Electron self-energy and generalized Drude formula for infrared conductivity of metals

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Götze and Wölfle (GW) [Phys. Rev. B **6**, 1226 (1972)] wrote the conductivity in terms of a memory function $M(\omega)$ as $\sigma(\omega+i\eta)=(ine^2/m)[\omega+M(\omega+i\eta)]^{-1}$, where $M(\omega+i\eta)=i/\tau$ in the Drude limit. The analytic properties of $-M(\omega+i\eta)$ are the same as those of the self-energy Σ of a retarded Green's function. In the approximate treatment of GW, $-M$ closely resembles a self-energy with differences, e.g., the imaginary part is twice too large. The correct relation between $-M$ and Σ is known for the electron-phonon case and is conjectured to be similar for other perturbations. When vertex corrections are ignored there is a known relation. A derivation using Matsubara temperature Green's functions is given.

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I. PRELIMINARIES

Holstein [1] used elementary arguments to show that in the infrared properties of metals there can be quantum effects (outside of the semiclassical Boltzmann approach) when the temperature is low enough and the probing frequency ω is degenerate with nonelectronic excitations, such as phonons. Such effects have been seen experimentally [2,3]. Götze and Wölfle (GW) [4] gave a nice simplified way to compute such effects in the optical response of metals using truncated equations of motion to compute the "memory function" $M(\omega+i\eta)$ defined as

$$\sigma(\omega+i\eta)=\frac{ine^2/m}{\omega+M(\omega+i\eta)}. \tag{1}$$

In the dc limit, their formulas correctly reproduce lowest-order variational solutions of the corresponding Boltzmann transport theories. Unfortunately, a systematic perturbation theory for $M(\omega+i\eta)$ is not known, and the GW approximation is therefore hard to improve. The GW results are slightly less accurate than the corresponding lowest-order results of Green's function theories.

The function $-M(\omega+i\eta)$ has causal analytic properties and, not surprisingly, bears a close resemblance to an electron self-energy $\Sigma(\vec{k},\omega+i\eta)$ for $\vec{k}$ points averaged over the Fermi surface. However, the imaginary part of Σ is $-1/2\tau$ whereas the imaginary part of $-M$ must be $-1/\tau$. This is not the only difference between $-M$ and Σ. Since the analogy between $-M$ and Σ is sometimes used for analysis of infrared spectra [5], it is important to understand just how good it actually is. A full formula seems not to have been derived and is beyond the ambition of this paper. A reasonable conjecture is that when anisotropy with k around the Fermi surface is not too important, then

$$\sigma(\omega+i\eta)=\frac{ine^2}{m\omega}\int_{-\infty}^{\infty}d\omega'\frac{f(\omega')-f(\omega'+\omega)}{\omega-\Sigma_{\rm ir}(\omega'+\omega+i\eta)+\Sigma_{\rm ir}^{*}(\omega'+i\eta)}, \tag{2}$$

where $f(\omega')=[\exp(\beta\omega')+1]^{-1}$ is the Fermi-Dirac function. Here $\Sigma_{\rm ir}$ is a modified version of Σ, averaged over the Fermi surface, but with an extra weighting factor, similar to the familiar transport factor $1-\cos\theta$. The actual weighting factor (in the solved electron-phonon case [6,7]) is found from a frequency-dependent nonlinear integral equation. Replacement of the weight factor by 1, turning $\Sigma_{\rm ir}$ into an ordinary but $\vec{k}$-averaged self-energy, should work fairly well in most cases. Scher [8] performed a numerical study which tends to confirm that the difference between $\Sigma_{\rm ir}$ and Σ is small. Sometimes the anisotropy of Σ around the Fermi surface is large. A modified version of Eq. (2) that deals approximately with such cases is presented at the end of the paper.

Equation (2) implies a relation between $-M(\omega+i\eta)$ and the self-energy which becomes more direct at low frequencies. Keeping the lowest order (in ω) terms, one gets a derivative of the Fermi-Dirac function $-\partial f(\omega')/\partial\omega'$, which can be approximated by the Dirac $\delta(\omega')$,

$$\begin{aligned}\sigma(\omega+i\eta)&\approx\frac{ine^2}{m}\int_{-\infty}^{\infty}d\omega'\left(-\frac{\partial f(\omega')}{\partial\omega'}\right)\\&\quad\times\frac{1}{\omega[1-d\Sigma_{\rm ir,1}(\omega')/d\omega']+2i\Sigma_{\rm ir,2}(\omega')}\\&\approx\frac{ine^2/m}{\omega-\omega\,d\Sigma_{\rm ir,1}(\omega)/d\omega+2i\Sigma_{\rm ir,2}(\omega)}.\end{aligned} \tag{3}$$

Therefore the real part of $-M$ at low frequencies is $\omega d\,\mathrm{Re}\,\Sigma_{\rm ir}(\omega)/d\omega$, and the imaginary part is $-2\,\mathrm{Im}\,\Sigma_{\rm ir}(\omega)$. If the interesting part of $\mathrm{Re}\,\Sigma$ is odd in ω and approximately linear, then M at very low ω is a lot like Σ except for the factor of 2 in the imaginary part.

In the dc limit, the result $\sigma=ne^2\tau/m$ is retrieved with $1/\tau=-2\,\mathrm{Im}\,\Sigma_{\rm ir}(\omega\to0)$. There are minor differences between this and the more exact result found from a solution of the Boltzmann transport equation. These differences arise from $\vec{k}$ dependence and disappear when the electron scattering is isotropic.

II. KUBO FORMULA

The starting point is the Kubo [9] formula for the conductivity. In an external electric field $\vec{E}(t)=\vec{E}\cos(\omega t)$, the current operator $j=-e\sum_k v_{kx}c_k^{\dagger}c_k$ acquires an expectation value of $\langle j(t)\rangle=\mathrm{Re}[\sigma(\omega+i\eta)\exp(-i\omega t)]E$ where the

linear-response coefficient $\sigma(\omega+i\eta)$ is

$$\sigma(\omega+i\eta)=\frac{i}{\omega}\left[r(\omega+i\eta)+\frac{ne^2}{m}\right], \tag{4}$$

$$r(\omega+i\eta)=i\int_0^\infty dt\, e^{i\omega t-\eta t}\langle[j(t),j(0)]\rangle. \tag{5}$$

The Hamiltonian $\mathcal{H}=\mathcal{H}_0+\mathcal{H}_1$ has the noninteracting part $\mathcal{H}_0=\sum_k \epsilon_k c_k^\dagger c_k$. The label k is short for the Bloch wave vector and other quantum numbers ($\vec{k}n\sigma$). The state k has energy ϵ_k and group velocity $\vec{v}_k$.

To obtain a Wick-ordered perturbation theory we use an imaginary time ($0\leqslant\sigma\leqslant\beta=1/k_BT$) version of $r(\omega)$,

$$r(i\omega_\mu)=-\int_0^\beta d\sigma\, e^{i\omega_\mu\sigma}\overline{\langle\hat{T}\,j(\sigma)j(0)\rangle}, \tag{6}$$

where $j(\sigma)=\exp(\sigma\mathcal{H})j\exp(-\sigma\mathcal{H})$. Angular brackets denote a canonical ensemble temperature average, and the overbar indicates, if necessary, an average over an ensemble of randomly distributed impurities. The Matsubara frequency ω_μ is $2\pi\mu/\beta$, and μ is an integer. When analytically continued from $i\omega_\mu$ to $\omega+i\eta$ just above the real ω axis (η is a positive infinitesimal) $r(i\omega_\mu)$ becomes $r(\omega+i\eta)$, the retarded correlation function needed for the Kubo formula.

All Feynman graphs for $r(i\omega_\mu)$ are formally summed in terms of the exact electron Green's function,

$$G(k,i\omega_\nu)=\frac{1}{i\omega_\nu-\epsilon_k-\Sigma(k,i\omega_\nu)}, \tag{7}$$

and the exact vertex function $\Gamma(k,k',i\omega_\mu,i\omega_\nu)$, where $\omega_\nu=2\pi(\nu+1/2)/\beta$. The exact answer is

$$r(i\omega_\mu)=-\frac{e^2}{\beta}\sum_{kk'\nu}v_{k'x}\Gamma(kk',i\omega_\mu,i\omega_\nu)\times G(k',i\omega_\nu+i\omega_\mu)G(k,i\omega_\nu). \tag{8}$$

Neither Σ nor Γ can be calculated exactly. A linearized Boltzmann equation is obtained when lowest-order results for Σ and Γ are treated consistently.

An explicit formula relating σ to Σ occurs when Γ is replaced by its lowest-order term,

$$\Gamma(kk',i\omega_\mu,i\omega_\nu)\to\Gamma_0=v_{kx}\delta(k,k'). \tag{9}$$

The corresponding answer for $\sigma(\omega+i\eta)$, denoted by $\sigma_0(\omega+i\eta)$ after continuing to the real frequency axis and averaging away the k dependence of $\Sigma(k,\omega+i\eta)$ is

$$\sigma_0(\omega+i\eta)=\frac{ine^2}{m\omega}\int_{-\infty}^\infty d\omega'\frac{f(\omega')-f(\omega'+\omega)}{\omega-\Sigma(\omega'+\omega+i\eta)+\Sigma^*(\omega'+i\eta)}. \tag{10}$$

This is the desired approximation, a simplification of the conjectured version Eq. (2). It is not particularly original. A derivation for a "local Fermi liquid" is given by Berthod *et al.* [10]. It seems worthwhile to present a simpler and more general discussion. A careful derivation of Eq. (10) is given in the next section.

Unlike the conjectured version Eq. (2), the approximation of Eq. (9) does not correctly reproduce the Boltzmann dc conductivity because of the omission of vertex corrections. This is related to the fact that the quasiparticle scattering rate $1/\tau=-2\,\mathrm{Im}\,\Sigma$ differs from the transport scattering rate $1/\tau_{\rm tr}=-2\,\mathrm{Im}\,\Sigma_{\rm ir}$ by a factor of the type $1-\cos\theta$. The "cos θ" correction (omitted if the integral equation part of the Boltzmann equation is neglected) takes into account that small angle θ scattering events ($\vec{k}\to\vec{k}'$) do not degrade the current efficiently and make smaller contributions to $1/\tau_{\rm tr}$ than to $1/\tau$. The difference, except at low temperatures, is likely to be numerically small since small-angle scattering does not usually play a dominant role. The version of this, applicable to electron-phonon-coupled superconductors, was given by Nam [11].

III. DERIVATION OF EQ. (10)

Starting by inserting Eq. (9) into Eq. (8),

$$r_0(i\omega_\mu)=-\frac{e^2}{\beta}\sum_k v_{kx}^2G(k,i\omega_\nu+i\omega_\mu)G(k,i\omega_\nu). \tag{11}$$

This approximation, labeled r_0, keeps in principle arbitrarily complicated self-energy graphs in G.

The spectral function is defined as

$$G(k,i\omega_\nu)=\int_{-\infty}^\infty d\omega\frac{A(k,\omega)}{i\omega_\nu-\omega}, \tag{12}$$

$$A(k,\omega)=-\frac{1}{\pi}\mathrm{Im}\,G(k,i\omega_\nu\to\omega+i\eta), \tag{13}$$

where $G(k,\omega+i\eta)$ is the retarded Green's function,

$$G(k,\omega+i\eta)=\frac{1}{\omega-\epsilon_k-\Sigma(k,\omega+i\eta)}, \tag{14}$$

and $\Sigma(k,\omega+i\eta)=\Delta(k,\omega)-i/2\tau(k,\omega)$ has imaginary part $1/2\tau$ non-negative. The approximate correlation function r_0 becomes

$$r_0(i\omega_\mu)=-\frac{e^2}{\beta}\sum_k v_{kx}^2\int_{-\infty}^\infty d\omega_1\int_{-\infty}^\infty d\omega_2A(k,\omega_1)A(k,\omega_2)\times\sum_\nu\left[\frac{1}{i\omega_\nu+i\omega_\mu-\omega_1}\frac{1}{i\omega_\nu-\omega_2}\right]. \tag{15}$$

The Matsubara sum can be performed exactly,

$$-\frac{1}{\beta}\sum_\nu\left[\frac{1}{i\omega_\nu+i\omega_\mu-\omega_1}\frac{1}{i\omega_\nu-\omega_2}\right]=\frac{f(\omega_2)-f(\omega_1)}{\omega_2-\omega_1+i\omega_\mu}. \tag{16}$$

The correlation function now is

$$r_0(i\omega_\mu)=-e^2\int_{-\infty}^\infty d\epsilon\sum_k v_{kx}^2\delta(\epsilon-\epsilon_k)\int_{-\infty}^\infty d\omega_1\times\int_{-\infty}^\infty d\omega_2A(k,\omega_1)A(k,\omega_2)\frac{f(\omega_2)-f(\omega_1)}{\omega_2-\omega_1+i\omega_\mu}, \tag{17}$$

where a gratuitous factor of $1=\int d\epsilon\,\delta(\epsilon-\epsilon_k)$ was inserted. From Eqs. (13) and (14), the spectral function has a rapid ϵ_k dependence,

$$A(k,\omega)=-(1/\pi)\mathrm{Im}[\omega-\epsilon_k-\Sigma(k,\omega+i\eta)]^{-1}. \tag{18}$$

But because of the δ function in the k sum,

$$\sum_k v_{kx}^2 \delta(\epsilon - \epsilon_k) A(k,\omega_1) A(k,\omega_2), \tag{19}$$

it is allowed to replace ϵ_k in the denominators of the spectral functions by ϵ. The rapid ϵ dependence in $A(k,\omega)$ must be treated carefully, but the remaining weak k dependence of $\Sigma(k,\omega+i\eta)$ in the denominator of $A(k,\omega)$ can often be treated less carefully. For many metals, the self-energies $\Sigma(k,\omega+i\eta)$ in the spectral functions $-(1/\pi)\mathrm{Im}(\omega-\epsilon-\Sigma)^{-1}$ vary weakly with $\vec{k}$ and can be replaced by their k average over the Fermi surface,

$$\Sigma(\omega+i\eta) = \sum_k \Sigma(k,\omega+i\eta)\delta(\epsilon_k) \Big/ \sum_k \delta(\epsilon_k). \tag{20}$$

In "conventional" s-wave superconductors, for example, anisotropy of the gap function $\Delta(k,\omega)$ is often surprisingly small, and the gap can be approximated well as $\Delta(\omega)$. The gap $\Delta(k,\omega)$ is a superconducting extension of the normal-state self-energy. Serious anisotropy is not forbidden and is known to occur in the $T_c = 39$-K superconductor MgB_2 [12], for example. A modified formula applicable to such cases is given at the end of the paper. Using Eq. (20), the k sum is

$$\begin{aligned}\sum_k v_{kx}^2 \delta(\epsilon-\epsilon_k) &= \frac{1}{\hbar^2}\sum_k \frac{\partial\epsilon_k}{\partial k_x}\left(-\frac{\partial f}{\partial k_x}\right) \\ &= \frac{1}{\hbar^2}\sum_k \frac{\partial^2\epsilon_k}{\partial k_x^2} f = [n/m]_{\mathrm{eff}}(\epsilon).\end{aligned} \tag{21}$$

Here the δ function was replaced by $-\partial f/\partial\epsilon_k$. An integration by parts was used to obtain the inverse effective mass $(\partial^2\epsilon_k/\partial k_x^2)/\hbar^2$ summed over all states lower in energy than ϵ.

The range of the remaining ϵ integration is nominally $(-\infty,\infty)$. However, the factors $A(k,\omega)$ are peaked at $\epsilon \approx \omega_1$ and $\epsilon \approx \omega_2$. Thus the integrand is large only if ω_1 and ω_2 have similar values. Because of the factor $[f(\omega_2)-f(\omega_1)]$, they must both lie near the Fermi energy (one below and one above.) Therefore the ϵ integral is dominated by ϵ near the Fermi energy. The value of $[n/m]_{\mathrm{eff}}(\epsilon)$ at the Fermi energy is $[n/m]_{\mathrm{eff}}$, the number of electrons divided by the effective mass averaged over all states below the Fermi energy. An equivalent formula is

$$[n/m]_{\mathrm{eff}} = \sum_k v_{kx}^2 \delta(\epsilon_k) = N(0)\langle v_x^2\rangle. \tag{22}$$

The current correlation function now is

$$\begin{aligned} r_0(i\omega_\mu) = \left[\frac{n}{m}\right]_{\mathrm{eff}} e^2 \int_{-\infty}^{\infty} d\epsilon \int_{-\infty}^{\infty} d\omega_1 \int_{-\infty}^{\infty} d\omega_2 \\ \times A(\epsilon,\omega_1)A(\epsilon,\omega_2)\frac{f(\omega_2)-f(\omega_1)}{\omega_2-\omega_1+i\omega_\mu}. \end{aligned} \tag{23}$$

It is necessary to integrate ϵ carefully over the Lorentzian peaks of $A(\epsilon,\omega_1)A(\epsilon,\omega_2)$. Cauchy's theorem can be used after closing the ϵ contour by an arc going to infinity in either the upper or the lower half-plane. The result is expressed by another identity,

$$\begin{aligned}\int_{-\infty}^{\infty} d\epsilon \left(\frac{1}{\pi}\right)\mathrm{Im}\left(\frac{1}{\omega_1-\epsilon-\Sigma_1}\right)\left(\frac{1}{\pi}\right)\mathrm{Im}\left(\frac{1}{\omega_2-\epsilon-\Sigma_2}\right) \\ = -\left(\frac{1}{\pi}\right)\mathrm{Im}\left(\frac{1}{\omega_1-\omega_2-\Sigma_1+\Sigma_2^*}\right).\end{aligned} \tag{24}$$

The proof is elementary but tedious. The current correlation function is now

$$\begin{aligned} r_0(i\omega_\mu) = \left[\frac{n}{m}\right]_{\mathrm{eff}} \frac{e^2}{\pi}\int_{-\infty}^{\infty} d\omega_1 \int_{-\infty}^{\infty} d\omega_2 \frac{f(\omega_2)-f(\omega_1)}{\omega_2-\omega_1+i\omega_\mu} \\ \times \mathrm{Im}\left(\frac{1}{\omega_1-\omega_2-\Sigma_1+\Sigma_2^*}\right). \end{aligned} \tag{25}$$

The function $r_0(\omega+i\eta)$ is now just $r_0(i\omega_\mu)$ with $i\omega_\mu$ replaced by $\omega+i\eta$. The only complex quantity in the formula for $r_0(\omega+i\eta)$ is the factor $(\omega_2-\omega_1+\omega+i\eta)^{-1}$, so the real part $\mathrm{Re}\,\sigma_0(\omega+i\eta) = \mathrm{Im}\,r_0(\omega+i\eta)/\omega$ [Eq. (4)] is

$$\begin{aligned}&\mathrm{Re}\,\sigma_0(\omega+i\eta) \\ &= \left[\frac{n}{m}\right]_{\mathrm{eff}} \frac{e^2}{\omega}\int_{-\infty}^{\infty} d\omega_1 \int_{-\infty}^{\infty} d\omega_2 [f(\omega_2)-f(\omega_1)] \\ &\quad \times \delta(\omega_2-\omega_1+\omega)\mathrm{Re}\left(\frac{i}{\omega_1-\omega_2-\Sigma_1+\Sigma_2^*}\right) \\ &= \left[\frac{n}{m}\right]_{\mathrm{eff}} e^2 \int_{-\infty}^{\infty} d\omega' \left[\frac{f(\omega')-f(\omega'+\omega)}{\omega}\right] \\ &\quad \times \mathrm{Re}\left(\frac{i}{\omega-\Sigma(\omega'+\omega+i\eta)+\Sigma^*(\omega'+i\eta)}\right).\end{aligned} \tag{26}$$

The function $\sigma_0(\omega+i\eta)$ is specified by the requirements of being analytic for $\mathrm{Im}\,\omega > 0$, vanishing sufficiently rapidly as $\omega \to \infty$, and agreeing with Eq. (26). It is necessary and sufficient to remove the real part designator from both sides. This is the derivation of Eq. (10).

Here is a modification of Eq. (10) that does not ignore the anisotropy of $\Sigma(k,\omega+i\eta)$ as $\vec{k}$ varies around the Fermi surface,

$$\begin{aligned}&\sigma_0(\omega+i\eta) \\ &= \frac{ie^2}{\omega}\int_{-\infty}^{\infty} d\omega' [f(\omega')-f(\omega'+\omega)] \\ &\quad \times \sum_k \frac{v_{kx}^2 \delta(\epsilon_k-\epsilon_F)}{\omega-\Sigma(k,\omega'+\omega+i\eta)+\Sigma^*(k,\omega'+i\eta)}.\end{aligned} \tag{27}$$

To derive this, go back to Eq. (17), but do not use the isotropic form Eq. (20) for Σ, and do not make use of Eq. (21). The factor $[n/m]_{\mathrm{eff}}$ no longer appears outside the integrals, but $\sum_k v_{kx}^2\delta(\epsilon_k-\epsilon)$ appears inside the $d\epsilon$ integral in Eq. (23). It is no longer possible to use Eq. (24), unless an approximation is made, namely, that the $\vec{k}$ dependence of v_{kx}^2 and of $\Sigma(k,\omega+i\eta)$ is not too rapid. There can be a large variation in both v_{kx}^2 and $\Sigma(k,\omega+i\eta)$ as $\vec{k}$ moves around the Fermi surface. However, the variation perpendicular to the Fermi surface as ϵ_k changes on the scale of the relevant infrared ω's must be small. Then one can ignore the ϵ dependence of both v_{kx}^2 and $\Sigma(k,\omega+i\eta)$

and recover the use of Eq. (24). Then Eq. (27) follows. A version of this approximation was used by Hussey *et al.* [13] for analysis of the normal state of cuprates.

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[1] T. Holstein, Optical and infrared volume absorptivity of metals, Phys. Rev. **96**, 535 (1954).

[2] R. R. Joyce and P. L. Richards, Phonon contribution to the far-infrared absorptivity of superconducting and normal lead, Phys. Rev. Lett. **24**, 1007 (1970).

[3] B. Farnworth and T. Timusk, Phonon density of states of superconducting lead, Phys. Rev. B **14**, 5119 (1976).

[4] W. Götze and P. Wölfle, Homogeneous dynamical conductivity of metals, Phys. Rev. B **6**, 1226 (1972).

[5] J. Huang, T. Timusk, and G. D. Gu, High transition temperature superconductivity in the absence of the magnetic resonance mode, Nature (London) **427**, 714 (2004).

[6] T. Holstein, Theory of transport phenomena in an electron-phonon gas, Ann. Phys. (N.Y.) **29**, 410 (1964).

[7] P. B. Allen, Electron-phonon effects in the infrared properties of metals, Phys. Rev. B **3**, 305 (1971).

[8] H. Scher, Far-infrared absorptivity of normal lead, Phys. Rev. Lett. **25**, 759 (1970).

[9] R. Kubo, Statistical-mechanical theory of irreversible processes. 1. general theory and simple applications to magnetic and conduction problems, J. Phys. Soc. Jpn. **12**, 570 (1957).

[10] C. Berthod, J. Mravlje, X. Deng, R. Zitko, D. van der Marel, and A. Georges, Non-Drude universal scaling laws for the optical response of local Fermi liquids, Phys. Rev. B **87**, 115109 (2013).

[11] S. B. Nam, Theory of electromagnetic properties of superconducting and normal systems. I, Phys. Rev. **156**, 470 (1967).

[12] H. J. Choi, D. Roundy, H. Sun, M. L. Cohen, and S. G. Louie, First-principles calculation of the superconducting transition in MgB_2 within the anisotropic Eliashberg formalism, Phys. Rev. B **66**, 020513 (2002).

[13] N. E. Hussey, J. C. Alexander, and R. A. Cooper, Optical response of high-Tc cuprates: Possible role of scattering rate saturation and in-plane anisotropy, Phys. Rev. B **74**, 214508 (2006).