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THERMOELETRRIC EFFECT IN HIGH-T_c SUPERCONDUCTORS: THE ROLE OF DENSITY OF STATES FLUCTUATIONS

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We study the effect of the density of states (DOS) fluctuations on the thermoelectric coefficient of highly anisotropic superconductor above critical temperature. It is shown that it is the DOS contribution which gives rise to the leading correction to thermoelectric coefficient in spite of previous results where the only Aslamazov–Larkin term was taken into account. This conclusion is valid for an arbitrary impurity concentration.

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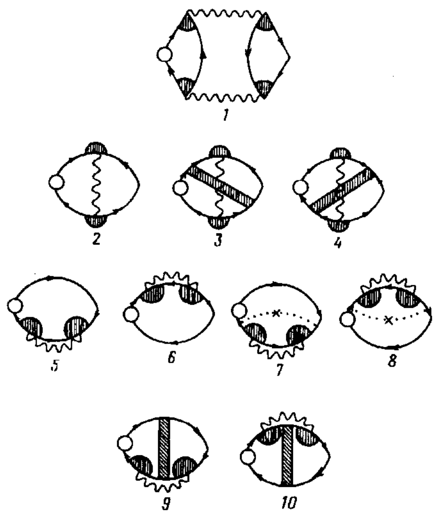
1. The problem of thermoelectric effect in fluctuation regime has been attracting the attention of theoreticians during more than twenty years, since the paper of Maki [1]. The main question which should be answered is whether the correction to thermoelectric coefficient β has the same temperature singularity in vicinity of critical temperature T_c as the correction to electrical conducticity σ or not. In the paper of Maki [1] the only logarithmically divergent contribution was predicted in two-dimentional (2D) case and its sign was found to be opposite to the sign of the normal state thermoelectric coefficient β_0. Later on, in a number of papers [2–4] it was claimed that temperature singularity of fluctuation correction to β is the same as it is for σ ($\propto (T-T_c)^{-1}$ in 2D). Finally, Reizer and Sergeev [5] have recently revised the problem using both quantum kinetic equation and linear response methods and have shown that, in the case of isotropic electron spectrum, strongly divergent contributions [2–4] are cancelled out for any dimensionality, while the final result has the same logarithmic singularity as it was found by Maki, but the opposite sign. We should emphasize that in all papers cited above the only Aslamazov–Larkin (AL) contribution was taken into account, while the anomalous Maki–Thompson (MT) term was shown to be absent [2, 5]. It was mentioned [5] that the non-correct evaluation of interaction corrections to heat-current operator in Refs. [2–4] produced the erroneously large terms which really are cancelled out within the adequate procedure. Due to this strong cancellation the AL term turns out to be less singular if compared with corresponding correction to conductivity [5].

From the other side, now it is well established that in every case where the senior AL and MT fluctuation corrections are suppressed by some reason, the contribution connected with fluctuation renormalization of one-electron density of states (DOS) can become important. As examples we can mention c-axis fluctuative transport [6, 7], NMR relaxation rate [8] and infrared optical conductivity [9]. In this communication we show that the analogous situation takes place also in the case of thermoelectric coefficient. In what follows we study the DOS contribution to the thermoelectric coefficient of superconductors with an arbitrary impurity concentration above T_c. We will be mostly interested in 2D case, but the generalization to the case of layered superconductor will be done at the end. We show that, although DOS term has the same temperature dependence as AL contribution [5], it turns out to be the leading fluctuation contribution both in clean and dirty cases due to its specific dependence on electron mean free path.



The Feynman diagrams for the fluctuation correction to thermoelectric coefficient are shown. Shaded partial circles are impurity vertex corrections, dashed curves with central crosses are additional impurity renormalizations, and shaded thick lines are additional impurity vertex corrections

2. We use units with $\hbar = c = k_B = 1$. We introduce the thermoelectric coefficient β in the framework of linear response theory as:

$$\beta = \lim_{\omega \to 0} \frac{\mathrm{Im}[Q^{(eh)R}(\omega)]}{T\omega} \tag{1}$$

where $Q^{(eh)R}(\omega)$ is the retarded Fourier component of the correlation function of electric and heat current operators. This correlation function in diagrammatic technique is represented by the two exact electron Green's functions loop with two external field vertices, the first, $-e\mathrm{v}$, associated with the electric current operator and the second one, $\frac{i}{2}(\epsilon_n + \epsilon_{n+\nu})\mathrm{v}$, associated with the heat current operator ($\epsilon_n = \pi T(2n+1)$ is fermionic Matsubara frequency and $\mathrm{v} = \partial\xi(\mathrm{p})/\partial\mathrm{p}$ with ξ being the quasiparticle energy). Taking into account the first order of perturbation theory in Cooper interaction and averaging over impurity configuration one can find ten diagrams presented in Fig. 1. The solid lines represent $G(\mathrm{p}, \epsilon_n) = 1/(i\tilde{\epsilon}_n - \xi(\mathrm{p}))$, the single-quasiparticle normal state Green's function averaged over impurities which contains the scattering lifetime τ ($\tilde{\epsilon}_n = \epsilon_n + 1/2\tau \mathrm{sign}\epsilon_n$). The shaded objects are the vertex impurity renormalization $\lambda(\mathrm{q}=0, \epsilon_n, \epsilon_{n'})$ (see [7]). The wavy line represents the fluctuation propagator $L(\mathrm{q}, \Omega_k)$:

$$L^{-1}(\mathrm{q}, \Omega_k) = -\rho\left[\ln\frac{T}{T_c} + \psi\left(\frac{1}{2} + \frac{|\Omega_k|}{4\pi T} + \frac{2\eta q^2}{\pi^2}\right) - \psi\left(\frac{1}{2}\right)\right] \tag{2}$$

where

$$\eta = -\frac{v_{\rm F}^2\tau^2}{2}\left[\psi\left(\frac{1}{2}+\frac{1}{4\pi T\tau}\right)-\psi\left(\frac{1}{2}\right)-\frac{1}{4\pi T\tau}\psi'\left(\frac{1}{2}\right)\right]$$

is a positive constant which enters into the current expression in Ginzburg–Landau theory in 2D case (ρ is one-electron density of states and $\psi(x)$ and $\psi'(x)$ are digamma function and its derivative, respectively). The first diagram describes the AL contribution to thermoelectric coefficient and was calculated in [5] with electron-hole asymmetry factor taken into account in fluctuation propagator. Diagrams 2-4 represent Maki-Thompson contribution. As it was mentioned in Refs. [2, 5], neither anomalous nor regular parts of this diagram contribute to β in any order of elecron-hole asymmetry. In what follows we will discuss the contribution from diagrams 5-10 which describes the correction to β due to DOS renormalization.

For diagrams 5 and 6 we have

$$\begin{aligned} Q^{(5+6)}(\omega_\nu) &= -2eT\sum_{\Omega_k}\int(d\mathrm{q})L(\mathrm{q},\Omega_k)T\sum_{\epsilon_n}\frac{i(\epsilon_{n+\nu}+\epsilon_n)}{2}\int(d\mathrm{p})v^2\times \\ &\times\left[\lambda^2(\epsilon_n,-\epsilon_n)G^2(\mathrm{p},\epsilon_n)G(\mathrm{q}-\mathrm{p},-\epsilon_n)G(\mathrm{p},\epsilon_{n+\nu})+\right. \qquad (3) \\ &+\left.\lambda^2(\epsilon_{n+\nu},-\epsilon_{n+\nu})G^2(\mathrm{p},\epsilon_{n+\nu})G(\mathrm{q}-\mathrm{p},-\epsilon_{n+\nu})G(\mathrm{p},\epsilon_n)\right]. \end{aligned}$$

(We use the shorthand notation $(d\mathrm{q}) = d^dq/(2\pi)^d$, where d is dimentionality). Evaluating Eq. (3) one naturally obtains zero result without taking into account the electron-hole asymmetry. The first possible source of this factor is contained in fluctuation propagator and was used in [5] for AL diagram. Our calculations show that for DOS contribution this correction to fluctuation propagator results in non-singular correction to β in 2D case and can be neglected. Another source of electron-hole asymmetry is connected with expansion of energy-dependent functions in power of $\xi/E_{\rm F}$ near Fermi level performing p-integration in Eq. (3) ($E_{\rm F}$ is the Fermi energy):

$$\rho v^2(\xi) = \rho v^2(0) + \xi\left[\frac{\partial(\rho v^2(\xi))}{\partial\xi}\right]_{\xi=0}. \qquad (4)$$

Only second term in Eq. (4) contributes to thermoelectric coefficient. Contribution of diagrams 7 and 8 can be calculated in analogous way. Diagrams 9-10 do not give any singular contribution to thermoelectric coefficient due to the vector character of external vertices and as a result an additional q^2 factor appears after p-integration. The same conclusion concerns MT-like diagram 3-4.

Performing integration over ξ we find the contribution of the important diagrams 5-8 in the form

$$Q^{(5-8)}(\omega_\nu) = \frac{eT^2}{4}\left[\frac{\partial(\rho v^2(\xi))}{\partial\xi}\right]_{\xi=0}\int(d\mathrm{q})L(\mathrm{q},0)(\Sigma_1+\Sigma_2+\Sigma_3), \qquad (5)$$

where we have separated sums over semi-infinite $(-\infty,-\nu-1]$, $[0,\infty)$ and finite $([-\nu,-1])$ intervals :

$$\Sigma_1 = 2\sum_{n=0}^{\infty}\frac{2\epsilon_n+\omega_\nu}{2\tilde\epsilon_n+\omega_\nu}\left(\frac{\tilde\epsilon_n+\omega_\nu}{(\epsilon_n+\omega_\nu)^2}+\frac{\tilde\epsilon}{\epsilon_n^2}\right),$$

$$\Sigma_2 = \frac{1}{(1/\tau+\omega_\nu)^2}\sum_{n=-\nu}^{-1}(2\epsilon_n+\omega_\nu)^2\left(\frac{\tilde{\epsilon}_{n+\nu}}{\epsilon_{n+\nu}^2}-\frac{\tilde{\epsilon}_n}{\epsilon_n^2}\right) \tag{6}$$

$$\Sigma_3 = (1+\omega_\nu\tau)\sum_{n=-\nu}^{-1}(2\epsilon_n+\omega_\nu)\left(\frac{1}{\epsilon_{n+\nu}^2}-\frac{1}{\epsilon_n^2}\right).$$

Σ_1 and Σ_2 are associated with diagram 5-6, while Σ_3 with diagram 7-8. Calculating sums (6) we are interested in terms which are linear in external frequency ω_ν. Sum Σ_1 turns out to be an analytical function of ω_ν and it is enough to expand it in Taylor series after analytical continuation $\omega_\nu \to -i\omega$. The last two sums over finite intervals require more attention because of their nontrivial ω_ν-dependence and before analytical continuation they have to be calculated rigorously. As a result:

$$\Sigma_1^R = \frac{i\omega}{4T^2}\ ;\ \Sigma_2^R = -\frac{2i\omega\tau}{\pi T}\ ;\ \Sigma_3^R = -\frac{i\omega}{2T^2}. \tag{7}$$

Finally, we perform integration over q and the total contribution associated with DOS renormalization in 2D case takes the form:

$$\beta^{\mathrm{DOS}} = \frac{1}{8\pi^2}\frac{eT_c}{v_{\mathrm{F}}^2\rho}\left[\frac{\partial(v^2\rho)}{\partial\xi}\right]_{\xi=0}\ln\left(\frac{T_c}{T-T_c}\right)\kappa(T_c\tau), \tag{8}$$

$$\begin{aligned}\kappa(T\tau) &= -\frac{1+\dfrac{\pi}{8T\tau}}{T\tau\left[\psi\left(\dfrac{1}{2}+\dfrac{1}{4\pi T\tau}\right)-\psi\left(\dfrac{1}{2}\right)-\dfrac{1}{4\pi T\tau}\psi'\left(\dfrac{1}{2}\right)\right]} = \\ &= \begin{cases}\dfrac{8\pi^2}{7\zeta(3)}T\tau \approx 9.4T\tau & \text{for } T\tau \gg 1\\ \dfrac{1}{T\tau} & \text{for } T\tau \ll 1\end{cases}\end{aligned} \tag{9}$$

To generalize this result to the important case of layered superconductor one has to replace $\ln(1/\epsilon) \to \ln[2/(\sqrt{\epsilon}+\sqrt{\epsilon+r})]$ ($\epsilon = (T-T_c)/T_c$ and r is an anisotropy parameter [7]) and to multiply Eq. (8) by $1/p_{\mathrm{F}}s$, where s is the interlayer distance. In the limiting case of 3D superconductor ($r \gg \epsilon$) both AL [5] and DOS contributions are not singular.

3. Comparing Eq. (8) with the results of [5] for AL contribution, we conclude, that in both limiting cases of clean and dirty systems the decrease of β due to fluctuation DOS renormalization dominates the thermoelectric transport due to AL process. Really, the total relative correction to thermoelectric coefficient in the case of 2D superconducting film of thickness s can be written in the form:

$$\frac{\beta^{\mathrm{DOS}}+\beta^{\mathrm{AL}}}{\beta_0} = -0.09\frac{1}{E_{\mathrm{F}}\tau}\frac{1}{p_{\mathrm{F}}s}\ln\left(\frac{T_c}{T-T_c}\right)\left[\kappa(T_c\tau)+10.6\ln\frac{\Theta_{\mathrm{D}}}{T_c}\right], \tag{10}$$

where the first term in square brackets corresponds to the DOS contribution (8) and the second term describes the AL contribution from Ref. [5] (Θ_{D} is Debye temperature). Assuming $\ln(\Theta_D/T_c) \approx 2$ one finds that DOS contribution dominates AL one for any value of impurity concentration: κ as a function of $T\tau$ has a minimum at $T\tau \approx 0.3$ and even at this point DOS term is larger. In both limiting cases $T\tau \ll 1$ and $T\tau \gg 1$ this difference strongly increases.

The temperature and impurity concentration dependencies of fluctuation corrections to β can be evaluated through a simple qualitative consideration. The thermoelectric coefficient may be estimated through the electrical conductivity σ as $\eta \sim (\epsilon^*/eT)f_{as}\sigma$, where ϵ^* is the characteristic energy involved in thermoelectric transport and f_{as} is the electron-hole asymmetry factor, which is defined as the ratio of the difference between numbers of electrons and holes to the total number of particles. Conductivity can be estimated as $\sigma \sim e^2\mathcal{N}\tau^*/m$, where $\mathcal{N}$, τ^* and m are the density, lifetime and mass of charge (and heat) carriers, respectively. In the case of AL contribution the heat carriers are nonequlibrium Cooper pairs with energy $\epsilon^* \sim T - T_c$ and density

$$\mathcal{N} \sim p_F^d \frac{T}{E_F} \ln \frac{T_c}{T - T_c}$$

and characteristic time, given by Ginzburg-Landau time $\tau^* \sim \tau_{\rm GL} = \frac{\pi}{8(T-T_c)}$. Thus in 2D case

$$\Delta\eta^{\rm AL} \sim (T - T_c)/(eT_c)f_{as}\Delta\sigma^{\rm AL} \sim ef_{as} \ln \frac{T_c}{T - T_c}.$$

One can easily get that the fluctuation correction due to AL process is less singular (logarithmic in 2D case) with respect to the corresponding correction to conductivity and does not depend on impurity scattering [5].

The analogous consideration of the single-particle DOS contribution ($\epsilon^* \sim T$, $\tau^* \sim \tau$) evidently results in the estimate

$$\beta \sim ef_{as}T_c\tau \ln \frac{T_c}{T - T_c}$$

which coincides with (8) in clean case. The dirty case is more sofisticated because the fluctuation density of states renormalization strongly depends on the character of the electron motion, especially in the case of diffusive motion [10]. The same density of states redistribution in the vicinity of Fermi level directly enters into the rigorous expression for β and it is not enough to write the fluctuation Cooper pair density $\mathcal{N}$ but it is necessary to take into account some convolution with $\delta\rho_{\rm fl}(\epsilon)$. This is what was actually done in the previous calculations.

Experimentally, although Seebeck coefficient $S = -\eta/\sigma$ is probably the easiest to measure among thermal transport coefficients, the comparison between experiment and theory is complicated by the fact that S cannot be calculated directly; it is rather a composite quantity of electrical conductivity and thermoelectric coefficient. As both η and σ have corrections due to superconducting fluctuations, total correction to Seebeck coefficient is given by

$$\Delta S = S_0 \left(\frac{\Delta\beta}{\beta_0} - \frac{\Delta\sigma}{\sigma_0} \right). \tag{11}$$

Both these contributions provide a positive correction $\Delta\beta$, thus resulting in the decrease of the absolute value of S at the edge of superconducting transition ($\Delta\beta/\beta_0 < 0$). As for fluctuation correction to conductivity $\Delta\sigma/\sigma_0 > 0$, we see from

Eq. (11) that thermodynamical fluctuations above T_c always reduce the overall Seebeck coefficient as temperature approaches T_c. So the very sharp maximum in the Seebeck coefficient of high-T_c materials experimentally observed in few papers [11] seems to be unrelated to fluctuation effects within our simple model even leaving aside the question about experimental reliability of these observations.

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