Connection between the heat capacity and the effective mass of the electrons in Fermi-liquid theory at finite temperatures

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The effect of electron-phonon interaction on the connection between the electronic heat capacity and the effective mass of the electrons in metals is investigated. It is shown that this connection is essentially nonlocal and is independent of the phonon spectrum $g(\omega) = \alpha^2(\omega)F(\omega)$. A simple differential relation is obtained between the heat capacity of the electrons in a metal and the known Fermi-liquid formula for the heat capacity of electrons.

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The effect of phonons on the electron Fermi liquid in a metal has been thoroughly investigated.[1,2,3] The problem of the connection between the heat capacity $C_e(T)$ and the effective mass $m^*(T)$ of the electrons in metals in the presence of a finite electron-phonon interaction has not been solved, however, to this day. Attempts of a direct generalization of the Landau Fermi-liquid theory were obviously ineffective, since the temperature corrections to $m^*(T)$ and $C_e(T)$, due to the electron-phonon interaction, are connected with the phonon spectrum $g(\omega) = \alpha^2(\omega)F(\omega)$ by integral relations with essentially different kernels.

Indeed, the temperature corrections to the effective mass and to the so-called slope coefficient $\gamma(T) = C_e(T)/T$ are given by[2,3]

$$\delta m^*(T)=[m^*(T)-m_0]/m_0=2\int_0^\infty d\omega g(\omega)G(T/\omega)/\omega, \quad (1)$$

$$\delta\gamma(T)=[\gamma(T)-\gamma_0]/\gamma_0=2\int_0^\infty d\omega g(\omega)Z(T/\omega)/\omega, \quad (2)$$

where m_0 is the effective mass in the absence of the electron-phonon interaction; $\gamma_0 = m_0 p_0/3$ is the "slope" in the absence of the electron phonon interaction:

$$G(x)=\int_0^\infty dz[1-(2xz)^2]^{-1}\,\mathrm{ch}^{-2}z=4\sum_{k=1,3,5...}^{\infty}\frac{yk}{[1+yk^2]^2}\Bigg|_{y=(\pi x)^2}; \quad (3)$$

$$Z(x)=\frac{1}{2J_2}\int_{-\infty}^{+\infty}\frac{dtt}{\mathrm{ch}^2 t}\int_0^\infty\frac{dt'}{\mathrm{ch}^2 t'}\frac{t+t'}{1-[2x(t+t')]^2}; \quad (4)$$

$$J_\alpha=\int_0^\infty dzz^\alpha\,\mathrm{ch}^{-2}z.$$

As seen from (1) and (2), the temperature corrections $\delta m^*(T)$ and $\delta\gamma(T)$ are actually different because of the substantial difference between the kernels $G(T/\omega)$ and $Z(T/\omega)$ (see Fig. 1). The asymptotic forms of $\delta m^*(T)$ and $\delta\gamma(T)$ are also different.[3,4,5]

Thus, at a finite electron-phonon interaction the heat capacity is not proportional to the electron effective mass. As for the known Fermi-liquid formula

$$C_{ef}(T)=m^*p_0T/3, \quad (5)$$

it is valid as $T\to 0$ and at $\omega_D \ll T \ll \varepsilon_F$. Consequently, the effect of the electron-phonon interaction is to deviate the temperature dependence of the heat capacity from linearity and to violate the proportionality of the effective mass to the heat capacity.

This is due to two opposing processes: an increase of the number of phonons in the "phonon cloud" of the electrons and the "spreading" of this cloud when the electronic-excitation energy increases with rising temperature. Thus, negative values of $\delta\gamma(T)$ at $T \gtrsim \omega_D/3$ are due to the rapid spreading of the "cloud" at these temperatures.

To find the sought connection between the effective mass and the heat capacity of the electrons it suffices to eliminate from (1) and (2) the phonon spectrum $g(\omega)$. This is easily done with the aid of Mellin integral transformations. Using them we can, for example, obtain from (2) the following relation for the Mellin transform of the correction $\delta\gamma(T)$, of the phonon spectrum $g(\omega)$ and, of the kernel $Z(x)$

$$M(\delta\gamma, s)=2M(g, s)M(Z, s), \quad (6)$$

where, by definition,

$$M(f,s)\equiv\int_0^\infty f(x)x^{s-1}\,dx$$

is the Mellin transform of the function $f(x)$. From (6) we ob-

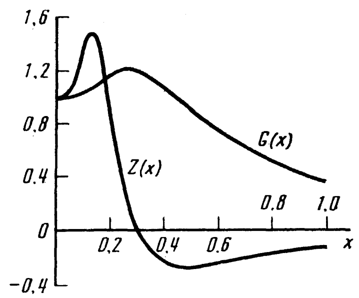

FIG. 1. It follows from a comparison of the kernels $G(x)$ and $Z(x)$ that the electron effective mass $m^*(T)$ is not proportional to their heat capacity $C_e(T)$.

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tain by taking the inverse Mellin transform, the phonon spectrum

$$g(\omega)=\frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty}\frac{M(\delta\gamma,s)}{M(Z,s)}\omega^{-s}\,ds, \tag{7}$$

where $0<c\equiv\mathrm{Re}\,s=\mathrm{const}<1$ is determined by the region of the existence of the transforms $M(g,s)$, $M(\delta\gamma,s)$, and $M(Z,s)$. Substituting now (7) in (1) and changing the order of integration, we obtain the formal relation between $m^*(T)$ and $C_e(T)$:

$$\delta m^*(T)=\frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty}\frac{M(\delta\gamma,s)}{R(s)}T^{-s}ds, \tag{8}$$

where $R(s)=M(Z,s)/M(G,s)$ is a universal function.

The connection obtained between the correction to the effective mass and the correction to the heat capacity is integral and depends strongly on the form of the universal function $R(s)$. In addition, Eq. (8) does not contain the phonon spectrum $g(\omega)$ and is therefore universal, i.e., valid for any metal with an isotropic Fermi surface. It follows from the last statement that relation (8) is valid, in particular, for the Einstein model, i.e., when the phonon spectrum is a δ-function $[g(\omega)=\lambda_0\delta(\omega/\omega_1-1)/2]$. Relation (8) becomes in this case the integral connection between the kernels $G(x)$ and $Z(x)$:

$$G(t)=\frac{1}{2\pi i}\int_{c-i\infty}\frac{M(Z,s)}{R(s)}t^{-s}ds;$$

$$M(Z,s)=\int_0^\infty dt\,t^{s-1}Z(t),\quad t=T/\omega_1. \tag{9}$$

Now the last relation contains no physical quantities, so that the problem of determining the connection between the effective mass and the heat capacity now becomes the purely mathematical problem of finding the relation between the kernel $G(x)$ and $Z(x)$ (see expressions (3) and (4) and Fig. 1).

Understandably, relations (8) and (9) by themselves are still not the solution of our problem, since they were obtained from the Fredholm equation (3) of the first kind, whose solution (7) is known[3,6] to be unstable. Further analysis is therefore necessary, at least to verify the stability of relations (8) and (9).

To simplify the analysis somewhat, we rewrite (9) in the form

$$Z(t)=\frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty}R(s)M(G,s)t^{-s}ds. \tag{10}$$

The universal function $R(s)$ is here in the numerator, and can be expressed with the aid of (3) and (4) in terms of the ratio of the integrals

$$R(s)=\frac{M(Z,s)}{M(G,s)}$$

$$=\int_{-\infty}^{+\infty}\frac{du\,u}{\mathrm{ch}^2 u}\int_0^\infty\frac{dv}{\mathrm{ch}^2 v}(u+v)^{1-s}\Big/2\int_0^\infty\frac{du\,u^2}{\mathrm{ch}^2 u}\int_0^\infty\frac{dv\,v^{-s}}{\mathrm{ch}^2 v}, \tag{11}$$

where $0<\mathrm{Re}\,s<1$. The integrals in the denominator can be expressed in terms of Riemann ζ functions. As for the double integral in the numerator, it can be calculated only approximately.

To estimate this integral we change to new variables, $x=u/v$ and $y=v$. Equation (11) then takes the form

$$R(s)=\int_{-\infty}^{+\infty}\int_0^{+\infty}\frac{dx\,dy\,x^2y^{3-s}}{\mathrm{ch}^2(xy)\,\mathrm{ch}^2 y}(1-s)$$

$$\times[Q(x)]^{-s}\left\{2\int_0^{+\infty}\frac{du\,u^2}{\mathrm{ch}^2 u}\int_0^{+\infty}\frac{dv\,v^{-s}}{\mathrm{ch}^2 v}\right\}^{-1},$$

$$Q(x)=\left[(1-s)\frac{x}{(1+x)^{1-s}-1}\right]^{1/s}. \tag{12}$$

Although the integration limits are infinite here, the presence of the hyperbolic cosines in the denominator and of x^2y^{3-s} in the numerator of (12) restrict effectively the integration to small regions bounded by the relations $|xy|\lesssim 1$, $y\lesssim 1$, $|x|\gtrsim y$, and $y\gtrsim 1$, inasmuch as $(0<\mathrm{Re}\,s<1$ in accord with (7). It follows from the indicated relations that the integral (12) builds up in small regions near the points with coordinates $(-1,1)$ and $(1,1)$, where the function $Q(x)$ varies slowly. The function $Q(x)$ within the effective integration region can therefore be replaced approximately by a constant and the universal function $R(s)$ takes the form

$$R(s)\approx(1-s)\left\{\int_0^\infty\frac{du\,u^2}{\mathrm{ch}^2 u}\int_0^\infty\frac{dv\,v^{-s}}{\mathrm{ch}^2 v}[Q(x_1)]^{-s}\right.$$

$$\left.+\int_0^\infty\frac{du\,u^2}{\mathrm{ch}^2 u}\int_0^\infty\frac{dv\,v^{-s}}{\mathrm{ch}^2 v}[Q(-x_2)]^{-s}\right\}$$

$$\times\left\{2\int_0^\infty\frac{du\,u^2}{\mathrm{ch}^2 u}\int_0^\infty\frac{dv\,v^{-s}}{\mathrm{ch}^2 v}\right\}^{-1}$$

$$=\tfrac{1}{2}(1-s)\{[Q(x_1)]^{-s}+[Q(-x_2)]^{-s}\}.$$

The function $R(s)$ depends thus on two constants, $Q(x_1)$ and $Q(-x_2)$, whose values are determined by obtaining the best fit of the exact value of the kernel $Z(t)$ to the approximate value of the integral (10).

As will be shown below, to find the approximate connection between the kernels $Z(x)$ and $G(x)$ we can assume that the values of the function $Q(x)$ at the points x_1 and $-x_2$ are identical, $Q(x_1)=Q(-x_2)=\Theta$, and the approximate expression for the universal function $R(s)$ takes the form

$$R(s)\approx(1-s)\Theta^{-s}. \tag{13}$$

Substituting the obtained value of $R(s)$ in (10) we have

$$Z(t)\approx\frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty}(1-s)M(G,s)(\Theta t)^{-s}ds. \tag{14}$$

The integral (14) is easy to evaluate and as a result, apart from an unknown scale factor Θ, we obtain the sought connection between the kernel $Z(x)$ and the kernel $G(x)$:

$$Z(x)\approx\frac{\partial}{\partial y}[yG(y)]|_{y=\Theta x}. \quad (15)$$

We estimate the scale factor from the asymptotic values of the kernels $Z(x)$ and $G(y)$ (Refs. 3 and 4):

$$Z(x)|_{x\ll 1}=1+\frac{12\pi^2}{5}x^2=1+\pi^2\Theta^2x^2=\frac{\partial}{\partial y}[yG]|_{y=\Theta x\ll 1},$$

from which it follows that $\Theta=(12/5)^{1/2}\approx 1.55\approx 1/0.65$. The high-temperature asymptotic values[3,5]

$$Z(x)|_{x\gg 1}=-\frac{0,152}{x^2}=-\frac{0,426}{x^2\Theta^2}=\frac{\partial}{\partial y}[yG]|_{y=\Theta x\gg 1}$$

yields $\Theta=(0.426/0.152)^{1/2}\approx 1.67$. It can be seen from these estimates that the scale factor, with good accuracy, equals $\Theta\approx 1.6\approx 1/0.6$. The kernel $Z(x)$ was compared with the derivative

$$\frac{\partial}{\partial y}[yG(y)]|_{y=\Theta x}$$

$$=4y\sum_{i=1}^{\infty}\left\{\frac{4(2i+1)}{[1+y(2i+1)^2]^3}-\frac{2i+1}{[1+y(2i+1)^2]^2}\right\}\Bigg|_{y=(\pi\Theta x)^2}$$

with computer for all x, at scale factors $\Theta=(12/5)^{1/2}\approx 1/0.65$ and $\Theta=1.67=1/0.6$. The calculation results are shown in Fig. 2, from which it follows that

$$Z(x)\approx\frac{\partial}{\partial y}[yG(y)]|_{y=x/0.6} \quad (16)$$

with an error less than 10% at the extremum points. This formula yields the sought connection between the kernels $Z(x)$ and $G(x)$.

It is easy to transform to the temperature dependences of $m^*(T)$ and $C_e(T)$. We put for this purpose $x=T/\omega$ and integrate both sides of (16) with respect to $d\omega g(\omega)/\omega$, as a result of which we get

$$\delta\gamma(T)=\frac{\gamma(T)-\gamma_0}{\gamma_0}\approx\frac{\partial}{\partial T'}[T'\delta m^*(T')]|_{T'=T/0.6}. \quad (17)$$

Using the definitions (1) and (2) of $\delta m^*(T)$ and $\delta\gamma(T)$ and the fact that $\gamma_0=m_0p_0/3$, we obtain the sought connection between the heat capacity $C_e(T)$ and the effective mass $m^*(T)$:

$$C_e(T)=\gamma(T)T, \quad (18)$$

where

$$\gamma(T)\approx\frac{\partial}{\partial T'}\left[\frac{m^*(T')p_0}{3}T'\right]\Bigg|_{T'=T/0.6}, \quad (19)$$

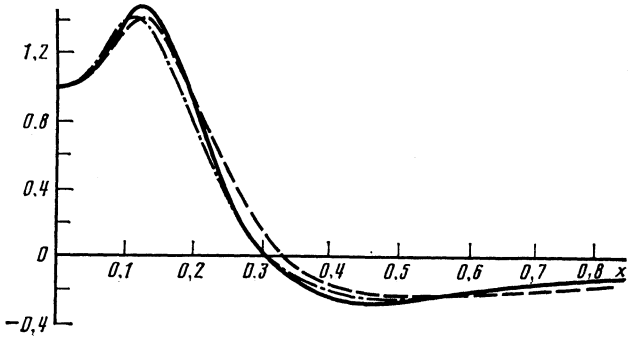

FIG. 2. A comparison of the kernel $Z(x)$ (solid curve) with the derivative $[yG(y)]'|_{y=\Theta x}$ at $\Theta=1/0.65$ (dashed curve) and $\Theta=1/0.6$ (dash-dot) points to validity of the approximate relation (19).

or

$$\gamma(T)\approx\frac{m^*(T')p_0}{3}\left[1+\frac{\partial\ln m^*(T')}{\partial\ln T'}\right]\Bigg|_{T'=T/0,6}. \quad (20)$$

As seen from the obtained relations, the connection (18)–(20) between the effective mass and the heat capacity, being linear and nonlocal, is independent of the phonon spectrum $g(\omega)=\alpha^2(\omega)F(\omega)$ even though it is caused by the electron-phonon interaction.

The region of applicability of the obtained relation is obviously limited to temperatures at which the concept of the effective mass of an electronic quasistatic excitation has meaning. On the other hand, relations (1)–(4) are valid only in the approximation where the Fermi surface is spherical, and relations (18)–(20) are therefore valid only within the framework of this approximation.

The simple differential connection obtained here between the heat capacity of the electrons and their effective mass makes it possible to determine experimentally the effective mass from measurements of the heat capacity at $T\lesssim\omega_D$, and to obtain at low temperatures $T\ll\omega_D$ the heat capacity of the electrons from effective-mass measurements. This indirect determination of the effective mass and of the heat capacity of the electrons is valuable because the accuracy of direct measurements of $m^*(T)$ at $T\lesssim\omega_D$ and of $C_e(T)$ at $T\ll\omega_D$ is low at present.

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[1]G. Grimvall, J. Phys. Chem. Sol. **29**, 1221 (1968).
[2]G. M. Éliashberg, Zh. Eksp. Teor. Fiz. **43**, 1105 (1962) [Sov. Phys. JETP **16**, 780 (1963)]
[3]G. O. Zaitsev and V. Z. Kresin, *ibid.* **74**, 1886 (1978) [**47**, 983 (1978)].
[4]N. F. Masharov, Fiz. Tverd. Tela (Leningrad) **16**, 3306 (1974) [Sov. Phys. Solid State **16**, 2147 (1974)].
[5]N. F. Masharov, *ibid.* **18**, 295 (1976) [**18**, 174 (1976)].
[6]I. M. Lifshitz, Zh. Eksp. Teor. Fiz. **26**, 551 (1954).

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