Renormalized Thermal Distribution Function in an Interacting Electron-Phonon System

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The electron-phonon interaction is used to demonstrate the important effect of interactions on the electronic distribution function at finite temperature. It is shown that the usual picture of "thermal (Fermi) smearing" is a greatly oversimplified one. The distribution function resulting from an Einstein spectrum with various coupling strengths is presented and interpreted, and an exact expression for the spin susceptibility is used to illustrate the utility of this novel viewpoint for thermodynamics.

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One of the primary characteristics of a metal at a finite temperature T is that the crystalline electronic eigenstates (labeled by index k) of energy E_k are occupied according to a thermal distribution $f(E_k)$. Almost universally in the theory of metals this distribution is taken to be that of *noninteracting* fermions, i.e., the Fermi-Dirac distribution $f_0(E_k)$. Typically this assumption appears as a thermal broadening ("Fermi smearing"), given by $-df_0(E)/dE$, of some quantity over a region around the Fermi energy E_F. The effect of interactions, if included at all, is not introduced into the occupation function. For systems where the density of states (DOS) function $N(E)$ varies sufficiently slowly near E_F thermal averaging is expected to be insensitive to the actual form of f. For varying DOS systems, however, of which the $A15$ class of compounds provides the canonical example,[1] the understanding of their anomalous thermal behavior may depend critically on the proper description of f and df/dE.

Two questions arise: What is the effect of interactions on the thermal distribution f, and is our understanding of thermodynamic properties clarified by a viewpoint which includes interactions in f? In this paper we use the example of the electron-phonon (EP) interaction to show that f, and thereby the interpretation of thermodynamic quantities, can be radically altered by interactions.

The distribution function $f(E_k)$ is defined as the thermal expectation of the number operator $\hat{n}_k$. For $T>0$, f is given in general in terms of the thermodynamic Green's function G by the relation[2]

$$f(E_k)=T\sum_{n=-\infty}^{\infty} G(k,i\omega_n)\exp i\omega_n\eta, \tag{1}$$

where $\omega_n=(2n+1)\pi T$ and η is a positive infinitesimal. (In our units $\hbar=k_B=1$, and for simplicity an isotropic approximation for electrons will be used.) It is easily verified that (i) in the absence of interactions, $f\to f_0$, and (ii) by converting the sum to a contour integral f can be written

$$f(E_k)=\int_{-\infty}^{\infty} d\omega f_0(\omega)A(k,\omega) \tag{2}$$

in terms of the spectral density A. Evidently $f=f_0$ *if and only* if A is a δ function at $\omega=E_k$. When A is broadened by interactions, f can differ considerably from f_0 (a result not often stated in quantum statistical theory texts), as I now explicitly demonstrate.

For simplicity let us initially consider a constant-DOS electronic system interacting with an Einstein phonon spectrum with EP spectral function α^2F given by

$$\alpha^2F(\omega)=(\lambda\Omega/2)\delta(\omega-\Omega), \tag{3}$$

where Ω is the Einstein frequency and λ is the EP coupling constant. A straightforward calculation of the electronic self-energy $\Sigma=M-i\Gamma$ on the real axis gives, with energies measured relative to E_F,

$$M(\omega)=-(\lambda\Omega/2)\mathrm{Re}\left\{\psi\left(\frac{1}{2}+\frac{\omega+\Omega}{2\pi i T}\right)+\psi\left(\frac{1}{2}+\frac{\omega-\Omega}{2\pi i T}\right)\right\}, \tag{4}$$

$$\Gamma(\omega)=(\pi\lambda\Omega/2)\{f_0(\Omega-\omega)+f_0(\Omega+\omega)+2n_0(\Omega)\}\,\mathrm{sgn}(\omega). \tag{5}$$

Here ψ and n_0 denote the digamma and Bose-Einstein functions, respectively. The spectral density is given simply by (ζ = chemical potential)

$$A(k,\omega)=\frac{1}{\pi}\left|\mathrm{Im}\,\frac{1}{\omega-(E_k-\zeta)-\Sigma(\omega)}\right|. \qquad (6)$$

In Fig. 1 I display $M(\omega)$ and $\Gamma(\omega)$ for several values of T. Spectral functions at $T=0$ have been studied previously by Engelsberg and Schrieffer[3] and by Shimojima and Ichimura,[4] who find that, even for $|E_k - E_F| \lesssim \Omega$, spectral weight is spread over a region of *several times* Ω around E_F. At $T>0$ this spread is further increased because of the increasing width $\Gamma(\omega)$ (Fig. 1). Neither of the previous studies have noted the affect of EP interactions on the distribution function.

The change in f due to EP interaction is represented most easily in unitless differential form $-T\,df/dE \equiv -f'$. The results, for several values of T and λ, are presented in Fig. 2 for $E>\zeta\equiv 0$. [Note that $f'(E)=f'(-E)$.] At $T=\Omega$ Fig. 2(a) indicates that increasing λ leads to the displacement of weight in $-f'(E)$ (i.e., occupation of bare electron and hole states) from the region $|E-\zeta| \lesssim 2\Omega$ to the higher excitation energy tails. At $T=\Omega/2$ [Fig. 2(b)] the behavior is similar. However, as the frequency dependence of Σ becomes sharper at $T \ll \Omega$ (Fig. 1), qualitatively new behavior—negative weighting near ζ—can occur at low energy, as shown in Fig. 2(c) for $T=\Omega/4$. This unusual behavior is exaggerated by the Einstein spectrum used here, although similar behavior may occur even for a realistic spectrum at lower temperatures. General features of $-f'$ include these: (a) at high energy $|E-\zeta| \gg \Omega$ it decreases as a Lorentzian of width $\Gamma \approx (\pi\lambda\Omega/2)[1+2n_0(\Omega)]$ rather than exponentially as does $-f_0'$, (b) at high $T \gtrsim \Omega$, $-f'$ is essentially Lorentzian [$\Gamma \approx \pi\lambda\Omega n_0(\Omega)$] everywhere, and (c) the behavior at $T=0$ is as given previously by Shimojima and Ichimura[4]: f possesses a discontinuity of $(1+\lambda)^{-1}$ at ζ, which indicates that the Fermi surface remains sharp, and $-f'$ has a δ-function contribution of corresponding amplitude, with the remaining weight $\lambda/(1+\lambda)$ displaced over the range

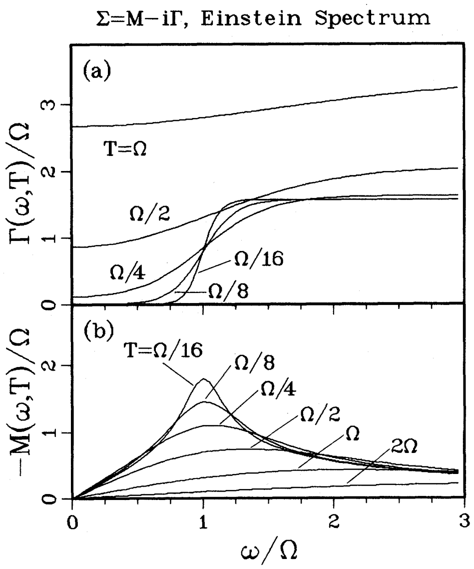

FIG. 1. Electron self-energy $\Sigma(\omega)=M(\omega)-i\Gamma(\omega)$ for an Einstein spectrum at energy Ω, for several temperatures T. The self-energies are proportional to λ and are shown for $\lambda=1$.

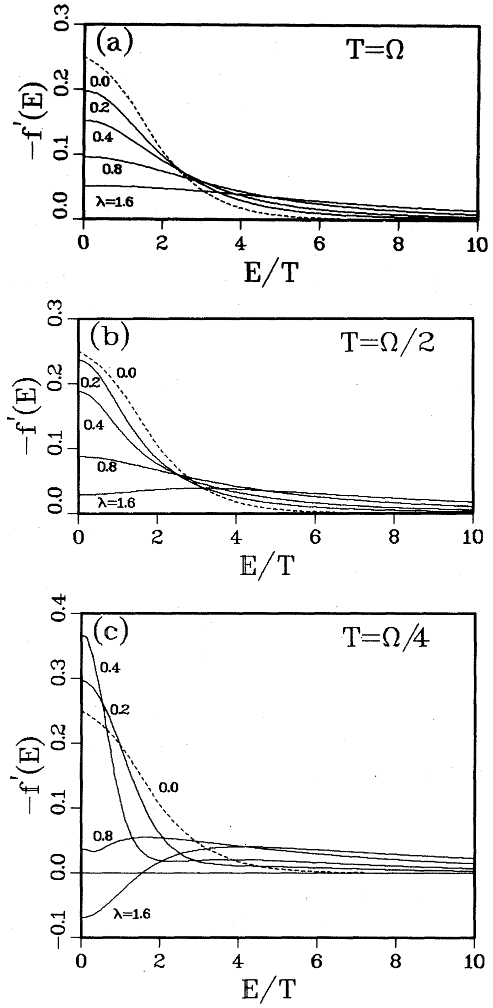

FIG. 2. The derivative $-f'(E)=-T\,df(E)/dE$ of the thermal distribution function f calculated from Eqs. (2) and (6) and the self-energies of Fig. 1, for several values of λ. The dashed line shows $-f'(=-f_0')$ in the absence of electron-phonon interaction ($\lambda=0$). Note that interactions broaden the thermal distribution considerably even for modest values of λ at all temperatures.

$|E-E_F| \sim \lambda\Omega$.

For systems in which the electronic spectrum varies on the scale of Ω, Σ becomes a functional[5] of $N(E)$ and the computation of f becomes correspondingly more involved. However, because of the substantial widths in the spectral density peaks for finite ω and/or T, the qualitative behavior of $-f'$ will generally reflect that of the constant-DOS model. The proper interpretation of thermodynamic properties, however, can be substantially altered in nonconstant-DOS systems, as will now be shown.

The case of the spin susceptibility χ_{sp} will be used to demonstrate that the renormalized thermal smearing function $-f'$, rather than $-f_0'$, often arises naturally in the formalism. That this should be the case is suggested by the relationship [Eq. (1)] between f and the (renormalized) Green's function G on the one hand, and the expansion of the thermodynamic potential, which is accomplished most concisely[6] in terms of G (rather than G_0), on the other. The conservation of electron number N_{el}, for example, is given naturally as the thermal redistribution of crystalline states:

$$N_{el} = 2\int dE\, f(E-\zeta)N(E), \tag{7}$$

although it can also be written

$$N_{el} = 2\int d\omega\, f_0(\omega-\zeta)\mathfrak{N}(\omega) \tag{7$'$}$$

in terms of a noninteracting electron distribution over a *broadened and renormalized* DOS[7] $\mathfrak{N}$ given by

$$\mathfrak{N}(\omega+\zeta) = \int dE\, N(E)A(E-\zeta,\omega). \tag{8}$$

This is simply a question of whether the ω or E integral is carried out first. However, from the magnetization $\mathfrak{M}$, given by[8]

$$\mathfrak{M} = \mu_B \sum_{\sigma=\pm} \sigma N_\sigma = \mu_B \sum_{\sigma=\pm} \sigma \int dE\, N(E) T \sum_n G_\sigma(E, i\omega_n) \exp i\omega_n \eta, \tag{9}$$

in terms of the number N_σ of spin σ electrons, χ_{sp} can be written *exactly* (within this isotropic treatment) as

$$\begin{aligned}\chi_{sp} = \frac{d\mathfrak{M}}{dH}\bigg|_{H=0} &= -\mu_B \sum_{\sigma=\pm} \sigma \int dE\, N(E) T \sum_n G_\sigma^2(E, i\omega_n) \frac{dG_\sigma^{-1}(E, i\omega_n)}{dH} \exp i\omega_n\eta \bigg|_{H=0} \\ &= 2\mu_B^2 \int dE\, N(E)\left[-\frac{df(E-\zeta)}{dE}\right][1+K(E,T)],\end{aligned} \tag{10}$$

where $-df/dE$ is identified by differentiating Eq. (1) with $G_\sigma^{-1}(E, i\omega_n) = i\omega_n - (E-\zeta-\sigma\mu_B H) - \Sigma_\sigma(i\omega_n)$, and the thermal average K of the field derivative of the self-energy is defined by

$$K(E,T) = -T\sum_n G^2(E, i\omega_n) \frac{d\Sigma_\sigma(i\omega_n)}{d(\sigma\mu_B H)}\bigg|_{H=0} \left[T\sum_n G^2(E, i\omega_n)\right]^{-1}. \tag{11}$$

Equation (10) gives an interpretation of χ_{sp} as arising from the bare DOS, appropriately enhanced by $1+K$ and averaged around ζ according to the *interacting* thermal smearing function. Equation (10) gives directly an enhancement due to the EP interaction of the T dependence of χ_{sp} arising from a peak in $N(E)$, as surmised by Bhatt[9] for low temperature.

Essentially all other interpretations of $\chi_{sp}(T)$ have assumed a form like Eq. (10) with $f \to f_0$. By means of the standard analytic continuation[2] to express the frequency sum in Eq. (9) in terms of an integral over real frequencies, χ_{sp} can be written *in terms of* f_0 as two contributions $\chi_{sp}^{(0)} + \chi_{sp}^{(1)}$:

$$\chi_{sp}^{(0)} = 2\mu_B^2 \int d\omega \left(-\frac{\partial f_0}{\partial\omega}\right)\mathfrak{N}(\omega+\zeta), \tag{10$'$}$$

which is *reminiscent of but not identical* to the first (unenhanced) term in Eq. (10), and the "enhancement"

$$\chi_{sp}^{(1)} = -\frac{2\mu_B^2}{\pi} \operatorname{Im}\int_{-\infty}^{\infty} d\omega \int dE\, N(E) G^R(E,\omega) \frac{\partial}{\partial\omega}\left\{f_0(\omega)\frac{\Sigma_H' - \Sigma_\omega'}{1-\Sigma_\omega'}\right\}, \tag{10$''$}$$

where $\Sigma_H' = d\Sigma_\sigma^R/d(\sigma\mu_B H)|_{H=0}$ and $\Sigma_\omega' = \partial\Sigma^R/\partial\omega$ (superscript R denotes retarded functions).

The simplicity of Eq. (10), and a general knowledge of the behavior of $-\partial f/\partial E$ from Fig. 2, allows one to identify the underlying causes of thermal anomalies in exotic systems. In V_3X compounds, for example, the strong T dependence of χ correlates closely[10] with high superconducting T_c, and thus with large λ, exactly as Eq. (10), with a peak in $N(E)$ near ζ and broadening proportional to λ, suggests. It is also evident that the incluence of the lattice should lead to an isotope effect on the critical temperature for itinerant-electron magnetism distinct from that proposed by Hopfield.[11] Neither of these properties is evident in the form given in Eqs. (10′) and (10″).

In terms of the two questions posed at the outset, (1) the behavior of f is qualitatively as shown in Fig. 2 and is of itself useful and perhaps necessary in interpreting thermodynamic behavior, and (2) f has been shown to arise simply and naturally in the expression for χ_{sp}. In general, each thermodynamic quantity must be investigated individually for a useful expression involving f and/or f_0. It is encouraging that Lee and Yang[12] have shown that thermodynamics can be formulated *exactly* in terms of f, although the author is unaware of any application of their very formal approach to metals.

A contrast can be drawn between the present viewpoint and that of Fermi-liquid theory.[7] The latter approach describes the *low-temperature* thermodynamic properties in terms of *noninteracting* quasiparticles described by f_0 and a *renormalized* quasiparticle density of states $\mathfrak{N}$. Typically $\mathfrak{N}$ is a constant for excitations of interest, and this approach has been very successful for *phenomenological* descriptions. It is proposed here that viewing the interactions as distributing the excitations over the noninteracting spectrum will prove a more useful approach when variation of $N(E)$ is important. This formulation provides a *conceptual* basis as well as a *computational* approach for the detailed understanding of many classes of interesting compounds.

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