Resistivity of Doped Two-Leg Spin Ladders

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In doped two-leg spin ladder systems, holes are expected to form charged bosonic pairs. We study charge transport in this system in the temperature range where the bosons can be described as weakly interacting quasi-particles. We consider boson-phonon and boson-impurity scattering processes. We suggest that due to the Ioffe-Regel resistivity saturation mechanism, the resistivity may exhibit a local maximum at intermediate temperatures. We propose that this may explain a similar feature found in recent experimental results.

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I. INTRODUCTION

One of the most exciting advances in the field of high $T_c$ superconductivity and in the theory of strongly correlated electrons in the last few years has been the experimental study and the theoretical understanding of pure and doped quantum spin ladders [1]. In contrast to the one dimensional (1D) antiferromagnetic (AF) Heisenberg chain, where the ground-state has an infinite correlation length, and exhibits a slow decay of the spin correlations, even -leg (undoped) ladders have spin-liquid ground-states with purely short-range spin correlations. The exponential decay of the spin-spin correlation is produced by a finite spin gap, i.e., a finite energy gap to the lowest $S = 1$ excitation in the infinite ladder. Even-leg ladders are the realization of the Resonant Valence Bond (RVB) quantum liquid of singlets proposed by Anderson in the context of 2D $S = 1/2$ AF Heisenberg systems [2].

Two-leg $S = 1/2$ ladders are found in vanadyl pyrophosphate $(VO)_2P_2O_7$ and in some cuprates like $SrCu_2O_3$. Spin susceptibility, neutron scattering, NMR and muon spin resonance measurements are consistent with a spin gap.

Even-leg ladders are especially interesting under doping because theory has revealed that holes should pair to form bosons, in a relative “d-wave” state, with a superconducting ground-state at finite doping [3]. Copper-oxide compounds exhibiting one dimensional features with both isolated $CuO_2$ chains and $Cu_2O_3$ ladders (pairs of $CuO_2$ chains linked by oxygen atoms between the coppers) have recently been found to be superconducting [3]. In the compound $Sr_2Cu_{12}O_{24}O_{41}$, a copper valency of $\simeq 2.2$, i.e., a hole density of 0.2 per ladder-Cu is estimated [3]. NMR and conductivity measurements have been conducted on the latter compound, and the existence of the spin-gap is clearly established for pressures smaller than 29 kbar [3].

Thus, in the normal state of two-leg compounds the charge carriers are likely to be bosons, restricted to move preferentially in one dimension (1D). The proposal that CuO-planes in high-$T_c$ cuprates are Bose conductors in the normal state has been extensively discussed in connection with Anderson’s RVB model [2]. However, it is still controversial. Besides, bosons in this context are strongly coupled to fermionic spinons via a gauge field [3]. The situation is clearer and simpler in the doped spin ladders, where the bosonic carriers are not coupled to low energy spin excitations. Materials in which these ladders occur are good candidates for true bosonic conductors.

At low enough energy, a one dimensional bose gas can be described in terms of density fluctuations with an energy spectrum which is linear in wave vector $\mathbf{k}$ [4]. A one dimensional bose gas can thus be mapped on a one dimensional Luttinger liquid of fermions, the transport properties of which are known [5]. In the presence of a random impurity potential, Anderson localization at low temperatures causes the resistivity to increase to infinity as a power law of the inverse temperature. At larger temperature a metallic behavior may step in, but no intermediate maximum is expected.

There is a characteristic energy scale above which the collective density oscillation picture ceases to be valid, and the bose gas can be described by the semiclassical quasi-particle picture [6]. Assume that the interaction potential between bosons can be modeled by $c\delta(x_i - x_j)$, where $c$ is a constant. Then the excitation spectrum remains that of independent quasi particles for $\hbar^2k^2/2m_e \gtrsim cn_b$, where $m_e$ is the boson mass and $n_b$ is the linear boson density. Thus for $k_BT > cn_b$ the 1D Bose particle transport phenomena can be described within a semi-classical approach. At low density and small interaction strength $c$, this temperature can be small. Below $k_BT \leq cn_b$ the collective mode description of the bose gas should hold and the transport should then be described accordingly [7].

One of us pointed out a long time ago [8] that in Bose conductors the condition for the validity of semiclassical transport theory - that the carriers mean free path is greater than their De Broglie thermal wavelength - is much weaker than that for ordinary (Fermi) conductors, for which the mean free path has only to be greater
than the mean distance between carriers. It was suggested in Ref. [3], on the basis of the Ioffe-Regel criterion [3], that when the mean free path is smaller than De Broglie’s thermal wavelength the resistivity saturates at a temperature-dependent value, which may be estimated by replacing the mean free path by De Broglie’s thermal wavelength in Drude’s formula for the resistivity.

The purpose of this note is to examine the consequences of the semiclassical picture on the resistivity of doped quantum spin ladder systems, in the spin gap regime. The hole pairs are treated as structureless bosonic particle: no account is taken of the d-wave like symmetry of their wave function [3]. In the following we examine the temperature dependent resistivity of a one dimensional boson liquid interacting weakly with phonons and with impurities. We propose that this straightforward analysis leads to a qualitative understanding of the experimental behavior of the electrical resistivity with temperature in doped quantum spin ladders [3].

II. RESISTIVITY

We assume that the free boson states are described by an energy band $\epsilon(k)$ the bandwidth of which for $k$ perpendicular to the ladders direction (c-direction) is small compared to $k_BT$. For motion along the ladders we assume that the bandwidth $W_c$ is large compared to $k_BT$. Under these assumptions we may approximate $\epsilon(k)$ by $\epsilon(k) = \hbar^2 k^2/2m_c$, where $-\pi/a_c \leq k_c \leq \pi/a_c$ is the component of $k$ along the ladders direction, $a_c$ is the period within the ladder and $m_c$ is the effective mass.

The calculation of the resistivity follows the traditional Boltzmann equation approach, as described by Ziman [3]. We consider the contributions from boson-impurity and boson-phonon scattering to the resistivity.

A. BOSON-IMPURITY SCATTERING

The expression for the impurity scattering contribution to the resistivity, $\rho_I$ is given by [13,14],

$$\rho_I = \frac{\int d^3k d^3k' [(k - k') \cdot \vec{u}]^2 P_i^k}{2k_BT \int d^3k' v_{k'}(k \cdot u) \frac{\partial n_k}{\partial \epsilon_k}} .$$

(2.1)

In Eq. (2.1) $\vec{u}$ is the bosons drift velocity along the ladders direction, $v_{k} = \partial\epsilon(k)/\partial k$ and $P_k^\alpha$ is the transition probability, given by

$$P_k^\alpha = \frac{2\pi}{\hbar} n_I | V_{b-i} |^2 \delta(\epsilon(k) - \epsilon(k')) n_k^b(1 + n_{k'}^b) ,$$

(2.2)

where $n_I$ is the number of impurities by $cm^3$ and $V_{b-i}$ is the boson-impurity interaction matrix element, assumed constant,

$$n_k^b = \frac{1}{e^{(\epsilon(k) - \mu)/k_BT} - 1}$$

(2.3)

is the boson occupation number, and $\mu$ is the chemical potential.

The relation between $\mu$ and the number of bosons per cm in the ladders, $n_b$, is obtained in the usual way, assuming non-interacting bosons [13]. We find

$$n_b \lambda_c = g_1/2(z) ,$$

(2.4)

where $\lambda_c = \sqrt{2\pi/m_c k_BT}$ is De Broglie’s thermal wavelength for motion along the ladders, $z = e^{\mu/k_BT}$ and $g_1/2 = \sum_{j=1}^\infty z^j/j^{1/2}$.

Carrying out the integrations in Eq. (2.1) we find that

$$\rho_I = \frac{m_c}{nq^2} \frac{2m_b n_I | V_{b-i} |^2}{\pi \hbar^2 n_b^2} n_0^b ,$$

(2.5)

where $n$ is the number of bosons per cm$^3$ and $n_0^b = z/(1-z)$ is the zero-momentum state occupation number [14]. Note that the $T$-dependence of $\rho_I$ come solely from the $n_0^b$ term. The latter is a monotonously decreasing function of $T$. The behavior of the impurity contribution to the resistivity with $T$ is unusual because it increases as $T$ decreases. This is a consequence of the bosonic 1D character of the problem.

B. BOSON-PHONON SCATTERING

The boson-phonon scattering contribution to the resistivity, $\rho_P$ is given by [13],

$$\rho_P = \frac{\int d^3kd^3k' |(k - k') \cdot \vec{u}|^2 P_k^\alpha}{k_BT \int d^3k' v_{k'}(k \cdot u) \frac{\partial n_k}{\partial \epsilon_k}} .$$

(2.6)

where $P_k^\alpha$ is the transition probability. Assuming a deformation potential-like interaction between the bosons and the phonons and a Debye phonon spectrum, with sound velocity $s$, this quantity is given by

$$P_k^\alpha = \frac{2\alpha}{\pi} \delta(\epsilon(k) - \epsilon(k') - \hbar s Q)$$

(2.7)

$$\times n_Q n_k n_b^b(1 + n_{k'}^b) ,$$

where $\alpha$ is a constant that characterises the boson-phonon interaction and $n_Q$ is the phonon occupation number.

We write $\rho_P$ as

$$\rho_P = \frac{m_c}{nq^2} \frac{\alpha k_D^4}{(2\pi)^3 s n_0} \left( \frac{T}{\Theta_D} \right)^4 J(T) ,$$

(2.8)

where $k_D$ is Debye’s wavevector, $\Theta_D = \hbar s k_D/k_B$ is Debye’s temperature,

$$J(T) = \int_0^\Theta_D d\xi \xi^4 n(\xi) \int_0^1 dp m(\chi - (\eta))(1 + n(\chi + (\eta))) ,$$

(2.9)
n(x) = (e^x - 1)^{-1} and χ±(η) = mc^2/2η^2 ± sQ/2 + Q^2η^2/8me - μ/k_BT.

At low temperatures, ΘD ≫ T, χ±(η) ≃ Q^2η^2/8me and it follows from Eqs. (2.8) and (2.9) that

\[ \rho_P \propto T^3 \eta_0^2. \]  

(2.10)

At high temperatures, T ≫ ΘD, and assuming that mc^2/k_BT ≪ 1 and ncλc ≪ 1 we find that

\[ \rho_P \propto T^{1/2}. \]  

(2.11)

C. Resistivity Saturation

The expressions for ρ used above, Eqs. (2.1) and (2.6), are valid as long as the mean free path for motion along the ladders ℓc is greater than λc. For ℓc < λc, resistivity saturation is believed to occur. An estimate of the saturation value of the resistivity ρSAT is obtained by substituting ℓc by λc in Drude’s formula ρ = mc/νT^2. Defining ℓc as ℓc = vT, where vT is the bosons thermal velocity, defined as vT = \sqrt{2(ε)/mc}, where ε is the bosons mean thermal velocity. Using the boson distribution Eq. (2.3) we find that

\[ v_T = \sqrt{\frac{k_BT}{mc}} \cdot \frac{g_{3/2}(z)}{g_{1/2}(z)}, \]  

(2.12)

where g_{3/2} = \sum_{j=1}^{∞} z^j / j^{3/2}. Thus

\[ \rho_{SAT} \sim \frac{mc^2k_BT}{(2\pi)^{1/2}\hbar ne^2} \cdot \frac{g_{3/2}(z)}{g_{1/2}(z)}. \]  

(2.13)

III. DISCUSSION

According to Eq. (2.13) ρSAT increases with increasing T, whereas ρI increases with decreasing T. Thus, if the boson-impurity interaction is sufficiently strong, there is a temperature below which ρI > ρSAT. Since, according to the Ioffe-Regel criterion the resistivity cannot be greater than ρSAT, saturation occurs and the resistivity curve follows ρSAT. Thus there is a resistivity maximum at a temperature T_0 that can be estimated as that for which ρI ≃ ρSAT. This is the main result of this paper. A typical resistivity curve predicted by our model is shown in Fig. 1. This figure also shows experimental resistivity data for Sr_xCa_{1-x}Cu_{2}O_{4} at 1.5GPa obtained in Ref. 5. In Fig. 1 the contributions to the resistivity from phonons, impurities and from the saturation mechanism are normalized as ρP(T = 100K) = ρSAT(T = 100K) = 22mΩ·cm and ρP(T = 200K) = 5mΩ·cm. These values for ρI and ρSAT are chosen so that the theoretical prediction coincides with the experimental one. The ρP curve is a smooth interpolation between the T ≪ ΘD and T ≫ ΘD behaviors, with ΘD = 200K. The value of ρP at T = ΘD = 200K is chosen for illustrative purposes only.

We propose that the local resistivity maximum observed in the Sr_xCa_{1-x}Cu_{2}O_{4} data at T ∼ 100K and several pressures [3] arises from the same mechanism as that for the 1D boson model discussed above. Thus, we interpret the decreasing resistivity curves below and above the temperature where it is maximum as resulting from resistivity saturation and from boson-impurity scattering, respectively. In order for this interpretation to be consistent it is necessary that, at T ∼ 100K, ρI ≃ ρSAT ∼ 20mΩ·cm. According to Eq. (2.13), this requires that mc/men ∼ 4.8 × 10^{-18} cm^3, where mc is the mass of the electron.

We show in Fig. 2 the mean free path along the ladder direction obtained from the Sr_xCa_{1-x}Cu_{2}O_{4} data at 1.5GPa [3] using the Drude formula for the resistivity and the definition of ℓc given in Sec. II C. In Fig. 2 the values of mc and n are chosen so that ℓc = λc at T = 100K. This requires, as discussed above, that mc/men = 4.8 × 10^{-18} cm^3. We choose mc/men = 180 and n = 3.7 × 10^{19} cm^{-3}, which is equivalent to 10^{-2} holes per ladder Cu atom. It is clear from Fig. 2 that there is a crossover around T = 100K from a regime of rapid variation of ℓc with T, that according to our interpretation results from boson-impurity scattering, to a regime of slow variation of ℓc with T, from T ∼ 100K to T ∼ 50K. The latter is consistent with the idea of resistivity saturation, as discussed in Ref. [3]. We also note that, according to our proposal, the boson-impurity scattering contribution to ℓc can be estimated for T < 100K by extrapolating the high-temperature ℓc × T data to lower T values. As shown in Fig. 2 this leads to a rapidly decreasing ℓc × T curve. This further indicates that, within the semiclassical picture, resistivity saturation is bound to occur in this compound, independent of the precise value of ℓc/λc at which it sets in.

The numerical values for mc and n obtained above are rough estimates. Nevertheless, our picture requires values of mc which are too large compared to those obtained from theoretical estimates for pure two-leg ladders [17] and values of n that are smaller than those reported in experiments (∼ 0.2 holes per ladder Cu). However, the possibility of large effective mass enhancement due to boson-phonon interaction effects, neglected in theoretical considerations, cannot be excluded. Besides, the Ioffe-Regel criterion gives only very rough order of magnitude estimates for the values of ℓc/λc and of ρ at saturation, so that the numerical values for mc and n used in our calculations may be uncertain by a large factor.

For the semiclassical picture to be valid a second condition must be met: the cross over temperature Θ to collective bosonic behavior must be smaller than the temperature at the resistivity maximum. Our order of magnitude estimate for this relies on the fact that the hole pair spatial extension is δ, so that the change in
binding energy $\Delta E$ of a pair when colliding with another one is $\Delta E \sim E_a / \delta$, because two hole pairs cannot occupy the same rung. Since $E \sim 200K$, we find $\theta = c n_b / k_B \sim E_n \delta (a_c / \delta) \sim 20K$. This value of $\theta$ further supports our proposal.

To conclude, we find that the simple minded semiclassical transport theory proposed here for the bosonic hole pairs in the quantum spin ladder system may account for the observed dependence of the resistivity on the temperature observed for $Sr_2Ca_{1-x}Cu_{24}O_{41}$. Our predictions can, in principle, be tested by changing the impurity concentration, $n_I$. According to our semiclassical model, increasing $n_I$ should shift the resistivity maximum to higher temperatures and increase its intensity, whereas decreasing $n_I$ should shift the maximum to lower temperatures and decrease its intensity.

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FIG. 1. Thick line: calculated resistivity versus temperature curve for $m_c = 180m_e$ and $10^{-2}$ holes per ladder Cu. Squares: $Sr_2Ca_{12}Cu_{24}O_{41}$ data. Dashed lines: individual contributions from phonons, impurities and the saturation mechanism (see text).

FIG. 2. Mean free path versus temperature for $Sr_2Ca_{12}Cu_{24}O_{41}$ at 1.5GPa. Dashed curve: extrapolation form high temperature data.
Fig. 1

$\rho (\text{m}\Omega \cdot \text{cm})$

$\rho_{\text{SAT}}$

$\rho_1$

$\rho_P$

$\rho_1 + \rho_P$

1.5 GPa (Ref. 5)
Fig. 2