Strongly Localized Electrons in a Magnetic Field: Exact Results on Quantum Interference and Magnetoconductance

Yeong-Lieh Lin[1,2] and Franco Nori[1]
[1]*Department of Physics, The University of Michigan, Ann Arbor, Michigan 48109-1120*
[2]*Department of Physics, West Virginia University, Morgantown, West Virginia 26506-6315**
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We study quantum interference effects on the transition strength for strongly localized electrons hopping on 2D square and 3D cubic lattices in a magnetic field **B**. In 2D, we obtain *closed-form* expressions for the tunneling probability between two *arbitrary* sites by exactly summing the corresponding phase factors of *all* directed paths connecting them. An *analytic* expression for the magnetoconductance, as an *explicit* function of the magnetic flux, is derived. In the experimentally important 3D case, we show how the interference patterns and the small-**B** behavior of the magnetoconductance vary according to the orientation of **B**. [S0031-9007(96)00395-X]

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Quantum interference (QI) effects between different electron paths in disordered electron systems have been a subject of intense study [1–8] because they play an important role in quantum transport; for instance, the QI of closed paths is central to *weak-localization* phenomena [1]. Recently, a growing interest exists on the effects of a magnetic field on *strongly localized* electrons with variable-range hopping (VRH) where striking QI phenomena have been observed in mesoscopic and macroscopic insulating materials. This strongly localized regime [2–8] is less well understood than the weak-localization case. Deep in the insulating regime, the major mechanism for transport is thermally activated hopping between the localized sites. In the VRH regime, localized electrons hop a long distance (the lower the temperature is, the farther away the electron tunnels) in order to find a localized site of close energy. The conductance of the sample is governed by one critical phonon-assisted hopping event [2]. During this critical tunneling process, the electron traverses many other impurities since the hopping length is typically many times larger than the localization length. It is important to emphasize that the electron preserves its phase memory while encountering these intermediate scatterers. This elastic multiple scattering is the origin of the QI effects associated with a single hopping event between the initial and final sites. The tunneling probability of one distant hop is therefore determined by the interference of many electron paths between the initial and final sites [2–7].

In this paper we investigate the QI of strongly localized electrons by doing *exact* summations over *all* directed paths between two *arbitrary* sites. For electrons propagating on a square lattice under a uniform potential, we derive an exact *closed-form* expression for the sum over paths. We also obtain an explicit formula for an experimentally important case, much less studied theoretically so far: the interference between paths on a 3D cubic lattice. In the presence of impurities, by computing the moments of the tunneling probability and employing the replica method, we derive a compact *analytic* result for the magnetoconductance (MC), which is applicable in any dimension. Our explicit field-dependent expression for the MC provides a precise description of the MC, including the low and high field limits. The period of oscillation of the MC is found to be equal to $hc/2e$. Also, a *positive* MC is clearly observed when turning on the field **B**. When the strength of **B** reaches a certain value, $B_{\rm sa}$, which is inversely proportional to twice the hopping length, the value of the MC becomes saturated. At very small fields, for two sites diagonally separated a distance r, the MC behaves as rB for quasi-1D systems, $r^{3/2}B$ in 2D with $\mathbf{B} = (0,0,B)$, and rB ($r^{3/2}B$) in 3D with **B** parallel (perpendicular) to the $(1,1,1)$ direction. The general expressions presented here (i) *contain, as particular cases*, several QI results [2–8] derived during the past decade (often by using either numerical or approximate methods), (ii) include QI to arbitrary points (m,n), instead of only diagonal sites (m,m), (iii) focus on 2D *and* 3D lattices, and (iv) can be extended to also include *backward* excursions (e.g., side windings) in the directed paths.

Exact results in this class of directed-path problems are valuable, and, for instance, can be useful to study other systems: (1) directed polymers in a disordered substrate, (2) interfaces in 2D, (3) light propagation in random media, and (4) charged bosons in 1D.

To study the magnetic-field effects on the tunneling probability of strongly localized electrons, we start from the tight-binding Hamiltonian $H = W\sum_i c_i^\dagger c_i + V\sum_{\langle ij\rangle} c_i^\dagger c_j e^{iA_{ij}}$, where $V/W \ll 1$ and $A_{ij} = 2\pi\int_i^j \mathbf{A}\cdot d\mathbf{l}$ is 2π times the line integral of the vector potential along the bond from i to j in units of $\Phi_0 = hc/e$. Consider two states, localized at sites i and f which are r bonds apart, and the shortest-length paths (with no backward excursions) connecting them, i.e., the *directed-path model*. By using a locator expansion, the Green's

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function (transition amplitude) between these two states can be expressed as $T_{if} = W(V/W)^r S^{(r)}$, with $S^{(r)} = \sum_\Gamma \exp(i\Phi_\Gamma)$, where Γ runs over all directed paths of r steps and Φ_Γ is the sum over phases of the bonds on the path. This directed-path model provides an excellent approximation to T_{if} in the extremely localized regime [2–8] since higher-order contributions involve terms proportional to $W(V/W)^{r+2l}$ ($l \geq 1$), which are negligible because $(V/W)^2$ is very small. Quantum interference, contained in $S^{(r)}$, arises because the phase factors of different paths connecting the initial and final sites interfere with each other. In this work, we focus on (i) the computation of the essential QI quantity $S^{(r)}$, (ii) the derivation of the MC in the disordered case, and (iii) the study of the full behavior of the MC—including the scaling in the low-field limit and the occurrence of saturation. It is important to keep in mind that the effect of a magnetic field on the MC follows the behavior of $S^{(r)}$.

Quantum interference on a 2D square lattice.—Let us choose $(0,0)$ to be the initial site and focus on sites (m,n) with $m,n \geq 0$. For forward-scattering paths of r steps, which exclude backward excursions, ending sites (m,n) satisfy $m+n=r$. Let $S_{m,n}$ $(=S^{(r)})$ be the sum over all directed paths of r steps on which an electron can hop from the origin to (m,n), each one weighted by its corresponding phase factor. Employing the symmetric gauge $\mathbf{A} = (-y,x)B/2$, and denoting the flux through an elementary plaquette (with an area equal to the square of the average distance, which is typically equal to or larger than the localization length, between two impurities) by $\phi/2\pi$, it is straightforward to construct the recursion relation $S_{m,n} = e^{-in\phi/2}S_{m-1,n} + e^{im\phi/2}S_{m,n-1}$. The factors in front of the S's account for the presence of the magnetic field. Enumerating the recursion relations for $S_{k_n,n}$ ($k_n = m-1,\ldots,0$) successively and using $S_{0,n}=1$, we obtain the relation $S_{m,n} = \sum_{k_n=0}^{m} e^{ik_n\phi/2} e^{-i(m-k_n)n\phi/2} S_{k_n,n-1}$. This equation states that the site (m,n) can be reached by moving one step upward from sites $(k_n, n-1)$ with $0 \leq k_n \leq m$, acquiring the phase $ik_n\phi/2$, then traversing $m-k_n$ steps from (k_n,n) to (m,n), each step with a phase $-in\phi/2$. By applying the above relation recursively and utilizing $S_{m,0}=1$, $S_{m,n}$ for $m,n\geq 1$ can be written as $S_{m,n}(\phi) = \exp(-imn\phi/2)L_{m,n}(\phi)$, and

$$L_{m,n}(\phi) = \sum_{k_n=0}^{m} \sum_{k_{n-1}=0}^{k_n} \cdots \sum_{k_1=0}^{k_2} e^{i(k_1+\cdots+k_{n-1}+k_n)\phi}. \quad (1)$$

Notice that each term in the summand corresponds to the overall phase factor associated with a directed path. When $\phi=0$, $S_{m,n}(0) = C_m^r \equiv N$ is just the total number of r-step paths between $(0,0)$ and (m,n).

After some calculations we obtain one of our main results, a very compact and elegant closed-form expression for $S_{m,n}(\phi)$,

$$S_{m,n}(\phi) = \frac{F_{m+n}(\phi)}{F_m(\phi)F_n(\phi)}, \; F_m(\phi) = \prod_{k=1}^{m} \sin\frac{k}{2}\,\phi. \quad (2)$$

Notice that the symmetry $S_{m,n} = S_{n,m}$ [apparent in Eq. (2)] is due to the square lattice geometry. In the very-low-flux limit $\phi \ll 1$, the logarithm of $S_{m,n}$, calculated *exactly* to order ϕ^2 (and omitting $\ln N$), is

$$\ln S_{m,n}(\phi) = -\tfrac{1}{24}mn(m+n+1)\phi^2, \quad (3)$$

and thus we obtain the familiar [2] harmonic shrinkage of the wave function.

$S_{m,m}$ has the richest interference effects because the number of paths ending at (m,m) and the areas they enclose are both the largest. We therefore examine more closely the behavior of the quantities $I_{2m}(\phi) \equiv S_{m,m}(\phi) = \prod_{k=1}^{m}[\sin(m+k/2)\phi]/[\sin(k/2)\phi]$. $I_{2m}(\phi)$ obeys the following properties: (i) 2π (4π) periodicity in ϕ for even (odd) m, (ii) $I_{2m}(2\pi-\phi) = I_{2m}(\phi)$ for $0 \leq \phi \leq \pi$ with m even, and (iii) $I_{2m}(2\pi \pm \phi) = -I_{2m}(\phi)$ for $0 \leq \phi \leq 2\pi$ with m odd. Furthermore, the zeros of $I_{2m}(\phi)$ are given by $\phi = 2\pi s/t$, for $(m+1/n+1) \leq t \leq (2m/2n+1)$, with $0 \leq n \leq (m-1/2)$, and the s's are prime to each allowed t. From the physical viewpoint, these flux values produce the complete cancellation of all phase factors (i.e., *fully destructive interference*). Indeed, as the magnetic field is turned on, $I_{2m}(\phi)$ rapidly drops to its first zero at $\phi/2\pi = 1/2m$ and then shows many small-magnitude fluctuations around zero.

Effects of disorder.—To incorporate the effects of random impurities, we now replace the on-site energy part (first term in H) by $\sum_i \epsilon_i c_i^\dagger c_i$. Now the ϵ_i are independent random variables which can take two values: $+W$ with probability μ and $-W$ with probability ν, where $\mu+\nu=1$. Because of disorder, the transition amplitude becomes $T_{if} = W(V/W)^r J_{m,n}$, with $J_{m,n} = \sum_\Gamma [\prod_{j\in\Gamma}(-W/\epsilon_j)]e^{i\Phi_\Gamma}$. For all directed paths ending at (m,n), electrons traverse r sites (the initial site is excluded). Each site visited now contributes an additional multiplicative factor of either $+1$ or -1 to the phase factor. Therefore, for a given path Γ, the probability for obtaining $\pm e^{i\Phi_\Gamma}$ is $[(\mu+\nu)^r \pm (\mu-\nu)^r]/2$. By exploiting Eq. (1), we derive a general expression for the disorder average of the tunneling probability (i.e., the transmission rate) as $\langle |J_{m,n}(\phi)|^2\rangle = N + (\mu-\nu)^{2r}[S_{m,n}^2(\phi) - N]$, where $\langle\cdots\rangle$ denotes averaging over all possible configurations of impurities. It is important to stress that the *conductivity* between i and f is proportional to $\langle |J_{m,n}(\phi)|^2\rangle$ [2–5].

For the most studied case so far, $\mu=\nu=1/2$, we can obtain analytical expressions for the moments $\langle |J_{m,n}(\phi)|^{2p}\rangle$ for any value of p. In general, $\langle |J_{m,n}(\phi)|^{2p}\rangle$ consist of terms involving N^k with $k=1,\ldots,p$. Hereafter, we omit the subscripts in J and S, and focus on the leading terms ($\propto N^p$), since they provide the most significant contribution to the moments, and hence the MC, when N is large. Recall that $S(0)=N$, therefore we need to consider all terms involving $S^{2k}(2\phi)N^{p-2k}$ in $\langle |J(\phi)|^{2p}\rangle$. We derive $\langle |J(0)|^{2p}\rangle = (2p-1)!!\,N^p$, and

$$\langle |J(\phi)|^{2p}\rangle = p!\,N^p\left\{\sum_{k=0}^{\infty}\frac{(2k)!\,C_{2k}^p}{(2^k k!)^2}\left[\frac{S(2\phi)}{N}\right]^{2k}\right\}. \quad (4)$$

Using these equations and employing the replica method, we obtain the log-averaged MC $L_{\rm MC} \equiv \langle \ln |J(\phi)|^2\rangle - \langle \ln |J(0)|^2\rangle$. The typical MC of a sample, $G(\phi) = \exp(\langle \ln |J(\phi)|^2\rangle)$, is then given by

$$\frac{G(\phi)}{G(0)} = \exp(L_{\rm MC}) = 1 + \sqrt{1 - \left[\frac{S(2\phi)}{N}\right]^2}. \quad (5)$$

Equation (5) is one of our main results. It provides a compact closed-form expression for the MC, as an *explicit* function of the magnetic flux. From Eq. (5) it becomes evident that a magnetic field leads to an increase in the *positive* MC: $G(\phi)/G(0)$ increases from 1 to a saturated value 2 [since $S(2\phi)$ decreases from N to 0] when the flux is turned on and increased. $G(\phi) = 2G(0)$ at the field ϕ that satisfies $S(2\phi) = 0$. Furthermore, it is clear that the MC varies *periodically* with the magnetic field and the periodicity in the flux is equal to $hc/2e$.

It is illuminating to draw attention to the close relationship between the behaviors of $I_{2m}(2\phi) = S_{m,m}(2\phi)$ and the corresponding $G(\phi)$. When $\phi = 0$, $[I_{2m}(0)/N]^2 = 1$, which is the *largest* value of $[I_{2m}(2\phi)/N]^2$ as a function of ϕ, and the MC is equal to the *smallest* value $G(0)$. When the magnetic field is increased from zero, $[I_{2m}(2\phi)/N]^2$ quickly approaches (more rapidly as m becomes larger) its *smallest* value, which is zero, at $\phi/2\pi = 1/4m$. At the same time, the MC rapidly increases to the *largest* value $2G(0)$. The physical implication of this is clear: fully constructive (destructive) interference in the case without disorder leads to the smallest (largest) hopping conduction in the presence of disorder. Moreover, when m (the system size is $m \times m$) is large, $G(\phi)/G(0)$ remains in the close vicinity of 2 for $\phi/2\pi > 1/4m$ in spite of the strong very-small-magnitude fluctuations of $I_{2m}(2\phi)/N$ around zero.

The saturated value of the magnetic field $B_{\rm sa}$ [i.e., the first field that makes $G(\phi) = 2G(0)$] is inversely proportional to twice the hopping length: the larger the system is, the smaller $B_{\rm sa}$ will be. In other words, as soon as the system, with hopping distance $r = 2m$, is penetrated by a total flux of $(1/2r)(r/2)^2 = r/8$ (in units of Φ_0), the MC reaches the saturation value $2G(0)$.

To examine the behavior of the MC in the low-flux limit, we first define the relative MC, $\Delta G(\phi) \equiv [G(\phi) - G(0)]/G(0)$. Since $\ln I_r = -r^2(r+1)\phi^2/96$ and $\ln S_{r-1,1} = -(r^2-1)\phi^2/24$ from Eq. (3), it follows then that, for very small fields, in 2D $\Delta G(\phi) \simeq \sqrt{3}\,r^{3/2}\phi/6$ and in ladder-type quasi-1D structures $\Delta G(\phi) \simeq \sqrt{3}\,r\phi/3$.

Our results for the MC are in good agreement with experimental measurements. For instance, a positive MC is observed in the VRH regime of both macroscopic In_2O_{3-x} samples and compensated n-type CdSe [9]. Moreover, saturation in the MC as the field is increased is also reported in Ref. [9].

The result for $G(\phi)$ presented in this work is consistent with theoretical studies based on an independent-directed-path formalism and a random matrix theory of the transition strengths [8]. The advantages of our results lie in that they (i) provide an explicit expression for the MC as a function of the magnetic field, and thus a straightforward determination of the period of oscillation, (ii) provide explicit scaling behaviors (i.e., the dependence on the hopping length as well as the orientation and strength of the field) of the low-flux MC in quasi-1D, 2D, and 3D systems, and (iii) allow a quantitative comparison with experimental data. It is important to emphasize that our analytic result for the MC is equally applicable to *any dimension,* since the essential ingredient in our expressions is the QI quantity $S^{(r)}$, which takes into account the dimensionality.

Quantum interference and the small-field magnetoconductance on a 3D cubic lattice.—Let $S_{m,n,l}$ ($= S^{(r)}$ in 3D) be the sum over all phase factors associated with directed paths of $m + n + l (= r)$ steps along which an electron may hop from (0,0,0) to the site (m,n,l) with m, n, and $l \geq 0$. The vector potential of (B_x, B_y, B_z) can be written as $\mathbf{A} = (zB_y - yB_z, xB_z - zB_x, yB_x - xB_y)/2$. Also, $a/2\pi$, $b/2\pi$, and $c/2\pi$ represent the three fluxes through the respective elementary plaquettes on the y-z, z-x, and x-y planes. To compute $S_{m,n,l}$, we start from the recursion relation $S_{m,n,l} = \sum_{p=0}^{m}\sum_{q=0}^{n} \times A_{p,q,l\to m,n,l}e^{i(qa-pb)/2}S_{p,q,l-1}$, where $A_{p,q,l\to m,n,l}$ is the sum over all directed paths starting from (p,q,l) and ending at (m,n,l). The physical meaning of this relation is clear: the site (m,n,l) is reached by taking one step from $(p,q,l-1)$ to (p,q,l), acquiring the phase $i(qa - pb)/2$, then traversing from (p,q,l) to (m,n,l) on the $z = l$ plane. We find that $A_{p,q,l\to m,n,l} = \exp\{i[(m-p)(lb-qc) + (n-q)(pc-la)]/2\}S_{m-p,n-q}(c)$. By applying the above equation l times, we obtain a general formula of $S_{m,n,l}$ for $m,n,l \geq 1$ in terms of the fluxes a, b, and c as

$$S_{m,n,l}(a,b,c) = e^{-i(nla+lmb+mnc)/2}\mathcal{L}_{m,n,l}(a,b,c), \quad (6)$$

$$\mathcal{L}_{m,n,l} = \left\{\prod_{j=1}^{l}\left[\sum_{p_j=0}^{p_{j+1}}\sum_{q_j=0}^{q_{j+1}} e^{i[q_j a+(m-p_j)b+p_j(q_{j+1}-q_j)c]} \times L_{p_{j+1}-p_j,q_{j+1}-q_j}(c)\right]\right\}L_{p_1,q_1}(c), \quad (7)$$

with $p_{l+1} \equiv m$, $q_{l+1} \equiv n$, and the $L_{p,q}(c)$'s are defined as in Eq. (1). In the absence of the flux, $S_{m,n,l} = (m+n+l)!/m!\,n!\,l! \equiv \mathcal{N}$ gives the total number of r-step paths connecting $(0,0,0)$ and (m,n,l). In the very-low-flux limit, *exactly* calculated to second order in the flux and omitting the term $\ln\mathcal{N}$, the 3D analog of the harmonic shrinkage of the wave function becomes

$$\ln S_{m,n,l} = -\tfrac{1}{24}[nla^2 + lmb^2 + mnc^2 + m(lb-nc)^2 + n(mc-la)^2 + l(na-mb)^2]. \quad (8)$$

In order to see how the interference patterns and the MC vary according to the orientation of the applied field, we now examine two special cases: $\mathbf{B}_{\parallel} = (1,1,1)(\phi/2\pi)$ and $\mathbf{B}_{\perp} = (1/2,1/2,-1)(\phi/2\pi)$, namely, fields parallel and perpendicular to the $(1,1,1)$ direction. We find that their $S_{m,m,m}$, designated, respectively, by $\mathcal{I}_r^{\parallel}$ and $\mathcal{I}_r^{\perp}$ (where $r = 3m$), exhibit quite different behaviors. Furthermore, they are insensitive to the commensurability of ϕ, unlike the case on a square lattice. Physically, this can be understood because paths have a higher probability of crossing (and thus interfering) in 2D than in 3D, thus making QI effects less pronounced in 3D than in 2D. A similar situation occurs classically (e.g., multiply scattered light in a random medium). For very small ϕ, $\ln \mathcal{I}_r^{\parallel} = -r^2\phi^2/72$ and $\ln \mathcal{I}_r^{\perp} = -r^2(r+1)\phi^2/144$. The 3D behavior of $\Delta G(\phi)$ thus becomes clear: $\simeq r\phi/3$ for $\mathbf{B}_{\parallel}$ and $\simeq \sqrt{2}\, r^{3/2}\phi/6$ for $\mathbf{B}_{\perp}$. These results can be interpreted as follows: the effective area exposed to $\mathbf{B}_{\parallel}$ is smaller ($\sim r$), similar to our quasi-1D case with $\Delta G(\phi) \propto r\phi$, while the effective area exposed to $\mathbf{B}_{\perp}$ is larger ($\sim r^{3/2}$), thus closer to the 2D case with $\Delta G(\phi) \propto r^{3/2}\phi$.

Average of the magnetoconductance over angles.—In a macroscopic sample, the conductance may be determined by *a few* (i.e., more than one) critical hopping events. As a result of this, the observed MC of the whole sample should then be the average of the MC associated with these critical hops [10]. Thus, in 3D systems, it is also important to take into account the randomness of the angles between the hopping direction and the orientation of the applied magnetic field. We therefore consider the following picture: the ending site of all hopping events (with the same hopping length r) is located at the body diagonal $(r/3, r/3, r/3)$, and the magnetic field can be adjusted between the parallel and perpendicular directions with respect to the vector $\mathbf{d} = (1,1,1)$. Our interest here is in the MC averaged over angles, denoted by $\overline{\Delta G}$, in the low-field limit. From Eq. (8), we obtain $\Delta G(B) = (2\pi/3\sqrt{3}) rB(1 + r\sin^2\omega)^{1/2}$, where B is the magnitude of the field and ω is the angle between $\mathbf{B}$ and $\mathbf{d}$. By averaging over the angle ω, we obtain

$$\overline{\Delta G}(B) = \frac{4}{3\sqrt{3}}\, r\sqrt{r+1}\, BE\left(\frac{\pi}{2}, \frac{\sqrt{r}}{\sqrt{r+1}}\right), \qquad (9)$$

where $E(\pi/2, \sqrt{r}/\sqrt{r+1})$ is the complete elliptic integral of the second kind. When r is large, $E \simeq 1$ and we therefore have $\overline{\Delta G}(B) \simeq (4/3\sqrt{3}) r^{3/2} B$. This means that the dominant contribution to the MC stems from the critical hop which is perpendicular to the field. This is understandable through our earlier observation that the effective area enclosed by the electron is largest when $\mathbf{B}$ is perpendicular to $\mathbf{d}$. From the above analysis, we conclude that in 3D macroscopic samples the low-field MC should in principle behave as $r^{3/2}B$.

Finally, we briefly address five issues. First, in addition to the dominant terms, we have also obtained the second-order contribution to the moments ($\propto N^{p-1}$) and the MC ($\propto 1/N$). The principal features in the behavior of the MC are not significantly modified: only the magnitude of the positive MC, including the saturation value, is slightly increased (though negligibly small). Second, we have also studied another model of disorder, ϵ_i uniformly distributed between $-W/2$ and $W/2$. The result for the MC remains the same. Third, returns to the origin become important for less strongly localized electrons, and their QI effects [11] can be incorporated in our approach. Fourth, the main limitations of our study are the following: no inclusion of spin-orbit scattering effects (for this see, e.g., Refs. [7,8] and references therein), and no explicit inclusion of the correlations between crossing paths, as discussed in Refs. [4,7]. However, these correlations are negligible when spin-orbit scattering is present [7]. Fifth, our result for $\Delta G(B)$ in 3D can be tested experimentally by measuring the MC of bulk samples for varying orientations of the field.

In summary, we present an investigation of QI phenomena and the magnetic-field effects on the MC for 2D and 3D systems in the VRH regime. We provide exact and explicit closed-form results for the forward-scattering paths which, in the strongly localized regime, give the dominant contribution to the hopping conduction.

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