Relation between Persistent Currents and the Scattering Matrix

Eric Akkermans,[(a)] Assa Auerbach,[(b)] Joseph E. Avron, and Boris Shapiro
Department of Physics, Technion–Israel Institute of Technology, Haifa, 32000, Israel
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We show that the differential contribution, at energy E, to the persistent currents of independent electrons in infinitely extended quantum systems is given by $(2\pi i)^{-1}\partial_\phi[\ln \det S(E,\phi)]dE$, where $S(E,\phi)$ is the (on-shell) scattering matrix. We apply this result to the calculation of the persistent currents in two examples: a mesoscopic loop connected to one infinitely long lead, and a phase pierced by a flux line. In the last example spin plays a remarkable role.

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In this Letter we consider the persistent currents in *infinitely extended* quantum systems of independent electrons in two dimensions. A persistent current is defined with respect to a point. It is given by the total current through a line that extends from that point to infinity, in the absence of currents through the external leads. We designate this point by a flux tube which is infinitesimally thin and which passes through the point. The flux denoted by ϕ may be either finite, or infinitesimal, $\phi=\mathbf{B}\cdot d\mathbf{s}$, where $\mathbf{B}$ is a finite magnetic field. Allowing the persistent-current definition to include the two limits provides a unified treatment of Aharonov-Bohm interference effects, and orbital magnetism.

Two classes of systems for which our considerations apply are (i) mesoscopic networks and (ii) continuous media. The mesoscopic networks are coupled to infinitely long, ordered leads (waveguides) with flux enclosed by the internal loops. The rings may have disordered potential associated with them. A simple example is shown in Fig. 1. An example of the second class is the persistent currents around the origin, pierced by a flux tube, for free electrons in the plane when all states below the Fermi energy are occupied.

The persistent currents in *finite* systems, and, in particular, in isolated rings, were first studied by Bloch in 1965 and subsequently by several authors,[1] and were observed by Levy *et al.*[2] In this case the persistent current carried by the nth eigenstate is $-dE_n(\phi)/d\phi$. For unbounded systems the spectrum will, in general, have both a discrete and a continuous part. The contribution of the discrete eigenvalues to the persistent currents is still given by $-dE_n(\phi)/d\phi$. Our purpose is to show that the scattering-state contribution to the persistent currents is

$$dI(E,\phi)=(2\pi i)^{-1}\partial_\phi[\ln \det S(E,\phi)]dE$$
$$=(1/\pi)\partial_\phi\left[\sum_j \delta_j(E,\phi)\right]dE\,, \qquad (1)$$

where $dI(E,\phi)$ is the differential contribution to the persistent current at energy E and $S(E,\phi)$ is the on-shell scattering matrix. The $\delta_j(E,\phi)$ are the scattering phase shifts [i.e., $\exp(2i\delta_j)$ are the eigenvalues of $S(E,\phi)$].

Here are some general properties of the persistent currents that can be read off directly from Eq. (1). First, since $S(E,\phi)$ is unitary, its determinant is of modulus 1, and the right-hand side of Eq. (1) is a real number. Second, as the determinant is unitary invariant, the persistent currents are gauge invariant, and periodic in ϕ with period $\phi_0\equiv h/e$. Third, in the special case that there are no magnetic fields besides the one associated with the flux ϕ, $S(E,\phi)=S^t(E,-\phi)$, by time reversal, where the superindex t denotes transpose. As a consequence, $\det S(E,\phi)$ is a symmetric function of ϕ, and the persistent currents are antisymmetric functions of ϕ, as expected on general grounds.

It is instructive to compare Eq. (1) for the persistent currents with the Landauer formula[3] for the conductance g, which expresses it as a certain function of the scattering matrix $g(S)$. The distinct features of these two formulas is that the Landauer formula does not involve derivatives with respect to ϕ and has the property that $g(S)=g(\exp(i\theta)S)$ with θ real valued, but otherwise arbitrary. Equation (1), in contrast, is linear in $d\theta/d\phi$. We learn that the conductance and persistent currents give complementary information on the scattering matrix.

Equation (1) is a consequence of an identity in scattering theory that relates the variation of the on-shell scattering matrix to the variation of the Hamiltonian H (we assume of course that H admits a good scattering

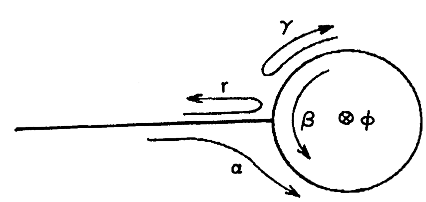

FIG. 1. An ideal one-dimensional ring, coupled to a perfect, infinite, one-mode wire. The vertex that couples the ring to the wire is described by the unitary matrix in Eq. (6). α, β, γ, and r are the entries in that matrix and their meaning is noted by the arrows.

theory):

$$\delta \ln \det S(E) = -(2\pi i)\mathrm{Tr}_E(\delta H). \quad (2)$$

det and Tr_E denote the determinant and the trace restricted to the energy shell (this is explained in some detail below). The study of det$S$ goes back to J. Schwinger, and Eq. (2) is related to, among others, Wigner's time-delay and Krein's formulas.[4]

We recall some basic facts of scattering theory that we need in order to explain the notation used above, and in order to outline the derivation of Eq. (2). Let $|E,\omega,\pm\rangle$ denote the incoming and outgoing scattering states at energy E.[5] ω labels the scattering channels. The simplest situations have a finite number of channels (this is the case for mesoscopic networks like the one in Fig. 1, where the number of channels is the total number of modes, at energy E, in the waveguide that extends to infinity). In the case of infinitely many channels, ω can be either a discrete or a continuous variable. For example, in potential scattering from noncentral potentials, it is natural to choose ω to denote the direction of the scattering state (i.e., a point on the sphere). The normalization we choose is $\langle E,\omega,\pm|E',\omega'\pm\rangle=\delta(E-E')\times\delta(\omega-\omega')$, in the case that ω is a continuous variable, and $\langle E,\omega,\pm|E',\omega'\pm\rangle=\delta(E-E')\delta_{\omega,\omega'}$ when it is discrete. For the sake of notation we assume below that ω is a discrete variable.

The *scattering matrix* is $S=\int(\sum_\omega|E,\omega,+\rangle\langle E,\omega,-|)dE$.[5] $\mathrm{Tr}_E(\cdot)$ in Eqs. (1) and (2), is defined by

$$\mathrm{Tr}_E(A)\equiv\sum_\omega\langle E,\omega,+|A|E,\omega,+\rangle. \quad (3)$$

For networks, the (on-shell) scattering matrix is the familiar unitary matrix that relates the incoming and outgoing channels of all external leads. The scattering states are normalized to carry unit current. In general, the on-shell scattering matrix is a unitary matrix —depending parametrically on E—with entries $S(E)_{\omega,\omega'}$. In order to write these matrix elements as matrix elements in the original basis $|E,\omega,\pm\rangle$ we need to factor a Dirac δ function from the scalar product. The derivation of Eq. (2) that we now describe shows how this factorization is done.

Let $|f,\omega,+\rangle\equiv\int dE\,f(E)|E,\omega,+\rangle$, with f square integrable, arbitrary, but *fixed*. S defines a unitary map, from the vector space spanned by $|f,\omega,-\rangle$ (as ω varies over the channels) to the vector space spanned by $|f,\omega,+\rangle$, whose matrix elements are $S(f)_{\omega,\omega'}=\langle f,\omega,-|f,\omega',+\rangle$. For this unitary matrix one has

$$\delta \ln \det S(f) = \mathrm{Tr}[S^\dagger(f)\delta S(f)] = \sum_\omega[\langle f,\omega,+|\delta(f,\omega,+)\rangle - \langle f,\omega,-|\delta(f,\omega,-)\rangle], \quad (4)$$

where we used the fact that $\delta(\langle f,\omega,-|f,\omega,-\rangle)=0$.

The basic fact that characterizes the incoming and outgoing scattering states is that they satisfy the integral equation

$$\delta|f,\omega,\pm\rangle=\int dE\,f(E)G_\pm(E)\delta H|E,\omega,\pm\rangle, \quad (5)$$

where $G_\pm(E)$ are the retarded and advanced Green functions, so that

$$G_\pm(E)|E',\omega,\pm\rangle=(E-E'\pm i\epsilon)^{-1}|E',\omega,\pm\rangle.$$

Inserting Eq. (5) into Eq. (4) and using the principal-value theorem gives Eq. (2) in the limit that $|f|^2$ approximates a δ function.

Equation (1) now follows from the fact that the current around the flux tube, in the state $|\psi\rangle$, is $I(\psi,\phi)=-\langle\psi|dH/d\phi|\psi\rangle$.

We shall now turn to two applications of Eq. (1). The first application deals with the persistent current in the simplest mesoscopic system and we shall rederive results first obtained by Büttiker by different means.[6] Consider an ideal one-dimensional ring of length L without disorder, attached to a perfect, infinite one-mode wire and threaded by an Aharonov-Bohm flux ϕ as in Fig. 1. The vertex that connects the loop to the wire is described by a 3×3 unitary matrix U which relates the ingoing and outgoing amplitudes at the vertex:

$$U\equiv\begin{pmatrix} r & \alpha & \alpha \\ \alpha & \beta & \gamma \\ \alpha & \gamma & \beta \end{pmatrix}. \quad (6)$$

The four real coefficients, α, β, γ, and r, are constrained by the three independent unitarity relations $r^2+2\alpha^2=1$, $\alpha^2+\beta^2+\gamma^2=1$, and $\alpha^2+2\beta\gamma=0$. The physical interpretation of r, α, β, and γ is indicated in Fig. 1. Since the infinite wire has one scattering channel, the on-shell scattering matrix of Eq. (1) is a complex number of modulus 1—the reflection amplitude—given by

$$S(E,\phi)=-D^*(kL,\phi/\phi_0)/D(kL,\phi/\phi_0),$$

where $E=\hbar^2k^2/2m$ and

$$D(x,y)\equiv\beta[\cos(x)-\cos(2\pi y)]-i\gamma\sin(x).$$

$S(E,\phi)$ is manifestly unitary, and

$$[\ln\det S(E,\phi)]'=(D^{*\prime}D-D'D^*)/|D|^2$$
$$=2i(\mathrm{Re}D)'(\mathrm{Im}D)/|D|^2$$

(the prime denotes derivative with respect to flux). From Eq. (1) we obtain for the persistent current I when all the states up to k_F are occupied

$$I=\frac{\hbar e\alpha^2}{\pi m}\int_0^{k_F}k\,dk\frac{\sin(kL)\sin(2\pi\phi/\phi_0)}{|D(kL,\phi/\phi_0)|^2}. \quad (7)$$

This equation contains a factor of 2 for the two spin states.

The limiting case of an ideal ring disconnected from the wire considered in Ref. 1, corresponds to the limit

$\alpha \to 0$, $\beta \to 1$, and $\gamma \to 0$. Since $\alpha \to 0$ multiplies the integral, the contribution to the persistent currents for most values of k will vanish and only those k which make the denominator of the integrand vanish can contribute. $D(kL,\phi)=0$ for $kL = 0 \bmod (2\pi)$, $\phi = 0 \bmod (\phi_0)$, and $kL = \pi \bmod (2\pi)$, $\phi = \frac{1}{2} \bmod (\phi_0)$. At these points the integrand approaches a sequence of δ functions that correspond to the contributions of the populated discrete energy levels of an isolated ring. One then recovers the standard expressions for the persistent currents in an isolated ring. It is noteworthy that the scattering data for an almost disconnected network convey information about the persistent currents carried by the (almost) bound states on the ring. This is reminiscent of what happens in the Levinson theorem in scattering theory. A similar analysis can be done for the one-dimensional ring with two leads, allowing an explicit comparison of the conductance and persistent current.[7]

As a second application we consider a macroscopic system of free electrons in the plane. We shall compute the persistent currents at zero temperature around, and due to, a flux line that pierces the plane. The corresponding scattering problem was considered in the original Aharonov-Bohm paper[8] for the spinless case and by Hagen[9] for the spin-$\frac{1}{2}$ case, which shows a delicate effect that has to do with the $\boldsymbol{\sigma}\cdot\mathbf{B}$ interaction, with B δ-function-like. As we shall see, this leads to the rather remarkable result that the contributions to the persistent currents from the two spin states *cancel,* rather than add, as it does in the previous example and as one might naively expect.

Let $0 \le \phi < \phi_0$. The phase shifts are[8,9]

$$\delta_m(\phi) = \begin{cases} (\pi/2)\phi/\phi_0, & \text{if } m=0 \text{ and } s_z = -\frac{1}{2}, \\ (\pi/2)(|m| - |m+\phi/\phi_0|), & \text{otherwise}. \end{cases} \tag{8}$$

The phase shifts correspond to a singular scattering problem because they do not decay as $|m| \to \infty$ and the sum in Eq. (1) is not absolutely convergent. A reasonable way to regularize the sum is to define it as $\lim_{m\to\infty}\sum_{|m|<M}$. The contributions to Eq. (1) from m and $-m$ cancel in pairs irrespective of spin and this leaves the contribution of $m=0$. In the spinless case $m=0$ gives a finite contribution, but in the spin-$\frac{1}{2}$ case the two spin states at $m=0$ carry *opposite* currents. The final result is

$$I = \begin{cases} -E_F/2\phi_0, & \text{if } 0<\phi<\phi_0 \text{ spinless}, \\ 0, & \text{spin } \frac{1}{2}, \end{cases} \tag{9}$$

where E_F is the Fermi energy. By the general antisymmetry and periodicity property, the nontrivial function in the spinless case extends to all ϕ as a periodic, antisymmetric step function.

We note that by similar arguments, the differential contribution to the current density $\mathbf{j}(\mathbf{x})$ is

$$d\mathbf{j}(\mathbf{x}) = \frac{dE}{2\pi i}\frac{\delta \ln \det S(E,\mathbf{A})}{\delta \mathbf{A}(\mathbf{x})}, \tag{10}$$

where $\mathbf{A}(\mathbf{x})$ is the vector potential.

We now close with a remark about how the persistent currents scale with the characteristic size of the system. For an isolated ring of length L, the persistent currents are known to scale like $O(1/L)$. On the other hand, for the two examples considered here, the persistent currents are typically of $O(1)$. This not surprising for electrons in the plane for there is no length scale in this problem besides k_F^{-1}. However, the mesoscopic networks such as those considered here do have a characteristic (large) length scale given by the size of the loop and it is not immediately obvious what protects the persistent currents from scaling like $1/L$ as they do for the isolated ring. To analyze this, note that in the examples considered above $(\pi i)^{-1}\ln\det S(E,\phi) = F(kL)$, with F a *periodic* function of its argument, and $k \equiv (2mE/\hbar^2)^{1/2}$. This turns out to be a general property of scattering matrices for networks with the generalized Neumann boundary conditions at the vertices (and commensurate lengths for the finite links in the network), and in addition, is the high-energy behavior for networks with point vertices even if the boundary conditions are not Neumann. In such networks, let $F(t) = \langle F\rangle + dP(t)/dt$ with P the periodic indefinite integral of F and $\langle F\rangle$ independent of k. Since the persistent current is $(\hbar^2/m)\int_0^{k_f} dk\, kF'(kL)$, integrating by parts one finds

$$I = \langle F\rangle' E_F + (\hbar^2 k_F/mL)P'(k_F L) + O(L^{-2}). \tag{11}$$

(The prime denotes derivative with respect to the flux.) We see that if $\langle F\rangle' \neq 0$, the persistent currents are proportional to E_F in the $L\to\infty$ limit. However, whenever $\langle F\rangle' = 0$, the persistent currents are proportional to k_F/L in the $L\to\infty$ limit and the scale of the system enters.

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[a]Permanent address: Centre de Recherches sur la Trés Basses Temperatures, CNRS, B.P. 166x, 38042, Grenoble CEDEX, France.

[b]Present address: Department of Physics, Boston University, Boston, MA 02215.

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