

Comparison of quantization of charge transport in periodic and open pumps

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We compare the charges transported in two systems, a spatially periodic and an open quantum pump, both depending periodically and adiabatically on time. The charge transported in a cycle was computed by Thouless [Phys. Rev. B **27**, 6083 (1983)] and by Büttiker *et al.* [Z. Phys. B: Condens. Matter **94**, 133 (1994)] in the two cases. We show that the results agree in the limit where the two physical situations become the same, i.e., that of a large open pump.

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I. INTRODUCTION

In this Brief Report, we compare two systems, depending periodically and adiabatically on time, which may exhibit quantized charge transport. We describe them in the simplest possible situation. The first one, which may be called a periodic quantum pump, is modeled as a one-dimensional Fermi gas moving in a potential which is periodic in space as well. Thouless¹ (see also Refs. 2 and 3) showed that charge transport is quantized provided that the Fermi energy remains in a gap throughout the cycle. The second system is an open quantum pump and consists of a dot connected to two leads, containing free Fermi gases. Particles impinging on the dot may be transmitted through or reflected by it. The charge transported in a cycle has been expressed by Büttiker *et al.*⁴ (see also Refs. 5 and 6) in terms of the scattering matrix at the Fermi energy. It is quantized in special cases only.⁷⁻⁹ At first sight, the descriptions of transport in periodic and open pumps may look unrelated because of the infinite (finite) extent of the two devices or even conflicting: in the first case, transport is attributed to energies way below the Fermi energy, which lies in a spectral gap; in the second, the scattering matrix matters only at the Fermi energy.

In order to compare the two approaches, we consider the pump obtained by truncating the potential of the periodic pump to finitely many periods and joining the ends to half-lines where particles move freely. In the limit where the number of periods grows large, we recover the original physical situation, and one would wish the two approaches to agree on the result. This is shown in this Brief Report.

A related comparison, though for finite dots, was made in Ref. 10, where the scattering approach of Ref. 4 was shown to agree with linear response theory, an instance of which is the approach by Thouless.

Transport in periodic systems of finite length, like those where the pump mechanism is realized by surface acoustic waves, can be discussed either by means of the approach of Büttiker *et al.*⁴ and Brouwer⁵ or, alternatively, when the wave extends over many wave lengths, by that of Thouless.¹ Several theoretical works¹¹⁻¹⁶ using the first approach find quantization of charge transport in some cases either analytically or numerically. Precise agreement with the result¹⁷ based on the second approach is found for a specific, exactly solvable, tight binding Hamiltonian in Ref. 16. The present work establishes a general equivalence between the two ap-

proaches. Experimental work on such system is presented in Refs. 18 and 19.

In Secs. II and III, we recall the results for periodic and open pumps, respectively, to the extent needed for the comparison, which is made in Sec. IV.

II. TRANSPORT IN PERIODIC PUMPS

We consider the Schrödinger Hamiltonian on the line \mathbb{R}_x ,

$$H(s) = -\frac{d^2}{dx^2} + V(x, s), \quad (1)$$

where V is doubly periodic: $V(x+L, s) = V(x, s)$ and $V(x, s+T) = V(x, s)$. Let $\psi_{nks}(x)$ be the solution of the time-independent Schrödinger equation

$$H(s)\psi_{nks} = E_{ns}(k)\psi_{nks},$$

with the Bloch boundary condition

$$\psi_{nks}(x+L) = e^{ikL}\psi_{nks}(x) \quad (k \in \mathbb{R} \bmod 2\pi/L)$$

and normalized with respect to the inner product

$$\langle \phi, \psi \rangle = \frac{1}{L} \int_0^L dx \bar{\phi}(x) \psi(x).$$

The index $n=1, 2, \dots$ labels the bands. The Fermi energy is assumed to lie in a spectral gap of $H(s)$ for all s .

Thouless discussed the evolution of the Fermi sea under the nonautonomous Hamiltonian $H(\omega t)$ in the adiabatic limit $\omega \rightarrow 0$. The charge transported through $x=0$ in a cycle of period T/ω is found to be

$$C = \sum_n^* \frac{i}{2\pi} \int_0^T ds \int_0^{2\pi/L} dk \left(\left\langle \frac{\partial \psi_{nks}}{\partial s}, \frac{\partial \psi_{nks}}{\partial k} \right\rangle - \left\langle \frac{\partial \psi_{nks}}{\partial k}, \frac{\partial \psi_{nks}}{\partial s} \right\rangle \right),$$

where the asterisk indicates that the sum extends over filled bands n only. Each of its terms is an integer defining the Chern number of the $U(1)$ fiber bundle ψ_{nks} over the torus $\mathbb{T} = \mathbb{R}^2/(T, 2\pi/L)$. That number reflects the obstruction to choosing the phase of ψ_{nks} in a continuous way on all of \mathbb{T} .

Thouless provided the following alternate definition of C related to the above by analytic continuation. At energies in a

gap and specifically at the Fermi energy, the solutions of the time-independent Schrödinger equation are unbounded, and two linearly independent ones may be picked by the condition

$$\psi_{\pm,s}(x+L) = (-1)^n e^{\pm \kappa x} \psi_{\pm,s}(x) \quad (2)$$

for some $\kappa = \kappa(s) > 0$, where n refers to the gap following the n th band. The functions ψ_{\pm} may be assumed real. Then, C equals the number of nodes of ψ_{-} traversing a reference point, say, $x=0$, as s completes a cycle. A node contributes positively if it runs from left to right.

III. TRANSPORT IN OPEN PUMPS

We consider the Hamiltonian [Eq. (1)] where $V(x,s)$ is now of compact support in x but still periodic in s . The autonomous dynamics it generates for a fixed value of s yields a scattering matrix

$$S(E,s) = (S_{ij})_{i,j=1}^2 = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix},$$

where the entry S_{ij} is the amplitude for a particle of energy E , incident from lead j to be scattered into lead i , or, more explicitly, t, r (t', r') are the transmission and reflection amplitudes for a wave incident from the left (right). We shall henceforth set $E=E_F$ and drop it from the notation.

Büttiker *et al.*⁴ investigated the motion of particles governed by the nonautonomous Hamiltonian $H(\omega t)$, again in the adiabatic limit. The charge delivered to lead j in a cycle is

$$\langle Q_j \rangle = \frac{i}{2\pi} \int_{s=0}^{s=T} [(dS)S^*]_{jj},$$

where $\langle \cdot \rangle$ denotes a quantum mechanical expectation value. For the same situation, Ivanov *et al.*²⁰ (following Ref. 21) computed the variance of the same quantity,

$$\begin{aligned} \langle \langle Q_j^2 \rangle \rangle &= \frac{1}{(2\pi)^2} \int_{-\infty}^{\infty} \int_0^T ds ds' \frac{1 - |[S(s)S^*(s')]_{jj}|^2}{(s-s')^2} \\ &= T^{-2} \int_0^T \int_0^T ds ds' \frac{1 - |[S(s)S^*(s')]_{jj}|^2}{\sin^2 \frac{2\pi}{T}(s-s')} \end{aligned}$$

(note that the denominator and the numerator both vanish quadratically at $s=s'$). For the left lead ($j=1$), this reads

$$\langle Q_1 \rangle = \frac{i}{2\pi} \int_{s=0}^{s=T} (\bar{r} dr + \bar{t}' dt'),$$

$$\langle \langle Q_1^2 \rangle \rangle = T^{-2} \int_0^T \int_0^T ds ds' \frac{1 - |[r(s)\bar{r}(s') + t'(s)\bar{t}'(s')]|^2}{\sin^2 \frac{2\pi}{T}(s-s')}. \quad (3)$$

It has been noticed⁹ that if the j th row of $S(s)$ changes with s by multiplication with a phase $u(s)$ ($|u(s)|=1$), then

$$\langle Q_j \rangle = \frac{i}{2\pi} \int_{s=0}^{s=T} \bar{u} du \quad (4)$$

is the negative of the winding number of u and $\langle \langle Q_j^2 \rangle \rangle = 0$, which means that the charge transport is quantized. For the left lead, that condition amounts to $z=r/t' \in \mathbb{C} \cup \{\infty\}$ remaining put as a point on the Riemann sphere.

IV. COMPARISON

We compare the periodic pump to the open one obtained from it by truncating the potential to N periods

$$H(s) = -\frac{d^2}{dx^2} + \chi_{[0,NL]}(x)V(x,s).$$

Let us determine the scattering matrix at the Fermi energy. For a wave incident from the left, the solution is of the form

$$e^{ipx} + r_N e^{-ipx} \quad (x \leq 0),$$

$$A_+ \psi_+(x) + A_- \psi_-(x) \quad (0 \leq x \leq NL),$$

$$t_N e^{ipx} \quad (x \geq NL),$$

with $p = \sqrt{E_F}$, ψ_{\pm} as specified in Eq. (2), and s temporarily omitted from the notation. Within the barrier, the Wronskian of this solution and ψ_+ (or ψ_-) is constant and, in particular, equal at $x=0$ and at $x=NL$. The matching conditions thus amount to

$$W(e^{ipx} + r_N e^{-ipx}, \psi_{\pm})|_{x=0} = W(t_N e^{ipx}, \psi_{\pm})|_{x=NL},$$

where $W(\phi, \psi)|_x = \phi(x)\psi'(x) - \phi'(x)\psi(x)$. Setting $W_{\pm} = W(e^{ipx}, \psi_{\pm})|_{x=0}$ and using

$$W(e^{-ipx}, \psi_{\pm})|_{x=0} = \bar{W}_{\pm},$$

$$W(e^{ipx}, \psi_{\pm})|_{x=NL} = (-1)^{nN} e^{\pm \kappa NL} e^{ipNL} W_{\pm},$$

we find

$$r_N = -u_- \frac{1 - e^{-2\kappa NL}}{1 - e^{-2\kappa NL} u_- u_+^{-1}},$$

$$t_N = (-1)^{nN} e^{-\kappa NL} e^{-ipNL} \frac{1 - u_- u_+^{-1}}{1 - e^{-2\kappa NL} u_- u_+^{-1}},$$

with

$$u_{\pm} = \frac{W_{\pm}}{\bar{W}_{\pm}} = \frac{\psi'_{\pm}(0) - ip\psi_{\pm}(0)}{\psi'_{\pm}(0) + ip\psi_{\pm}(0)}. \quad (5)$$

Since ψ_{\pm} is real, we have $|u_{\pm}|=1$. Owing to the invariance of the Hamiltonian under time reversal, S is symmetric, i.e., $t'_N = t_N$. In the limit of a long barrier, we have

$$r = \lim_{N \rightarrow \infty} r_N = -u_-, \quad t' = \lim_{N \rightarrow \infty} t'_N = 0,$$

and the condition for quantized transport is attained exponentially fast in N . Restoring the dependence on s , the charge

[Eqs. (3) or (4)] delivered to the left lead becomes

$$\lim_{N \rightarrow \infty} \langle Q_1 \rangle = \frac{i}{2\pi} \int_{s=0}^{s=T} (\bar{r} dr + \bar{r}' dt') = \frac{i}{2\pi} \int_{s=0}^{s=T} \bar{u}_- du_-,$$

which, up to the sign, is the winding number of the phase $u_-(s)$. The charge crossing $x=0$ in the positive direction is thus given by the winding number itself.

Finally, we show that this result agrees with the Chern number of Thouless, as characterized at the end of Sec II.

Whenever a node of $\psi_{-,s}$ crosses $x=0$ from the left, $\partial\psi_-/\partial s|_{x=0}$ and $\partial\psi_-/\partial x|_{x=0}$ have opposite signs. Hence, $u_-(s)$, which moves along the unit circle [see Eq. (5)], crosses $u=1$ from below, counting +1 to its winding number; nodes crossing $x=0$ from the right contribute -1.

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