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Theoretical calculation of the resistivity of the High-Tc superconductors

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Abstract : Working within the Anderson lattice model, we calculate the first correction to the mean field theory and evaluate the self-energy Σ of the carriers. The resistivity is then given by Drude's formula $\rho = m^*/ne^2\tau$ where $\tau^{-1} = 2 \text{ Im } \Sigma$.

1. Introduction

As shown by the observations, the interaction between the oxygen and copper atoms, within their two-dimensional layers, seems to play the leading role for a new microscopic mechanism leading to the pairing of the holes. We consider then the typical Anderson lattice model, used in heavy fermion systems [1], which can describe all electronic structure effects.

2. Description of the model and some ideas about the calculations

The Anderson Hamiltonian, in the slave boson representation, writes [2, 3] :

$$H = \sum_{k\sigma} \varepsilon_k c^+_{k\sigma} c_{k\sigma} + \sum_i E_o b^+_i b_i + \sum_{i\sigma} E_1 d^+_{i\sigma} d_{i\sigma} + \sum_i E_2 a^+_i a_i + \sum_{ik\sigma} V_k [b_i d^+_{i\sigma} c_{k\sigma} e^{ikr_i} + a_i d^+_{i\sigma} c^+_{k-\sigma} e^{-ikr_i} \operatorname{sgn}\sigma + \text{h.c.}] \quad (1)$$

Here the $c_{k\sigma}$ are fermion operators for holes of spin σ in the o-band; E_1, E_o and E_2 are the energies of the d^9, d^{10} and d^8 Cu-states respectively represented by the localised fermion $d_{i\sigma}$ and by the bosons b_i and a_i respectively. The matrix elements $V_k = \langle od|V|k\alpha\rangle$ define the hopping amplitude from an atomic d-state at the origin to an itinerant o-state in the band α. Newns and Rasolt [2] worked out a mean field theory of this model. They could estimate the critical temperature and its dependence in the doping. Performing a 1/N expansion, where $N = 2\sigma+1$ is the spin degeneracy, we consider the first order correction and calculate the self-energy of the holes.

On a microscopic level, the resistivity is due to the scattering of the holes by many different processes but in our model, the most important one appears to be the scattering by the a-boson[4]. The main contribution to the self-energy writes :

$$\Sigma(p,\omega_n) = -V^2/\beta \sum_{i\omega_v} \sum_q D(q,i\omega_v)\, G(p+q,i\omega_n+i\omega_v) \quad (2)$$

where G is the quasi-hole propagator ($G^{-1}(p,\omega) = \omega - \xi(p)$ where $\xi(p) = p^2/2m^* - \mu$) and D is the a-boson propagator, given by

$$D^{-1}(q,i\omega_v) = -i\omega_v + U_{eff} - NV^2/\beta \sum_{i\omega_n} \sum_k [\, G_{dd}(q-k, i\omega_v - i\omega_n) G_{cc}(k,i\omega_n) + G_{cd}(q-k,i\omega_v-i\omega_n) G_{cd}(k,i)\,] \quad (3)$$

Performing the integration over the momentum and frequencies of the localised d- and itinerant c-electrons, we find [4], in the approximation ω_v , $v^*_F q \ll 4\pi KT$:

$$D^{-1}(q,i\omega_v) = A\,[\, B \ln(T/Tc) - i\omega_v + C\, q^2 \,] \quad (4)$$

where $A = \dfrac{s_o^2}{s_o^2 + \varepsilon_d^2} \dfrac{NV^2 N_s \rho_o}{8\pi KT}$ $\quad B = \dfrac{4\pi KT}{\pi^3}$ $\quad C = \dfrac{7\zeta(3)}{\pi^2} \dfrac{v^{*2}_F}{4\pi KT}$

The parameters ε_d and s_o were calculated self-consistently in the mean field theory [2] while V ≈2eV and ρ_o ≈0.25eV^{-1} are given by band structure calculations [2] . The effective Fermi velocity is $v^*_F = m/m^*\, v_F \approx 0.2\, v_F$ and N_s is the number of unit cells. Introducing (3) in (2) and performing the usual integrals over momentum and energy , one finds :

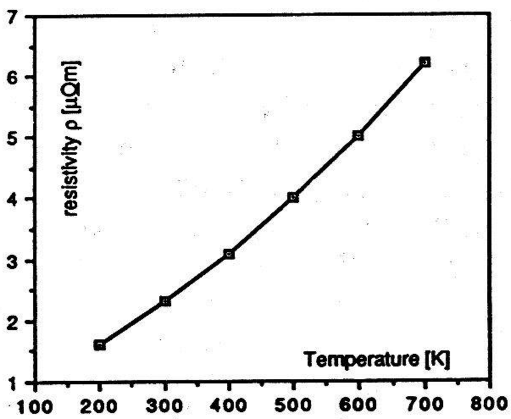
$$\rho = \frac{m^*}{ne^2\tau_a} = \frac{m^*}{ne^2}\frac{2}{\hbar}\,\mathrm{Im}\,\Sigma = \frac{m^*}{\hbar ne^2}\frac{4V^2}{(hv^*_F)^2 A}E(\overline{x})$$

$$\text{where } E(\overline{x}) = \int_{-\mu}^{\infty} dz\, \frac{e^z}{(1+e^z)^2}\int_0^{\overline{x}} dx \int_{-x-z}^{x-z} dy \frac{xy}{[(0.5\ln T/Tc + x^2/4\pi)^2 + y^2]}\frac{[n_F(y+z) + n_B(y)]}{\sqrt{x^2-(y+z)^2}}$$

with $z = \omega / KT$, $y = \omega' / KT$, $x = v^*_F q / KT$ and $\overline{x} = v^*_F\overline{q} / KT$

3. Results and discussion

In the above expression, there is one single free parameter $\overline{x} = v^*_F\, \overline{q} / KT$ which means that nothing in the theory fixes the value of the cut-off $\overline{q}$ of the a-boson momentum. The temperature dependence of the resistivity is very much sensitive to the value of this parameter, but if we choose the value $\overline{x} = 1$, which satisfies all the approximations done in the calculations, the resistivity is almost linear in the temperaure (see graph) as shown in the experiments [5]. Moreover, for n=3*10^{27} m^{-3} [5], its value is very close to the experimental one [5] $\rho^{exp}(T=300) \approx 4$ µΩm. We should of course understand the meaning of the relation $\overline{q} = KT/v^*_F$ if it has any and also analyse carefully Hall experiments to know more about the density n, taken here as a constant. Besides the results, the above calculation is interesting since it considers one of the many theories on the market of the High-Tc and we have to understand the normal state in order to know more about the superconducting state.



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