Failure of Migdal's approximation in electron transport

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The role of vertex corrections, associated with electron-phonon interactions, for electron scattering in metals is studied quantitatively. It is found that the correction, proportional to $(m/M)^{1/2}$, is multiplied by a large numerical factor, ~ 30. As a consequence the residual resistivity of a metal is not left unchanged by electron-phonon interactions. The resistivity suffers an increase by a factor $\sim(1+0.16\lambda)$, where λ is the mass renormalization caused by electron-phonon interactions. The coefficient of λ depends on the square root of the ratio v/v_F of sound velocity to Fermi velocity, and the value 0.16 is obtained for the ratio $\frac{1}{200}$.

I. INTRODUCTION

Electron-phonon interactions might be expected to have a significant influence on electron transport over and above direct scattering processes at finite temperatures. For example, the residual resistivity of a metal, i.e., at $T=0$,

$$\rho_0=\frac{m^*}{ne^2\tau} , \tag{1}$$

varies as $(m^*)^2$ since the impurity-potential scattering rate, $1/\tau$, is proportional to the electronic density of states at the Fermi surface. The explicit factor m^* in Eq. (1) arises from the fact that the group velocity of an electron at the Fermi surface is

$$v_F=\hbar k_F/m^* , \tag{2}$$

which results in a proportionate current reduction if m^* is greater than m.

It is well known that electron-phonon interactions cause a renormalization of the effective mass:[1]

$$m^*=m(1+\lambda) , \tag{3}$$

where m is the band mass and λ is the mass-renormalization parameter. Naively one might expect that ρ_0 would (as a consequence) be increased by a factor $(1+\lambda)^2$; but this is not the case.[2] The scattering rate is reduced by a compensating factor of $(1+\lambda)^{-2}$ in the approximation proposed by Migdal.[3] The purpose of this study is to explore the extent to which Migdal's approximation fails, since any deviation can lead to a new temperature-dependent contribution to the electrical resistivity at very low temperatures, even if all of the scattering is *elastic*.[4] This work was prompted by recent high-precision resistivity studies of simple metals,[5] which have indicated a need for further theoretical exploration.

II. ELECTRONS DRESSED WITH PHONONS

In the presence of electron-phonon interactions the energy of an electron suffers a shift $\Sigma(\mathbf{k})$, the self-energy correction, relative to its band energy $\varepsilon(\mathbf{k})$:

$$E(\mathbf{k})=\varepsilon(\mathbf{k})+\Sigma(\mathbf{k}) . \tag{4}$$

In second-order, Brillouin-Wigner perturbation theory,

$$\Sigma(\mathbf{k})=\sum_{\mathbf{q}}\frac{|g(q)|^2}{E-\varepsilon(\mathbf{k}-\mathbf{q})-\hbar\omega(\mathbf{q})} - \sum_{\mathbf{q}}\frac{|g(q)|^2}{\varepsilon(\mathbf{k}+\mathbf{q})-E-\hbar\omega(\mathbf{q})} , \tag{5}$$

where $g(q)$ is the electron-phonon-scattering matrix element for momentum $\mathbf{q}$. The first term arises from virtual emission of phonons by the electron $\mathbf{k}$, which then recoils to *empty* states $\{\mathbf{k}-\mathbf{q}\}$. The second term arises from the suppression of virtual transitions from *occupied* states $\{\mathbf{k}+\mathbf{q}\}$ to the (now) filled state $\mathbf{k}$. [The quasiparticle energy $E(\mathbf{k})$ is the difference between the total energy of the $(N+1)$-electron system ($\mathbf{k}$ occupied) and the N-electron system ($\mathbf{k}$ empty).]

The influence of $\Sigma(\mathbf{k})$ on the density of states $N(E)$ is easily found since $N(E)\sim(dE/dk)^{-1}$.

$$\frac{dE}{dk}=\frac{d\varepsilon}{dk}+\frac{d\Sigma}{dE}\frac{dE}{dk} ; \tag{6}$$

so, on solving for dE/dk in Eq. (6),

$$\frac{dE}{dk}=\frac{d\varepsilon}{dk}\left[1-\frac{d\Sigma}{dE}\right]^{-1} . \tag{7}$$

Accordingly,

$$\frac{m^*}{m}=1-\frac{d\Sigma}{dE} . \tag{8}$$

From Eq. (3) it follows that $\lambda=-d\Sigma/dE$; whereupon λ can be calculated directly by differentiating Eq. (5):

$$\lambda(E)=\sum_{\mathbf{q}}\left[\left[\frac{g(\mathbf{q})}{E-\varepsilon(\mathbf{k}-\mathbf{q})-\hbar\omega(\mathbf{q})}\right]^2 + \left[\frac{g(\mathbf{q})}{\varepsilon(\mathbf{k}+\mathbf{q})-E-\hbar\omega(\mathbf{q})}\right]^2\right] . \tag{9}$$

Again, the first term is summed for $\mathbf{k}-\mathbf{q}$ empty and the second for $\mathbf{k}+\mathbf{q}$ occupied.

Equation (9) can be evaluated numerically for a free-electron model, but see the Appendix. We show in Fig. 1, $\lambda(E)$ versus E near E_F. The area, $\int \lambda(E)dE$, is necessarily zero since the self-energy correction merely alters the density-of-states distribution, but conserves the total number of quantum states. The electron-phonon-interaction matrix element was taken to be

$$g(q)=Aq[\omega(q)]^{-1/2}, \quad 0<q<q_D \ , \tag{10}$$

which is appropriate for a "jellium" model. (q_D is the radius of the Debye sphere.) We modified the Debye frequency spectrum ($\sim\omega^2$) to avoid the unrealistic, singular cut off at $\hbar\omega=\Theta$, which would result in infinite values for $\lambda(E)$ at $E_F\pm\Theta$. Instead we used a phonon frequency distribution,

$$F(\omega)=B\sin^2\left[\frac{\pi\hbar\omega}{2\Theta}\right]\cos\left[\frac{\pi\hbar\omega}{2\Theta}\right] , \tag{11}$$

which falls continuously to zero at the cut off, $\hbar\omega=\Theta$. This spectrum corresponds to $\hbar\omega=(2\Theta/\pi)\sin^{-1}(q/q_D)$. One should note that $\lambda(E)$ has a *minimum* at E_F. It is this minimum which leads to a $T^3\ln(\Theta/T)$ contribution to the *electronic* heat capacity.[6] It will also cause *elastic* impurity scattering to contribute a $T^2\ln(\Theta/T)$ term to the electrical resistivity.[4] The behavior of $\lambda(E)$ shown in Fig. 1 is typical of results obtained from calculations on specific metals.[7]

Consider now an N-electron system at $T=0$, and let Ψ_N be its wave function, including virtual excitations caused by the electron-phonon interaction. If, for example, an extra electron is added to the system in state $\mathbf{k}$, above E_F, the wave function of the $(N+1)$-electron system will be

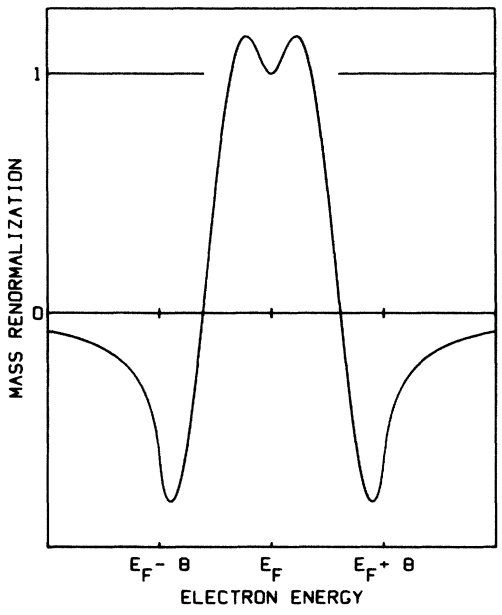

FIG. 1. Mass-renormalization parameter $\lambda(E)$ divided by $\lambda(E_F)$ near the Fermi energy E_F. (Θ is the Debye energy.)

$$\Psi_{N+1}\sim A_{\mathbf{k}}^*\Psi_N \ , \tag{12}$$

where the dressed-electron creation operator is

$$A_{\mathbf{k}}^*=z\left[a_{\mathbf{k}}^*+\sum_{\mathbf{q}}\frac{g(\mathbf{q})}{E(\mathbf{k})-\varepsilon(\mathbf{k}-\mathbf{q})-\hbar\omega(\mathbf{q})}a_{\mathbf{k}-\mathbf{q}}^*b_{\mathbf{q}}^*+\sum_{\mathbf{q}}\frac{g(\mathbf{q})}{E(\mathbf{k})-\varepsilon(\mathbf{k}+\mathbf{q})+\hbar\omega(\mathbf{q})}a_{\mathbf{k}+\mathbf{q}}^*b_{\mathbf{q}}\right] . \tag{13}$$

The first term creates a (bare) electron in $\mathbf{k}$, and the second term creates its phonon dressing. The third term annihilates the phonon dressing of Ψ_N which arose because the state $\mathbf{k}$ was (originally) empty; it restores an electron to $\mathbf{k}+\mathbf{q}$, which was emptied by virtual emission of the phonon $\mathbf{q}$ (now annihilated). z is the quasiparticle renormalization factor:

$$\frac{1}{z^2}=1+\sum_{\mathbf{q}}\left[\left[\frac{g(\mathbf{q})}{E(\mathbf{k})-\varepsilon(\mathbf{k}-\mathbf{q})-\hbar\omega(\mathbf{q})}\right]^2+\left[\frac{g(\mathbf{q})}{\varepsilon(\mathbf{k}+\mathbf{q})-E(\mathbf{k})-\hbar\omega(\mathbf{q})}\right]^2\right] . \tag{14}$$

When one compares Eqs. (9) and (14), it is evident that

$$\frac{1}{z^2}=1+\lambda \ , \tag{15}$$

which is the Ward identity. [See also Eq. (3).]

III. SCATTERING OF DRESSED ELECTRONS BY A POTENTIAL

Suppose there are scattering potentials $V(\mathbf{r})$, having Fourier transform $V(Q)$, which give rise to the residual resistivity. The distribution function $f(\mathbf{k})$ of the Boltzmann transport equation describes the occupation probability of dressed electrons. So the collision operator (arising from the impurity potentials) depends on the (complete) matrix elements

$$M_{\mathbf{k}',\mathbf{k}}=\langle A_{\mathbf{k}'}^*\Psi_N \mid V(\mathbf{r}) \mid A_{\mathbf{k}}^*\Psi_N\rangle \ , \tag{16}$$

instead of the "bare" matrix element

$$V(Q)=\langle \mathbf{k}' \mid V(\mathbf{r}) \mid \mathbf{k}\rangle \ , \tag{17}$$

where $\mathbf{k}'=\mathbf{k}+\mathbf{Q}$. It follows from Eqs. (13) and (16) that,

$$M_{\mathbf{k}',\mathbf{k}}=z^2V(Q)[1+\Lambda(\mathbf{k}',\mathbf{k})] \ , \tag{18}$$

where Λ, the "vertex correction" arises from the "dressing" terms of Eq. (13):

$$\Lambda(\mathbf{Q})=\sum_{\mathbf{q}}\left[\frac{|g(\mathbf{q})|^2}{\Delta_1(\mathbf{k})\Delta_1(\mathbf{k}')}+\frac{|g(\mathbf{q})|^2}{\Delta_2(\mathbf{k})\Delta_2(\mathbf{k}')}\right] . \tag{19}$$

Here Δ_1 and Δ_2 are the energy denominators of the second and third terms in Eq. (13).

The residual resistivity is now proportional to the square of the matrix elements, Eq. (17), as well as to the m^*/m factors mentioned in Sec. I. Accordingly,

$$\rho_0=\frac{m}{ne^2\tau_0}\left[\frac{m^*}{m}\right]^2 z^4(1+\Lambda)^2 \ , \tag{20}$$

where τ_0 is the relaxation time computed without consideration of electron-phonon interactions. From Eqs. (3) and (15),

$$\rho_0=\frac{m}{ne^2\tau_0}(1+\Lambda)^2 , \tag{21}$$

since the mass-renormalization factors and the wave-function renormalization factors cancel. The only modification of the residual resistivity that remains arises from the vertex correction, Λ.

Migdal's theorem is the observation that Λ is $\sim(m/M)^{1/2}$, where M is the atomic mass, and so can be safely neglected. In this event the well-known result that electron-phonon interactions do not alter ρ_0 appears justified.[2] However, such a conclusion assumes that the numerical factor multiplying $(m/M)^{1/2}$ is near unity. In the following section we shall calculate the effect of vertex corrections and shall find that the numerical factor is ~ 30.

We first examine Eq. (19) and consider the special case when $\mathbf{k}'-\mathbf{k}$ is near zero. Then from Eqs. (9) and (19),

$$\lim_{Q\to 0}\Lambda(Q)=\lambda . \tag{22}$$

The failure of Migdal's approximation is 100% in this limit, as originally noted by Migdal.[3] If the scattering centers causing the residual resistivity were very large objects, having only Fourier components near $Q=0$, then ρ_0 would be increased by $(1+\lambda)^2$, in accord with the naive surmise mentioned in Sec. I.

IV. Q DEPENDENCE OF THE VERTEX CORRECTION

In the foregoing section we have noticed that, for very small Q, the scattering matrix element of a dressed electron receives a proportionate contribution from the dressed components. In such an event, the $(1+\Lambda)$ factor cancels the z^2 factor in Eq. (18), so the matrix element is the same as that for a bare electron. For larger Q, however, the confluences of the singular factors associated with $\Delta_1(k)$ and $\Delta_1(k')$, etc., no longer obtain. Accordingly, the numerical value of Λ, Eq. (18), becomes smaller than λ. The physical meaning is that the virtual-phonon dressing of the initial state $\mathbf{k}$ loses most of its overlap with the dressing of the final state $\mathbf{k}'$. The scattering matrix element is then dominated by the bare part, $z^2\langle\mathbf{k}'\,|\,V\,|\,\mathbf{k}\rangle$. (Migdal's approximation retains *only* this contribution.)

We have calculated $\Lambda(Q)$ in order to quantify the failure of Migdal's approximation. The threefold integration, d^3q, in Eq. (19) can be evaluated numerically after an initial analytic integration over the azimuthal angle defined relative to the polar axis $\mathbf{Q}$. E was taken equal to the Fermi energy E_F, and the phonon spectrum was extended: $0<q<2k_F$, in order to include umklapp processes. Such an extension requires that the electron-phonon-interaction matrix element, Eq. (10), be replaced by one having the periodicity of the reciprocal lattice. We employed the approximation

$$|g(q)|^2=A'\sin(\pi q/G) , \tag{23}$$

where $\mathbf{G}$ was taken to be a (1,1,0) reciprocal-lattice vector of a bcc monovalent metal. Dispersion of the velocity of sound, v, was neglected in the energy denominators, Δ.

The relative importance of $\Lambda(Q)$ depends on the ratio, v/v_F, of sound velocity to Fermi velocity. For a ratio, $\frac{1}{200}$, a heuristic fit to the numerical values obtained was,

$$J(Q)\equiv\frac{\Lambda}{\lambda}\cong\left[1+220\left[\frac{Q}{2k_F}\right]+360\left[\frac{Q}{2k_F}\right]^2\right]^{-1/2} . \tag{24}$$

This deviation from Migdal's approximation is shown in Fig. 2. One should note that the deviation falls rapidly from 100% at $Q=0$, as expected, but remains quite significant ($\sim 7\%$) near $Q=k_F$. The value near k_F varies approximately as $(v/v_F)^{1/2}$. (The *ratio* of Λ to λ, Eq. (24), is independent of interaction strength in first-order Born approximation.)

Equation (24) can be used to calculate the effect of the vertex correction on, say, the residual resistivity. The result depends, of course, on the scattering potential assumed. For illustrative purposes we consider

$$V(r)=B\exp(-r^2/r_s^2) , \tag{25}$$

where r_s is the radius of the Wigner-Seitz sphere, i.e., $k_Fr_s=(9\pi/4)^{1/3}$. Accordingly,

$$V(Q)=B'\exp(-r_s^2Q^2/4) . \tag{26}$$

The residual resistivity, *with* Migdal's approximation, is proportional to

$$I_0=\int_0^{\pi}[V(Q)]^2(1-\cos\theta)\sin\theta\,d\theta , \tag{27}$$

where θ is the scattering angle, i.e.,

$$Q=2k_F\sin(\theta/2) . \tag{28}$$

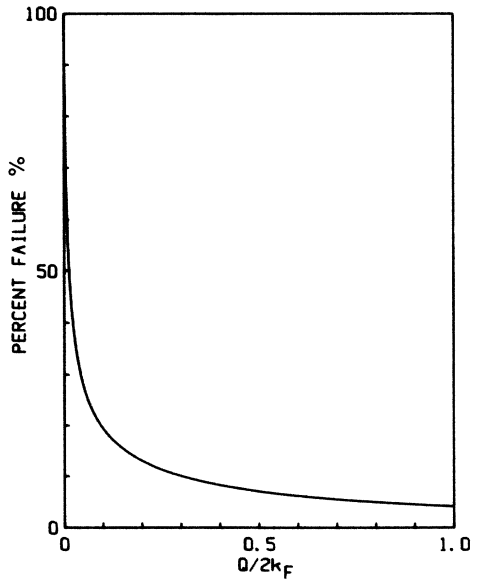

FIG. 2. Vertex correction $\Lambda(Q)$, divided by $\lambda(E_F)$, as a function of momentum transfer Q.

When including the vertex corrections, the residual resistivity is proportional to,

$$I=\int_0^{\pi}[V(Q)]^2(1-\cos\theta)[1+2\lambda J(Q)]\sin\theta\, d\theta \ . \quad (29)$$

We have neglected the quadratic term, $(\lambda J)^2$. The ratio of I to I_0 is easily evaluated from Eqs. (24)–(29):

$$I/I_0 \cong 1+0.16\lambda \ . \quad (30)$$

This is the factor by which the *residual* resistivity would be increased as a consequence of electron-phonon interactions.

The coefficient, 0.16, of λ in Eq. (30) is approximately proportional to $(v/v_F)^{1/2}$. It is rather insensitive to the functional form of $V(r)$, Eq. (25). For a δ-function potential (isotropic scattering) it has a value of ~ 0.11. For scattering arising from atomic displacements surrounding an impurity,[8] it can exceed 0.20. Since $(m/M)^{1/2} \sim 0.005$, the vertex correction to ρ_0 is approximately 30 times larger than the original order-of-magnitude estimates.

V. CONCLUSIONS

Numerical study of vertex corrections for electron transport reveals that they are large enough to be of physical significance. In a subsequent work, we have found that such corrections cause a new, measurable contribution to the low-temperature resistivity, proportional to $T^2\ln(\Theta/T)$, which arises solely from *elastic* scattering.[4]

ACKNOWLEDGMENT

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APPENDIX

The integrals in Eqs. (5) and (9) are both singular. The principal value is the correct interpretation of Eq. (5). $\lambda(E)$, given *symbolically* by Eq. (9), can only be obtained by differentiation after the principal-value evaluation of Eq. (5) has been accomplished analytically.

A simple example of the questions involved may clarify the meaning. Consider

$$y(a)=\int_{-1}^{1}\frac{dx}{x-a} \ ,$$

where $|a|<1$. Formally,

$$\frac{dy}{da}=\int_{-1}^{1}\frac{dx}{(x-a)^2}$$

appears to be positive (by inspection of the integrand). However, the principal-value interpretation of the integral for $y(a)$ leads to

$$y(a)=\ln\left|\frac{1-a}{1+a}\right| \ .$$

Whereupon, by differentiation,

$$\frac{dy}{da}=\frac{-2}{1-a^2} \ ,$$

which is negative for $|a|<1$. Interestingly, this last (and correct) result is also obtained if the integral for dy/da is evaluated formally, without noticing the singularity of the integrand.

The integrals displayed in this paper were evaluated with appropriate care.

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