Anisotropic Localization Effect in Layered Materials

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Abstract

We investigate localization properties in the highly anisotropic and intrinsically disordered layered material, which is analogous to high-$T_c$ cuprates. By varying the anisotropy of the system which is parameterized by the interlayer hopping $t_p$, we find a crossover from two-dimensional (2D) to three-dimensional (3D) behavior at a critical hopping amplitude $t_{pc}$, where a mobility edge starts to appear. We show that below the mobility edge, anisotropic localization effect may exist for a finite size system, when the $ab$-plane localization length is longer than the system size and the $c$-axis localization length is shorter than the system size. Nevertheless, we argue that such anisotropic localization can not account for the “semiconductor” like behavior of the $c$-axis resistivity of high $T_c$ cuprates.

PACS numbers: 71.30.+h, 74.25.Fy, 74.80.Dm
It has been controversial whether anisotropic localization could exist in intrinsically disordered layered systems such as the high-\(T_c\) cuprates [1,2]. There are two interesting theoretical issues: first, whether it is possible at all for a three-dimensional (3D) system to be localized in one direction and extended in the other two directions; secondly, if it is possible, whether this anisotropic localization effect can account for the \(c\)-axis resistivity in high \(T_c\) cuprates. In this paper, we address both issues.

According to the scaling theory of metal-insulator transition [3], for an infinite 2D system, no matter how weak the disorder is, there is no real metallic behavior, the system is localized. In the presence of inelastic scattering, however, when the length scale of inelastic scattering \(L_{in}\) is smaller than the localization length \(\xi\), electron loses its phase coherence before it can finish the back scattering process, thus localization can not be realized. This is the so called finite size effect, the system has the same physical property as if it has a size of order of \(L_{in}\). In a physical system, the inelastic scattering length \(L_{in}\) is a function of temperature which decreases as temperature increases, thus effectively, one can mimic the effect of temperature by changing the cutoff length of the system. If the localization length is longer than the cutoff length, the system would have metallic behavior; otherwise, it would behave as an insulator. This is the reason why two-dimensional electron systems in semiconductor heterostructures have very high mobility. One expects that anisotropic transport behavior (such as in high \(T_c\) cuprates) could arise in a finite-size (or at finite temperature) anisotropic system (which has different localization lengths along different directions) even if the system is below the mobility edge.

While a 2D system is always localized, it is known that there is a mobility edge in 3D system, where metal insulator transition occurs [3]. We model the highly anisotropic and disordered layered material by an anisotropic tight binding lattice, which is parameterized by hopping \(t\) (which is set to be 1 throughout this paper) in the \(ab\)-plane and \(tp\) along the \(c\)-axis. In the limit of \(tp = 0\), the system is equivalent to a set of disconnected 2D planes, and therefore has no mobility edge. While at \(tp/t = 1\), the model describes an isotropic 3D system, there is a well defined mobility edge, whose position is in principle a function
of disorder. It is interesting to investigate the localization properties in the intermediate regime \((0 < t_p/t < 1)\). Previous work [4] on this model has shown that the mobility edge immediately emerges once a finite \(t_p\) is introduced. However, in the presence of strong disorders, the situation is more complicated. One expects that the mobility edge appears only when \(t_p\) exceeds a critical value \(t_{p_c}\) which is a function of the disorder. Equivalently, if one fixes the energy to be at the band center \(E = 0\), and changes \(t_p\), one expects a metal-insulator transition at \(t_p = t_{p_c}\), since \(E = 0\) is where the extended states start to form once the mobility edge appears. This effect is somewhat similar to the effect studied by Clark et al. [5], in which they find a critical hopping amplitude between two coupled Luttinger Chains, which separates coherent from incoherent tunneling between two chains.

In this paper, we systematically investigate the possible anisotropic localization effect in layered materials. The conductances for a cubic sample (along both \(c\)-axis and \(ab\)-plane) are calculated by using the Landauer-Büttiker formula. Our numerical results show that upon increasing the strength of interplane hopping through a critical \(t_{p_c}\), \(c\)-axis conductance changes from semiconductor like to metallic, provided that the \(ab\)-plane is sufficiently disordered (characterized by disorder strength \(W\)), yet metallic. We attribute this phenomenon to the highly anisotropic localization effect – a metal-insulator transition along \(c\)-axis for a finite-size sample. We also calculate the finite-size localization length along the \(c\)-axis using the transfer matrix technique. By carrying out a finite-size scaling analysis, we found a 2D to 3D crossover where a mobility edge starts to emerge when \(c\)-axis hopping is above the same critical \(t_{p_c}\). For highly anisotropic system (such as \(tp < 0.3t\)), the critical \(t_{p_c}\) could be determined from a universal relation \(W/t_{p_c} \sim 30 – 40\). We discuss the relevance of this anisotropic localization effect to the anisotropic transport phenomena in high-\(T_c\) cuprates.

In the following, we briefly outline our model and technique to calculate the conductance. We model our anisotropic three-dimensional system in a cubic geometry with a finite width \((M)\) square lattice with nearest neighbor hopping. The disorder potential is modeled by the on-site white-noise potential \(V_{ijm}\) \((i, j\) denote the column and chain indices, \(m\) denotes the plane index) ranging from \(-W/2\) to \(W/2\). The interplane hopping along \(c\)-axis \(t_p\) is different
from the $ab$-plane hopping amplitude $t$. We calculate the conductance in both $ab$-plane and $c$-axis, for different degree of anisotropy levels $tp/t \sim 0 - 0.5$. The Hamiltonian of this system can be written as:

$$
\mathcal{H} = \sum_{ijm} V_{ijm} |ijm><ijm| - t \sum_m \sum_{<ijkl>} [|ijm><klm| + c.c.] - tp \sum_{ijm} [|ijm><ijm| + 1| + c.c.],
$$

where $<ij;kl>$ indicates nearest neighbors on the $m$th plane. From now on, we choose $ab$-plane hopping amplitude $t$ as the energy unit ($t = 1$ throughout the paper). The dc conductance at Fermi energy $E$ for a cubic sample is calculated using the Landauer-Büttiker formula [6]:

$$
g = \frac{e^2}{h} \text{Tr} T^\dagger(E) T(E),
$$

where $T(E)$ is the transmission matrix which is related to the retarded Greens function $G^+(0,L)$ across the disordered sample (along direction $L$ in a $M \times M \times L$ sample). The retarded single particle Greens function can be calculated using the recursive Greens-function algorithm [4].

We present in Fig.1, the calculated resistance (1,000 sample ensemble average) as function of the inverse of the sample size (which could mimic the effect of temperature) for both $ab$-plane and $c$-axis, with different strength of disorder $W$. All the calculations are at the band center, where energy $E = 0$. From Fig.1, we can see that for $W = 2, 4, 6,$ and 8, the in-plane resistance increases with $1/M$, displaying a metallic behavior, even more so (the slope increases) as the hopping amplitude $tp$ in the $c$-axis increases. While the $c$-axis resistance may change from metallic to insulating by changing $tp$. For example, for $W = 2$, the $c$-axis resistance $R$ is metallic-like for $tp \geq 0.05$, while for $tp \leq 0.02$, $R$ increases with sample size $M$, the system appears to be localized along $c$ direction. In this case, there seems to be a critical hopping amplitude $tp_c \sim 0.03 - 0.04$ that separates the localized and the metallic conduction along the $c$-axis. As we go to higher degree of disorder, $tp_c$ increases. This
anisotropic localization effect (the system is only localized along c-axis) does not violate
the scaling theory of localization [3] which states that there only exists a single mobility
edge for any disordered system even if it is highly anisotropic (as shown in recent numerical
calculations [3]), i.e. for large enough system, ab-plane would undergo the metal-insulator
transition at the same $t_{pc}$ as along the c-axis. Below the mobility edge, the localization
length in the ab-plane is extremely large, thus the system could have metallic behavior
along ab-plane if the sample size is smaller than the localization length. Nevertheless, if
the system is big enough, we expect the ab-plane would have insulating behavior [4]. It is
worth mentioning that above the mobility edge (when $tp > t_{pc}$), the calculated conductance
in both ab-plane and c-axis increase linearly with the increasing sample size $M$, indicating
typical 3D Drude conductance behavior.

The finite size correction to the conductivities of an anisotropic system has been calcu-
lated by Wölffe and Bhatt, [10] from evaluating the maximally crossed diagrams by assum-
ing both anisotropic single particle energy dispersions and anisotropic impurity scatterings.
Their results show that backscattering gives rise to a diffusive correction to the metallic con-
ductivity, and that the effects of anisotropy near the weak coupling (metallic) fixed point can
be completely absorbed into an anisotropic diffusion coefficient. More recent work by Szott
et al has microscopically derived the anisotropic diffusion constants from the anisotropic
impurity scattering rates for the superlattice semiconductor, and concluded that the con-
ductivity for superlattices still has the diffusive form. [11] Nevertheless, these above work did
not address the 2D-3D transition found in our numerical calculations. To be more specific,
it is shown that the contribution from backscattering (weak localization correction) reduces
the conductivity differently in 2D and 3D. [12]

\[
\sigma_{3D}(M) = \frac{ne^2\tau}{m^*} - \frac{e^2}{\hbar\pi^2} \left[ \frac{1}{l} - \frac{1}{M} \right] \\
\sigma_{2D}(M) = \frac{ne^2\tau}{m^*} - \frac{e^2}{\hbar\pi^2} \ln \left[ \frac{M}{l} \right]
\]

(3a) (3b)

where $l$ is the mean free path. Therefore, we expect that in our anisotropic layered system,
the weak localization correction would have a crossover from logarithmic behavior to $1/M$
as $tp$ increases from 0 (pure 2D system) to 1 (isotropic 3D system). On the other hand, our numerical data show that above the mobility edge (when $tp > tp_c$), the calculated conductance in both $ab$-plane and $c$-axis increase linearly with the increasing sample size $M$, exhibiting a typical 3D Drude conductance. For large sample sizes, the breaking away from linear behavior in our data compare favorably to a negative weak localization correction in the conductivity. However, strong finite size effect and statistical fluctuations do not allow us to make a quantitative comparison with the analytic results of Refs [10] and [11].

In order to study the transition between 2D and 3D behaviors by tuning $tp$ in our anisotropic tight-binding model, we need to calculate the localization length directly. We now introduce the technique to calculate the localization length in a long square bar geometry ($M \times M \times L$) along the $c$-axis. For a specific energy $E$, a transfer matrix $T_m$ can be easily set up mapping the wavefunction amplitudes at plane $m-1$ and $m$ to those at plane $m+1$, i.e.

$$
\begin{pmatrix}
\psi_{m+1} \\
\psi_m \\
\psi_{m-1}
\end{pmatrix} =
T_m
\begin{pmatrix}
\psi_m \\
\psi_{m-1}
\end{pmatrix} =
\begin{pmatrix}
\frac{H_m - E}{tp}
& -I \\
I
& 0
\end{pmatrix}
\begin{pmatrix}
\psi_m \\
\psi_{m-1}
\end{pmatrix},
$$

(4)

where $H_m$ is the Hamiltonian for the $m$th plane, $I$ is a $M^2 \times M^2$ unit matrix. Using a standard iteration algorithm [13], we can calculate the Lyapunov exponents for the transfer matrix $T_m$. The localization length $\lambda_M(E)$ for energy $E$ at finite width $M$ is then given by the inverse of the smallest Lyapunov exponent. We choose sample length $L(\approx 1000)$ to be long enough so that the self-averaging effect automatically takes care of the ensemble statistical fluctuations. In our calculation, we fix the energy at $E = 0$ and change the hopping amplitude $tp$ for sample size $M = 4 \sim 16$.

To obtain the thermodynamic properties of the system, we carry out a finite-size scaling analysis of the renormalized localization length $\lambda_M/M$, which satisfies a simple scaling law. As shown in Fig.2, all $\lambda_M/M$ data for different disorder and hopping amplitude $tp$ fall on the same curve which can be written as:

$$
\lambda_M(W, tp)/M = f[\xi(W, tp)/M]
$$

(5)
where $\xi(W, tp)$ is a characteristic length which depends on $W$ (or energy $E$) but not on $M$. Similar to the scaling analysis for an isotropic 3D system [14], the scaling function has two branches. The scaling parameter associated with the lower branch corresponds to the thermodynamic localization length, i.e. $\xi = \lambda_\infty$. The one associated with the upper branch belongs to the extended regime and identifies with the resistivity of the system [14]. The scaling parameter should diverge at the critical point which separates the two branches in the scaling function indicating a metal-insulator transition. The inset of Fig.2 plot the scaling parameter $\xi$ as a function of $W/tp$ for all the $W$ and $tp$ shown in the scaling curve. We can see that for the highly anisotropic system we considered ($tp/t < 0.5$), the scaling parameter is a universal function of $W/tp$. At $W/tp \sim 30 - 40$, $\xi$ diverges, showing a typical Anderson metal-insulator transition. We now compare to Fig.1, where the critical hopping amplitude separating the metallic and localized regimes for $W = 2, 4, 6, 8$ all seem to be pinned at $W/tp_c \sim 30 - 40$. Thus we argue for this highly anisotropic tight-binding model ($tp < 0.5$), a typical metal-insulator transition occurs at certain $tp_c(W)$, where $W/tp_c$ is a universal number independent of hopping $tp$ and on-site disorder $W$.

Here we should emphasize that the relation $W/tp_c \sim 30 - 40$ is only true for highly anisotropic system where $tp << t$. (We fix $t = 1$ in this paper.) However, for systems with modest anisotropy, namely $0.5 < tp/t < 1$, we do not expect that the relation $W/tp_c \sim 30 - 40$ to be relevant. In fact, we find that $W/tp_c \approx 16$ for isotropic system (i.e. $tp = t$), which is consistent with previous works [14]. For the strong anisotropic system we have studied, where $tp/t < 0.5$, the system is closer to 2D, the mobility edge is mostly determined by the small amount of interlayer hopping $tp$, while the in-plane hopping $t$ plays a much weaker role in determining the critical point of $W/tp_c$ other than setting the energy scale of both $W$ and $tp$. As the system becomes less anisotropic, $tp$ and $t$ become compatible, therefore should both determine the mobility edge. Thus we find for $tp/t < 0.5$, the mobility edge appears at $W/tp_c \sim 30 - 40$ and $W/t \sim 2 - 8$; when anisotropy decreases, at $0.5 < tp/t < 1$, it is only natural that these two ratios merge closer, and eventually, at $tp = t$, we have $W/tp_c = W/t \sim 16$. Another way to understand this is to write the critical ratio $W/tp_c$ as
function of \(tp/t\) which characterizes the anisotropy of the system, we find \(W/tp_c = 30 - 40\) at \(tp/t \ll 1\), and \(W/tp_c = 16\) at \(tp/t = 1\). We expect a smooth crossover in the intermediate anisotropy regime of \(0.5 < tp/t < 1\). Our results show that \(W/tp_c\) is overall \(t\)-dependent, while in the strong anisotropic limit of \(tp/t < 0.5\), the \(t\)-dependence of \(W/tp_c\) becomes much weaker.

In conclusion, we observe a crossover from 2D to 3D behavior in the highly anisotropic layered system when the interlayer hopping amplitude exceeds a critical value. This crossover behavior of localization from 2D to 3D has been studied by various researchers, such as in Ref. 4. However, we have investigated the non-trivial consequences of this crossover behavior by directly calculating the conductance of finite-size samples. Anisotropic transport properties (such as temperature dependence) could arise from the anisotropic localization properties. We have shown that even when the system is below the mobility edge, in the presence of inelastic scattering which provides a cutoff length scale, it is possible to observe localization in the \(c\)-direction (if the localization length along \(c\)-axis is shorter than the cut-off length) and metallic behavior in the \(ab\)-plane (if the localization length in the \(ab\)-pane is longer than the cut-off length) for highly anisotropic systems.

A natural applicable system where the above anisotropic localization may occur is the layered high \(T_c\) cuprates, where the \(c\)-axis resistivity indeed shows a “semiconductor-like” upturn at low temperatures for Bi\(_2\)Sr\(_2\)CaCu\(_2\)O\(_8\) and underdoped La\(_{2-x}\)Sr\(_x\)CuO\(_4\) and YBa\(_2\)Cu\(_3\)O\(_{6+x}\), while the upturns disappear upon doping. Nevertheless, optical far-infrared and Raman experiment [15] suggest that the \(c\)-axis scattering rate \(1/\tau_c\) for typical YBa\(_2\)Cu\(_3\)O\(_{6+x}\) is of the order of 100meV, while the \(c\)-axis hopping amplitude \(tp \sim 10\)meV. Thus it appears that the ratio of disorder (should not be larger than \(1/\tau_c\) if there is any) and \(c\)-axis hopping \(W/tp < W/tp_c\). Moreover, the typical \(ab\)-plane hopping energy is of the order of 100meV, leaving \(W/t < 1\). Therefore, these cuprates are well above the mobility edge, and the \(c\)-axis transport should be on the metallic side. Details of the \(c\)-axis scattering rate and the hopping rate for each individual cuprate at different dopings are listed in Ref. [16]. Furthermore, unlike the simple model we present here, there is a strong \(ab\)-plane fluctuation
which increases with temperature, unless at very low $T$, this planar fluctuation will destroy the phase coherence so that back scattering can not occur \[^{2}\]. Therefore, we argue that the $c$-axis resistivity of high-$T_c$ cuprates can not be associated with the anisotropic localization phenomena we discussed above. An reasonable understanding of the $c$-axis resistivity data is given in the recent work of Ref. \[^{16}\]. Nevertheless, this does not exclude the possibility that localization (either $c$-axis or $ab$-plane) may occur in some extremely dirty samples or films or at doping concentration in closely proximity of the insulating phase of cuprates.

We acknowledge stimulating conversations with A.J. Leggett, P. Philips, K. Levin, J. Miller, and Q.M. Li. This work is supported by NSF-DMR-91-20000 and 94-16926 through the Science and Technology Center of Superconductivity.
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[9] Strictly speaking, one can only discuss metal-insulator transition in the thermodynamic limit where insulating states have finite localization length. Practically, however, one could investigate the localization properties using the finite size technique. By probing the sample size dependence of the transport properties for large enough sample, one could distinguish localized states from extended ones according to the arguments given in Ref.3. In doing so, however, it is important to make sure that the sample size is big enough so that the asymptotic behavior is reached, because if the sample size is much smaller than the thermodynamic localization length, even a localized state would have a metallic behavior.

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FIGURES

FIG. 1. Sample size dependent resistance for a cubic sample for different disorder strength (a) $W = 2$; (b) $W = 4$; (c) $W = 6$; (d) $W = 8$.

FIG. 2. The scaling function, $\lambda_M/M$ vs $\xi/M$. The $\xi(W,tp)$ shown in the inset turns out to be a universal function of $W/tp$. 
