}}{(\eta_k - \epsilon_{k^*} - \hbar \omega)}.$$

The total energy of $\widetilde{\Psi}_{0 k_0}$ becomes

$$E_{0 k_0} = \sum_{k'} \eta_{k'} + \eta_{k_0} = E_0 + \epsilon_{k_0} + \sum_{k'' q \lambda} g_{k_0 k'' q \lambda} \alpha_{k'' k_0, q \lambda} - \sum_{k'} g_{k_0 k', q \lambda} \alpha_{k_0 k', q \lambda}.$$

The quasiparticle energy $E_{k_0}$ of the state $c_{k_0}$ is then

$$E_{k_0} = \epsilon_{k_0} + \sum_{k'' q \lambda} g_{k_0 k'' q \lambda} \alpha_{k'' k_0, q \lambda} - \sum_{k'} g_{k_0 k', q \lambda} \alpha_{k_0 k', q \lambda},$$

which yields

$$E_{k_0} = \epsilon_{k_0} + \sum_{k'' q \lambda} \frac{|g_{k_0 k'' q \lambda}|^2}{(\eta_{k_0} - \epsilon_{k_0} - \hbar \omega)} - \sum_{k'} \frac{|g_{k_0 k', q \lambda}|^2}{(\eta_{k'} - \epsilon_{k_0} - \hbar \omega)}.$$

(C1)

If one compares this expression for $E_{k_0}$ with the Green’s function expression in Eq. (A1), one recognizes differences in the energy denominators. In the Green’s function expression, the $k_0$ energy in the denominators is given by $E_{k_0}$. There, the transition from $k'$ to $k_0$ is replaced by a transition from $k_0$ to $k'$. The physics behind this is not obvious. As a matter of fact, Schrieffer uses in his book both approaches in parallel in the discussion of the electron-phonon self-energy.