Allowed Charge Transfers between Coherent Conductors Driven by a Time-Dependent Scatterer

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We derive constraints on the statistics of the charge transfer between two conductors in the model of arbitrary time-dependent instant scattering of noninteracting fermions at zero temperature. The constraints are formulated in terms of analytic properties of the generating function: its zeros must lie on the negative real axis. This result generalizes existing studies for scattering by a time-independent scatterer under time-dependent bias voltage.

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I. Introduction.—The concept of full counting statistics (FCS) for charge transfer in coherent conductors has been introduced in Ref. [1]. While the average current through small junctions may usually be understood in classical terms, its fluctuations reflect the quantum nature of electrons; even in the model of noninteracting electrons, the fluctuations of the current are nonclassical due to the electronic Fermi statistics [2]. Generally, one studies the statistical distribution of the charge transfer between several conductors coupled by a time-dependent scattering matrix. In the simplest case (considered in this Letter), there are only two leads, and therefore the charge transfer may be statistically described by the probabilities p_q to transfer exactly q electrons from the left to the right lead (here q is an integer number, either positive or negative). The leads are assumed to provide a thermal source of incoming electrons with the Fermi occupation number $n_F(E)$. In the context of coherent quantum manipulation, one of the most interesting setups is that of an "adiabatic pumping" where the scattering matrix varies slowly compared to the characteristic scattering time [3]. Neglecting the scattering time amounts to considering the scattering matrix to be independent of the energy E, i.e., local in time [4]. In this approximation, in the model of noninteracting electrons, a general expression (the so-called "determinant formula") for the charge-transfer statistics $\{p_q\}$ in terms of the time evolution of the single-particle scattering matrix $S(t)$ has been derived [1,5].

Remarkably, recent progress has been made in understanding the implications of the old results for the FCS in the particular case of the bias voltage applied to a fixed scatterer [6]. In this "bias-voltage" problem, the scattering matrix $S(t)$ is changed along a one-dimensional trajectory parametrized by the U(1) phase $\phi(t) = \int V(t)dt$, where $V(t)$ is the applied voltage. Within this model, nontrivial constraints have been derived for the charge-transfer statistics. Namely, not every set of probabilities $\{p_q\}$ is allowed, but only those for which the zeros of the generating function,

$$\chi(\lambda) = \sum_{q=-\infty}^{+\infty} p_q e^{i\lambda q}, \tag{1}$$

obey certain restrictions (see our discussion below).

II. Main result.—Inspired by this work [6], we derive similar (weaker) constraints for the more general case of adiabatic pumping [3]: an arbitrary time-dependent scattering matrix $S(t)$ with any number of channels. We restrict our consideration to the case of two conducting leads and to zero temperature. Under those conditions, we find that the generating function (1) may take zero values only for a discrete set of λ such that $u = e^{i\lambda}$ belongs to the negative real axis $(-\infty, 0)$. Furthermore, we find that the generating function $\chi(\lambda)$ (and therefore the full charge-transfer statistics) is uniquely determined by its zeros u_k, up to an overall integer charge transfer $\chi(u) \mapsto u^N \chi(u)$. These statements constitute the main finding of our Letter.

As a simple illustration of the derived constraint, consider a charge-transfer statistics with the only nonzero probabilities $p_{-1,0,1} = 1/3$. While this statistics appears *a priori* reasonable, it follows from our results that it can never be produced for any time-dependent scattering matrix $S(t)$ with any number of channels between two conductors (since such a statistics would correspond to the pair of complex roots $u = e^{\pm i2\pi/3}$).

III. Determinant formula and its regularization.—The generating function (1), in the approximation of noninteracting electrons and of instant scattering, is given by the determinant formula [1,4,5,7],

$$\chi(\lambda) = \det[1 + n_F(S^\dagger e^{i\lambda P_3} S e^{-i\lambda P_3} - 1)], \tag{2}$$

where S is the time-dependent single-particle scattering matrix. At each moment of time, $S(t) \in U(2M)$, where M is the number of conducting channels in each of the two conductors. The operator $P_3 = \mathrm{diag}(\mathbf{1}_M, \mathbf{0}_M)$ is the projector counting the charge in the right conductor. The operator n_F is the Fermi distribution function in the conductors. In this Letter, we consider only the case of zero temperature, and so $n_F(E) = \theta(-E)$ is the step function in the frequency representation (in the time representation, $n_F(t,t') = i/[2\pi(t - t' + i0)]$). Since the electrons are noninteracting, we treat them as spinless fermions (the spin may be trivially included as a channel index).

The determinant (2) is understood as that of an infinite-dimensional operator acting both in the time domain and in the $2M$-channel space. In its original form (2), the determinant is ill-defined: while the operator tends to $\mathbf{1}$ at infinite positive energies, it goes to another unitary matrix, $S^\dagger e^{i\lambda P_3} S e^{-i\lambda P_3}$, at infinite negative energies. Therefore the determinant requires a proper regularization [4]. A consistent way to regularize the determinant has been proposed in Ref. [8] (their regularization is also equivalent to that used in Ref. [9]). At zero temperature, the Fermi distribution operator is a projector $n_F^2 = n_F$, and the regularized determinant may be written in a particularly simple form [8],

$$\chi(\lambda) = \det\{e^{-i\lambda P_3 n_F}[1 - P_3 + P_3 S e^{i\lambda n_F} S^\dagger]\}. \tag{3}$$

There is a subtle point in calculating the FCS in the situation where charge counting is performed over a finite time interval: in this case, there are contributions to the noise arising from the starting and ending of the measurement, even in the absence of scattering [1,5]. This noise grows logarithmically with the observation time. To eliminate this contribution from the switching-on and switching-off, one often considers a *periodic* signal $S(t)$ (e.g., by repeating the same signal with a large time period). In this periodic formulation, at large number of periods N_p, the asymptotic behavior of $\chi(\lambda)$ is given by [4] $\chi(\lambda) \sim [\chi_0(\lambda)]^{N_p}$, where $\chi_0(\lambda) = \exp[\lim_{N_p\to\infty} \frac{1}{N_p} \times \ln\chi(\lambda)]$ is the counting statistics *per period*. The generating function $\chi(\lambda)$ may be computed with the same formula (3), but with the finite time interval closed into a loop with the periodic boundary conditions. We further consider this periodic setup and omit the subscript 0 by using the notation $\chi(\lambda)$ for the charge-transfer statistics per period.

To write the operators in (3) in the matrix form, one can perform a Fourier transform in time (introducing discrete quasienergies). In the quasienergy basis, the operators are represented as infinite-dimensional discrete matrices. We assume that the dependence $S(t)$ is sufficiently smooth, so that it induces only short-range transitions between quasienergies [10]. Then the operator in (3) rapidly approaches $\mathbf{1}$ away from the Fermi level, and the determinant converges for all values of λ. Thus we conclude that $\chi(u)$ is a single-valued analytic function of $u = e^{i\lambda}$ for any $u \in C\backslash\{0\}$.

IV. Determinant formula in z representation.—For our discussion, it will be convenient to rewrite (3) in a different form. We parametrize the $2M \times 2M$ unitary S matrix by two complex $2M \times M$ matrices z and $\tilde{z}$ as

$$S^\dagger = (z|\tilde{z}), \tag{4}$$

subject to the constraints $z^\dagger z = \tilde{z}^\dagger \tilde{z} = \mathbf{1}_M$ and $z^\dagger \tilde{z} = \mathbf{0}_M$. These constraints guarantee the unitarity of the S matrix.

Substituting (4) into (3) and using the explicit form of the charge operator P_3, we immediately obtain

$$\chi(\lambda) = \det(e^{-i\lambda n_F} z^\dagger e^{i\lambda n_F} z). \tag{5}$$

Notice that the determinant size in the channel space is $M \times M$ in (5) versus $2M \times 2M$ in (3).

Furthermore, $\chi(\lambda)$ has a symmetry with respect to the right gauge transformation $z \mapsto zU_M(t)$ for any time-dependent unitary $M \times M$ matrix $U_M(t)$. Under this transformation, $\chi(\lambda)$ gets multiplied by $\det(U_M e^{-i\lambda n_F} U_M^\dagger e^{i\lambda n_F}) = \exp[i\lambda \mathrm{Tr}(n_F - U_M n_F U_M^\dagger)] = \exp[i\lambda \int \frac{dt}{2\pi} \mathrm{tr}(U_M i\partial_t U_M^\dagger)]$. Because of the periodicity of $U_M(t)$, the integral in the last expression is an integer number, and it affects only the overall shift of the total pumped charge. We conclude that, up to this integer, the FCS depends only on z modulo $U(M)$ gauge transformations. The latter space may be described as $U(2M)/[U(M) \times U(M)]$ and contains $2M^2$ real parameters [instead of $4M^2$ real parameters in $S \in U(2M)$]. It may be convenient to parametrize it with $\hat{N}(t) = 2zz^\dagger - 1$, a $2M \times 2M$ traceless Hermitian matrix obeying the constraint $\hat{N}^2(t) = \mathbf{1}_{2M}$ (this matrix was introduced in Ref. [12]). Physically, the gauge invariance described above corresponds to the independence of FCS on the scattering separately in the right outgoing states [12].

In addition to gauge rotations, (5) is also insensitive to global (time-independent) left rotations $z \mapsto U_{2M} z$, which correspond to global rotations of $\hat{N}(t)$ [13].

V. Derivation of the main result.—To derive our main result we rewrite (5) as

$$\chi(u) = \det[1 + (u^{-1} - 1)n_F][1 + (u - 1)n_F^z], \tag{6}$$

where $n_F^z = z^\dagger n_F z$, and we have used $n_F^2 = n_F$.

The first factor in (6) does not involve any information about the time-dependent scattering. Its only role is to provide a reference point: the position of the Fermi level. The dependence on the evolution of S matrix enters through n_F^z, which has a $M \times M$ matrix structure and tends to $\mathbf{0}_M$ and to $\mathbf{1}_M$ at infinite positive and infinite negative energies, respectively.

We can show that (6) is fully determined by the spectrum of n_F^z, up to an overall constant charge transfer. Indeed, we can rewrite (6) as

$$\begin{aligned}\chi(\lambda) &= \det[(e^{-i\lambda n_F} e^{i\lambda n_F^z})\{e^{-i\lambda n_F^z}[1 + (u - 1)n_F^z]\}] \\ &= \det(e^{-i\lambda n_F} e^{i\lambda n_F^z}) \det\{e^{-i\lambda n_F^z}[1 + (u - 1)n_F^z]\} \\ &= e^{i\lambda \mathrm{Tr}(n_F^z - n_F)} \det\{e^{-i\lambda n_F^z}[1 + (u - 1)n_F^z]\},\end{aligned} \tag{7}$$

where the determinant of the product can be written as the product of the determinants, since both operators behave properly (tend to $\mathbf{1}_M$) at infinite energies, and the last transformation is justified, since $n_F^z - n_F$ rapidly tends to zero at infinite energies. The trace in the first factor of the last expression equals the total transferred charge (generally noninteger) [8] $\mathrm{Tr}(n_F^z - n_F) = Q$. The second factor in (7) depends *only* on the spectrum of n_F^z.

For a periodic time dependence of $S(t)$, the operator n_F^z may be represented in the quasienergy basis as a discrete infinite Hermitian matrix. It tends to **0** at large positive energies and to **1** at large negative energies. Its spectrum is discrete and takes real values between 0 and 1, with possible accumulation points at 0 and 1 [14]. If we denote the eigenvalues of n_F^z as n_α^z, Eq. (7) implies the following expression for the generating function:

$$\chi(u) = e^{i\lambda Q} \prod_\alpha e^{-i\lambda n_\alpha^z}[1 + (u-1)n_\alpha^z]. \tag{8}$$

Notice that while this formula involves $\lambda = -i \ln u$, it is a single-valued function of u on $C0\}$. As explained above, this expression is valid up to a constant integer charge transfer.

It is obvious from (6) that the spectrum of n_F^z is in one-to-one correspondence with the positions of zeros of $\chi(u)$,

$$u_\alpha = 1 - (n_\alpha^z)^{-1}. \tag{9}$$

Since the spectrum of n_F^z is real and lies between 0 and 1, we conclude that the zeros of $\chi(u)$ must all lie on the negative real axis. This argument finishes the demonstration of the main result of this Letter.

VI. Example of forbidden charge transfers.—We can illustrate our result with an example of a charge transfer that cannot be realized in our scattering system. Consider the following particular example of FCS:

$$\chi(u) = 1 - 2F + F(u + u^{-1}), \tag{10}$$

where $0 \le F \le 1/2$. The corresponding nonvanishing probabilities $p_{\pm 1} = F$, $p_0 = 1 - 2F$ are normalized and non-negative. However, the roots of (10) are real only for $F \le 1/4$. Therefore, the statistics (10) with $1/4 < F \le 1/2$ cannot be produced by any evolution of scattering matrix at zero temperature.

VII. Allowed charge transfers.—While the condition of real negative zeros of $\chi(u)$ is a necessary condition for an allowed FCS, it is also apparently a sufficient condition. Indeed, for any finite set of negative real u_α, the statistics

$$\chi(u) = u^{N_1} \prod_{\alpha=1}^{N_2} \frac{u - u_\alpha}{1 - u_\alpha} \tag{11}$$

[which is identical to (8) with $N_1 = Q - \sum_\alpha n_\alpha^z$] can be trivially realized in a system with $N_2 + 1$ channels by using single-particle-transfer pulses as described in Ref. [4] (one channel per each u_α plus one channel for the overall integer transfer N_1).

Moreover, this FCS may also be arbitrarily closely approximated in a *single-channel* system by sending individual well-separated pulses for each of the required zeros, u_α. Indeed, in a single-channel system, the FCS is determined by the time evolution of the vector $\mathrm{Tr}\hat{N}\sigma$ on the two-dimensional sphere, as shown in Ref. [12]). Motion of this vector along a circular trajectory of a given area (on the sphere) is equivalent to the "bias-voltage" problem with a fixed channel transparency determined by the area enclosed by the contour. This "bias-voltage" problem has been considered in Ref. [4] where it has been shown that an arbitrarily sharp Lorentzian voltage pulse produces the elementary charge transfer $\chi(u) = (u - u_\alpha)/(1 - u_\alpha)$. By superimposing such pulses, well separated in time, along circles of different areas, we can approximate the required statistics (11) arbitrarily close.

Furthermore, since we can make this approximation for any finite number of roots N_2, and the possible infinite sets of roots have accumulation points only at $u_\alpha \to 0$ and $u_\alpha \to -\infty$, we can also approximate arbitrarily close any statistics (8) with an infinite set of roots, provided they converge sufficiently rapidly to $n_\alpha^z \to 0$ and $n_\alpha^z \to 1$ [for the convergence of (8) it is sufficient to require that n_α^z converge not slower than $|\alpha|^{-\eta}$ with $\eta > 1$ at their accumulation points]. We leave it as a mathematical problem to determine the precise requirements on the convergence and the conditions under which the generating function (8) may be reproduced *exactly* by a suitable evolution of the S matrix.

VIII. Bias-voltage case.—With this result in mind, we would like to comment on the existing results for the problem with a *restricted* evolution of the scattering matrix, namely, the "bias-voltage" case [6]. In this restricted problem, the transparencies of the channels are fixed, and the evolution of the S matrix is determined by the single parameter $\phi(t) = \int V(t)dt$. The time dependence of z in this setup is given by $z = e^{i\phi(t)P_3} z_0$, where z_0 is a fixed $2M \times M$ matrix. As follows from the results of Ref. [6], for this restricted evolution of the scattering matrix, there is an additional constraint on the positions of u_α. Namely, there are two types of roots u_α: ordinary ("typical" in notation of Ref. [6]) and anomalous. Ordinary roots come in inversion-symmetric pairs $(u_\alpha, 1/u_\alpha)$. In addition, there are M anomalous roots, each having the same multiplicity $|W|$, where W is the winding number of $\phi(t)$ (we assume that it is integer). They are located either at $-g_i/(1 - g_i)$ or at $-(1 - g_i)/g_i$, depending on whether W is positive or negative. Here g_i are the channel transparencies given by the eigenvalues of $z_0^\dagger P_3 z_0$.

We can easily rederive this result within our formalism with a procedure analogous to that in Ref. [6]. Consider for simplicity only one channel with transparency g. Then

$$n_F^z = (1 - g)n_F + g n_F^\phi, \tag{12}$$

where $n_F^\phi = e^{-i\phi} n_F e^{i\phi}$. The symmetry of the spectrum of n_F^z (at zero temperature) can be demonstrated with the use of the algebra of four operators,

$$Q_+ = n_F + n_F^\phi - 1, \qquad Q_- = n_F - n_F^\phi,$$
$$Q_3 = i[n_F, n_F^\phi] = iQ_-Q_+, \qquad C = Q_-^2 = 1 - Q_+^2. \tag{13}$$

The operators Q_+, Q_-, and Q_3 anticommute with each other, and the operator C commutes with them (this algebra relies only on n_F and n_F^ϕ being projectors). Obviously C also commutes with

$$n_F^z = \frac{1}{2} + \frac{1}{2}Q_+ + \left(\frac{1}{2} - g\right)Q_- = \frac{1}{2} \pm \sqrt{\frac{1}{4} - g(1-g)C}, \quad (14)$$

and they can be diagonalized simultaneously [the last equality in (14) should be understood as a relation between eigenvalues, with different sign choices for different eigenvectors]. Let Ψ be a common eigenvector of C and n_F^z with the eigenvalues C_α and n_α^z, respectively. The vector $Q_3\Psi$, if nonzero, has the eigenvalue $1 - n_\alpha^z$, which produces [according to (9)] a pair of ordinary roots $(u_\alpha, 1/u_\alpha)$. If $Q_3\Psi = 0$, then one easily proves that either $Q_-\Psi$ or $Q_+\Psi$ is zero. If $Q_-\Psi = 0$, then $C_\alpha = 0$, and this corresponds to n_α^z equal to 0 or 1, without any contribution to FCS. Finally, the zero modes $Q_+\Psi = 0$ produce an anomalous contribution with $C_\alpha = 1$.

One can prove that, for a phase winding W, there are exactly $|W|$ zero modes of Q_+. Assuming a non-negative W (without loss of generality), zero modes of Q_+ must be simultaneously eigenstates of n_F and of n_F^ϕ with eigenvalues 1 and 0, respectively. Such eigenstates are easily constructed explicitly by using the decomposition $e^{i\phi(t)} = e^{i[W\omega t + \phi_+(t) + \phi_-(t)]}$, where $\phi_\pm$ are the positive- and negative-frequency parts, and ω is the driving frequency. One finds that the space of zero modes is then spanned by $\psi_k = e^{-ik\omega t - i\phi_-(t)}$ for $k = 1, 2, \ldots, W$. The corresponding eigenvalue n_α^z does not have a pair, but is W-fold degenerate $n_\alpha^z = 1 - g$. Similarly, for $W < 0$, one finds $|W|$ zero modes of Q_+ with $n_F = 0$ and $n_F^\phi = 1$, which produces $n_\alpha^z = g$.

In terms of the generating function, the separation into the inversion-symmetric (ordinary) and anomalous (depending only on the average charge transfer) parts may be written as (for $W \geq 0$)

$$\chi(u) = [1 + g(u-1)]^W \chi_{\text{inv}}(u), \qquad \chi_{\text{inv}}(u^{-1}) = \chi_{\text{inv}}(u). \quad (15)$$

With some algebraic manipulations, one can also derive an explicitly inversion-symmetric formula for χ_{inv},

$$\chi_{\text{inv}}(u) = \det[1 + g(1-g)(u + u^{-1} - 2)(1 - n_F)n_F^\phi] \quad (16)$$

(this expression also assumes $W \geq 0$). This formula may be viewed as a compact form of the product over eigenvalues obtained in Ref. [6]. Note that this separation of the two contributions is specific to the "bias-voltage" case at zero temperature.

IX. Conclusion.—We have derived constraints on the charge-transfer statistics between two conductors in the limit of instant scattering and at zero temperature. Our findings generalize the results obtained previously for the case of a fixed scatterer with a time-dependent voltage [6]. The allowed statistics is characterized by negative real zeros of the characteristic function $\chi(u)$. While we have not performed a similar analysis of the problem at finite temperature, we conjecture that the singularities of $\log\chi(u)$ remain restricted to the negative real axis even at finite temperature, but develop a cut instead of a discrete set of branching points. The available simplest examples of the charge-transfer statistics at finite temperature support this conjecture.

Similar to Ref. [6], our result (8) can be interpreted as a decomposition of the charge transfer into independent tunneling events—binomial processes. The effective channel transparencies of these events are the eigenvalues of n_F^z depending on the time evolution of the scattering matrix. This interpretation suggests that the physical origin of this result lies in the assumed absence of interactions between electrons and that it may break down once interaction is taken into account [15].

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