Distinctive features in the kinetic coefficients of high-T_c superconductors according to a generalized Hubbard model

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Equations for superconductivity with a finite relaxation time with spin flip are analyzed. This relaxation time depends on the temperature. This factor is responsible for features in the kinetic coefficients of high-T_c superconductors which distinguish them from conventional superconductors. Numerical estimates are derived on the basis of a strong-repulsion Hubbard model.

The absence of a maximum from the temperature dependence of the absorption of electromagnetic waves, the absence of a corresponding maximum for the nuclear-spin relaxation rate, and the anomalous temperature dependence of the energy gap and the acoustic absorption are the basic experimental results which distinguish the high-T_c

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superconductors from conventional ones. All these distinctive features can be explained on the basis of a spin-dependent electron–electron scattering amplitude. This amplitude determines a finite relaxation time τ_s and a depairing parameter ζ, both of which are strong functions of the temperature.

In the Hubbard–Emery–Hirsch models, relaxation effects are seen even in the two-loop approximation, so the system of equations for the anomalous ($\widetilde{\Delta}$) and normal ($\widetilde{\omega}$) self-energy parts resembles the equation for superconductors with a paramagnetic impurity:[1]

$$\widetilde{\Delta}_\omega=\Delta+T\sum_{\omega'} K_2(|\omega'-\omega|)\psi_{\omega'}/\sqrt{1+\psi_{\omega'}^2},$$
$$\widetilde{\omega}_\omega=\omega+T\sum_{\omega'} K_1(|\omega'-\omega|)\mathrm{sgn}\,\omega'/\sqrt{1+\psi_{\omega'}^2}, \tag{1}$$

where $\Delta = gT\Sigma_\omega\psi_\omega/\sqrt{1+\psi_\psi^2}$, $\omega_n = (2n+1)\pi T$, and $\psi_\omega = \widetilde{\Delta}_\omega/|\widetilde{\omega}_\omega|$.

The kernels $K_{1,2}(\Omega)$ can be found by averaging the zero-sound vertex part over all possible values of the momentum transfer.

The logarithmic singularity at small ω is cut off by the quantity $1/\tau_s$, which we can find by linearizing Eqs. (1) with respect to the function ψ_ω:

$$\left[|\omega|+T\,\mathrm{sgn}\,\omega\sum_{\omega'}\mathrm{sgn}\,\omega' K_1(|\omega'-\omega|)\right]\psi_\omega=T\sum_{\omega'}K_2(|\omega'-\omega|)\psi_{\omega'}+\Delta. \tag{2}$$

Using the Euler–Maclaurin summation formula, we find, for low temperatures,

$$\frac{1}{\tau_s}=\frac{\pi T^2}{3}[K_2'(0)-K_1'(0)]. \tag{3}$$

In the high-temperature limit, the reciprocal of the relaxation time is proportional to the temperature and is determined by the values of kernels $K_{1,2}$ at a zero frequency transfer:

$$\frac{1}{\tau_s}=T[K_1(0)-K_2(0)]. \tag{4}$$

In contrast with superconductors with a paramagnetic impurity, the reciprocal of the relaxation time, $1/\tau_s$, depends strongly on the temperature T in this case, and it vanishes as $T\to 0$. All physical properties ultimately depend on the depairing parameter $\zeta=1/(2\pi T\tau_s)$, which reaches its maximum value ζ_m at a high temperature.

In the Hubbard model with an infinite repulsion we have the estimate

$$\zeta_m=[\epsilon_0\rho_0(\epsilon_0)]^2(3+f)/\pi f^2,\quad f=1-\frac{n}{2}, \tag{5}$$

where the parameter ϵ_0 is related to the electron density $n=2f\int^{\epsilon_0}\rho_0(\epsilon)\,d\epsilon$ through the equation of state, and $\rho_0(\epsilon)$ is the seed density of states.

According to (5), the quantity ζ_m is not greatly different from unity. In the simplest model with $\rho_0=1/2$ we thus have $\zeta_m=(3+f)/4\pi f^2$, so the maximum value is reached with $n=1$. In this case we have $\zeta=7/2\pi=1.114$. For a square lattice at the edge of the band we would have $\zeta_m=14/\pi^3=0.452$, but the absolute maximum is reached at intermediate values of n.

In our model, the relaxation time τ_s is infinite at $T=0$, so the size of the energy gap, Δ_0, is given by the standard BCS expression. The transition temperature T_c, on the other hand, is determined by the relaxation time at $T=T_c$. Correspondingly, we have a relation which is convenient for comparison with experiment:

$$\frac{2\Delta_0}{T_c}=8\pi\exp\left[\psi\left(\frac{1}{2}+\zeta\right)\right]. \tag{6}$$

Here and below, $\zeta=1/2\tau_s T_c$, $\psi(x)=\Gamma'(x)/\Gamma(x)$, and $\psi^{(K)}(x)$ is the polygamma function.

The existence of a finite depairing parameter explains some experimental results which contradict the BCS theory. For example, the relative relaxation rate of the nuclear spins near the transition point is found in terms of the order parameter Δ and the parameter ζ (Refs. 2 and 3, for example):

$$\frac{R_s}{R_n}=1+\left(\frac{\Delta}{2\pi T}\right)^2\left[\psi^{(1)}\left(\frac{1}{2}+\zeta\right)+3\zeta\psi^{(2)}\left(\frac{1}{2}+\zeta\right)\right]/2\zeta. \tag{7}$$

According to the GLAG theory, we have

$$\left(\frac{\Delta}{2\pi T}\right)^2=4\left(\frac{T_c-T}{T_c}\right)\frac{\left[1+\dfrac{\partial\zeta}{\partial(\ln T_c)}\psi^{(1)}\left(\dfrac{1}{2}+\zeta\right)\right]}{-\psi^{(2)}\left(\dfrac{1}{2}+\zeta\right)-\dfrac{\zeta}{3}\psi^{(3)}\left(\dfrac{1}{2}+\zeta\right)}. \tag{8}$$

With increasing ζ, the slope of the relaxation rate versus the temperature changes sign as early as $\zeta=0.13$. For larger values, curve (7) has a positive slope, which reaches a maximum value of 12 in the limit $\zeta\gg1$.

There is a corresponding situation for the magnetic susceptibility. According to Ref. 4, the relative susceptibility depends on only τ_s, not the mean free path:

$$\frac{\chi_s}{\chi_n}=1-\left(\frac{\Delta}{2\pi T}\right)^2\frac{3}{2\zeta^2}\left\{\frac{3}{2}\left[\psi\left(\frac{1}{2}+\zeta\right)-\psi\left(\frac{1}{2}+\frac{\zeta}{3}\right)\right]-\zeta\psi^{(1)}\left(\frac{1}{2}+\zeta\right)\right\}. \tag{9}$$

In the limit $\zeta\to0$ we find the result found previously by Yosida:

$$\frac{\chi_s}{\chi_n}=1-2\frac{T_c-T}{T_c}. \tag{10}$$

With increasing value of the parameter ζ, the angular coefficient increases, and it reaches a maximum at $\zeta\gg1$:

$$\frac{\chi_s}{\chi_n}=1-9\frac{T_c-T}{T_c}\ln\left(\frac{27}{e^2}\right)\approx1-11.68\left(\frac{T_c-T}{T_c}\right). \tag{11}$$

According to experiments on the Knight shift[5] and nuclear spin relaxation[6] in $YBa_2Cu_3O_7$, the slopes of curves (9) and (7) as $T \to T_c$ are 3.3 and 5.0, respectively; correspondingly, we find $\zeta = 0.45$.

We can impose the same experimental test on the relative magnitude of the imaginary part of the magnetic susceptibility calculated for T_c:

$$\frac{\operatorname{Im} \chi_s}{\operatorname{Im} \chi_n} = 1 - \frac{3\Delta^2}{8(\pi T)^2 \zeta} \left\{ \left[\psi^{(1)}\left(\frac{1}{2} + \frac{\zeta}{3}\right) - \psi^{(1)}\left(\frac{1}{2} + \zeta\right) \right] + \frac{2}{3}\zeta \psi^{(2)}\left(\frac{1}{2} + \zeta\right) \right\}, \tag{12}$$

where $\operatorname{Im} \chi_n = 3\omega_0 \tau_s / 4$, and ω_0 is the frequency of the external magnetic field.

Relations (9) and (12) were derived by summing ladder diagrams which arise when a spin–spin electron correlation function is averaged. According to (12), this correlation function is of a relaxation nature in both the normal and superconducting phases.

In a study of the absorption of sound we find a completely different physical situation. Even in the normal phase we must deal with diffusion effects, which are manifested in a calculation of the density–density correlation function.[7] When there is a spin flip in the superconducting phase, a new type of relaxation, with a time $\propto \zeta T_c \Delta^{-2}$, appears. The polarization operator put in dimensionless form by division by the one-particle density of states has a substantial spatial dispersion and also a substantial temporal dispersion:

$$\Pi_\omega(q) = Dq^2/(Dq^2 - i\omega) + \left(\frac{\Delta}{2\pi T}\right)^2 \beta_\omega^{-1} \left[\frac{\psi^{(1)}(\frac{1}{2} + \zeta_+)}{\zeta_+} - \frac{\psi^{(1)}(\frac{1}{2} + \zeta_+ \sqrt{1+\beta_\omega})}{\zeta_+ \sqrt{1+\beta_\omega}} \right]$$

$$+ \beta_\omega \zeta_+ \frac{\psi^{(1)}(\frac{1}{2} + \zeta_+ \sqrt{1+\beta_\omega})}{\sqrt{1+\beta_\omega}}, \tag{13}$$

where

$$\zeta_+ = \zeta - \frac{i\omega}{2\pi T}, \quad \beta_\omega = \frac{2i\Delta^2 \left(\frac{1}{\tau_s} - \frac{i\omega}{4}\right)}{(\omega + iDq^2)\left(\frac{1}{\tau_s} - \frac{i\omega}{2}\right)^2}.$$

Accordingly, despite the condition that ω be small in comparison with T_c, the quantity β_ω can vary over a wide range. The first term corresponds to a diffusion mechanism for absorption in the normal phase.

At low frequencies, $\omega \ll v_s^2 / \tau v_0^2$, and except in the close vicinity of the transition point, with $1 \gg (\frac{\Delta}{2\pi T})^2 \gg \frac{\zeta\omega}{2\pi T}$, the quantity in (13) tends toward its quasistatic value

$$\Pi_\omega = 1 + \frac{i\omega D}{v_s^2} + \frac{i\omega \zeta \pi T^2}{\Delta^2}. \tag{14}$$

At low frequencies we thus find an acoustic absorption which is strengthened by relaxation in the superconducting phase:

$$\gamma_{\omega}=\lambda\frac{\omega^{2}}{2}\left(\frac{D}{v_{s}^{2}}+\frac{1}{2\Delta^{2}\tau_{s}}\right). \tag{15}$$

Here λ is the BCS constant, and v_s is the longitudinal sound velocity. As the temperature is varied at a given frequency ω, the acoustic absorption increases toward the transition point and goes through a maximum. In the immediate vicinity of the transition point, $v_s/\tau v_0 \gg \zeta\omega \gg \Delta^2/2\pi T$, the correction for anomalous absorption becomes small again:

$$\Pi_{\omega}=\frac{Dq^{2}}{Dq^{2}-i\omega}+\left(\frac{\Delta}{2\pi T}\right)^{2}\left\{\frac{4i\pi T}{\omega}\psi^{(1)}\left(\frac{1}{2}+\zeta\right)+\frac{1}{2\zeta}\left[\psi^{(1)}\left(\frac{1}{2}+\zeta\right)-\zeta\psi^{(2)}\left(\frac{1}{2}+\zeta\right)\right]\right\}. \tag{16}$$

In the immediate vicinity of the transition point, the anomalous correction to the absorption thus increases with distance from the transition point, and its magnitude does not depend on the frequency of the sound wave:

$$\gamma_{\omega}=\lambda\left\{\frac{\omega^{2}Dv_{s}^{2}}{2(v_{s}^{4}+D^{2}\omega^{2})}+\frac{\Delta^{2}}{2\pi T}\psi^{(1)}\left(\frac{1}{2}+\zeta\right)\right\}. \tag{17}$$

This effect has been observed[8] in the compound $YBa_2Cu_3O_7$ at a frequency of 15 MHz. The shift of the maximum away from T_c on the temperature dependence was 4%.

The following expression describes the entire temperature dependence and frequency dependence of the absorption of longitudinal sound:

$$\gamma_{\omega}=\gamma_{\omega}^{(n)}+\lambda\left(\frac{\Delta}{2\pi T}\right)^{2}\left\{\left(\frac{1}{\zeta\lambda_{\omega}}+\frac{4\pi T}{\omega}\right)\operatorname{Re}\frac{\psi^{(1)}(\frac{1}{2}+\zeta\sqrt{1+i\lambda_{\omega}})}{\sqrt{1+i\lambda_{\omega}}}-\frac{\psi^{(1)}(\frac{1}{2}+\zeta)}{\zeta\lambda_{\omega}}\right\}, \tag{18}$$

where $\lambda_{\omega}=\Delta^2/(\zeta\omega\pi T)$, $\gamma_{\omega}^{(n)}$ is the absorption coefficient in the normal phase.

The current–current correlation function does not have an anomalous frequency dependence, since it is not related to the diffusion singularity. In the low-frequency limit it has a correction determined by the two relaxation times τ_s and τ. In the very dirty limit, however, the relaxation time τ "withdraws" into the determination of the conductivity σ, so we find the same result as in (7):

$$\frac{\operatorname{Im}Q}{\omega\sigma}=\frac{R_{s}}{R_{n}}. \tag{19}$$

The agreement of curves (7) and (19), without any maximum as a function of the temperature, has been demonstrated in experiments[9] on $YBa_2Cu_3O_7$.

The fact that there is no Hebel–Slichter maximum and the fact that there is an anomalous absorption of longitudinal sound cannot be explained by introducing an extremely strong electron–phonon coupling.[10] The Éliashberg equations written in the form in (1) have $K_1=K_2$. As a result, there is a pronounced cancellation of quasielastic processes; elastic processes are completely cancelled out. These circumstances are responsible for the slight blurring of the peak in the density of states in conventional superconductors with a strong electron-phonon coupling. The electron–phonon coupling does not lead to a relaxation of the electron spins, nor does it lead to an anomalous absorption of ultrasound. The correlation functions associated with heat fluxes have corrections which depend on the depairing parameter ζ, but their magnitude and sign are the same as those predicted by the theory of a strong electron–phonon coupling.

Determining the temperature dependence over a broad range below the transition point requires finding of the specific correlation functions $K_{1,2}(\Omega)$ and then solving integral equations (1). It has been shown that near the transition point all the thermodynamic, kinetic, and magnetic properties of superconductors are determined by the GLAG equations and by Eqs. (7)–(19), which depend on the parameter ζ calculated for $T=T_c$.

This parameter can be found from a measurable quantity with the help of Eq. (6). It turns out that experimental data which cannot be explained by the BCS theory can be reconciled in a qualitative sense with values $0.13<\zeta\lesssim 1/2$. Such values correspond to fairly high values of $2\Delta_0/T_c$, from 7 to 14. The values of $2\Delta_0/T_c$ which have been measured for the high-T_c superconductors run from 4 to 11, i.e., over an interval lower than the preceding interval.

[1] A. A. Abrikosov and L. P. Gor'kov, Zh. Eksp. Teor. Fiz. **39**, 1781 (1960) [Sov. Phys. JETP **12**, 1243 (1960)].
[2] R. O. Zaĭtsev, Fiz. Tverd. Tela (Leningrad) **31**(5), 52 (1989) [Sov. Phys. Solid State **31**, 749 (1989)].
[3] K. Maki, in *Superconductivity*, Vol. 2 (ed. R. D. Parks), New York, 1969, p. 1035.
[4] L. P. Gor'kov and A. I. Rusinov, Zh. Eksp. Teor. Fiz. **46**, 1363 (1964) [Sov. Phys. JETP **19**, 922 (1964)].
[5] S. E. Barrett *et al.*, Phys. Rev. B **41**, 6283 (1990).
[6] P. C. Hammel *et al.*, Phys. Rev. Lett. **63**, 1992 (1989).
[7] L. P. Gor'kov and G. M. Éliashberg, Zh. Eksp. Teor. Fiz. **54**, 612 (1968) [Sov. Phys. JETP **27**, 328 (1968)].
[8] H. P. Baum *et al.*, Phys. Rev. B **37**, 3675 (1988).
[9] R. T. Collins *et al.*, Phys. Rev. B **43**, 8701 (1991).
[10] F. Marsiglio, Phys. Rev. B **44**, 5373 (1991).

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