Bull. Mater. Sci., Vol. 14, No. 4, August 1991, pp. 1003–1005. © Printed in India.

Is high-T_c superconductor an undegenerated doped semiconductor?

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Abstract. The model of electron spectrum of HTS is suggested. It is supposed that the main feature of the spectrum is the presence of a narrow local pair level placed near the top of the filled two-dimensional (2D) electron band. Holes in this band are the result of thermal activation of electrons from the band to the pair level. The temperature dependences of resistivity and Hall constant of HTS in this model are in agreement with experiment on YBCO. The possibility of a first-order phase transition in such a system is considered.

Keywords. Concentration of carriers; undegenerated doped semiconductor; first-order phase transition.

Recently Kapitulnik (1988) has established that the temperature dependences of both reciprocal Hall constant $R_H^{-1}(T)$ and resistivity $\rho(T)(T>T_c)$ of the high-quality $YBa_2Cu_3O_7$ samples have the simplest forms $R_H^{-1}(T)=bT$ and $\rho(T)=aT$, where a and b are constants. At the same time Pauli susceptibility $\chi_0(T)$ of $YBa_2Cu_3O_7$ is practically temperature-independent (Bezinge *et al* 1988). For the single band model $R_H^{-1}(T)=nec$, but the temperature dependence $R_H^{-1}(T)$ evidences against applicability of such model for $YBa_2Cu_3O_7$. On the other hand, the charge carriers redistribution between different bands with temperature variation contradicts the temperature independence of χ_0. From our point of view the only way to resolve this contradiction is to suppose that the transition of carriers occurs between two-dimensional free carriers band and a pair level. Density of states N of 2D-band is independent of carrier concentration n.

We suggest that the energy spectrum of $YBa_2Cu_3O_7$ (and other high-T_c superconductors) consist of an acceptor-type pair level placed near the upper edge of the filled electron 2D-band. The position of this level is determined by oxygen concentration. Oxygen atoms in the chains play a role of the contaminations with double electron centres. In this case the carriers (holes) appear under thermal excitation of electrons from the filled band to the pair level according to reaction $O^\circ + 2e \rightleftarrows O^{2-}$. It is convenient to consider this electron spectrum in the hole presentation, when the hole-2D band is empty at $T=0$ and the carriers appear in the band from the hole pair level E_0. Assuming that the chemical potential μ of carriers is pinning at the pair level E_0 one can obtain that the concentration $n=rNk_BT\ln(1+\exp\mu/k_BT)$, where μ is measured from the bottom of the hole band, r is the number of equivalent extrema in the Brillouin zone. If the pair level coincides with the bottom of hole band (it probably takes place for $YBa_2Cu_3O_7$) and $n=rNk_B\,T\ln 2$. This result agrees with Hall's measurements for $rN \simeq 50$ states/eV cell. The same values of rN have also been obtained from specific heat jump and Pauli susceptibility.

As it is supposed, the main contribution to resistivity is due to the electron–electron scattering. The temperature dependence of resistivity may be obtained from Drude relation $\rho = m^*\nu/ne^2$, where m^* is the effective mass of holes and ν the collision frequency. ν is proportional to the concentration of scattering centres, i.e. n, and also to the number of final states for interacting holes which in turn is proportional to their average energy $\tilde{\varepsilon}$. The temperature change of $\tilde{\varepsilon}$ determines completely the $\rho(T)$ dependence. As in general $\tilde{\varepsilon} - \mu \simeq T$ then for $\mu = 0$, $\tilde{\varepsilon} \simeq T$ and $\rho(T) \sim T$ independently on n (that occurs in $YBa_2Cu_3O_7$). If $\mu \neq 0$, for example, for $YBa_2Cu_3O_{7-x}$ with $x > 0$ ($\mu > 0$) and $Y_2Ba_4Cu_8O_{16-y}$ ($\mu < 0$)—then $\tilde{\varepsilon} \simeq T + \mu$. This results in linear dependence $\rho(T) \sim (T + \mu)$ extrapolated to negative values of T in the first case and to positive values of $T \sim \mu$ in the second.

The superconductivity in the system arises in undegenerated gas of holes interacting with the pair level, which plays the Fermi surface role. The double electron centres with local attractive interaction may be responsible for high-T_c superconductivity (Khomskii and Zvezdin 1988). The superconducting transition in such a system can realize as the first-order phase transition. At $T > T_c$ the concentrations both of holes (in 2D-band) and hole pairs (on local level) are determined by equality of reaction rates in the direct and opposite directions. On the other hand it is improbable that such distribution of concentrations is optimal for superconductivity. It may be of advantage near T_c to change the correlation hole concentrations in band and on pair level, i.e. for example to transfer a part of holes from the band to the pair level. The resulting excess energy is compensated by the superconducting condensation energy. This can be explained from figure 1, where the free energy of system F is plotted as a function of concentration of hole pairs n_p ($T > T_c$). The equilibrium concentration $n_{p0}(T)$ corresponds to $F(n_p)$-curve minimum and determines the superconducting temperature T_{c0}. At $T \gtrsim T_{c0}$ near n_{p0} the $F(n_p)$-dependence will be changed because of negative contribution of condensation energy $\Delta F \sim N\Delta^2(n_p, T)$. Here $\Delta(n_p, T)$ is the superconducting gap. If we suppose that T_c increases near n_{p0} as a function of concentration n_p, we obtain $F(n_p)$ for $T \gtrsim T_{c0}$ as shown in figure 1. The dependences $F(n_p)$ at various temperatures $T_1 > T_2 > T_3$ are shown by dotted lines. At $T \lesssim T_2$ the additional minimum appears on $F(n_p)$-curve that corresponds to non-zero $\Delta = \Delta(T_2, n_p)$. This second minimum will decrease with fall of temperature. In such system large fluctuations of hole pairs density can take place at $T \to T_3$ ($F(n_{p0}) = F(n_{p3})$) being stabilized by the superconducting condensation energy. T_3 is to be taken as the experimentally determined transition temperature T_c, so the superconducting state with $n = n_3$ is more advantageous. At this temperature the first-order phase transition in superconducting state with non-zero gap Δ can take place. The jump of Δ was observed in experiments on IR-reflectivity (Collins *et al* 1987) and electron tunneling (Geerk *et al* 1988). Such transition may result in the modification of other characteristics of the system: elastic modula (Golovashkin *et al* 1987), interatomic

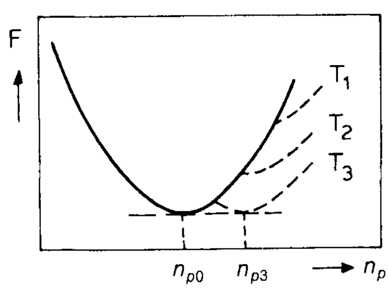

Figure 1. The dependence of free energy of system on hole pairs concentration. The solid curve corresponds to $T > T_{c0}$. The dashed lines correspond to the temperatures $T_1 > T_2 > T_3$ in the vicinity T_{c0}.

distances (Shäfer *et al* 1988) and Raman spectra (Tomsen *et al* 1988). As at $T = T_c$ the system transforms in the state with non-zero Δ, corresponding to the larger $T_c' \simeq T_2$, the ratio $2\Delta(0)/kT_c$ may essentially exceed the true value.

The influence of magnetic field on such system is determined by decreasing of free energy gain due to transition in superconducting state. However, this influence will be different in dependence on the dimension of arising superconducting region.

In particular, the regions with dimensions less than coherent length $\xi \ll \lambda$ (λ is the magnetic penetration length) are practically independent of the magnetic field, because the field penetrates completely in these regions. Therefore, in magnetic field at $T = T_3$ the state with superconducting lamellar regions with dimensions ξ is possible. In ordinary second-type superconductor the nucleation of superconducting regions takes place in fields $H(T) \leqslant \phi_0/\xi^2(T)$ and $H(T_c) = 0$. In our case the coherent length in the arising superconducting regions has at once a finite value, i.e. at $T = T_3$ the superconducting nucleation will occur even in a large field. Below T_3 in magnetic field the superconducting layers ($\sim \xi$ thick) directed along the field may exist in normal matrix.

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