Comparison of quantization of charge transport in periodic and open pumps

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Abstract

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, respectively by Büttiker et al. 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.

1 Introduction

In this note 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 modelled as a 1-dimensional Fermi gas moving in a potential which is periodic in space as well. Thouless [9] showed that charge transport is quantized provided 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. [3] (see also [4, 10]) in terms of the scattering matrix at Fermi energy. It is quantized in special cases only [1, 8, 2]. At first sight the descriptions of transport in periodic and open pumps may look unrelated, because of the infinite, resp.

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 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 paper.

A related comparison, though for finite dots, was made in [5], where the scattering approach of [3] was shown to agree with linear response theory, an instance of which is the approach by Thouless.

In Sections 2 and 3 we recall the results for periodic and open pumps respectively, to the extent needed for the comparison, which is made in Section 4.

2 Transport in periodic pumps

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

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

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 Bloch boundary condition

$$\psi_{nks}(x+L) = \mathrm{e}^{\mathrm{i}kL}\psi_{nks}(x)\,, \qquad (k \in \mathbb{R} \mod 2\pi/L)$$

and normalized with respect to the inner product

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

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

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

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

where the star 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 provides 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

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

for some $\kappa = \kappa(s) > 0$, where n refers to the gap following the n-th band. The functions $\psi_\pm$ 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.

3 Transport in open pumps

We consider the Hamiltonian (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

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

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 (resp. t', r') are the transmission and reflection amplitudes for a wave incident from the left (resp. right). We shall henceforth set $E = E_F$ and drop it from the notation.

Büttiker et al. [3] investigate the motion of particles governed by the non-autonomous Hamiltonian $H(\omega t)$, again in the adiabatic limit. The charge delivered to lead j in a cycle is

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

where $\langle\cdot\rangle$ denotes a quantum mechanical expectation value. For the same situation Ivanov et al. [6] (following [7]) computed the variance of the same quantity

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

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

$$\begin{aligned}
\langle Q_1 \rangle &= \frac{\mathrm{i}}{2\pi} \int_{s=0}^{s=T} \left(\overline{r} dr + \overline{t}' dt'\right), \qquad (3) \\
\langle\!\langle Q_1^2 \rangle\!\rangle &= T^2 \int_0^T \int_0^T ds\, ds' \, \frac{1 - |\big(r(s)\overline{r}(s') + t'(s)\overline{t}'(s')\big)|^2}{\sin^2 \frac{2\pi}{T}(s-s')}\,.
\end{aligned}$$

It has been noticed [2] that if the j-th row of $S(s)$ changes with s by multiplication with a phase $u(s)$ ($|u(s)| = 1$), then

$$\langle Q_j \rangle = \frac{\mathrm{i}}{2\pi} \int_{s=0}^{s=T} \overline{u}\, du \qquad (4)$$

is the negative of the winding number of u, and $\langle\!\langle Q_j^2 \rangle\!\rangle = 0$, meaning 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.

4 The 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

$$\begin{cases} \mathrm{e}^{\mathrm{i}px} + r_N \mathrm{e}^{-\mathrm{i}px} & , \quad (x \le 0) \\ A_+\psi_+(x) + A_-\psi_-(x) & , \quad (0 \le x \le NL) \\ t_N \mathrm{e}^{\mathrm{i}px} & , \quad (x \ge NL) \end{cases}$$

with $p = \sqrt{E_F}$, $\psi_\pm$ as specified in (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

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

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

$$W(\mathrm{e}^{-\mathrm{i}px}, \psi_\pm)|_{x=0} = \overline{W}_\pm , \qquad W(\mathrm{e}^{\mathrm{i}px}, \psi_\pm)|_{x=NL} = (-1)^{nN} \mathrm{e}^{\pm\kappa NL} \mathrm{e}^{\mathrm{i}pNL} W_\pm ,$$

we find

$$\begin{aligned} r_N &= -u_- \frac{1 - \mathrm{e}^{-2\kappa NL}}{1 - \mathrm{e}^{-2\kappa NL} u_- u_+^{-1}} , \\ t_N &= (-1)^{nN} \mathrm{e}^{-\kappa NL} \mathrm{e}^{-\mathrm{i}pNL} \frac{1 - u_- u_+^{-1}}{1 - \mathrm{e}^{-2\kappa NL} u_- u_+^{-1}} \end{aligned}$$

with

$$u_\pm = \frac{W_\pm}{\overline{W}_\pm} = \frac{\psi_\pm'(0) - \mathrm{i}p\psi_\pm(0)}{\psi_\pm'(0) + \mathrm{i}p\psi_\pm(0)} . \tag{5}$$

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

$$r = \lim_{N\to\infty} r_N = -u_- , \qquad t' = \lim_{N\to\infty} t_N' = 0 ,$$

and the condition for quantized transport is attained exponentially fast in N. Restoring the dependence on s, the charge (3) or (4) delivered to the left lead becomes

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

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 Section 2. 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 (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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