Spin-Orbit Scattering for Localized Electrons: Absence of Negative Magnetoconductance

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The distribution of hopping conductances in the strongly localized regime in the presence of both a magnetic field and spin-orbit (SO) scattering is calculated via an analytic independent-directed-path formalism and a locator expansion which includes all correlations between paths. Both methods lead to a positive magnetoconductance for all strengths of SO scattering, contrary to recent random-matrix-theory predictions. Extensive numerical simulations demonstrate that the crossover from negative to positive magnetoconductance occurs as the system size exceeds the localization length.

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In the last ten years there has emerged a coherent theory of the conductance and its fluctuations in the metallic, weakly localized regime, which involves effects of potential scattering, magnetic field, and spin-orbit (SO) scattering, and agrees very well with experiments.[1] In particular, there is a positive magnetoconductance (MC) in the absence of SO scattering, and a negative MC in the presence of strong SO scattering. Similarly, in the strongly localized regime, where transport is via variable-range hopping,[2] both experiments and theories yield positive MC in the absence of SO scattering.[3] In further analogy to the weakly localized regime, it was recently predicted,[4] based on random-matrix theory, that in the insulating phase the MC in the presence of SO scattering is negative. In this Letter we give conclusive evidence to the contrary: The MC becomes positive as the system size exceeds the localization length, no matter how large the latter is, or how strong the SO scattering becomes.

First, we calculate the distribution of the hopping conductances in the strongly localized regime in the presence of both a magnetic field and SO scattering. This is done via three approaches: (a) a general formalism, based on independent forward-scattering paths; (b) a locator expansion, which includes all correlations between paths; and (c) extensive numerical simulations. All three methods lead to a positive MC for all strengths of SO scattering. We show that these results follow from symmetry considerations and thus are insensitive to details of the model. By extending the numerical simulations into the metallic regime, we show that the change of sign of the MC occurs when the system size is equal to the localization length.

The microscopic model for hopping in the presence of SO scattering and a uniform magnetic field consists of an Anderson Hamiltonian[5] defined on a d-dimensional lattice, with disordered on-site energies taken from a symmetric distribution of width W, and with hopping matrix elements which include SO scattering:[6,7]

$$H=\sum_{l,\sigma}\epsilon_l|\Psi_l^\sigma\rangle\langle\Psi_l^\sigma|+\sum_{\langle lm\rangle\sigma\sigma'}Ve^{i\phi_{lm}}S_{lm}^{\sigma\sigma'}|\Psi_l^\sigma\rangle\langle\Psi_m^{\sigma'}|+\text{H.c.} \quad (1)$$

Here $\langle lm\rangle$ denotes nearest-neighbor sites l and m, $|\Psi_l^\sigma\rangle$ is the spinor wave function at site l with spin σ, and ϕ_{lm} is the magnetic phase associated with the bond $\langle lm\rangle$ (V is assumed to be constant). Because of the time-reversal invariance of the SO interaction, the on-site term is diagonal in spin space, and S_{lm}, the SO-scattering matrix, is given by[6,7]

$$\begin{pmatrix}\alpha_{lm} & \beta_{lm}\\ -\beta_{lm}^* & \alpha_{lm}^*\end{pmatrix},$$

with $\det(S_{lm})=1$. In this model the SO disorder (i.e., the distribution of α_{lm} and β_{lm}) is independent of the site disorder (ϵ_i).

Let i and f be two sites between which the electron hops (i.e., $\epsilon_i\sim\epsilon_f$). The amplitude at site f of the eigenfunction centered at site i is given by $\langle\Psi_f^{\sigma'}|S|\Psi_i^\sigma\rangle$, with

$$S=\sum_{k=0}^{\infty}(V/W)^{L+2k}\sum_{p\in\Gamma_k}j_pS_pe^{i\phi_p}, \quad (2)$$

where L is the shortest length between sites i and f. Γ_k denotes the set of all n_k paths of length $L+2k$, connecting i and f; each path consists of an ordered set of sites $\{l\}$ and bonds $\{\langle lm\rangle\}$. In Eq. (2), the path parameters j_p, S_p, and $\exp(i\phi_p)$ are given by $j_p=1/\prod_{l\in p}[(\epsilon_i-\epsilon_l)/W]$, $\phi_p=\sum_{\langle lm\rangle\in p}\phi_{lm}$, and

$$S_p=\prod_{\langle lm\rangle\in p}S_{lm}\equiv\begin{pmatrix}\alpha_p & \beta_p\\ -\beta_p^* & \alpha_p^*\end{pmatrix}.$$

In the random-resistor-network theory[8] for transport in the variable-range-hopping regime, the conductance is determined by the distribution of the wave-function overlaps between hopping sites. To treat magnetic-field effects in variable-range hopping, Nguyen, Spivak, and Shklovskii[9] calculated numerically the distribution of wave-function overlaps starting from (2), including only forward-scattering paths and with no SO scattering, for i and f along the diagonal ([11] direction). In this case only the n_0 shortest paths [belonging to Γ_0 in (2)] are relevant. Within this directed-path model, now including SO scattering, the probability of finding the electron at site f (averaged over initial spin directions and summed over final spin directions) is $J^2 e^{-2L/\xi}$, where ξ is the localization length, and

$$J^2 = \tfrac{1}{2} e^{2L/\xi} \mathrm{Tr}\{S^+ S\} = \sum_{q=1}^{8} J_q^2 . \quad (3)$$

In Eq. (3), $J_q = n_0^{-1/2} \sum_{p \in \Gamma_0} j_p \chi_{qp}$, where, for each path, the eight components of the vector χ_{qp} are given by the tensorial product $(\cos\phi_p, \sin\phi_p) \otimes (\mathrm{Re}\alpha_p, \mathrm{Im}\alpha_p, \mathrm{Re}\beta_p, \mathrm{Im}\beta_p)$.

We first calculate the distribution of overlaps $P(J^2)$ analytically, following the approach of Sivan and coworkers,[10] in which correlations between paths are neglected, and the real path amplitudes j_p are taken from a Gaussian distribution of zero mean and unit standard deviation. It is then straightforward to calculate the joint distribution function of $\mathbf{J} \equiv (J_1, \ldots, J_8)$,

$$P(\mathbf{J}, \Lambda) = \frac{1}{(2\pi)^4} \frac{1}{\det(\Lambda)^{1/2}} \exp(-\tfrac{1}{2} \mathbf{J} \Lambda^{-1} \mathbf{J}) , \quad (4)$$

where the "phase" matrix $\Lambda_{qq'} = n_0^{-1} \sum_{p=1}^{n_0} \chi_{qp} \chi_{q'p}$ represents a particular magnetic field and a particular configuration of SO scattering (to be averaged upon later). It is convenient to evaluate first the Laplace transform of $P(J^2, \Lambda)$,

$$\tilde{P}(s,\Lambda) \equiv \int_0^\infty dJ^2 e^{-sJ^2} \int d\mathbf{J}\, P(\mathbf{J}) \delta(J^2 - |\mathbf{J}|^2) = \prod_{q=1}^{8} \frac{1}{(2\lambda_q s + 1)^{1/2}} , \quad (5)$$

where λ_q are the eigenvalues of Λ and obey $\sum_{q=1}^{8} \lambda_q = 1$.

As the number of paths n_0 grows, the phase matrix Λ converges towards its average over the SO scattering $\bar{\Lambda}$, with corrections of order $1/n_0$. Then $\tilde{P}(s)$, the Laplace transform of the total distribution of wave-function overlaps $P(J^2)$, is given by

$$\tilde{P}(s) = \prod_{q=1}^{8} \frac{1}{(2\lambda_q s + 1)^{1/2}} + O(1/n_0) , \quad (6)$$

where λ_q are now the eigenvalues of $\bar{\Lambda}$. For the cases (a) $H=0$, SO=0, (b) $H \neq 0$, SO=0, (c) $H=0$, SO$\neq$0, and (d) $H \neq 0$, SO$\neq$0, $\bar{\Lambda}$ has, respectively, (a) 1, (b) 2, (c) 4, and (d) 8 nonzero eigenvalues. In general, the 8 eigenvalues of $\bar{\Lambda}$ are given by $R^2 a^2$, $R^2 b^2$, $\frac{1}{3}(1-R^2) a^2$, $\frac{1}{3}(1-R^2) b^2$, where the last two eigenvalues have threefold degeneracy and where[11] $b^2 = n_0^{-1} \sum_{p=1}^{n_0} \sin^2\phi_p$, $a^2 = 1 - b^2$, and $R^2 = \langle (\mathrm{Re}\alpha_p)^2 \rangle$ ($\langle \cdots \rangle$ indicates an average over SO scattering). b^2 increases from 0 to $\frac{1}{2}$ with increasing magnetic field.[10] $R^2 = 1$ means no SO scattering, while in the strong-SO-scattering limit[7] $R^2 = \frac{1}{4}$. In the strong-field and strong SO limits of (b)-(d) above, all nonzero eigenvalues of $\bar{\Lambda}$ are equal. Hence, the number of eigenvalues and their values are determined by the *symmetry* of the system: The lower the symmetry, the larger the number of eigenvalues and the smaller their values.

In principle, from the above eigenvalues, one can construct the distribution function $P(J^2)$. (Indeed, for the case with no SO scattering, one reproduces the distribution function found in Ref. 10.) However, one can calculate most transport properties directly from the Laplace transform (6). Of particular importance is the sign of the MC, which depends on the width of the distribution: A narrower distribution implies fewer pairs of sites with very low hopping rates and, consequently, a higher average conductance.[10] Since $\langle J^2 \rangle = d^2 \tilde{P}(s)/ds^2|_{s=0}$, the width is given by $\sum_q 2\lambda_q^2$, and is equal to 2, 1, $\frac{1}{2}$, and $\frac{1}{4}$, for the limiting cases of (a), (b), (c), and (d) above, respectively. Evidently, a magnetic field always reduces the width of the distribution and we expect *a positive magnetoconductance for all values of spin-orbit scattering.* This result is in perfect agreement with the results in the weakly localized regime,[12] where strong SO scattering reduces the width of the distribution of conductances by a factor of 4 and, independently, a strong magnetic field reduces the width by a factor of 2. In that regime the width determines the amplitude of the conductance fluctuations,[13] whereas in the strongly localized regime the width affects the average conductance as well.

To determine quantitatively the MC in the limits of zero and strong SO scattering, we note that deep in the strongly localized regime[9,14] $\sigma(H) = \sigma_0 \exp\langle \ln(J^2) \rangle$. The logarithmic average can be calculated directly from the Laplace transform $\tilde{P}(s)$ in (6). For the case with no SO scattering, we find $\langle \ln(J^2) \rangle = -\gamma - \ln(2) + \ln(1+2ab)$, where $\gamma \simeq 0.577$ is the Euler constant. This implies a positive MC, linear in the magnetic field, $\sigma(H)/\sigma(0) = 1 + 2ab$, in agreement with previous theoretical[9,14] and experimental[15] results ($b \propto H$ at small magnetic field). As pointed out by Nguyen, Spivak, and Shklovskii,[9] the main contribution to the average of the logarithm comes from the neighborhood of $J^2 = 0$, and a linear MC occurs if, without a magnetic field, $P(J^2 = 0) \neq 0$. From (6) it follows that $P(J^2=0) \neq 0$ only for zero SO scattering. Physically, $P(J^2=0)=0$ in the presence of SO scattering follows from the vanishing probability for completely destructive interference in the two spin directions simultaneously. Thus the linearity or nonlinearity of the MC is determined by the symmetry of the system, and we expect a quadratic dependence of the MC at small fields in the presence of SO scattering. In the limit of strong SO scattering,

$$\langle \ln(J^2) \rangle = -\gamma + \ln\left[\frac{ab}{2}\right] + \frac{6a^2b^2 - 1}{(b^2 - a^2)^3} \ln\left[\frac{a}{b}\right] + \frac{a^4 + b^4}{(b^2 - a^2)^2} . \quad (7)$$

As expected from the arguments above, the resulting MC is positive and quadratic at small magnetic fields, $\sigma(H)/\sigma(0) = 1 + b^2$. The MC, for zero and for strong SO scattering, is plotted[16] in Fig. 1. Note that the MC is smaller in the presence of SO scattering. For the four

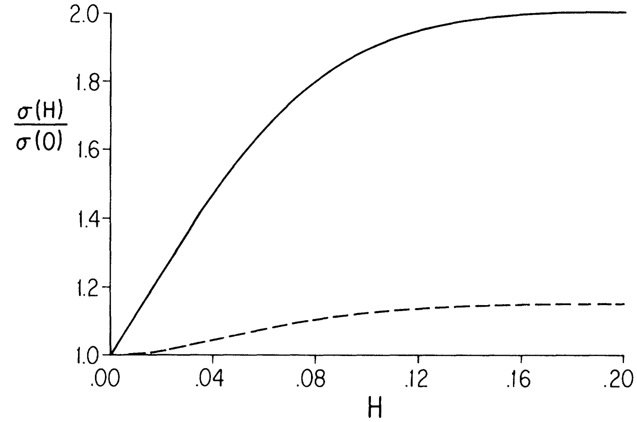

FIG. 1. Magnetoconductance in the variable-range-hopping regime in the independent-directed-path model. Both with (dashed line) and without (solid line) spin-orbit scattering, the magnetoconductance is strictly positive. The magnetic field is plotted in units of ϕ_0/A, where $\phi_0 = hc/e$ and A is the area enclosed by a typical pair of paths (Ref. 16).

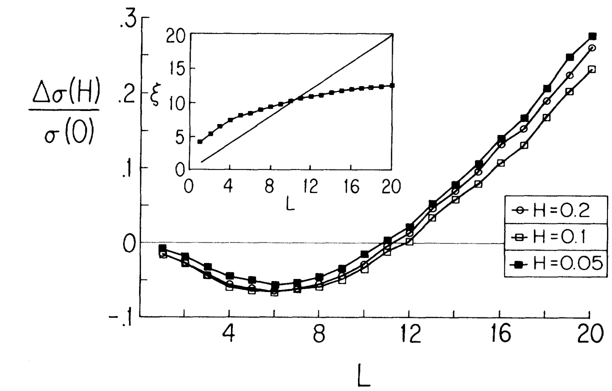

FIG. 2. Relative magnetoconductance (MC) along a strip of length L, width $m=5$, and disorder $W/V=4$, for several values of magnetic field (measured in flux quanta per plaquette). Each point represents average over 15000 realizations. The MC changes sign at L_{co}, which obeys $L_{co} = \xi(L_{co}) \simeq 11$ (see text). Inset: The L dependence of the localization length for the same strip.

extreme cases above, where all q^* nonzero eigenvalues are equal, $\langle \ln(J^2) \rangle = \Psi(q^*/2) - \ln(q^*/2)$, where Ψ is the digamma function. Thus the conductance indeed increases with the number of nonzero eigenvalues; i.e., the lower the symmetry, the larger the conductance.

In the low-field regime where $b \ll \sigma/\sigma_0$, i.e., either close to the metal-insulator transition or at very small magnetic fields, one should use the percolation condition for the random-resistor network[8] in order to expand[10] σ in terms of H^2. In that regime one always finds quadratic MC, and the coefficient of H^2 is given by

$$\frac{db^2}{dH^2}\left[\frac{\sigma_0}{\sigma}\frac{I_{n,\beta}}{I_{n+1,\beta}} - 1\right],$$

where

$$I_{n,\beta} = \int_1^\infty \ln^{2d+1}(x) e^{-\beta x \sigma/2\sigma_0} x^n \, dx ,$$

with $n = -\frac{3}{2}$, $\beta = 1$ ($n=0$, $\beta=4$) for zero (strong) SO scattering. As before, the coefficient of H^2 is positive in the deeply localized regime,[10] and the SO scattering decreases the magnitude of the MC.

So far, we have ignored correlations[17] between different trajectories. In order to check analytically that such correlations do not change the sign of the MC, we choose the sites i and f in (2) to be in the [10] direction and drop the restriction to forward-scattering paths. In this case there is a single shortest path of length L between the hopping sites. This permits us to perform a locator expansion[5,18] of the overlap matrix S. Expanding (2) to fourth order in V/W, we find,[19] upon averaging,

$$\frac{\sigma(H)}{\sigma(0)} = 1 + 2\left(\frac{V}{W}\right)^4 \sum_{p \in \Gamma_1} \left\langle \frac{j_p^2}{j_0^2} \right\rangle \langle (\mathrm{Re}\,\alpha_p)^2 \rangle \sin^2\phi_p . \quad (8)$$

The averages in (8) still contain all correlations between different trajectories. Our previous conclusions, based on the independent-directed-path approximation, are unchanged by the inclusion of correlations between paths: The MC in the strongly localized regime is *positive and quadratic* for all values of SO scattering, and the magnitude of the MC decreases as the SO scattering increases.

For homogeneously disordered systems, near the metal-insulator transition, backscattering processes, which were neglected in the directed-path approach, are relevant to the hopping conductance.[20] The only analytic results concerning the dependence of σ on H, in this regime, rely on scaling theory,[21] which provides no information on the sign of the effect. To investigate the MC in this regime we have performed extensive numerical simulations to calculate the transmission coefficient $T(H)$ and the conductance $\sigma(H) \sim \exp\langle \ln T(H) \rangle$, along a strip of tight-binding sites (1) (with periodic boundary conditions in the transversal direction), as a function of length L, width M, amount of disorder W/V, and magnetic field H, for strong SO scattering. In Fig. 2, the relative MC is plotted as a function of L, for several values of H. As expected, in the weakly localized regime ($L \ll \xi$) the MC is negative, but becomes positive for $L > \xi$. The crossover length L_{co}, where the MC changes sign, is determined by the localization length according to[22]

$$L_{co} = \xi(L_{co}) \quad (9)$$

(see inset, $L_{co} \simeq 11$). The numerical simulations demonstrate that Eq. (9) holds independently of the amount of disorder, its distribution, or the width of the strip. *For any disorder,* the sign of the MC in the presence of SO scattering changes sign from negative to positive as the sample length L exceeds ξ. Importantly, since $\xi \gg 1$, backscattering processes make a significant contribution to the simulations. Nevertheless, the MC is found to be positive for $L > \xi$, as predicted by our directed-path approach for $L \gg \xi$.

In contrast to suggestions made in Ref. 4 concerning this work, our main result, namely, a positive MC for $L > \xi$ in the presence of SO scattering, holds even when the magnetic flux through an area defined by the localization length is larger than the quantum flux, ϕ_0.[23] In Fig. 2, for example, the total flux through the area $m \times \xi \simeq 5 \times 12 = 60$ is about $12\phi_0$ for the curve with 0.2 flux quanta per plaquette.

To conclude, we have treated a microscopic model for spin-orbit scattering and magnetic-field effects in the variable-range-hopping regime. Our results, both analytical and numerical, predict a *positive* magnetoconductance for all values of SO scattering. The crossover from negative to positive MC occurs as the system size exceeds the localization length. Since in order to observe variable-range hopping the hopping length must be at least a few times the localization length, our results conclusively indicate that in homogeneously disordered systems one should always observe a positive MC in the variable-range-hopping regime. Interestingly, recent experiments[4,24] exhibited negative MC in the (noninteracting) variable-range-hopping regime. While the negative MC in these systems can be attributed to macroscopic disorder and the contribution of weakly localized islands in the samples, we hope that our results will stimulate further experiments in order to resolve this question.

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