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Electronic conduction in highly anisotropic systems

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Abstract:

We have calculated the ratio of conductivities along the chains and perpendicular to the chains in highly anisotropic quasi-one-dimensional systems. The electronic motion along the transverse direction is viewed as a coherent inter-chain tunnelling between neighbouring chains blocked by repeated intra-chain incoherent scatterings. Our results predict intrinsically the same temperature dependence for both conductivities. It also predicts a linear dependence of the anisotropy ratio on the carrier concentration, which is absent in the earlier treatments of the same problem.

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The conduction in highly anisotropic systems exhibit some unusual striking features. In the recently discovered high T_c layered oxides the transport properties are different in different directions; metallic transport in the ab plane and non metallic (or metallic) transport along the c-axis [1-3]. Especially the c-axis resistivity of $YBa_2Cu_3C_{7-\delta}$ is known to be metallic [4] with $(d\rho_c/dT) > 0$. This is some what unusual given the fact that the resistivities of the samples are much larger than the Mott's maximum metallic resistance (or even Mooij value [5])and yet they show the metallic behaviour. The observed value of the c-axis resistivity is much larger than (10 to 100 times) the Ioffe-Regel-Mott limit which provides a criterion for metals in a conventional Boltzmann type of band transport. Generally in disordered systems it is well established that, when the value of the resistance is larger than the Mott's maximum resistance ($\sim 100\mu\Omega cm$), the incipient localization sets in. In this regime one expects the negative temperature coefficient for resistance (TCR) arising due to suppression of the quantum interference by the inelastic phonon scattering. The negative TCR may also arise due the breakdown of the adiabatic approximation in the metallic phase leading to phonon-assisted tunnelling [5]. However, the high-T_c compound mentioned above shows completely the opposite trend for TCR compared to all other disordered systems. In such pure anisotropic systems effect of localization seems to be less important. It should be noted that the localization being purely quantum mechanical coherent back scattering phenomena that requires electron to retain its local coherence in all directions. Thus it is not possible to have states localized in one-direction only. Similar problem seems to arise in quasi one-dimensional systems [6]. For instance, in tetrathiafulvalene-tetracyanoquinodimethane (TTF-TCNQ) crystals. In these systems band width anisotropy between a direction (between the chains) and b direction (along the chains) is roughtly of the order of $t_a/t_b \sim 0.01$. In these systems conduction is metallic in both directions. The resistivity is a few $m\Omega$cm

along the chains and several Ω cm between the chains at room temperature. Even though the mean free path perpendicular to the chains is much shorter than the lattice constant, $d\rho_a/dT > 0$. This behaviour calls for a new mechanism for transport other than the simple Boltzmann type band transport for highly anisotropic systems. Soda et al [6] have explained this in a simple picture, supposing coherent on-chain and incoherent inter-chain couplings. In the following based on the same picture we derive an expression for ratio of the conductivities (resistivities) along longitudinal and transverse direction. However, our final result differs from the earlier one with an additional factor arising due to the effective number of carriers involved in the motion along the transverse directions.

We proceed here along the same lines as our recent treatment on the c-axis resistivity in layered compounds [7]. We generalize our treatment to quasi-one dimensional anisotropic systems. For simplicity we consider first the two dimensional anisotropic conductor. In this case we have one-dimensional chains along the b directions (or $\|$ direction) and they are weakly coupled along the a direction (or $\perp$ directions). In our treatment intra-chain electron transport is characterized by a Boltzmann-like mean free path. The intrachain resistivity comes entirely from the mean free lifetime τ, and is given by the Drude relation $\rho_{\|} = m^*_{\|}/ne^2\tau$, where $m^*_{\|}$ is the in-chain electron effective mass. The intra-chain inelastic scatterings characterized by τ interrupt and therefore, block the coherent tunnelling of the electrons to the neighbouring chains-under the influence of tunnelling matrix element $t_\perp$. This blocking of coherent motion modifies $t_\perp$ to $t_\perp^2\tau/\hbar$ for $t_\perp\tau/\hbar << 1$. The latter inequality simply assumes that the large number of intra-chain scattering takes place before an inter-chain tunnelling occurs. This is equivalent to having large anisotropy, $\rho_\perp/\rho_{\|} >> 1$, which will be assumed throughout. With these conditions successive inter-chain tunnelling events are incoherent (or uncorrelated) and therefore it is sufficient to consider tunnelling between just two neighbouring chains,

lebeled 1 and 2 say.

The Hamiltonian in our model is given in obvious notation, $H = H_0 + H'$, with

$$H_0 = \sum_{K,\sigma} \epsilon_K\, C^+_{1,K\sigma} C_{1,K\sigma} + \sum_{K,\sigma} \epsilon_k\, C^+_{2,K\sigma} C_{2,K\sigma}$$
$$+ t_\perp \sum (C^+_{2,K\sigma} C_{1,K\sigma} + hc), \qquad (1)$$

where H' is the unspecified intra-chain inelastic scattering term leading to the finite lifetime τ for the transport along the chains. The energy dispersion relation along the 1-d chains is given by $\epsilon_K = -2t_{\|} cos Kb$, where b is the lattice spacing along the chains. In absence of H', if we consider a situaiton where at time t = 0 the electron with a quasi-momentum K is on the chain 1, then at later time t the probability of electron to persist on the same plane P_{11} is given by $P_{11} = cos^2(t_\perp t/\hbar)$. With the introduction of H'_0 this coherence between the chains is lost. Consequently the survival probability P_{11} for the electron to persist in the chain 1 is given by

$$P_{11} = exp[-\frac{2t_\perp^2 \tau}{\hbar^2} t] \qquad (2)$$

For the details of the evaluation of P_{11} see ,ref[7,8]. Here τ is the mean free lifetime of the electron in the chain. From the equation (2) one can easily get the inter chain transition rate W (or the hopping probability) as $W = (2t_\perp^2 \tau/\hbar^2)$. Soda et al [6] have also obtained the same expression for the hopping probability between the chains. However, to calculate the transverse conductivity they assume Einstein relation between the conductivity and diffusion coefficient (D). In their calculation transverse diffusion constant D is given at once by $D = a^2 W$, where a is a lattice constant along the transverse direction. It should be noted that this procedure subsumes that the number of electrons involved in transport along the longitudinal direction are same as those involved in the transverse direction, which is not true. It has recently been shown [9] explicitly using the anisotropic tight

binding Hamiltonian that the density of mobile carriers along the transverse direction is much less than that along the longitudinal direction. In an anisotropic system when the density of electron increases, the electrons can no longer be described by plane waves in transverse direction due to the Bragg reflection. This is because the Fermi surface will touch the Brillouin zone boundary along $K_\perp = \pm\pi$ first. Hence only the fraction of electron of the order of $(t_\perp/t_\parallel)n$ can contribute to the electrical conductivity in the transverse direction. To calculate the transverse conductivity we proceed along the line now well known in the theory of quantum transport in mesoscopic systems. Let an electric field E be applied perpendicular to the pair of chains seperated by the distance a. This will generate a chemical potential difference $\Delta\mu = eaE$ between the two chains. Naturally this will expose number of $\Delta\mu g_{1d}$ of unoccupied states per unit length into which the electrons are free to make the inter-chain transitions. Here g_{1d} is the 1-d density of states per unit length. Now the inter-chain current density will be given by $j = e(\Delta\mu g_{1d})W$. Thus the transverse resistivity is given by $\rho_\perp \equiv (E/j)$, substituting the value for W we get

$$\rho_\perp = (\hbar^2/2e^2 a g_{1d} t_\perp^2 \tau) \tag{3}$$

This is our final result for the transverse resistivity for the two dimensional anisotropic quasi-one-dimensional system. As mentioned earlier the longitudinal resistivity is given by the Drude relation $\rho_\parallel = m_\parallel^*/ne^2\tau$. One can easily generalize the relation (3) to 3-dimensional anisotropic quasi-one-dimensional conductors, where the $\rho_\perp(d=3)$ is given by $\rho_\perp(d=3) = (\hbar^2/2e^2 g_{1d} t_\perp^2 \tau)$. For the further calculation of ratio of resistivities we make some simple approximations. First the energy dispersion relation $\in (K) = -2t_\parallel \cos Kb$ gives a values for the effective mass $m_\parallel^*$ to be $m_\parallel^* = (\hbar^2/2t_\parallel b^2)$. Since the band width of 1-d chain is given by $4t_\parallel$ we take the value for g_{1d} to be an averaged value $g_{1d} = 1/2t_\parallel b$, including the spin. With these values one can immediately get the

anisotropic ratio of resistivities, namely

$$\rho_\perp/\rho_\parallel = 2(b/a)^2(t_\parallel/t_\perp)^2\delta \tag{4}$$

This relation is independent of the dimensionality and δ is the number of transport charge carriers per site in the chain given by (nab) and (na^2b) for two and three dimensional quasi-one-dimensional conductors respectively.

Our result (4) differs from that of Soda et al [6] by an extra factor of δ. For the three dimensional anisotropic layered compounds [7] factor 4 appears instead of 2 in right hand side of equation (4). Interestingly our result predicts a linear dependence of the anisotropic ratio on the carrier concentration δ, which should be experimentally a verifiable feature. The temperature dependence of $\rho_\perp$ is similar to that of $\rho_\parallel$, as the factor τ enters in the same way in the expressions for both cases. The additional temperature dependence in $\rho_\perp$ may arise due to the renormalization of the tunnelling matrix element $t_\perp$ due to adiabatic phonons. For the discussion on this phonon renormalization of $t_\perp$ and the role of disorder on $\rho_\parallel$ and $\rho_\perp$ we refer to our earlier work [7] for the details. At present we are exploring to extend our work to other transport properties of highly anisotropic systems such as Hal coefficient and electronic thermal conduction.

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