Electron-Phonon Mass Enhancement in Multi-Layers

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Abstract

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 is investigated whether the mass enhancement can be manipulated in multi-layers of two metals with strong and weak electron-phonon interaction. 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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1 Introduction

A strong electron-phonon interaction (EPI) alters the electronic properties of a metal rather dramatically [3], [1]. It enhances the electron density of states in the vicinity of the Fermi energy. 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 $Z = (1 + \lambda) \approx 2.6$. 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 multi-layers 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 one 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 $k'$ below the Fermi energy can virtually emit a phonon $(q, \lambda)$ and make a transition into a satellite state $k''$ above the Fermi energy. This process does not fulfill energy conservation since the satellite state $\epsilon_{k''}^* a_{q,\lambda}^*$ has an excess energy of $\Delta E = \epsilon_{k''} + \hbar \omega_{q,\lambda} - \epsilon_{k'}$. The satellite causes a finite electron occupation of the states $k''$ above the Fermi surface and a finite hole occupation of the states $k'$ below the Fermi surface.

In Fig.1 an electron is introduced into a state $k_0$ directly above the Fermi energy. It changes the occupation of the $k_0$-state only by $Z^{-1} < 1$ because this state was already partially occupied, and after the introduction into the state $k_0$ part of the electron makes virtual transitions into the other states above the Fermi energy. This reduces the occupation of the state $k_0$. 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 $k_0$ above the Fermi energy has two contributions:

- The pre-occupation of the state $k_0$ is larger than 0: The state $k_0$ is already partially occupied before an additional electron is introduced.

- The post-occupation of the state $k_0$ 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.

Fig. 1: The occupation as a function of momentum (energy) for a strong-coupling metal. At the Fermi momentum (energy) the jump in occupation at zero temperature is $1/Z$.

Since the occupation of the state $k_0$ changes only by $Z^{-1}$ the energy (of the quasi-particle in $k_0$) is only $\varepsilon_{k_0}/Z$. Therefore the quasi-particle energies are closer together and their density of states is enhanced by the factor $Z$.

In appendix A1 a short review is given of the treatment of the electron-phonon mass enhancement with Green functions. The discussed physical interpretation of the mass enhancement in terms of pre- and post-occupation is sketched. However, the Green function method cannot be easily expanded to multi-layers. Therefore in this paper I use self-consistant perturbation theory.

In part II the electron-phonon interaction and matrix element in multi-layers is derived. In part III the amplitudes of the electron-phonon satellites are discussed. In a multi-layer these satellites interfere in real space. This is discussed in part IV. In appendix A2 the ground-state wave function in the presence of electron-phonon interaction is derived in self-consistent perturbation theory. Finally appendix A3 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 multi-layer the 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 to future work.

Abbreviations: EPI = electron-phonon interaction, EPME = electron-phonon matrix element.

2 Electron-Phonon Interaction in Multi-Layers

Now the question is: 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 this question we investigate a very simple model of a double layer.

2.1 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 \( N^s_z \) layers and lies in the range \( 0 \leq z \leq d_s = N^s_z a \), and the metal W has \( N^w_z \) layers in the regime \( d_s \leq z \leq d_s + d_w = L_z = N_z a \), where \( d_w = N^w_z a \) and \( N_z \) is the total number of layers in the z-direction. For normalization reasons the double film has a finite but large extension in the x- and y-direction 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 multi-layer 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 \( N = N_x N_y (N^s_z + N^w_z) \).

- 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 \( k_i = \nu_i 2\pi/L_i, \) \( (i = x, y, z) \). \( (The \ quantization \ in \ the \ z\text{-}direction \ extends \ over \ the \ total \ thickness \ L_z = d_s + d_w). \)

- 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 \( q_i = \mu_i 2\pi/L_i, \) \( (i = x, y, z) \). Here \( \mu_i \) lies in the range \(-N_i/2 < \mu_i \leq N_i/2\).

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 \([1],[2]\). 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 integer.

In the lower strong-coupling film for \( 0 \leq z \leq d_s \) the atoms have an (somewhat artificial) electron potential

\[ U(r) = V(r - r_n) - V(r - R_n) \]

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

\[ U(r) \approx \sum_{n_s} (u_n \cdot \nabla) V(r - R_n) = i \sum_{n_s} \sum_{p} (u_n \cdot p) V_p e^{i p (r - R_n)} \]

where the sum over \( n_s \) 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 \( (-q', \lambda) \).

\[ u_n = \frac{1}{\sqrt{N}} \sum_{q',\lambda} e^{i q' R_n} (a_{q',\lambda} + a^*_{-q',\lambda}) \]
where $\mathbf{e}_{q',\lambda}$ is the unit vector of polarization $\lambda$. This yields the electron-phonon interaction Hamiltonian

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

(1)

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

$$g_{k_2-k_1,q',\lambda} = i\sqrt{N} \left( \frac{\hbar}{2M\omega_{q',\lambda}} \right)^{1/2} \left( (\mathbf{k}_2-\mathbf{k}_1) \cdot \mathbf{e}_{q',\lambda} \right) V_{k_2-k_1} S_f \left( \mathbf{q'}-\left( \mathbf{k}_2-\mathbf{k}_1 \right) \right)$$

(2)

where the structure factor $S_f (\mathbf{Q})$ [with $\mathbf{Q} = \mathbf{q'}-\left( \mathbf{k}_2-\mathbf{k}_1 \right)$] is given by

$$S_f (\mathbf{Q}) = \frac{1}{N} \sum_{n_s} e^{i\mathbf{Q} \mathbf{r}_n} = \frac{N_x N_y}{N} \sum_{G_x,G_y} \delta_{Q_x,G_x} \delta_{Q_y,G_y} \sum_{n_z=0}^{N_z} e^{iQ_z a_{n_z}}$$

(3)

$$= \sum_{G_x,G_y} \delta_{Q_x,G_x} \delta_{Q_y,G_y} \frac{1}{N_z} \frac{1 - e^{iQ_z a_{N_z}}}{1 - e^{iQ_z a}}$$

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 $g_{k_2-k_1,q',\lambda}^0$. Its structure factor $S_f^0 (\mathbf{Q}) = \sum_{\mathbf{G}} \delta_{\mathbf{Q},\mathbf{G}}$ with $\mathbf{Q} = \mathbf{q'}-\left( \mathbf{k}_2-\mathbf{k}_1 \right)$ fulfills conservation of lattice momentum

$$g_{k_2-k_1,q',\lambda}^0 = i\sqrt{N} \left( \frac{\hbar}{2M\omega_{q',\lambda}} \right)^{1/2} \left( (\mathbf{k}_2-\mathbf{k}_1) \cdot \mathbf{e}_{q',\lambda} \right) V_{k_2-k_1} S_f^0 \left( \mathbf{q'}-\left( \mathbf{k}_2-\mathbf{k}_1 \right) \right)$$

(4)

For those electron-phonon processes in the multi-layer which conserve the lattice momentum, i.e., when $\mathbf{k}_2-\mathbf{k}_1 = \mathbf{q'}+\mathbf{G}$, one obtains

$$g_{k_2-k_1,q',\lambda} = N_z \frac{g_{k_2-k_1,q',\lambda}^0}{g_{k_2-k_1,q',\lambda}^0} = \frac{d_s}{d_s + d_w} g_{k_2-k_1,q',\lambda}^0$$

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

### 3 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 $|\Psi_0\rangle = \prod_{k' < k_F} c_{k'}^\dagger |\Phi_0\rangle$

where $|\Phi_0\rangle$ is the vacuum. We select from the full Fermi sphere an occupied state $k'$. (In the following the states such $k$ will be sometimes denoted by their creation operators such as $c_k^\dagger$). 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 $\alpha_{k'', k', q}$. The resulting ground state $\tilde{|\Psi_0\rangle}$ in the presence of EPI is derived in the appendix A2 in self-consistent perturbation theory. One obtains for the amplitude of the satellites

$$\alpha_{k'', k', q, \lambda} = \frac{g_{k'' - k', - q, \lambda}}{(\eta_{k'}^0 - \varepsilon_{k''} - \hbar \omega)}$$

where $\eta_{k'}^0$ is given in appendix A2 by the self-consistent equation (12).

This means that a state $c_{k'}^\dagger$ with the occupation "1" generates satellites $c_{k'', q}^\dagger a_{q, \lambda}^\dagger$ 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

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

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

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.

4 The interference of the satellite wave functions in a multi-layer

In a multi-layer 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 $G \neq 0$. Then,
in a homogeneous metal, one obtains for a given \( k' \)-state within the Fermi sphere and a given phonon state \((q, \lambda)\) just one satellite state \( c_{k''}^* a_{q, \lambda}^* \) with \( k'' = k' - q \). This is different for the double layer. Here \( k'' \) can take many possible values,

\[
k'' = k' - q + \nu \frac{2\pi}{d_s + d_w} \hat{z} = k''_0 + \nu g
\]

where \( k''_0 = k' - q \) and \( g = \frac{2\pi}{d_s + d_w} \hat{z} \). We call the states \( c_{k''_0}^* c_k^* a_{q, \lambda}^* \) with the amplitude \( g_{-q + \nu g} \left( \eta_{k''} - \varepsilon_{k''_0 + \nu g} - \hbar \omega \right) \) a family of satellite states. Each member of the family has the same electron hole \( k' \) and the same phonon \((q, \lambda)\). The members only differ in the wave number of the state \( k'' \) by \( \nu g \). The states of a family are coherent and can interfere. Their phases differ by \( \exp (i\nu gz) \). This yields a modulation of the amplitude of \( \left| c_{k''_0}^* c_k^* a_{q, \lambda}^* \Psi_0 \right| \) in real space.

The total amplitude of the family \( \left| c_{k''_0}^* c_k^* a_{q, \lambda}^* \Psi_0 \right| \) of hole-electron-phonon states in real space is

\[
A_{k''_0, k', q, \lambda} (r) = c_k^* c_{k''_0}^* a_{q, \lambda}^* e^{i\nu gr} = \sum \nu g_{-q + \nu g} \left( \eta_{k''} - \varepsilon_{k''_0 + \nu g} - \hbar \omega \right) e^{i\nu gr}
\]

With \( Q_z = -q_z - (k''_z - k'_z) = -g\nu \) we obtain with equ. (2)

\[
= i \sqrt{N} \left( \frac{\hbar}{2 M \omega_{q, \lambda}} \right)^{1/2} \sum \nu g_{-q + \nu g} \left( \eta_{k''} - \varepsilon_{k''_0 + \nu g} - \hbar \omega \right) e^{i\nu gz}
\]

Before we evaluate this result in more detail we consider two extreme cases:

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

\[
A_{k''_0, k', q, \lambda} (r) = i \sqrt{N} \left( \frac{\hbar}{2 M \omega_{q, \lambda}} \right)^{1/2} \left( -q \cdot e_{q, \lambda} \right) V_{-q + \nu g} \left( \eta_{k'} - \varepsilon_{k''_0 + \nu g} - \hbar \omega \right) e^{i\nu gz}
\]

\[
= \frac{N_z^s}{N_z} \frac{g^0_{-q, q, \lambda}}{\left( \eta_{k'} - \varepsilon_{k''_0} - \hbar \omega \right)}
\]

where \( g^0_{-q, q, \lambda} \) 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
ds/(ds + dw). 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 $\nu g$ can be neglected in the expressions $(\eta k' - \varepsilon k''_0 + \nu g - \hbar \omega)$ and $((-q + \nu g) \cdot e_{q,\lambda}) V_{-q + \nu g}$ then we obtain

$$A_{k'-q,k',q,\lambda}(r) = i\sqrt{N} \left( \frac{\hbar}{2M\omega_{q,\lambda}} \right)^{1/2} \left( \frac{-q \cdot e_{q,\lambda}}{(\eta k' - \varepsilon k''_0 - \hbar \omega)} \right) V_{-q}$$

$$\ast \sum_{N_z/2}^{N_z/2} \frac{1}{N_z} \frac{1 - \exp \left(-\frac{2\pi i\nu N_z^+}{N_z} \right)}{1 - \exp \left(-\frac{2\pi i\nu}{N_z} \right)} \exp \left(\frac{2\pi i\nu}{L_z} z \right)$$

This yields

$$A_{k'-q,k',q,\lambda}(r) = \frac{g_{q,-q,\lambda}^0}{(\eta k' - \varepsilon k''_0 - \hbar \omega)} S(z)$$

$$S(z) = \sum_{N_z/2}^{N_z/2} \frac{1}{N_z} \frac{1 - \exp \left(-\frac{2\pi i\nu N_z^+}{N_z} \right)}{1 - \exp \left(-\frac{2\pi i\nu}{N_z} \right)} \exp \left(\frac{2\pi i\nu}{L_z} z \right)$$

where $S(z)$ is essentially a step function which is equal to one in the strong-coupling metal $S$ and zero in the normal metal $W$. In Fig.2 the function $S(z/a)$ is shown for a multi-layer with $N_z^s = 10$ and $N_z^w = 8$. If the conditions for case (2) are fulfilled the state $k''_0$ 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
Fig. 2: The amplitude of the electronic part of the electron-phonon satellite (with the wave function $e^{-i\mathbf{k}'_0 \mathbf{r}}$) is restricted to the strong-coupling metal S and vanishes in the normal metal W.

For a realistic evaluation we consider a sandwich of 10 atomic layers of S and 8 atomic layers of W. For S and W we use the electronic density and Debye temperature of Pb with $\varepsilon_F = 9.5\,\text{eV}$, $k_F = 1.6 \times 10^{10}\,\text{m}^{-1}$ and $\Theta_D = 90\,\text{K}$ but assume a simple cubic lattice with $a = 3.28 \times 10^{-10}\,\text{m}$. The vector $g$ has the value of $1.9 \times 10^9\,\text{m}^{-1}$.

Fig. 3 shows a typical electron-phonon process. The electron in the state $\mathbf{k}'$ below the Fermi surface emits a phonon $(\mathbf{q}, \lambda)$ and makes a transition into a state $\mathbf{k}''$ above the Fermi surface. The amplitude in the satellite state is proportional to the inverse energy denominator $(\eta_{\mathbf{k}'} - \varepsilon_{\mathbf{k}''} - \hbar \omega)^{-1}$. Therefore the main contribution is from the regime where $|\varepsilon_{\mathbf{k}''}|, |\varepsilon_{\mathbf{k}'}| \ll \hbar \omega_D$ and the states $\mathbf{k}'$ and $\mathbf{k}''$ lie close the Fermi energy.
Fig. 3: The $k_z$-planes of a double layer with periodic boundary conditions. Both metals have the same electron band structure. The films have strong and zero electron-phonon interaction. The arrows show transitions from state $k'$ to $k''$ with a virtual phonon ($q, \lambda$). For given $k', q$ there are several final states $k'' = k' - q + \nu 2\pi \hat{z} / (d_u + d_w)$ permitted. The amplitude of these states are coherent and interfere.

In one scenario the main satellite state $k''_0$ lies close to the $z$-direction. In this case the sub-states $k'' = k''_0 + \nu g$ with negative $\nu$ are occupied and not available. The sub-states with positive $\nu$ lie above the Fermi energy by an energy of $\delta E(\nu) = \nu \varepsilon_F \frac{q}{2k_F} \approx 0.06 \nu \varepsilon_F$. Since the Fermi energy corresponds to a temperature of about $1.1 \times 10^6 K$ the next sub-state $k'' = k''_0 + g$ lies above the Fermi level by an energy corresponding to $6600 K$. This is very large compared to the Debye temperature of 90K. Because of the large energy denominator $(\eta_k - \varepsilon_k'' - \hbar \omega)^{-1}$ the sub-states with $k'' = k''_0 + \nu g$ can be
neglected. In this direction only the main state $k''_0$ 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 $k''_0$ lies in the x-direction. This is shown in Fig.3 on the left side where $k''_0$ point in the negative x-direction. Here the states $k'' = k''_0 + \nu g$ are available. Their energy separation from the state $k''_0$ is given by $\delta E (\nu) = (\hbar \nu g)^2 / (2m) = (\nu g / k_F)^2 \varepsilon_F \approx 0.014 \nu^2 \varepsilon_F \approx \nu^2 1540 K$. Again this value lies considerably above the Debye temperature of 90K. However when we increase the thicknesses $d_s$ and $d_w$ by a factor 10 then $\delta E$ reduces to 15K and the sub-satellites 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 $(d_s + d_w) = N_z a$:

- $N_z < 50$: The electron-phonon matrix element is reduced by the factor $p = N^s_z / (N^s_z + N^w_z)$. Both films are equally enhanced but the enhancement factor is reduced by $p^2$.

- $50 < N_z < 300$: The occupation of a state $k''_0$ depends critically on the direction of $k''_0$; for $k''_0$ parallel to the z-direction its occupation is the same in S and W. Here one still has an averaged EPME. For $k''_0$ parallel to the film plane the occupation of $k''_0$ in S takes its full value while it approaches zero in W. The enhanced density of states in both films is highly anisotropic.

- $N_z > 300$: The occupation of the state $k''_0$ 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 quasi-particle state $k_0$ 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 $k_0$ is strongly reduced. One obtains as before the thin film regime for $N_z < 50$ where the EPME is averaged over the two metals and the bulk limit for $N_z > 300$ where the individual bulk mass enhancement are reinstated. In the intermediate thickness range one has a slow transition between the two extremes.
5 Conclusions

In this paper mass enhancement is investigated in double and multi-layers 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 $k_0$ above the Fermi energy changes the occupation of this state by less than one. This is for two reasons: (i) the state $k_0$ was (even at $T = 0$) already partially occupied due to electron transitions 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 multi-layers 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 $c_{k''}^*$ 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 pre-occupation of the electron state $k_0$. This results in very interesting properties of the mass enhancement in multi-layers 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 or multi layer 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.
A Appendix

A.1 Connection with Green 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-function method. Here one calculates the self-energy of an additional electron $k_0$ just above the Fermi energy (see for example [2], [3], [1]). This has two contributions. Fig.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

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

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Fig.4: The two contributions to the self energy and the mass enhancement
The inverse dressed Green function has then the form

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

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

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

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. \( k_0 = k_F^+ \) then we have the relation

\[ E_{k_0}^+ = \Sigma \left( k_F^+, E_{k_F^+} \right) \]

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

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

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

This yields for for the quasi-particle energy

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

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

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

\[ G \left( k_0, E \right) = \frac{1}{E - \varepsilon_{k_0} - E \frac{\partial}{\partial E} \text{Re} \Sigma \left( k_F^+, E_{k_F^+} \right) + i\Gamma_{k_0}} \]
or
\[ G(k_0, E) = \frac{1}{Z} \frac{1}{\frac{\varepsilon_{k_0}}{E} + i \frac{\Gamma_{k_0}}{Z} + E - \varepsilon_{k_0}} \]
where
\[ Z = \left(1 - \frac{\partial}{\partial E} \Sigma \left(k_F^+, E_{k_F^+}\right)\right) > 1 \]
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 \( \Sigma_a \) and obtain for \(-\partial \text{Re} \Sigma_a \left(k_F^+, E_{k_F^+}\right) / \partial E\).

\[-\frac{\partial}{\partial E} \sum_{k''} \frac{|g_{k''-k_0,-q}\lambda|^2}{E - \varepsilon_{k''} - \hbar \omega} |E_{k_F} = \sum_{k''} \frac{|g_{k''-k_0,-q}\lambda|^2}{\left(E_{k_F^+} - \varepsilon_{k''} - \hbar \omega\right)^2} \]

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).

### A.2 Satellite states in the ground state

At \( T = 0 \) in the absence of the electron-phonon interaction all states within the Fermi sphere with \( k \leq k_F \) (\( k_F \) is the Fermi wave number) are occupied and all other states are empty. We denote this ground state of the electron system as \( |\Psi_0\rangle = \prod_{k' < k_F} c_{k'}^\dagger |\Phi_0\rangle \). We have virtual electron-phonon emissions 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

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

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

The amplitude of the satellites we denote as \( \alpha_{k'', k', q} \). This state is not normalized.
For the new ground state we make the product ansatz

$$
\tilde{\Psi}_0(t) = \left[ \prod_{k'} \left( 1 + \sum_{k''} \alpha_{k'',k',q',\lambda} c^*_{k''} c_{k',q',\lambda} \right) |\tilde{\Psi}_0\rangle \right] e^{-\frac{i}{\hbar} E_0 t}
$$

(9)

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

$$
H = \sum_p \varepsilon_p c^*_p c_p + \sum_{p_1,p_2,q',\lambda} g_{p_2-p_1,q',\lambda} c_{p_2}^* c_{p_1} (a_{q',\lambda} + a^*_{-q',\lambda})
$$

The Schroedinger equation is

$$
H \tilde{\Psi}_0 = E_0 \tilde{\Psi}_0
$$

In order for $\tilde{\Psi}_0$ in equ. (9) to be an approximate eigenstate of the hamiltonian to first order in the electron-phonon interaction $g_{p_2-p_1,q',\lambda}$ the states

$$
\left( c^*_{k'} + \sum_{k''} \alpha_{k'',k',q',\lambda} c^*_{k''} c_{k',q',\lambda} \right) |\Phi_0\rangle
$$

must be (approximate) eigenstates of the hamiltonian, i.e.

$$
H \left( c^*_{k'} + \sum_{k''} \alpha_{k'',k',q',\lambda} c^*_{k''} c_{k',q',\lambda} \right) |\Phi_0\rangle = \eta^0_{k'} \left( c^*_{k'} + \sum_{k''} \alpha_{k'',k',q',\lambda} c^*_{k''} c_{k',q',\lambda} \right) |\Phi_0\rangle
$$

This yields

$$
\eta^0_{k'} \left( c^*_{k'} + \sum_{k''} \alpha_{k'',k',q',\lambda} c^*_{k''} c_{k',q',\lambda} \right) |\Phi_0\rangle
$$

$$
= \sum_{k''} \left[ \varepsilon_{k'} + \sum_{k''} \varepsilon_{k''} + \sum_{k''} \alpha_{k'',k',q',q''} c^*_{k''} c_{k',q',\lambda} \right]
$$

(10)

$$
\eta^0_{k'} \alpha_{k',k',q',\lambda} = (\varepsilon_{k'} + \hbar \omega) \alpha_{k'',k',q',\lambda} + g_{k''-k',\lambda} a_{q',\lambda}
$$

It follows that

$$
\alpha_{k'',k',q',\lambda} = \frac{g_{k''-k',\lambda}}{(\eta^0_{k'} - \varepsilon_{k'} - \hbar \omega)}
$$

(11)

with the self-consistency condition

$$
\eta^0_{k'} = \varepsilon_{k'} + \sum_{k''} |g_{k''-k',\lambda}|^2 \frac{(\eta^0_{k'} - \varepsilon_{k''} - \hbar \omega)}{(\eta^0_{k'} - \varepsilon_{k''} - \hbar \omega)}
$$

(12)
There are two approximations involved in the product ansatz: (a) The Pauli principle excludes for \( \tilde{c}^{*}_{k_1'} \tilde{c}^{*}_{k_2'} = (c^{*}_{k_1'} + \sum_{k_1, q_1, \lambda} \alpha_{k_1', k_1, q_1, \lambda} c^{*}_{k_1, q_1, \lambda}) \ast (c^{*}_{k_2'} + \sum_{k_2, q_2, \lambda} \alpha_{k_2', k_2, q_2, \lambda} c^{*}_{k_2, q_2, \lambda}) \) the double occupancy of the state \( c^{*}_{k_1} c^{*}_{k_2} \) for \( k_1 = k_2 \). (b) The electron-phonon interaction can introduce a transition from the state \( c^{*}_{k_1} \) into the satellite of \( \tilde{c}^{*}_{k_1} \) yielding a state \( c^{*}_{k_1} c^{*}_{q_1, \lambda} c^{*}_{k_1} a^{*}_{q_2, \lambda} \). This state is neglected.

The total ground-state energy in this approximation is

\[ E_0 = \sum_{k'} \eta^{0}_{k'} \]

The occupation of the states \( c^{*}_{k'} a^{*}_{q, \lambda} \) is given by

\[ |\alpha_{k'', k', q, \lambda}|^2 = \frac{|g_{k'' - k', -q, \lambda}|^2}{(\eta^{0}_{k'} - \kappa_{k'} - \hbar\omega)^2} \]

To normalize each state \( \tilde{c}^{*}_{k'} \) it has to be divided by \( \left[ 1 + \sum_{k'', q, \lambda} \frac{|g_{k'' - k', -q, \lambda}|^2}{(\eta^{0}_{k'} - \kappa_{k'} - \hbar\omega)^2} \right]^{1/2} \).

It should be emphasized that the energy \( \eta^{0}_{k'} \) is not the energy of a hole at \( k' \). It is here only a mathematical abbreviation.

### A.3 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

\[ \tilde{\Psi}_{0; k_0} = \tilde{c}^{*}_{k_0} \prod_{k'} \tilde{c}^{*}_{k'} |\Phi_0\rangle \]

with \( \tilde{c}^{*}_{k'} = (c^{*}_{k'} + \sum_{k'', q, \lambda} \alpha_{k'', k', q, \lambda} c^{*}_{k', q, \lambda} a^{*}_{q, \lambda}) \) where \( k'' \neq k_0 \).

When we derive the corresponding Schrödinger equations we obtain for \( |k'| < k_F \)

\[ \alpha_{k'', k', q, \lambda} = \frac{g_{k'' - k', -q, \lambda}}{(\eta_{k'} - \kappa_{k'} - \hbar\omega)} \]

\[ \eta_{k'} = \kappa_{k'} + \sum_{k'', q, \lambda} g_{k'' - k', q, \lambda} \alpha_{k'', k', q, \lambda} - g_{k' - k_0, q, \lambda} \alpha_{k_0, k', q, \lambda} \]
The amplitude $\alpha_{k'',k',q,\lambda}$ has a slightly different energy denominator compared with the ground state since $\eta_{k'}$ 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 $\tilde{c}_{k_0} = \left( \epsilon_{k_0}^* + \sum_{k'',q,\lambda} \alpha_{k'',k_0,0,0} c_{k'',q,\lambda}^* \right)$ one obtains in analogy

$$
\alpha_{k'',k_0,0,\lambda} = \frac{g_{k''-k_0,-q,\lambda}}{(\eta_{k_0} - \epsilon_{k''} - \hbar \omega)}
$$

The total energy of $\tilde{\Psi}_{0;0,k_0}$ becomes

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

The quasi-particle energy $E_{k_0}$ of the state $c_{k_0}$ is then

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

which yields

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

(13)

If one compares this expression for $E_{k_0}$ with the Green function expression in equ. one recognizes differences in the energy denominators. In the Green 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 Superconductor book both approaches in parallel in the discussion of the electron-phonon self energy.

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