Magnetic-Field Effects on Strongly Localized Electrons

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The magnetic-field response of strongly localized electrons is probed by examining the quantum interference of forward-scattering paths. With no disorder, there is a rich structure in the tunneling rate, which is sensitively dependent upon commensurability of the flux per plaquette with the flux quantum. With nonmagnetic impurities, there is a positive magnetoconductance, and the localization length appears to increase as $B^{1/2}$. With impurities breaking time-reversal symmetry, the distribution of tunneling rates is not changed by the magnetic field.

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Recently, there has been much emphasis on the influence of quantum-mechanical effects on small devices. An important example is provided by the reproducible fluctuations observed in the conductivity of small wires as a function of changing magnetic field or external voltage. However, most studies of such fluctuations have focused on metallic wires, or systems close to the metal-to-insulator transition.[1] By contrast, there is much less understanding of characteristic fluctuations on the insulating side,[2] where the main mechanism for conductivity is variable-range hopping.[3] The transmission (hopping) rate between two sites is obtained by summing over all the tunneling paths connecting them, and as such is a random variable. An important question is how the distribution function for this variable is modified by a magnetic field. This forms the main topic of this paper, and is relevant to various magnetoconductance measurements.

For electrons tunneling under a *nonrandom potential,* introduction of a magnetic field leads to a negative magnetoconductance (MC). This is due to destructive quantum interference between the various tunneling paths. However, even in this case, there are very characteristic fluctuations in the transmission probability. Periodic or quasiperiodic tunneling rates (as a function of distance) are obtained, depending on whether the flux per plaquette is rational or irrational. In a *random impurity potential,* there are no longer simple phase relations between contributions of different paths. The tunneling rates again fluctuate in the presence of a magnetic field, but there is an overall positive MC. This is somewhat surprising as the traditional explanation of a positive MC[4] relies on backscattering paths that are unimportant in the strongly localized regime. Instead we offer an explanation relying only on forward-scattering paths. Our results are obtained by using transfer-matrix methods to sum the contributions of such paths. This approach provides both an efficient numerical tool and an analytical understanding of the results. Our observations are relevant to the decay of gap states into a bulk (no randomness), and to the conductivity of doped semiconductors (with randomness).

The localization transition in the Anderson Hamiltonian

$$\mathcal{H}=\sum_i \epsilon_i a_i^\dagger a_i+\sum_{\langle ij\rangle} V_{ij} a_i^\dagger a_j \tag{1}$$

can be studied by performing a "locator" expansion,[5] valid in the limit $|V_{ij}|=V\ll E-\epsilon_i$, where ϵ_i is a random site energy and E is the electron energy. Indeed, for $V=0$, the eigenstates are just the single-site states, and the localization length is zero. For $V/(E-\epsilon_i)\ll 1$, various quantities can be obtained perturbatively around this solution; e.g., the Green's function (overlap) between initial $|i\rangle$ and final $|f\rangle$ sites is

$$\langle i|G(E)|f\rangle=\sum_\Gamma \prod_{i_\Gamma} \frac{Ve^{iA}}{E-\epsilon_{i_\Gamma}}. \tag{2}$$

The terms in the perturbation series can be illustrated graphically by paths Γ connecting the end points, and i_Γ are the sites along each path. (A is a magnetic vector potential defined on the bonds.) The sum over these paths is convergent up to the delocalization transition, beyond which very long paths dominate the sum. In the strongly localized regime, however, since there are additional factors of $V/(E-\epsilon_i)\ll 1$ for each link in the path, only the shortest paths need to be considered. This reduction to the shortest (forward-scattering or directed) paths is a considerable simplification, and allows us to obtain some interesting results in the strongly localized regime. For sites separated by a distance t along a diagonal of the square lattice, Eq. (2) can be rewritten as

$$\langle i|G(E)|f\rangle=\left(\frac{V}{E}\right)^t J(t),\quad J(t)=\sum_\Gamma \prod_{i_\Gamma} \frac{e^{iA}}{1-\epsilon_{i_\Gamma}/E}, \tag{3}$$

where the sum is now only over the directed paths, as shown in Fig. 1. There is an overall exponential decay

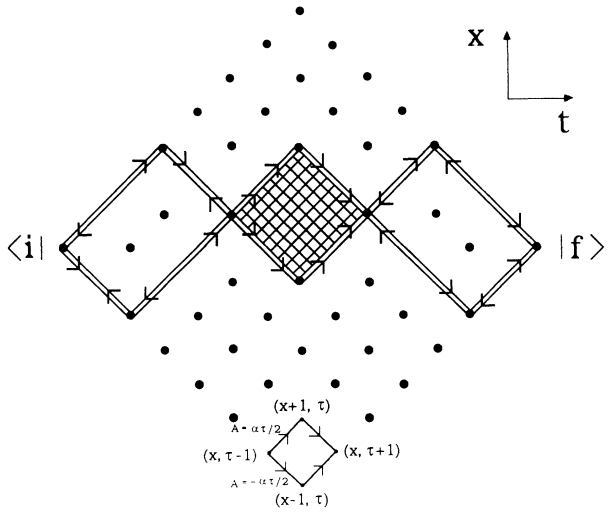

FIG. 1. Directed paths of length t connecting diagonally separated points on a square lattice. The figure shows the pairing of paths due to the averaging process; the arrows indicate whether paths are charged (arrows in same direction) or neutral (arrows in opposite direction). The "diagonal staggered gauge" choice is also indicated.

proportional to the length of each path, and all the interference information is contained in the sum $J(t)$. This latter quantity is calculated numerically and theoretically by the transfer-matrix method.

We first consider the nonrandom case with all $\epsilon_i = 0$. The magnetic-field response of *extended* states can be obtained from the work of Hofstadter.[6] Here we focus on the behavior of *localized* states. In the absence of a magnetic field ($B = A = 0$), clearly $J(t) = t!/[(t/2)!]^2 \sim 2^t$. With $B \neq 0$, there is a destructive interference between paths due to the dephasing factor of $\exp(iB\mathcal{A})$, where $\mathcal{A}$ is the area enclosed by paths, leading to a negative MC. However, as Fig. 2 indicates, the resulting interference patterns can be quite complicated. We define a quantity $W(x,\tau)$, which is the sum over contributions of all paths connecting the origin to the point (x,τ). This quantity can be calculated recursively in τ with the use of a transfer matrix $T(\tau)$. With the appropriate choice of gauge, the transfer matrix will have no x dependence (but will depend on τ). This choice, the "diagonal staggered gauge," corresponds to $A(\tau) = \pm \alpha\tau/2$ (Fig. 1), with $\alpha = 2\pi\phi/\phi_0$ being the fractional flux per plaquette. The resulting transfer matrix between columns τ and $\tau+1$,

$$\langle x \,|\, T(\tau) \,|\, x' \rangle = \exp\left(\frac{-i\alpha\tau}{2}\right)\delta_{x,x'+1} + \exp\left(\frac{i\alpha\tau}{2}\right)\delta_{x,x'-1},$$

is easily diagonalized by Fourier transforms for each τ. As the matrices for different τ commute, their product is also thus diagonalized. Finally, $J(B,t) = W(0,t) = \langle 0 |$

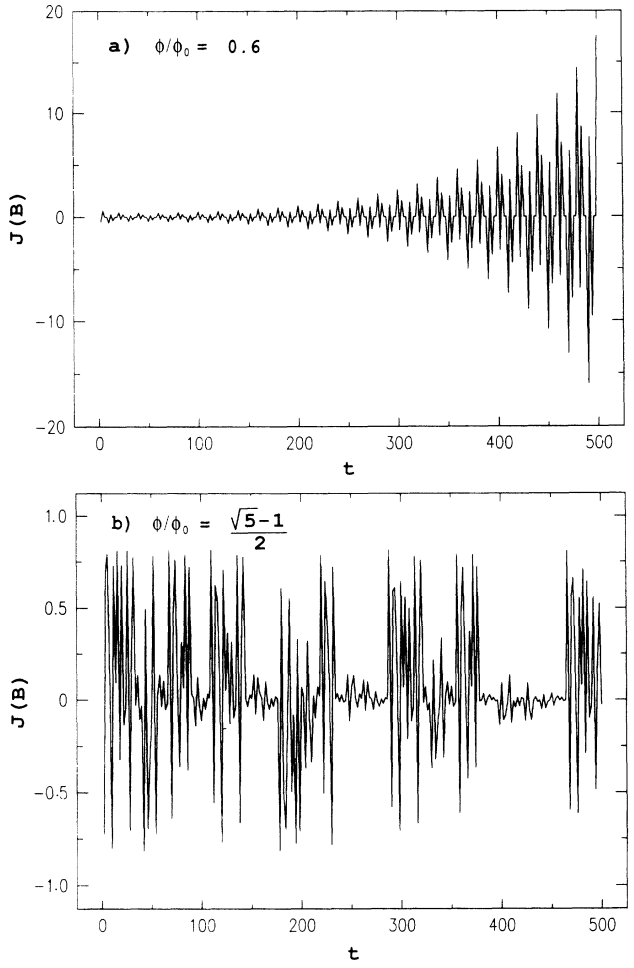

FIG. 2. Behavior of $J(t,B)$ for large fields. The flux per plaquette is (a) rational, $\phi/\phi_0 = 0.6$, and (b) irrational, $\phi/\phi_0 = (\sqrt{5}-1)/2$ (golden mean).

$\times \prod_{\tau=1}^{t} T(\tau) \,|\, 0\rangle$ is given by

$$J(t,B) = \sum_p \prod_{\tau=1}^{t} 2\cos\left(\frac{\alpha\tau}{2} - p\right). \tag{4}$$

(The allowed values of p, with periodic boundary conditions on N sites, are $\pm 2\pi k/N$.)

Equation (4) embodies various distinct behaviors. For small fields such that less than one flux unit goes through the entire "sample" (between the hopping end points), it can be shown that $\ln|J(B)| - \ln|J(0)| \sim B^2 t^3$. This behavior can be justified by regarding the important paths as executing a random walk ($\delta x \sim t^{1/2}$) in the transverse direction. The behavior of $J(t,B)$ for large fields, when many flux units penetrate the sample, is more complicated and crucially dependent on whether or not the flux per plaquette is rational or irrational. In the rational case, $\alpha = 2\pi/q$, there is a periodicity of $t = 2q$, where the value of J is repeated (except for an exponential rise). This is indicated for $\phi/\phi_0 = 0.6$ in Fig. 2(a).

When α is irrational, the sequence of transmission rates appears quite random, as illustrated in Fig. 2(b) for $\phi/\phi_0=(\sqrt{5}-1)/2=0.618\ldots$.

A *positive* MC has been observed in a number of recent studies of doped semiconductors in the variable-range-hopping regime.[2,7] To account for these observations, Nguyen, Spivak, and Shklovskii (NSS) introduced a model with site energies $\epsilon_i=\pm\epsilon$ with equal probability.[8] This model has been the subject of several recent theoretical studies,[9-11] but the origin of its positive MC had not been convincingly established. There are two bands of width roughly $2V$ centered at $E=\pm\epsilon$, outside of which the eigenstates are localized. For simplicity, we shall focus on $E=0$, which is deep in the localized regime (we have checked that the qualitative behavior is the same for other energies E). In this case each site crossed by the path contributes a factor $\eta_i=\pm 1$ to the sum for J in Eq. (3). For a given realization of randomness, the transfer matrix can be used to *exactly* calculate this sum. The results for many realizations of randomness then form a histogram for the probability $P[J(t,B)]$. We applied[11] this method to the case $B=0$ recently, and found that $P[J]$ becomes very broad with increasing t. In fact, our results indicated that $\langle\ln|J|\rangle=(0.322\pm0.001)t$, while $\langle\ln|J|^2\rangle-\langle\ln|J|\rangle^2\sim(0.46\pm0.05)^2t^{2/3}$; i.e., the distribution for $\ln J$ has a mean increasing linearly with t, and fluctuations that scale as $t^{1/3}$. The same procedure was extended to the case $B\neq0$, and the typical field dependences are shown in Fig. 3. [As J becomes a complex variable in a field, we have plotted the magnitude $\ln|J(t,B)|$.] We see that the average value increases with B, indicating a positive MC, as expected. Furthermore, we find that $P[\ln J(t,B)]$ maintains its functional form at finite B, except that the average moves to higher values, while fluctuations decrease (still scaling as $t^{1/3}$, but with a smaller coefficient).

The usual explanation for a positive MC, close to the localization transition, relies on the decreased weight of backscattering paths.[4] Since in our formulation such paths have been explicitly excluded, an alternative explanation is necessary. In previous work,[11] we established that to properly understand the numerically calculated shape of $P[\ln|J(0,t)|]$, it is essential to keep track of the correlations between paths. This can be done theoretically by a replica analysis of the moments $\langle J^{2n}\rangle$ (all odd moments vanish by symmetry). This is done by drawing $2n$ paths connecting the end points. They are then paired up into n double paths by the averaging process (Fig. 1). For $B=0$, upon each intersection the double paths can exchange partners, resulting in a degeneracy factor of 3 that can be interpreted as an exchange attraction. This attraction leads to formation of a bound state of the n paired paths.[12] The partition function, calculated by the transfer-matrix method,[11] is

$$\langle J^{2n}(t)\rangle=2^{nt}\exp[\rho n(n^2-1)t], \tag{5}$$

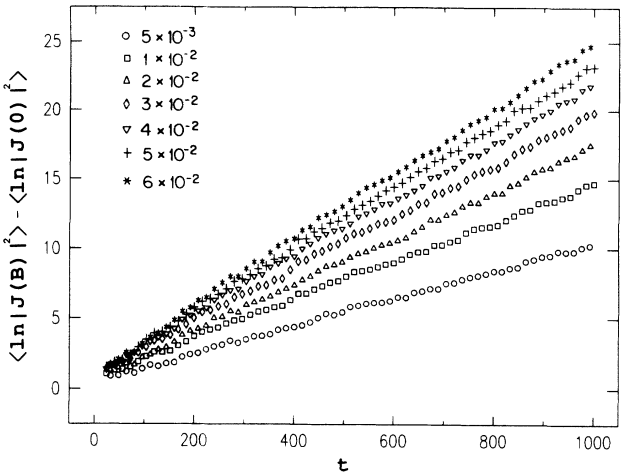

FIG. 3. Average value of the logarithm of the sums over directed paths vs the length t relative to the case $B=0$.

with $\rho=\rho_0=0.053\pm0.002$ from numerical simulations. Here we extend the replica analysis to $B\neq0$, by examining $\langle(JJ^*)^n\rangle$. Two types of paired paths are encountered: (i) Partners are taken one from J and one from J^*. Such pairs (referred to as neutral) do not feel the field since $e^{iA}e^{-iA}=1$. (ii) Both partners are taken from J or from J^*. Such paths (referred to as charged) feel a strong interference from the field corresponding to e^{2iA} or e^{-2iA}. It is reasonable to assume that because of their strong self-interference [see Eq. (4)], charged paths of long length do not contribute appreciably to $\langle J^{2n}\rangle$, and that dominant contributions come from neutral paths. However, between successive intersections of two neutral paths, short segments of charged paths can be present (see Fig. 1). If the area enclosed between intersections is $\mathcal{A}$, then the overall multiplicity factor becomes $4+2\times\cos(2B\mathcal{A})$. This is a decrease in the attraction from the value of $2\times3=6$ in the absence of a magnetic field. The net effect of integrating out charged segments is thus to reduce the effective attraction between neutral pairs. This leads to a reduction in the binding energy ρ in Eq. (5), simultaneously increasing the mean (the linear term), and decreasing fluctuations (the cubic term).

In fact, since Eq. (5) represents a one-parameter distribution, the changes in mean and variance should be perfectly correlated. This has indeed been tested numerically, and Fig. 4 shows the respective coefficients of the mean and variance for different values of the field B. Our numerical results for small B (but t large enough so that many flux units penetrate the sample[13]) are consistent with

$$\rho(B)=\rho_0-(0.15\pm0.03)(\phi/\phi_0)^{1/2}.$$

This implies $J(t,B)=J(t,Bt^2)$; i.e., the important area for the field is the whole sample, rather than a portion of it. This dependence agrees with the reduction of the lo-

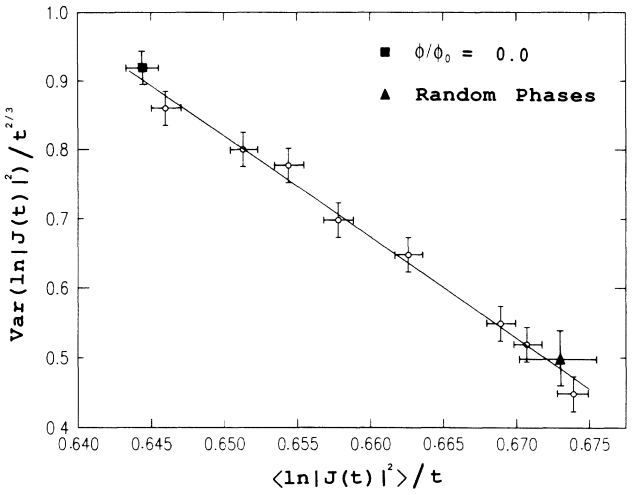

FIG. 4. Numerical tests for correlations between the mean and the variance of $P[J(t,B)]$ for different values of B. The random-phase point is also included.

calization length predicted at the localization transition.[4] Currently, we can offer no explanation of this dependence from the replica analysis.

A finite magnetic field breaks time-reversal symmetry by introducing complex phases for each path. It has been argued that this effect is equivalent to replacing the sign ($\pm$) randomness with a complex-phase ($e^{i\theta}$ with $0<\theta<2\pi$) randomness.[4,8,9] We also simulated the latter model, and found that it shows no MC. This can be easily explained in the replica language: After the averaging over random phases only the neutral paths survive, and such paths do not couple to the magnetic field. Indeed by totally eliminating the charged paths, we achieve an extreme limit of the reduced attraction between neutral paths that was described earlier—it is easy to check that the exchange attraction upon the crossing of two neutral paths is just 2. As Fig. 4 indicates, the model with random phases occurs as the extreme limit of the distributions found for the $\pm$ model in a field. Thus, the random-phase model does not directly correspond to the original disordered NSS model in a field. It may, however, be relevant to magnetic impurities that break the time-reversal symmetry of the original Hamiltonian.[14] Yet another indication of the phase correlations inherent to the magnetic field is the equality of $\langle J^2(B,t)\rangle$ with $\pm$ impurities with $J(2B,t)$ in the nonrandom problem, an identity easily established by replica analysis, and confirmed by numerical simulations.

In conclusion, we have numerically and analytically investigated the MC of electrons in the strongly localized regime. In the nonrandom case the probability of hopping a distance t initially decays as B^2t^3 when the flux through the sample is small. For larger fluxes an intricate pattern develops that is very sensitive to the commensurability of the flux per plaquette with the quantum flux. In the presence of nonmagnetic impurities we find a positive MC, which in the large-flux limit grows as $B^{1/2}$. The details of these calculations and their implications for experiments and theories of electron transport will be given elsewhere.

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