Energy spectrum and persistent current in one-dimensional rings

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The correlations in the energy spectrum and persistent current of electrons in one-dimensional disordered rings threaded by an Aharonov-Bohm magnetic flux are shown to be so strong that the current of any level is sufficient to cancel the sum of the contributions of all previous levels. Hence, the sign of the sum of the n lowest single-level currents alternates as a function of n. A new relation between the real part of the inverse transmission coefficient and the energy spectrum is also derived.

I. INTRODUCTION

Consider electrons in a one-dimensional ring without leads threaded by an Aharonov-Bohm flux. If the ring is smaller than the phase coherence length, then quantum coherence effects will be important. Some phenomena will depend on the structure of the discrete energy spectrum. An example is persistent currents in such rings.[1] Advances in semiconductor technology have begun to make it possible to study such systems experimentally. Here we discuss some general properties of the energy levels. We show that strong correlations exist between the slopes of the levels as function of flux, such that the total persistent current as function of filling alternates in sign from one filling to the next.

The model that we use is the Anderson model, which is a tight-binding model with diagonal disorder. However, the results hold also for other models, such as models with off-diagonal disorder, or free electrons in a random potential. The Hamiltonian for the Anderson model is

$$H=\sum_{i=1}^{N}\varepsilon_i a_i^{+}a_i - V\sum_{i=1}^{N-1}(a_i^{+}a_{i+1}+a_{i+1}^{+}a_i) - Ve^{i(2\pi\phi/\phi_0)}a_N^{+}a_1 - Ve^{-i(2\pi\phi/\phi_0)}a_1^{+}a_N \ . \quad (1.1)$$

Here, ϕ is the magnetic flux enclosed by the ring, $\phi_0=hc/e$ the flux quantum, and N is the number of lattice sites as well as the number of levels in the system. In the following we set $V=1$, so that energies are measured in units of V. We consider the case of nonmagnetic impurities and neglect spin degeneracy and electron-electron interactions.

The magnetic flux ϕ enters the Hamiltonian (1.1) explicitly and the wave functions satisfy periodic boundary condition. It is mathematically equivalent to consider the above Hamiltonian at zero flux with the flux then entering via the phase-shifted boundary condition,[2]

$$\psi(N+n)=\exp\left[\frac{i2\pi\phi}{\phi_0}\right]\psi(n) \ . \quad (1.2)$$

In this case one can change the boundary condition continuously by varying the flux ϕ.

Byers and Yang[2] showed in 1961 that the energy spectrum E_n of the system is periodic in the magnetic flux with period ϕ_0, and that the persistent current of each level is determined by the slope of the level versus flux,

$$I_n=-c\frac{\partial E_n}{\partial\phi} \ . \quad (1.3)$$

In 1983, Büttiker, Imry, and Landauer[1] addressed the question of the persistent current from the mesoscopic-physics point of view. They mapped the problem onto the band-structure problem of a one-dimensional infinite crystal. The idea is the following. After the electron circles the ring once, it sees exactly the same potential as before, but now has acquired an additional phase $2\pi\phi/\phi_0$. The situation is equivalent to the one described by the Bloch theorem. Hence the energy-flux diagram is equivalent to the band structure (E versus ka) of a one-dimensional infinite crystal. Also the fact that the $E_n(\phi)$ have alternating slopes from level to level was already noticed by these authors. Imry[3] discusses this point further, starting from results for the band structure of one-dimensional infinite crystals. He concludes that $E_n(\phi)$ cannot have an absolute minimum or maximum except at $\phi=0$ and $\phi=n\phi_0/2$.

Random matrix theory also applies here.[4] The Anderson Hamiltonian (1.1) falls into the class of the orthogonal ensemble when the flux is zero or an integer multiple of half flux quantum, and into the class of the unitary ensemble for other values of the flux. Two interesting results are the level repulsion and the extraordinary small fluctuation of the number of levels within some typical energy range, if the localization length is not much shorter than the ring circumference.

Thouless pointed out to us that the first $(N-1)$th moments of the spectrum are flux independent.[5] A way to see this moment condition is as follows. The Hamiltonian contains on-site terms plus nearest-neighbor hopping terms. Physically, every time the Hamiltonian operator acts on the electron wave function, the electron can either remain sitting at the same site or hop to the next site. In order to contribute to the diagonal terms of the mth power of the Hamiltonian, the electron must return to its initial site after exactly m steps, each step being one sit or one hop. In a sequence of sits and hops, although

the electron may cross the site with the flux and so acquire an additional phase $2\pi\phi/\phi_0$, it can hop back across that site and cancel that phase. The only way that it can go back to the initial site without canceling the phase due to the flux is to hop around the ring, which requires at least N hops. So up to the $(N-1)$th power of the Hamiltonian, the diagonal terms cannot contain terms that depend on the flux.

It is interesting to see what the above moment condition implies. First of all, it imposes $(N-1)$ constraints, which means that the energy spectrum is a very rigid function of ϕ. With one additional relation between the energies (e.g., the knowledge of one energy), one could then, in principle, solve for the whole spectrum. In practice these are nonlinear equations, which have been studied under the name "moment equations."[5] If one takes their derivative with respect to ϕ, one obtains $(N-1)$ homogeneous linear equations for the currents, with coefficients depending on the energies. Hence, if the whole spectrum plus one current were known, one could solve for the other currents. This approach yields useful information about the current. However, in the following we shall use an alternative approach, which yields all of this plus additional information.

II. TRANSFER-MATRIX MATCHING METHOD

The approach we use for finding the energy levels is the transfer-matrix method. The method is discussed in Anderson and Lee.[6] Later it was applied by us to investigate the persistent current in a one-dimensional ring.[7] We discuss it further here, concentrating on the general properties of the system.

The transfer-matrix method for finding the energy levels of electrons in a ring consists of two steps. In step 1, imagine the ring being cut open and stretched out to form a straight wire. Starting with some trial wave function of energy E on the first two sites (ψ_1 and ψ_2), one can obtain the wave function on the next site (ψ_3) by solving the eigenvalue equation $H\psi=E\psi$. [We let the flux enter via the boundary condition Eq. (1.2), so that H is flux independent.] The result is $\psi_3=(\varepsilon_2-E)\psi_2-\psi_1$, ε_2 being the random site energy. This procedure is repeated until the two sites corresponding to the starting sites are reached, now with the wave functions ψ_{N+1} and ψ_{N+2}, respectively. The result is written in terms of the transfer matrix T in real space,

$$\begin{bmatrix}\psi_{N+1}\\ \psi_{N+2}\end{bmatrix}=T\begin{bmatrix}\psi_1\\ \psi_2\end{bmatrix}\equiv\begin{bmatrix}T_{11} & T_{12}\\ T_{21} & T_{22}\end{bmatrix}\begin{bmatrix}\psi_1\\ \psi_2\end{bmatrix}. \tag{2.1}$$

From the construction, one sees that the elements of the T matrix are polynomials in E of at most order N. The procedure can also be formulated in k space. Then the transfer matrix T connects the amplitudes of right- and left-traveling waves (A and B) at the left end of the wire to the corresponding amplitudes (C and D) at the right end,

$$\begin{bmatrix}C\\ D\end{bmatrix}=T\begin{bmatrix}A\\ B\end{bmatrix}=\begin{bmatrix}1/t^* & r/t\\ r^*/t^* & 1/t\end{bmatrix}\begin{bmatrix}A\\ B\end{bmatrix}. \tag{2.2}$$

Here, t and r are the total transmission and reflection coefficients for waves entering from the left. Now we consider step 2 of the transfer-matrix matching method. For a level to exist at energy E, the wave function ψ must also satisfy the boundary condition (1.2). This is possible if and only if the T matrix has an eigenvalue equal to $\exp(i2\pi\phi/\phi_0)$. Mathematically, $\det[T-\exp(i2\pi\phi/\phi_0)]=0$. This matching condition for a level to exist reduces to the following simple equation:[6]

$$f(E)\equiv\mathrm{Re}\left[\frac{1}{t}\right]=\cos\left[\frac{2\pi\phi}{\phi_0}\right]. \tag{2.3}$$

The expression for the current is also very simple,[7]

$$I_n=\frac{e}{\hbar}\frac{\sin(2\pi\phi/\phi_0)}{f'(E_n)}. \tag{2.4}$$

Alternatively, one can work in real space and the matching function $f(E)$ would then be equal to one-half times the trace of the T matrix. From the above construction of the T matrix, one knows that the elements of the T matrix are polynomials in E of order not larger than N. Since the number of levels is N, the above implies that $f(E)$ is a polynomial in E of order exactly equal to N. Hence the function $\exp(-i2\pi\phi/\phi_0)\det[T-\exp(i2\pi\phi/\phi_0)]$, which is equal to $2\,\mathrm{Re}(1/t)-2\cos(2\pi\phi/\phi_0)$, must be proportional to $\prod_n(E_n-E)\equiv\det(H-E)$. Both functions vanish at the energies of the levels. By comparing the coefficients of the $\cos(2\pi\phi/\phi_0)$, one finds that the proportionality constant is 1. So our main result is

$$f(E)\equiv\mathrm{Re}\left[\frac{1}{t}\right]=\cos\left[\frac{2\pi\phi}{\phi_0}\right]+\tfrac{1}{2}\prod_{n=1}^{N}[E_n(\phi)-E]. \tag{2.5}$$

This is a useful new relationship between the energy levels of the electron in the ring and the total transmission coefficient around the ring, in either clockwise or anticlockwise direction. Since $f(E)$ is independent of flux, one may consider without loss of generality $\phi=\frac{1}{4}\phi_0$ and write $f(E)=\frac{1}{2}\prod_{n=1}^{N}[E_n(\frac{1}{4}\phi_0)-E]$. The energies of all levels $E_n(\frac{1}{4}\phi_0)$ are real. From the above one infers that the matching function $f(E)$ has the following exact properties. (i) There are N zeroes, at $E=E_n(\frac{1}{4}\phi_0)$. (ii) There is only one turning point between any two adjacent zeroes. Hence there are $(N-1)$ turning points. (iii) At those turning points $|f(E)|$ must be at least 1, as implied by the definition $f(E)=\mathrm{Re}(1/t)$ and $|t|\le 1$.

The above properties may seem a mild restriction. However, by asking how close one can move the energy E_n towards E_{n+1} without violating these constraints (keeping all other E_m fixed), we find that there must be a minimum energy separation between these two levels. If one tried to reduce the separation further, one would force $|f(E)|$ at one of the turning points to be less than 1. Moreover, there are long-range correlations in the spectrum. If one puts E_n and E_{n+1} at the minimum separation such that $|f(E)|$ at the turning point between these levels is equal to 1, one cannot move any other levels

closer to this pair without forcing $|f(E)|$ at this turning point to be less than 1. This gives a rough picture for viewing level repulsion and level rigidity.

For general flux, Eq. (2.3) defines the energy levels. Graphically, one may consider $f(E)$ versus E intersected with a constant equal to $\cos(2\pi\phi/\phi_0)$.

Since $f(E)$ is an oscillating function of the energy with an amplitude not less than one, Eqs. (2.3) and (2.4) imply the following general results.

Case 1. The flux is not equal to zero or an integer multiple of a half flux quantum. Then the energy levels are nondegenerate, and the currents of the levels are nonzero and alternate in sign from level to level.

Case 2. The flux is equal to zero or an integer multiple of a half flux quantum. In general the energy levels are nondegenerate and have zero current. In the peculiar "resonance" case $t=\pm 1$ ($t=1$ for even integer multiples of a half flux quantum and $t=-1$ for odd integer multiples), the levels are twofold degenerate and their currents add up to zero.

The first result follows because at these fluxes the magnitude of the right-hand side of Eq. (2.3) is less than 1 and therefore Eq. (2.3) cannot have multiple solutions. The behavior of the current can be deduced from Eq. (2.4). The result follows since $f'(E)$ is finite, nonzero, and alternates in sign from level to level. The second result follows by considering under which conditions multiple solutions of Eq. (2.3) are possible. A double solution is possible if and only if $t=\pm 1$ at that energy and for those fluxes. From Eq. (2.4), nonzero current requires $f'(E)=0$, and this coincides with the conditions for degeneracy. The sum of the currents of two degenerate energy levels is zero because $f'(E)$, being determined solely by the curvature of $f(E)$, is antisymmetric very close to that energy.

From Eqs. (2.3)–(2.5), one derives that the single-level current is

$$I_n=\frac{2e}{\hbar}\frac{1}{\prod'_m[E_m(\phi)-E_n(\phi)]}\sin\left[\frac{2\pi\phi}{\phi_0}\right]. \tag{2.6}$$

This result also follows from the moment condition. Equation (2.6) implies some of the results derived above. It demonstrates explicitly that in the absence of degeneracy the single-level currents I_n are alternating in sign with n. Likewise, one current being zero implies that all other currents must vanish, etc.

Next we consider the total current. First we define the total current up to the nth level as the sum of the currents of the first n level. We shall see that the total current is also very rigid, namely, it is alternating in sign with n.

To derive this result, first we rewrite the single-level current in terms of a parameter E,

$$I_n\propto\frac{-1}{2\pi i}\oint\frac{1}{\prod(E_m-E)}dE\ , \tag{2.7}$$

where the integral is over a closed path which encloses only the pole at $E=E_n$. Then the total current can be expressed as

$$I_{\text{total}}\propto\frac{-1}{2\pi i}\int_C\frac{1}{\prod(E_m-E)}dE\ , \tag{2.8}$$

where the contour C encloses the first n poles. Alternatively, one can integrate over the real axis by shifting the first n poles by a small positive imaginary part, and the others by a small negative imaginary part. The integrand is similar in form to the standard Green's function.

The integrand has poles on the real axis only, see Fig. 1. We will deform the contour in the following way. Define an angle θ_n by $E_n-E=|E_n-E|\exp(i\theta_n)$, with $-\pi<\theta_n\le\pi$. Then the integrand in Eq. (2.8) can be rewritten as $\exp(-i\sum\theta_m)/\prod|E_m-E|$. Now consider the set of $(N-1)$ lines defined by $\sum\theta_m=\pm l\pi$, $l=1,2,\ldots,N-1$, in the complex E plane. Ignore the real axis for the moment. One finds that between any two adjacent poles E_m and E_{m+1} there passes exactly one of the above-mentioned lines. These lines have the following properties. (i) They are mirror symmetric across the real axis, since the E_n are real. (ii) They never cross one another, since $\sum\theta_m$ is the imaginary part of the analytic function $\ln\prod(E_m-E)$. (iii) All lines start from infinity in the lower half plane and end at infinity in the upper half plane. (iv) If one follows any one line from the lower half plane to the upper half plane, the real part of E along the line is increasing on one side of the real axis but decreasing on the other, whereas the imaginary part of E is always increasing. Obviously, one can choose these lines to be the contours of integration in the expression for the total current. For the total current up the nth level the contour to be chosen is the line passing between E_n and E_{n+1} and the direction is from the lower half plane to the upper half plane. The integrand in Eq. (2.8) for the total current has the following properties. (a) It is real and does not change sign along a contour, since $\sum\theta_m=\pm l\pi$ and l is fixed. (b) It is symmetric across the real axis along a contour. (c) The sign of the integrand alternates with n, since when n changes by 1 the contour index l changes by 1. By combining these properties of the integrand with those of the contour lines stated above, especially (i) and (iv), one concludes that the real part of the integral in Eq.

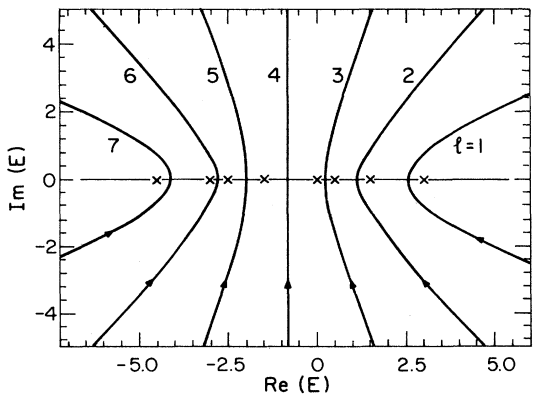

FIG. 1. Schematic representation of the poles (×) and contours of integration in Eq. (2.8). (Figure obtained for a ring with $N=8$ sites.)

(2.8) vanishes by symmetry, while the imaginary part alternates in sign with n. Therefore the total current I_{total} is always real and alternates in sign with n.

The last result is very interesting since it implies that the total current has the same sign but is smaller in magnitude than the current of the last level. The correlations in the spectrum are so strong that the current of any level is sufficient to cancel the sum of the contributions of all previous levels.

III. OTHER CONSIDERATIONS

Some of the above properties of single-level currents can also be understood from another viewpoint. Here we give a mathematical explanation for why the current cannot be zero at $\phi \neq n\phi_0/2$. The flux enters the problem via the phase-shifted boundary condition for the wave functions, Eq. (1.2). When $\phi \neq n\phi_0/2$, the phase factor is a complex number. This implies that none of the eigenfunctions can be chosen real on every site, which in turn implies nonzero current.

We give another reason why at $\phi = n\phi_0/2$, when the energy levels are doubly degenerate, the sum of their currents is zero. Those fluxes correspond to either periodic or antiperiodic boundary conditions for the wave function. The Hamiltonian and the phase factor in the boundary condition are real. So in case of double degeneracy one can choose a pair of real orthonormal wave functions as a basis. Since they are real, they carry zero current. Other bases are possible, and their wave functions may carry currents. However, when both of the two degenerate energy levels are filled, the sum of the currents must be zero since the result should not depend on the basis.

IV. SUMMARY

We have derived a useful relationship between the transmission coefficient and the energy levels for electrons in a one-dimensional ring. An understanding was developed for two important properties of the spectrum, namely, level repulsion and spectral rigidity. We find that the energy levels can be degenerate only if both the flux is equal to zero or $n\phi_0/2$ and the transmission coefficient is equal to ± 1 at that energy. For all other values of the flux, we find that the sign of the single-level current I_n alternates with n and that the total current I_{total} has the sign of the current of the last occupied level. This strong correlation is remarkable.

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