High- T_c superconductivity in the d - p electron system

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Abstract. The relaxation time with spin flip τ_s and the parameters ξ , δ , κ of superconducting phase have been calculated on the basis of the kinematical mechanism of superconductivity in strongly correlated oxide models. An inter-relation between the superconducting gap Δ_0 and the specific heat jump Δ_c allowing the experimental verification was obtained and the Ginsburg-Landau equation derived.

Keywords. Kinematical mechanism of superconductivity; parameters of superconducting phase; Ginsburg-Landau theory.

1. Introduction

At present, the electron structure of high-temperature superconductors is most adequately described using the correlated electron system. The representation of interaction where the one-particle hamiltonian with intra-atomic correlations is related to a zero approximation allows the distinguishing of the spectrum of quasi-fermions $\xi_{\vec{p}}$ determined by the poles of one-particle Green's function. From this spectrum we can obtain the density of electron states D and the tensor of reciprocal electron mass calculated for the Fermi level:

$$D = \sum_{\vec{p}} \delta(\xi_{\vec{p}}),$$

$$\frac{1}{m_{\alpha\beta}} = \sum_{\vec{p}} \delta(\xi_{\vec{p}}) \frac{\delta \xi_{\vec{p}}}{\delta p_{\alpha}} \frac{\delta \xi_{\vec{p}}}{\delta p_{\beta}} \frac{d}{2\mu D}, \quad (1)$$

where d is the dimension of lattice and μ is the chemical potential.

The study of non-phonon mechanisms of superconductivity using the models of Hubbard (Zaitsev and Ivanov 1987), Emery and Hirsch (Ivanov and Zaitsev 1988, 1989), and Anderson (Newns *et al* 1988) revealed the possibility of singlet coupling even in the limit of infinite Hubbard energy. In this case we have $\xi_{\vec{p}} = (1 - n/2)t_{\vec{p}} - \mu$ (Hubbard 1963), where n is number of electrons per atom in the non-magnetic phase and $t_{\vec{p}}$ is the energy of non-interacting electrons.

2. HTSC mechanism

Strong Hubbard repulsion, $I \gg t$, leads to the narrowing of the initial energy band $t(p)$, which is schematically shown in figure 1. With a low number of electrons, $n \ll 1$, no bound states are formed during the pair collision, which results in an increase of electron energies and in the kinematical repulsion of electrons at the bottom of the band. At the same time, in the top part of the band, where $n \gtrsim 1$, the interaction of electrons decreases their energies and, therefore, the attractions of electrons must take place. Thus, the Hubbard repulsion and Pauli principle, excluding a great number of

Figure 1. Schematic diagram showing the narrowing of the energy band of electron excitations due to extremely strong intra-atomic Hubbard's correlations for n electrons per atom. Z is the number of nearest neighbours.

lattice sites from the translational motion of electrons for $n \gtrsim 1$, lead to a pair attraction of the neighbouring electrons with antiparallel spins, forming Cooper's electron pairs. This effect, proportional to t , is the essence of the kinematical mechanism of superconductivity (Zaitsev and Ivanov 1987; Takahashi 1988). The magnitude of superconducting gap is determined by the BCS type formula:

$$\Delta_0 = 2\varepsilon \cdot \exp(-\Lambda_0^{-1}), \Lambda_0 = Dg_0, \quad (2)$$

where ε and g_0 are specified by the particular superconductor model (Zaitsev and Ivanov 1987; Ivanov and Zaitsev 1988, 1989). However, the characteristics of superconducting phase near T_c and the T_c value itself are determined by the renormalized interaction constant:

$$\Lambda^{-1} = \Lambda_0^{-1} + \psi(\frac{1}{2} + y) - \psi(\frac{1}{2}), \pi T_c = 2\varepsilon \gamma \cdot \exp(-\Lambda^{-1}). \quad (3)$$

3. Decay time τ_s in the d - p electron system

Expression (3) was obtained by analogy with the theory of superconductivity with paramagnetic admixture (Abrikosov and Gor'kov 1960), but involve a different, decreased and temperature-dependent, dimensionless parameter $y = 1/(2\pi T_c \tau_s)$ where τ_s^{-1} is the reciprocal decay time of electrons with spin inversion (Ivanov and Zaitsev 1989). In the general case, τ_s is expressed through the spin correlation functions. In the one-loop approximation assuming a low value of mean-square fluctuations, we obtain for the Emery-Hirsch model:

$$\tau_s^{-1} = \frac{\pi D(E_p E_d)^2}{2\mu^2} \left(\frac{K_p}{f_p^2 \cdot d} + \frac{K_d}{f_d^2} \right), \quad (4)$$

where $E_{d,p}$ are the energies of $3d(x^2 - y^2)$ and $2p_{x,y}$ electrons measured from the Fermi level, $f_p = 1 - 3n_p/4$ and $f_d = 1 - n_d/2$, $n_{p,d}$ being the doping parameters of Hubbard's p - and lower d -sub-bands. Once the lower d -sub-band is completely occupied and the upper Hubbard's sub-band of d -electrons is being filled, then $n_d > 1$, and f_d should be replaced by $f_d = n_d/2$, and E_d by $E_d + I_d$. If the value (4) is calculated as the probability of transition with a change of spin projection, the initial and final states $\bar{p}$ and $\bar{p}'$, are independently averaged on the same energy surface:

$$K_{p,d} = T \sum_{\bar{p}, \bar{p}'} \delta(\xi_{\bar{p}}) \delta(\xi_{\bar{p}'}) \chi(\bar{P} - \bar{P}') \cdot D^{-2}. \quad (5)$$

In the general case $\chi_{p,d}$ is the dimensionless spin susceptibility of p,d -electrons. The logarithmic approximation used allows us to restrict the consideration to the static

contribution:

$$\chi_{\bar{p},d}(\bar{q}) = \sum_{\bar{z}} \int_0^{T^{-1}} [\exp(-i\bar{q}\bar{z}) \langle \delta \hat{S}_{p,d}(\bar{z}, t) \delta \hat{S}_{p,d}(0, 0) \rangle] dt \quad (6)$$

For the Hubbard model, the magnetic susceptibility (6) has been calculated by Hubbard and Jain (1968) and turned out to be weakly dependent on temperature in the metallic phase. A similar situation takes place in the Emery-Hirsch model for non-integer $n_{p,d}$ values. For non-integer $n_{p,d}$ in the static limit the temperature dependence of τ_s is determined by the factor T in (5), while the dimensionless parameter y tends to unity.

4. Superconducting phase characteristics

Near T_c , the equations of superconductivity are determined by τ and τ_s , which should be calculated for $T = T_c$. The Ginsburg-Landau coefficients α and b depend on y , changing neither sign nor the order of magnitude:

$$\alpha(T - T_c)\psi^* - \hat{\partial}_i \hat{\partial}_n \Psi^* (4m_{in})^{-1} + b|\psi|^2\psi^* = 0. \quad (7)$$

In (8) $\hat{\partial}_n = \nabla_n + 2ieA_n$, while α and b have the form:

$$\begin{aligned} \alpha &= D \left[1 + \frac{dy}{d \ln T_c} \psi'(\tfrac{1}{2} + y) \right]^2 \cdot \frac{1}{2CT_c} \\ b &= D \left[-\psi''(\tfrac{1}{2} + y) - \frac{y}{3} \psi'''(\tfrac{1}{2} + y) \right] \frac{1}{(8\pi CT_c)^2}, \end{aligned} \quad (8)$$

where the value

$$C = 2\pi T_c \mu D \sum_{\omega = (2n+1)\pi T} \left(\omega + \frac{1}{2\tau} \right)^{-1} \left(\omega + \frac{1}{2\tau_s} \right)^{-2} \frac{1}{d} \quad (9)$$

determines the relation between ψ^* and Δ , so that the superconducting current density has the London's form taking into account the anisotropy:

$$j_k = \frac{ie}{2m_{kl}} (\psi \hat{\partial}_l \psi^* - \psi^* \hat{\partial}_l \psi), \quad |\psi|^2 = C|\Delta|^2. \quad (10)$$

Equation (10) allows the determination of the reciprocal square value of the penetration depth of a weak magnetic field:

$$\delta_{kl}^{-2} = 8\pi e^2 \alpha(T - T_c) (bm_{kl})^{-1}. \quad (11)$$

In the "dirty" limit, where:

$$C = \mu D \tau \psi'(\tfrac{1}{2} + y) \cdot (d\pi T_c)^{-1}, \quad (12)$$

the tensor of reciprocal penetration depth is related to the tensor of conductivity σ_{kl} .

$$\delta_{kl}^{-2} = \frac{(8\pi)^2 (T_c - T) \sigma_{kl} \left[1 + \frac{dy}{d \ln T_c} \psi'(\tfrac{1}{2} + y) \right] \psi'(\tfrac{1}{2} + y)}{-\psi''(\tfrac{1}{2} + y) - \frac{y}{3} \psi'''(\tfrac{1}{2} + y)}. \quad (13)$$

In (13), the coefficient at the tensor of resistivity ρ_{kl} decreases as the parameter y increases. Similarly, for the square of coherence length in the "dirty" limit we have:

$$\xi_{kl}^2 = \frac{\hbar^2}{4m_{kl}\alpha|T - T_c|} = \frac{\sigma_{kl}\psi'(\frac{1}{2} + y)}{8\pi De^2|T_c - T| \left[1 + \frac{dy}{d \ln T_c} \psi'(\frac{1}{2} + y) \right]}. \quad (14)$$

From the comparison of (13) and (14) we derive the dimensionless tensor of Ginsburg-Landau theory:

$$\kappa_{kl} = (\delta_{kl}^2 \xi_{kl}^{-2})^{1/2} = \frac{|e| \bar{C} \rho_{kl}}{\sqrt{8\pi} \psi'(\frac{1}{2} + y)} \left\{ D \left[-\psi''(\frac{1}{2} + y) - \frac{y}{3} \psi'''(\frac{1}{2} + y) \right] \right\}^{1/2}. \quad (15)$$

The Ginsburg-Landau parameter characterizing the second-order superconductors exhibits a slow decrease as the parameter y increases.

5. Conclusion

The calculations on the basis of the kinematical HTSC mechanism phase diagrams have some predictive power (Ivanov and Zaitsev 1988, 1989). In the low-temperature range, $T \ll T_c$, the microscopic theory of superconductivity has the BCS form. Excluding the parameter y from equations for the heat capacity jump Δ_c and $2\Delta_0/T_c$ we arrive to the inter-relation, presented by figure 2. Experimental verification of this dependence would be of interest.

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Figure 2. Dependence of relative specific heat jump $\Delta c/c_n$ at T_c on the value of superconducting gap Δ_0 calculated for the kinematical mechanism of high-temperature superconductivity. $\ln \gamma = 0.577$ is the Euler number, $\zeta(3) = 1.2$ is the Riemann zeta function.

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