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Thermoelectric power of high-T_c superconductors: superconducting fluctuations and the marginal Fermi-liquid hypothesis

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Abstract. Some common trends observed in the temperature variation of the thermoelectric power (TEP) of high-T_c materials are theoretically analysed. In the first part of the analysis, we calculate the dominant effect of superconducting fluctuations on TEP, assuming that the conduction process occurs in two dimensions. In the second part of the analysis, we show that, by including the self-energy proposed in the marginal Fermi-liquid hypothesis along with that arising from superconducting fluctuations, one can understand the main features of the temperature variation of TEP. The magnitude of TEP given by the formula derived here is also of the right order.

1. Introduction

In common with other transport properties, the thermoelectric power (TEP) of high-T_c materials exhibits a very interesting behaviour [1–12], whose fascination lies in the fact that it is very different from that of ordinary metals. A large number of high-T_c materials have been investigated, and, though there are differences of behaviour between different families of materials, some common trends can be discerned, which we summarize as follows. (i) For a number of materials, the TEP has a positive sign, but at the same time it decreases with increasing temperature. This is quite contrary to Mott's formula, according to which the sign and slope of the thermopower should be the same. A similar anomaly is seen in some materials with negative TEP. (ii) Related to the above observation is the point that the linear extrapolation of the high-temperature thermopower shows a large zero-temperature intercept, which is again contrary to the expectation that TEP should tend to zero as the temperature tends to zero (in the absence of intervention of the superconducting transition). (iii) The TEP vanishes continuously as the transition temperature T_c is approached and moreover shows a rather broad peak a little above T_c. A schematic variation of TEP with temperature can be seen in figure 3.

In an earlier paper [12], we have addressed the points (i) and (ii) by calculating the thermoelectric power using the hypothesis of marginal Fermi-liquid theory. The formula obtained there provides a fair account of the behaviour in the temperature range from a few degrees above T_c to about room temperature, with reasonable parameter values. The purpose of this paper is to address point (iii) above and to derive a comprehensive formula that will enable us to understand all the above-mentioned features. The important point to which we wish to draw attention is that the drop of thermopower to zero value at T_c invariably occurs over a finite temperature range, and this implies that the process driving TEP to zero value sets in somewhat above T_c. This process in all likelihood involves the

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precursor superconducting fluctuations, whose importance in these systems can be argued for in other ways as mentioned later in the paper. Thus we believe that the observed broad peak simply results because the superconducting fluctuations above T_c cause a turn-around in the rising (falling) trend in the hole (electron) superconducting temperature somewhat above T_c. While at this stage it is perhaps too ambitious to present a single theoretical scheme that explains TEP in the entire temperature range, we calculate the dominant effects of pairing fluctuations on TEP for a simple metal, and then include the normal-state anomalous behaviour by incorporating the self-energy proposed in the marginal Fermi-liquid hypothesis [13]. In view of the fact that knowledge of high-T_c materials is not yet sufficient to be able to assert a minimal microscopic model, the scope of our considerations is somewhat limited. We have tried to examine the consequences of the above-mentioned physical ideas in the simplest possible theoretical scheme and then to compare such results with the experimental results to extract certain parameters of theoretical interest. We hope that the consistency checks on these parameters will provide clues as to the key elements of the correct model.

One other possible explanation of the precursor peak that has been often mentioned in the literature is that it is due to a phonon-drag effect. In simple metals, similar broad peaks are known to occur around a temperature $T_D/5$, where T_D is the Debye temperature. A typical value of T_D for compounds of the family $YBa_2Cu_3O_7$ is 500 K, so the observed peak is in the right range. However, there is experimental evidence that discounts this explanation. Radhakrishnan *et al* [14] report TEP measurements on a series of compounds $YBa_2(Cu_{1-y}Zn_y)_3O_{7-x}$. By zinc substitution for copper, T_c varies from 90 to 50 K, while T_D is not expected to alter much, yet the TEP peak is still found to occur close to T_c.

The superconducting fluctuations are clearly important for high-T_c materials for the following two reasons: (i) the conduction process is two dimensional, and (ii) the coherence length of these superconductors is quite small. The theory for the effect of superconducting fluctuations has been studied for a long time, starting with the pioneering calculations of Aslamosov and Larkin [15]. In principle, one should generalize these calculations for the appropriate Kubo formulae for thermopower. However, such a fully fledged calculation is very complicated. So, in this paper we content ourselves with a microscopic calculation, which we believe incorporates the most significant effect of superconducting fluctuations on TEP, which drives it to zero value continuously as $T \to T_c$. This effect is essentially a one-particle effect arising due to velocity and density-of-states renormalization by superconducting fluctuations. Through in our later discussion we employ the Kubo formula, the main physical point can be easily discussed by considering the Mott formula, which is

$$S = \frac{\pi^2 k_B^2 T}{3e\epsilon_F}\left(\frac{\partial \ln \sigma(\epsilon)}{\partial \ln \epsilon}\right)_{\epsilon=\epsilon_F} \tag{1.1}$$

where $\sigma(\epsilon)$ is the conductivity regarded as a function of Fermi energy and the derivative is taken at the Fermi energy ϵ_F. Further, for simple metals

$$\sigma(\epsilon) = (e^2/3\hbar)\rho(\epsilon)v^2(\epsilon)\tau(\epsilon) \tag{1.2}$$

where $\rho(\epsilon)$, $v(\epsilon)$ and $\tau(\epsilon)$ denote single-particle density of states, velocity and mean collision time, respectively. In the normal state $\rho(\epsilon) \propto \epsilon^{1/2}$, while in the superconducting state $\rho(\epsilon)$ is zero within a gap around ϵ_F. So, clearly, as the transition temperature is approached from above, the superconducting fluctuations are expected to make $\rho(\epsilon)$ and $v(\epsilon)$ strong functions of temperature. The effect of this renormalization exhibits itself through the energy derivative in equation (1.1). As first noted by Opsal *et al* [16], the effect of velocity renormalization shows up in thermopower, in contrast with conductivity, where it gets cancelled out.

Our theory is based on incorporation of superconducting fluctuations in the single-particle propagator $G(p, \epsilon)$ for the quasiparticles of the system. For our purpose, the actual mechanism that gives rise to pairing fluctuations is not very important, as the result obtained depends upon the anomalous (order-parameter) susceptibility, whose form (apart from the values of the parameters) is quite general. So, while we do the explicit calculation in the simple interaction model of Bardeen, Cooper and Schrieffer (BCS), we believe that the results obtained are of wider generality in the sense that, instead of obtaining the parameters contained in the final formula from the model, one can obtain them directly from the experimentally measurable quantities.

The remainder of the paper is organized as follows. In section 2, we describe the basic scheme of the calculation of thermopower in terms of Kubo formulae and give the main approximation used in the calculation. Section 3 describes our scheme for incorporating superconducting fluctuations in the transport coefficients. Here we essentially calculate the single-particle self-energy, which is then used in the formula of section 2 to obtain the thermopower. The vertex corrections are omitted completely. Finally, in section 4, we describe a way of incorporating the normal-state correlations by employing the marginal Fermi-liquid hypothesis. The paper is concluded in section 5 with some remarks summarizing the results and indications for future work.

2. Theoretical formalism

In this section our goal is to obtain a formula for TEP that is suitable for the purpose of this analysis. The analysis presented involves several approximations, as the idea is to obtain what we regard as the main and general features of the TEP behaviour. The diffusion component of thermopower, S_d, with which we are concerned here can be expressed as a ratio of two coefficients obtained from Kubo-type correlators as follows [17]:

$$S_d = -(1/T)(L_{11}/L_{12}) \tag{2.1}$$

where L_{11} and L_{12} are obtained from the current–current correlators of the form

$$L_{11}(z_n) = \frac{1}{\beta z_n d\Omega} \int_0^\beta \mathrm{d}\tau \, \exp(z_n\tau)\langle T(J_e(\tau) \cdot J_e(0))\rangle \tag{2.2}$$

$$L_{12}(z_n) = \frac{1}{\beta z_n d\Omega} \int_0^\beta \mathrm{d}\tau \, \exp(z_n\tau)\langle T(J_Q(\tau) \cdot J_e(0))\rangle \tag{2.3}$$

where z_n denotes the Matsubara frequency $\mathrm{i}\pi(2n+1)/\beta$, d the dimensionality, Ω the volume and J_e and J_Q denote respectively the electric current and the heat current operators. The coefficients L_{11} and L_{12} are obtained by the following limiting procedure [17]:

$$L = \lim_{\omega \to 0} L(z_n \to \omega + \mathrm{i}\delta). \tag{2.4}$$

The electric current operator in terms of creation and annihilation operators $c_{ks}^\dagger$ and c_{ks} is given by

$$J_e = e \sum_{k,s} \frac{\hbar k}{m^*} c_{ks}^\dagger c_{ks} \tag{2.5}$$

where m^* stands for the effective mass of the carrier, k for its wavevector and s for its spin. For the heat current current operator J_Q we use the truncated form

$$J_Q = e \sum_{k,s} \frac{\hbar k}{m^*} \xi_k c_{ks}^\dagger c_{ks} \tag{2.6}$$

where $\xi_k = \hbar^2 k^2/2m^* - \epsilon_F$. There are other contributions to J_Q [17, 18], but we do not include them, as expression (2.6) seems adequate for the qualitative effects being considered here. Substituting equations (2.2) and (2.3) and following the known procedure [17], one arrives at the expressions for L_{11} and L_{12} given below:

$$L_{11} = \frac{2\hbar^2 e^2}{dm^{*2}} \frac{1}{\Omega} \sum_k k^2 \int \frac{d\epsilon}{2\pi} \left(-\frac{d f_0(\epsilon)}{d\epsilon}\right) G_r(k,\epsilon) G_a(k,\epsilon) \gamma(k, \epsilon - i\delta, \epsilon + i\delta) \tag{2.7}$$

$$L_{12} = \frac{2\hbar^2 e^2}{dm^{*2}} \frac{1}{\Omega} \sum_k \xi_k k^2 \int \frac{d\epsilon}{2\pi} \left(-\frac{d f_0(\epsilon)}{d\epsilon}\right) G_r(k,\epsilon) G_a(k,\epsilon) \gamma(k, \epsilon - i\delta, \epsilon + i\delta). \tag{2.8}$$

Here $f_0(\epsilon)$ is the Fermi function, γ is related to the vertex function, d is the dimensionality of the system, and G_r and G_a are respectively the retarded and advanced single-particle propagators, which can be written as

$$G_{r(a)} = [\epsilon - \xi_k - \Sigma(k, \epsilon \pm i\delta)]^{-1} \tag{2.9}$$

where the + (−) sign goes with r (a). Further, we will write Σ in terms of its real and imaginary parts,

$$\Sigma(k, \epsilon \pm i\delta) = \Sigma_R(k,\epsilon) \mp i\Gamma(k,\epsilon). \tag{2.10}$$

For evaluation of equations (2.7) and (2.8), we shall employ the following drastic approximations. First, we neglect the vertex corrections by setting $\gamma(k, \epsilon - i\delta, \epsilon + i\delta)$ to be unity. Secondly, we replace $\Gamma(k,\epsilon)$ by a constant value $\Gamma(k_F, 0)$. Finally, we assume that the k dependence of Σ comes only through ξ_k, as will be shown in later sections. The neglect of vertex corrections is not justified in most situations. For example, in the calculation of impurity resistance it replaces the single-particle relaxation time by transport relaxation time. Furthermore, as shown by Aslamosov and Larkin [15], the vertex corrections play a key role in calculating conductivity fluctuations. However, for TEP we find that the leading effect already emerges from the single-particle self-energy, and since relaxation time cancels out of the TEP formula, its corrections are not as significant. The neglect of the energy dependence of $\Gamma(k,\epsilon)$ is not correct in general, but is justified from the explicit expression in this case. With these approximations, equations (2.7) and (2.8) can be written as

$$L_{11} = \frac{2\hbar^2 e^2}{2m^{*2}\Gamma} \int \mathrm{d}\xi_k\, \rho_d(\xi_k) k^2 \int \frac{\mathrm{d}\epsilon}{2\pi} \left(-\frac{\mathrm{d}f_0}{\mathrm{d}\epsilon}\right) \frac{\Gamma}{[\epsilon - \xi_k - \Sigma_{\mathrm{R}}(\xi_k, \epsilon)]^2 + \Gamma^2} \tag{2.11}$$

$$L_{12} = \frac{2\hbar^2 e^2}{2m^{*2}\Gamma} \int \mathrm{d}\xi_k\, \rho_d(\xi_k) k^2 \xi_k \int \frac{\mathrm{d}\epsilon}{2\pi} \left(-\frac{\mathrm{d}f_0}{\mathrm{d}\epsilon}\right) \frac{\Gamma}{[\epsilon - \xi_k - \Sigma_{\mathrm{R}}(\xi_k, \epsilon)]^2 + \Gamma^2} \tag{2.12}$$

where $\rho_d(\xi_k)$ is the density of states in d dimensions. Further evaluation of these expressions is done by working to leading order in $\Gamma(\xi_k, 0)$, which enables us to replace the Lorentzian by δ-functions. This yields

$$\begin{aligned} L_{11} &= \frac{2\hbar^2 e^2}{dm^{*2}} \int \mathrm{d}\xi_k \frac{\rho_d(\xi_k) k^2}{\Gamma(\xi_k)} \int \mathrm{d}e \left(-\frac{\partial f_0}{\partial e}\right) \delta(e - \xi_k - \Sigma_k(\xi_k, e)) \\ &= \frac{\hbar^2 e^2}{dm^{*2}} \int \mathrm{d}\xi_k \frac{\rho_d(\xi_k) k^2}{\Gamma(\xi_k)} \left(-\frac{\partial f_0}{\mathrm{d}E_k}\right) \frac{1}{1 - \Sigma'_{\mathrm{R2}}(\xi_k, 0)} \end{aligned} \tag{2.13}$$

where

$$\Sigma'_{\mathrm{R2}}(\xi_k, E_k) = \partial \Sigma_{\mathrm{R}}(\xi_k, E_k)/\partial E_k \tag{2.14}$$

and

$$E_k = \xi_k + \Sigma_{\mathrm{R}}(\xi_k, E_k). \tag{2.15}$$

Similarly

$$L_{12} = \frac{\hbar^2 e^2}{dm^{*2}} \int \mathrm{d}\xi_k \frac{\rho_d(\xi_k) k^2 \xi_k}{\Gamma(\xi_k)} \left(-\frac{\partial f_0}{\partial E_k}\right) \frac{1}{1 - \Sigma'_{\mathrm{R2}}(\xi_k, 0)}. \tag{2.16}$$

Equations (2.13) and (2.16) are now evaluated in the degeneracy limit by resorting to Sommerfeld expansion. For conductivity, i.e. L_{11}, one obtains a contribution to the leading order, i.e.

$$L_{11} = \frac{\hbar^2 e^2}{dm^{*2}} \frac{\rho_d(0) k_{\mathrm{F}}^2}{\Gamma} \frac{1}{1 - \Sigma'_{\mathrm{R2}}(0, 0)} \left(\frac{\partial \xi_k}{\partial E_k}\right)_0. \tag{2.17}$$

From equation (2.15)

$$\partial E_k / \partial \xi_k = [1 + \Sigma'_{\mathrm{R1}}(\xi_k, E_k)]/[1 - \Sigma'_{\mathrm{R2}}(\xi_k, E_k)] \tag{2.18}$$

where

$$\Sigma'_{\mathrm{R1}}(\xi_k, E_k) = \partial \Sigma_{\mathrm{R}}(\xi_k, E_k)/\partial \xi_k. \tag{2.19}$$

Substituting equation (2.18) into equation (2.17), one finds

$$L_{11} = \frac{ne^2}{m^*\Gamma} \frac{1}{1+\Sigma'_{R1}(0,0)}. \tag{2.20}$$

As is well known, in the evaluation of L_{12} one gets a zero contribution from the leading order of the Sommerfeld expansion. Thus expanding $\rho_d k^2$ about the Fermi energy, we derive the following expression for the parabolic energy band:

$$\begin{aligned} L_{12} &= \frac{2e}{dm^*} \int \mathrm{d}E_k \left(-\frac{\partial f_0}{\partial E_k}\right) \xi_k \rho_d(0) \epsilon_F \left(1 + \frac{d}{2\epsilon_F}\xi_k\right) \frac{\mathrm{d}\xi_k/\mathrm{d}E_k}{1-\Sigma'_{R2}(\xi_k - 0)} \\ &= \frac{ne}{m^*T} \frac{\pi^2 k_B^2 T^2}{3\epsilon_F} \frac{1}{1+\Sigma'_{R1}(0,0)} \left(\frac{\partial \xi_k}{\partial E_k}\right)_0^2. \end{aligned} \tag{2.21}$$

From equations (2.20), (2.21) and (2.18), we finally arrive at the following expression for S_d:

$$S_d = \frac{\pi^2 k_B}{3e} \left(\frac{k_B T}{\epsilon_F}\right) \left(\frac{1-\Sigma'_{R2}(0,0)}{1+\Sigma'_{R1}(0,0)}\right)^2. \tag{2.22}$$

This expression will be used in the following sections.

3. Superconducting fluctuations

In this section we evaluate the contribution to single-particle self-energy arising due to superconducting fluctuations. We perform the calculation in the simple interaction model of BCS (see e.g. [19]). But we believe that the results have a wider validity, as what is basically involved is the order parameter or anomalous susceptibility of the normal state, and this susceptibility has a general form in which only certain parameters have model-dependent values. We consider a model in which quasiparticles with energy–momentum (ξ_k, $\boldsymbol{k}$) (where ξ_k is measured with respect to Fermi energy ϵ_F) interact attractively with a strength λ within the energy range $|\xi_k| \leqslant \hbar\omega_D$. We further assume that the quasiparticles also suffer elastic scattering from impurities, which leads to a lifetime τ for the particles at the Fermi surface. The simplest way to include the effect of virtual pairing is to consider the set of diagrams for self-energy shown in figure 1. This set of diagrams incorporates the instability of the normal state to pairing as it occurs in the vertex function of the particle–particle channel. These can also be thought of in terms of the random-phase approximation for the anomalous susceptibility whose divergence signals the onset of superconductivity.

The self-energy corresponding to these diagrams is given by

$$\Sigma(\boldsymbol{p}, z_n) = \frac{1}{\beta\Omega} \sum_{\boldsymbol{K},z} t(z, \boldsymbol{K}, \boldsymbol{K}/2-\boldsymbol{p}, \boldsymbol{K}/2-\boldsymbol{p}) g(\boldsymbol{K}-\boldsymbol{p}, z-z_n) \tag{3.1}$$

where $g(\boldsymbol{q}, z)$ denotes the unperturbed single-particle propagator (including impurity scattering) given by

$$g(\boldsymbol{q}, z) = [z - \xi_q + \mathrm{i}\tau_q^{-1}(\operatorname{sgn}\xi_q)]^{-1} \tag{3.2}$$

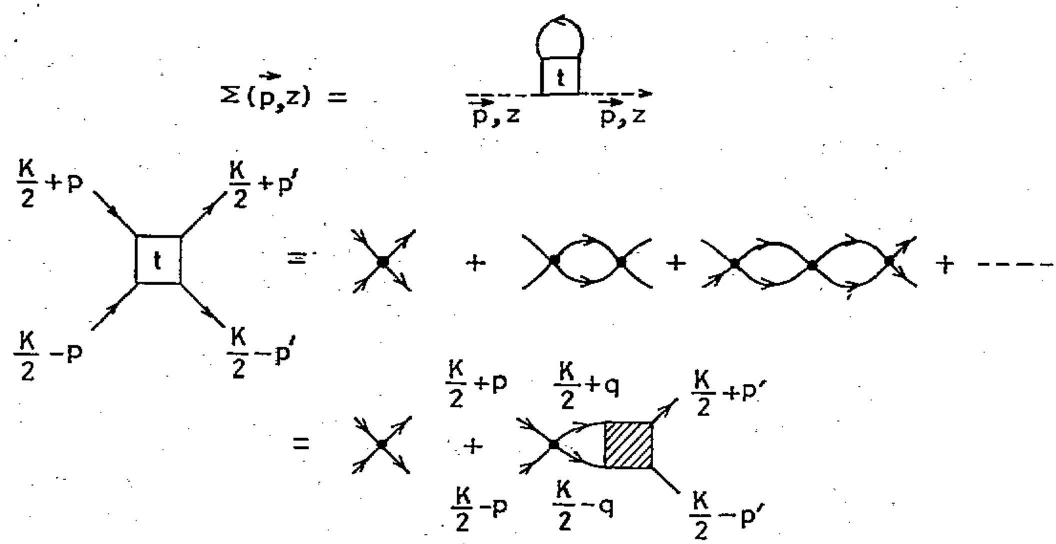

Figure 1. The diagrammatic series for $\Sigma(\boldsymbol{p}, z)$ and the representation for the integral equations for $t(\boldsymbol{K}, z)$. In the figure K stands for $(\boldsymbol{K}, z)$.

where τ_q is the lifetime of the state due to scattering from impurities and t denotes the ladder sum of repeated particle–particle scattering shown in figure 1. For the present case, the t-matrix equation and its solution are given as [19]

$$t(z, \boldsymbol{K}, \boldsymbol{p}, \boldsymbol{p}) = \lambda - \frac{\lambda}{\beta\Omega}\sum_{\boldsymbol{p}'', z''} g(\boldsymbol{K}/2 - \boldsymbol{p}'', z - z'') g(\boldsymbol{K}/2 + \boldsymbol{p}'', z'') t(z, \boldsymbol{K}, \boldsymbol{p}'', \boldsymbol{p}')$$
$$= \lambda/[1 + \lambda\chi_a(\boldsymbol{K}, z)] \tag{3.3}$$

where

$$\chi_a(\boldsymbol{K}, z) = \frac{1}{2\beta\Omega}\sum_{\boldsymbol{p}'', z''} g(\boldsymbol{K}/2 - \boldsymbol{p}'', z - z'') g(\boldsymbol{K}/2 + \boldsymbol{p}'', z'')$$
$$= \frac{1}{\Omega}\sum_{\boldsymbol{p}}\int \frac{d\epsilon}{2\pi}\{f_0(\epsilon) g(\boldsymbol{K}/2 - \boldsymbol{p}, z - \epsilon)\,\mathrm{Im}\, g(\boldsymbol{K}/2 + \boldsymbol{p}, \epsilon)$$
$$- [1 - f_0(\epsilon)] g(\boldsymbol{K}/2 + \boldsymbol{p}, z - \epsilon)\,\mathrm{Im}\, g(\boldsymbol{K}/2 - \boldsymbol{p}, \epsilon)\}. \tag{3.4}$$

Note that in this model t depends only on z and $\boldsymbol{K}$, which correspond to the total frequency and momentum of the particle pair. Now recall that $t(z = 0, \boldsymbol{K} = 0)$ exhibits the superconducting instability, as given by [19]

$$t(0, 0) = \frac{\lambda}{1 + \lambda\rho_d(\epsilon_F)\ln\{(\beta\omega_D\gamma/\pi)[1 + 1/(4\omega_d^2\tau^2)]\}} \tag{3.5}$$

that is

$$t(0, 0) = -\frac{1}{\rho_d(\epsilon_F)\ln(T/T_c)} \tag{3.6}$$

where γ is the Euler constant and in the small τ^{-1} limit

$$k_B T_c = (\hbar\omega_D\gamma/\pi)\exp\{-[|\lambda|\rho_d(0)]^{-1}\} \tag{3.7}$$

which is the well known BCS expression for the transition temperature. The main physical consequences of the analysis clearly come from the small-K behaviour of $t(\omega, K)$. In this limit $\chi_a(\omega, K)$ can be evaluated as

$$\chi_a(\omega, K) = \rho(0)[\ln(\beta\omega_D\gamma/\pi) + i(\pi/8)\beta\omega - \tfrac{1}{6}K^2V_F^2\tau^2] \tag{3.8}$$

which leads to

$$t(\omega, K) = -\frac{1}{\rho(0)[\ln(T/T_c) + K^2\xi^2 - i\pi\beta\omega/8]} \tag{3.9}$$

with $\xi^2 = V_F^2\tau^2/6$.

The frequency sum in equation (3.1) can be easily done to yield

$$\Sigma(p, z_n) = \int \frac{d\omega}{\pi}[f_0(\epsilon)t(z_n + \epsilon, K)\,\mathrm{Im}\,g(K - p, \epsilon) - f_B(\epsilon) \times \mathrm{Im}\,t(\epsilon, K)g(\epsilon - z_n, K - p)] \tag{3.10}$$

where $f_B(\epsilon)$ denotes the Bose–Einstein factor $(e^{\beta\epsilon} - 1)^{-1}$.

The first term of this expression corresponds to the physical effect that we discussed earlier, that is, it describes the effect that near T_c the quasiparticle energy gets renormalized as the quasiparticle (hole) free state gets strongly mixed with a state in which it is paired with another particle (hole) from the Fermi sea. The second part containing the Bose factor is an additional effect of superconducting fluctuations. In two dimensions, the second factor gives rise to a divergence, which corresponds to absence of superconducting ordering in accordance with the Mermin–Wagner theorem. In the present context such a divergence has to be suppressed owing to the overall three-dimensional nature of the problem, so we believe this term to be unimportant apart from an overall shift of the chemical potential.

The evaluation of the first term in the self-energy is straightforward. Substituting for t yields

$$\Sigma(p, E) = -\frac{1}{\Omega\rho_d(0)}\sum_K f_0(\xi_{K-p})\frac{1}{(\mu + K^2\xi^2) - (i\pi\beta/8)(E + \xi_{K-p})} \tag{3.11}$$

where μ stands for $\ln(T/T_c) \simeq (T - T_c)/T_c$. Performing the momentum sum in two dimensions, keeping in mind that the important contributions come from $K \simeq 0$, which allows us to approximate $\xi_{K-p} \simeq \xi_p$, we obtain the leading contributions for the real and imaginary parts of the self-energy to be

$$\Sigma_R(p, E) \simeq \frac{1}{4\pi\xi^2\rho_2(0)} f_0(\xi_p)\ln\left(\frac{\mu^2 + [(\pi\beta/8)(E + \xi_p)]^2}{K_m^2\xi^2}\right) \tag{3.12}$$

$$\Gamma(p, E) \simeq -\frac{1}{4\pi\xi^2\rho_2(0)} f_0(\xi_p)\left[\frac{\pi}{2} - \tan^{-1}\left(\frac{8\mu}{\pi\beta(E + \xi_p)}\right)\right] + \tau_q^{-1} \tag{3.13}$$

where K_m denotes the upper limit for the K sum. Note that near the Fermi level $\Gamma \simeq \tau^{-1}$, which justifies ignoring its momentum–energy dependence in the formula for TEP. We can now use equation (3.12) in the formula for TEP given in equation (2.22). Noting that the derivative of Σ_R with respect to E vanishes at $E = 0$, we obtain the following formula:

$$S_d = \frac{\pi^2 k_B}{3e}\left(\frac{k_B T}{\epsilon_F}\right)\frac{1}{[1-(\lambda_T/4\pi\xi^2)\ln\mu]^2} \tag{3.14}$$

where $\lambda_T^2 = \hbar^2/(2m^* k_B T)$. The most important feature of this formula is that it shows how the superconducting fluctuations drive the thermoelectric power to zero value at T_c. The temperature range over which this happens is clearly decided by the coherence length ξ. The parameters involved in the formula are T_c, m^*, ϵ_F and ξ. Using typical values of these parameters, i.e. $T_c \simeq 110$ K, $m^* = 2m$, $\epsilon_F = 40\,000$ K and $\xi = 20$ Å, a plot of the formula given in equation (3.14) is shown as curve (a) in figure 2.

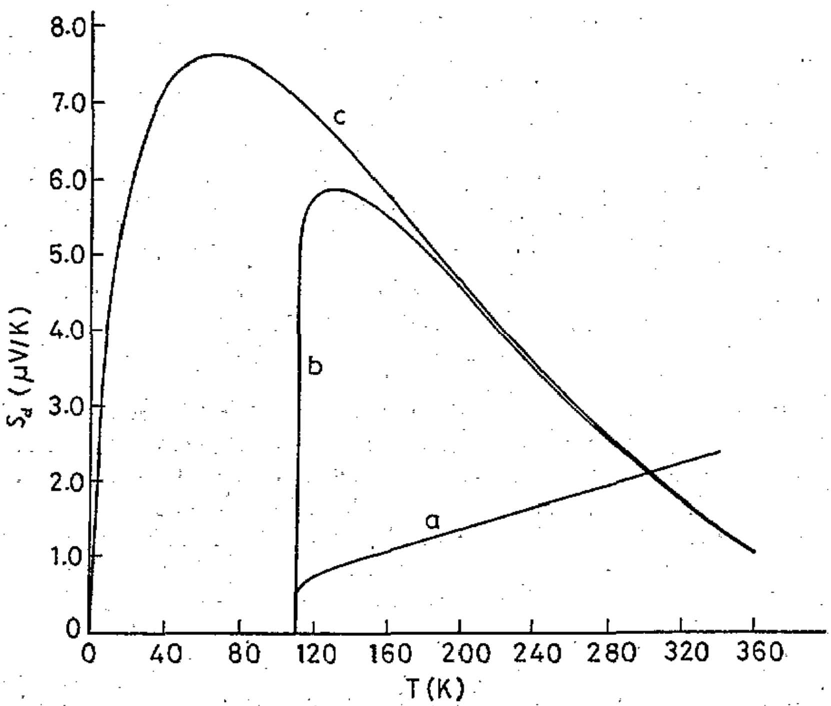

Figure 2. (a) The temperature variations of thermopower according to equation (3.14); (b) the same variation according to equation (4.3); (c) the variation when we include only the marginal Fermi-liquid self-energy. The parameters used for these plots are: $T_c = 110$ K, $m^* = 2m$, $\epsilon_F = 40\,000$ K, $\xi = 20$ Å, $\lambda = 2$ and $\hbar\omega_c = 600$ K.

4. Normal-state correlations

In the above derivation we have considered superconducting fluctuations within the standard Fermi-liquid description. This is not quite adequate to understand the typical behaviour of figure 3. So we clearly need to include correlations that are responsible for anomalies in various normal-state transport properties. In the absence of any first-principles description of the normal-state properties, we have chosen to employ the marginal Fermi-liquid (MFL) hypothesis, which has been used with some success to understand a variety of normal-state properties [13]. The MFL hypothesis consists of assuming the following form of the self-energy:

$$\Sigma_{\mathrm{MFL}}(\boldsymbol{k},\epsilon) = \lambda[\epsilon \ln(x/\hbar\omega_{\mathrm{c}}) - \mathrm{i}\pi x/2] \tag{4.1a}$$

$$x = \max(|\epsilon|, 2k_{\mathrm{B}}T) \tag{4.1b}$$

where λ is a dimensionless coupling constant and $\hbar\omega_{\mathrm{c}}$ is a cut-off frequency such that the above expression is valid only for $\epsilon < \hbar\omega_{\mathrm{c}}$. Note that this self-energy does not depend upon the momentum variable. So we propose that, to obtain a better account of normal-state behaviour, we include equation (4.1) in the self-energy of our propagator $G(\boldsymbol{k},\epsilon)$ and write

$$\Sigma(\boldsymbol{k},\epsilon) = \Sigma_{\mathrm{MFL}}(\epsilon) + \Sigma_{\mathrm{SCF}}(\xi_{k},\epsilon) \tag{4.2}$$

where $\Sigma_{\mathrm{SCF}}(\xi_{k},\epsilon)$ is given by equation (3.10). This proposal amounts to perturbative inclusion of a process causing superconducting fluctuations and a process leading to MFL behaviour in the Fermi-liquid theory. If we now use equation (4.2) in the formula for S_{d}, i.e. equation (2.22), one notes that Σ_{MFL} enters only in the numerator and thus simply contributes a factor multiplying the expression contained in equation (3.14). The final resulting expression for S_{d} thus becomes

$$S_{\mathrm{d}} = \frac{\pi^2 k_{\mathrm{B}}}{3e}\left(\frac{k_{\mathrm{B}}T}{\epsilon_{\mathrm{F}}}\right)\frac{[1-\lambda\ln(2k_{\mathrm{B}}T/\hbar\omega_{\mathrm{c}})]^2}{[1-(\lambda_T^2/4\pi\xi^2)\ln\mu]^2}. \tag{4.3}$$

In our earlier work [12] we had considered the effect of MFL correlations only and found a fairly good quantitative agreement with thermopower data in some bismuth-based superconductors. There we obtained the values of parameters like λ, $\hbar\omega_{\mathrm{c}}$ and ϵ_{F} using fits to data on conductivity as well as on thermopower. Using typical values $\lambda = 2$, $\hbar\omega_{\mathrm{c}} = 600$ K and $\epsilon_{\mathrm{F}} = 40\,000$ K, we exhibit a plot of equation (4.3) as curve (b) in figure 2. To make the role of various terms explicit, we have also included the plot (as curve (c) in figure 2) in which only MFL correlations are included. Since a variety of data has been reported in the literature, which ranges from exhibiting a rather broad hump to a sharp peak close to T_{c}, we point out that a small variation in parameters like λ and $\hbar\omega_{\mathrm{c}}$ can allow this range of behaviour. Figure 3 shows plots showing three such choices. It should be remarked that the value of the cut-off energy that is required to obtain the observed trends is 20% lower than the authors of the MFL hypothesis expect it to be [20]. Further, it should be noted that the magnitudes obtained in our formula are indeed of the right order, and the observed magnitude variations can be easily accommodated with small variations in parameters like ϵ_{F}, λ and $\hbar\omega_{\mathrm{c}}$.

5. Conclusions

We see from the plots of figures 2 and 3 that some of the main features of thermopower data on a number of high-T_{c} superconductors can be understood on the basis of the

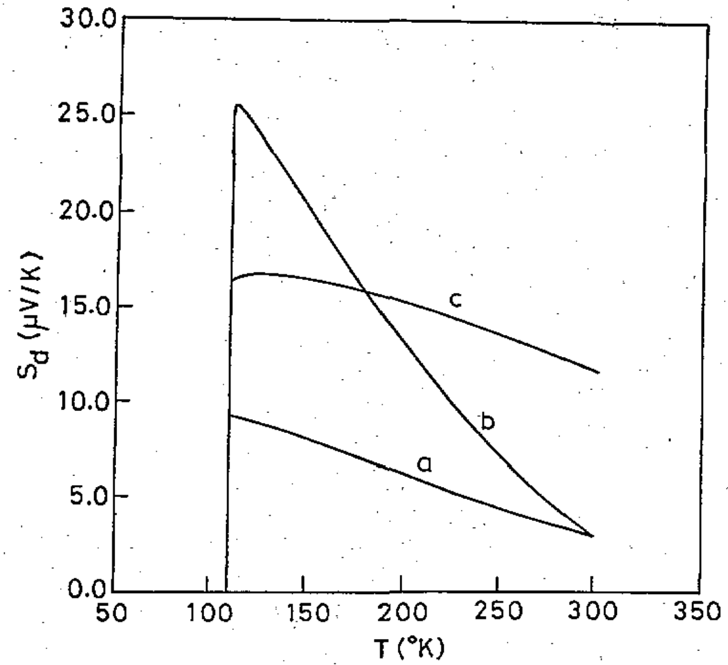

Figure 3. Three plots of the formula for thermopower variation with temperature to show the effect of variation of marginal Fermi-liquid parameters λ and $\hbar\omega_c$: (a) $\lambda = 2$, $\hbar\omega_c = 600$ K; (b) $\lambda = 4$, $\hbar\omega_c = 600$ K; (c) $\lambda = 2$, $\hbar\omega_c = 1000$ K. The other parameters are common: $\epsilon_F = 30\,000$ K and $m^* = 2m$.

formula derived in this paper. In spite of the simplifications and approximations made in the derivation of the formula for S_d, we feel that the agreement with the experiments at a quantitative level suggests that the superconducting fluctuations due to reduced dimensionality and small coherence length do indeed play a role in the continuous vanishing of TEP at T_c, whereas the large departure from the Fermi-liquid-like behaviour at higher temperatures seems to require a drastic proposal like the MFL hypothesis. This approach can be refined and extended. In particular, in many compounds the thermopower changes sign at higher temperatures. This is conjectured to be due to conduction in two or more bands. We propose to examine this aspect in future.

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