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Transport through quantum dots: A supersymmetry approach to transmission eigenvalue statistics

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We study quantum transport through ballistic cavities coupled to two electron reservoirs by point contacts. We develop a powerful method, based on supersymmetry, to calculate exactly transmission eigenvalue statistics in the presence of tunnel barriers and for a small number of open scattering channels. We calculate the transmission eigenvalue density for ballistic point contacts and find it to be consistent with a distribution of transmission eigenvalues given by the Jacobi ensemble from random-matrix theory. We also calculate explicitly the transmission eigenvalue density for quantum dots with tunneling point contacts. [S0163-1829(98)51044-2]

Modern submicrometer electron beam lithography has been used to manufacture devices in which phase-coherent electrons can travel ballistically at low temperature. One of such devices is a quantum dot, which consists of a conducting island, spatially confined by electrostatic gates, and connected to electron reservoirs by point contacts.^{1–5} A great deal of the interest in such systems stems from the remarkable connection between quantum chaos and mesoscopic transport. Several experiments and numerical simulations have to date produced convincing evidence that transport in ballistic quantum dots can be understood by using concepts and models from the theory of quantum chaotic scattering.

Motivated by these results, the first theoretical efforts to account for transport characteristics in ballistic quantum dots have made use of semiclassical methods⁶ akin to those of the fairly successful periodic orbit theory of closed chaotic systems. More recently, other approaches such as randommatrix theory⁷ and Efetov's supersymmetry^{8,9} have been used to describe transport in quantum dots in various regimes.

In this work, we describe a systematic nonperturbative method for studying certain transport functions in ballistic quantum dots. The method is based on a known combination of random-matrix theory with supersymmetry. Specifically, we construct a map of the density of eigenvalues of tt^{\dagger} , where *t* is the transmission matrix, onto a supersymmetric nonlinear σ model. We thus calculate exactly the density of these transmission eigenvalues for systems with broken time-reversal symmetry, with a small number of scattering channels, and in the presence of tunnel barriers. Extensions of our method to systems with time-reversal symmetry and/or spin-orbit scattering are straightforward.

The random-matrix theory that we shall be using builds on a phenomenological maximum-entropy principle, which applies whenever the dynamics of the system is sufficiently complex for the existence of an intrinsic equilibration time scale beyond which most microscopic details become irrelevant. In this situation, the presence of certain universal symmetries are sufficient to establish a complete statistical description of the system's observables by means of an appropriate distribution function that maximizes the information entropy. In quantum dots the ergodic time τ_{erg} plays the role of this equilibration time and thus the replacement of the Hamiltonian of the system by a random matrix, with the same universal symmetries, is justified on time scales $t \gg \tau_{erg}$. A rigorous microscopic proof of the validity of random-matrix theory on such time scales for disordered metallic grains has been put forward by Efetov.⁸ Extensions of the zero-dimensional supersymmetric nonlinear σ model introduced in Ref. 8 have been used in connection with the problem of chaotic scattering. Such extensions have been particularly successful in describing quantum transport in quantum dots.⁹⁻¹²

An altogether different way of studying chaotic scattering in quantum dots is to use the maximum-entropy principle to obtain directly the distribution of the S-matrix elements, without any reference to an underlying Hamiltonian. This has been put forward in Ref. 13. It was demonstrated that in chaotic scattering transmission eigenvalues play a role similar to that of the energy eigenvalues in closed chaotic systems. It was shown that the joint-distribution of transmission eigenvalues exhibits level repulsion and is completely determined by universal symmetries of the system. The great advantage of this approach is that, as a consequence of the Landauer-Büttiker scattering theory, transmission eigenvalue densities and correlation functions can be used to evaluate averages and correlators of several observables. The conductance, for instance is simply $G = G_0 \sum_{n=1}^{N} \tau_n$, where τ_n are the transmission eigenvalues, N is the number of scattering channels and $G_0 = 2e^2/h$. Many other useful observables can be written in the general form $A = \sum_{n=1}^{N} a(\tau_n)$. This approach has been successful in describing some important particular cases, such as (i) ballistic point contacts, where orthogonal polynomial methods can be used, (ii) single mode leads, where transmission eigenvalue correlations vanish, and (iii) semiclassical limit, where $N \ge 1$ and perturbation theory applies. Unfortunately not much is known about the transmission eigenvalue density and correlation functions in more general situations, such as quantum dots with tunnel barriers and a small number of scattering channels. The main reason for this state of affairs seems to be the lack of a systematic

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nonperturbative approach to calculate them. This situation is rather unsatisfactory since many relevant experiments are performed under these more general conditions. In this work we present such a method.

Our model system for the quantum dot consists of a ballistic cavity coupled by nonideal point contacts to two semiinfinite perfectly conducting leads. Following the approach of Ref. 14, we write the scattering matrix of the system as

$$S = 1 - 2\pi i W^{\dagger} D^{-1} W, \qquad (1)$$

in which $D \equiv E_F - H + i\pi W W^{\dagger} + i0^{+}$, E_F is the Fermi energy, *H* is a complex Hermitian random matrix, and *W* is a nonrandom $M \times (N_1 + N_2)$ rectangular matrix describing the coupling between the *M* states inside the dot and the modes in the two leads. The structure of *W* is

$$(W)_{\mu n} = \begin{cases} (W_1)_{\mu n}; & n = 1, 2, \dots, N_1 \\ (W_2)_{\mu n}; & n = N_1 + 1, \dots, N_1 + N_2, \end{cases}$$

where W_1 and W_2 describe the coupling to leads 1 and 2, respectively, and N_1 and N_2 are the number of modes in each lead. It is convenient to reduce the number of coupling parameters by defining transmission coefficients $T_n^{(1)} = 1$ $-|\langle r \rangle_{nn}|^2$ and $T_n^{(2)} = 1 - |\langle r' \rangle_{nn}|^2$, where *r* and *r'* are random reflection matrices defined by the identity

$$S = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix}, \tag{2}$$

and by assuming the orthogonality conditions: $W_1^{\dagger}W_1$ = MX, $W_2^{\dagger}W_2 = MY$, $W_1^{\dagger}W_2 = 0 = W_2^{\dagger}W_1$, where X= diag (x_1, \ldots, x_{N_1}) and Y =diag (y_1, \ldots, y_{N_2}) .

In the usual supersymmetry approach the next step would be to use the Landauer theory and write observables, such as the conductance $G = G_0 tr(tt^{\dagger})$, in terms of the random elements of the *S* matrix. After an appropriate field-theoretic representation of the product of elements of the *S* matrix is constructed, a mapping onto a supersymmetric nonlinear σ model follows by taking $M \rightarrow \infty$.

In this work we shall instead construct a representation for the density of transmission eigenvalues. Consider the following generating function:

$$Z(P) = \operatorname{Sdet}^{-1}(\mathcal{D} + J) \tag{3}$$

$$= \exp[-\operatorname{tr} \ln(1 - \nu_1 t t^{\dagger}) + \operatorname{tr} \ln(1 - \nu_0 t t^{\dagger})], \qquad (4)$$

where $\mathcal{D} = \text{diag}(D, D, D^{\dagger}, D^{\dagger}), J = i \pi (W_1 W_1^{\dagger}) \otimes (P - L), L$ = diag(1, 1, -1, -1) and

$$P = \begin{pmatrix} 1 - 2\nu & -2i\sqrt{\nu(1 - \nu)} \\ 2i\sqrt{\nu(1 - \nu)} & 2\nu - 1 \end{pmatrix},$$
 (5)

in which $\nu = \text{diag}(\nu_1, \nu_0)$. The operator Sdet above stands for the superdeterminant (we use the {1,2}-block notation of Ref. 14). The density of transmission eigenvalues, which by definition is the average $\rho(\tau) = \langle \Sigma_n \delta(\tau - \tau_n) \rangle$, can be generated from Z(P) as follows:

$$\rho(\tau) = -\frac{1}{\pi\tau^2} \operatorname{Im}\{h[1/(\tau+i0^+)]\},\tag{6}$$

where

$$h(z) = \frac{\partial \langle Z(P) \rangle}{\partial \nu_1} \bigg|_{\nu_1 = z = \nu_0} = \left\langle \operatorname{tr} \left(\frac{t t^{\dagger}}{1 - z t t^{\dagger}} \right) \right\rangle.$$
(7)

We remark that a similar generating function has been used in Refs. 15 and 16 for studying a different system.

We proceed by representing the average of Z(P) as an integral over a supermatrix field σ

$$\langle Z(P) \rangle = \int d\sigma \exp(\mathcal{L}(P,\sigma)),$$
 (8)

where

$$\mathcal{L}(P,\sigma) = -\frac{M}{2} \operatorname{Str} \sigma^2 - \operatorname{Str} \ln(E_F + i \pi (WW^{\dagger}) \otimes L + J - M \sigma \Delta / \pi).$$

with Δ denoting the mean energy-level spacing in the cavity. The integration measure $d\sigma$ in Eq. (8) is the usual flat Berezin measure of supermathematics.¹⁷ The great advantage of this supersymmetry representation is that since Z(0)=1, we can circumvent the need to use the replica trick, which, as shown in Ref. 18, fails to describe the nonperturbative regime of this system. In the limit of $M \rightarrow \infty$ the massive longitudinal components of σ can be integrated out and we are left with massless transverse fields Q that define a manifold of saddle points (a coset space). The final result can be written as the coset integral

$$\langle Z(P)\rangle = \int_{Q^2=1} \mathcal{D}Q \mathcal{Z}_P(Q),$$

where Q is a 4×4 supermatrix and

$$\mathcal{Z}_{P}(Q) = \prod_{n=1}^{N_{1}} \operatorname{Sdet}^{-1}(1 + \beta_{n}^{(1)}QP) \prod_{m=1}^{N_{2}} \operatorname{Sdet}^{-1}(1 + \beta_{m}^{(2)}QL).$$

The parameters $\beta_n^{(j)}$ (j=1,2) are related to the transmission coefficients via $T_n^{(j)} = 4\beta_n^{(j)}/(1+\beta_n^{(j)})^2$.

Since our system has broken time-reversal symmetry progress can be made by introducing Efetov's coordinates,⁹ in terms of which the explicit form of the integration measure reads

$$\mathcal{D}Q = -\frac{d\lambda_1 d\lambda_0}{(\lambda_1 - \lambda_0)^2} d\varphi_1 d\varphi_0 d\eta_1^* d\eta_1 d\eta_2^* d\eta_2, \qquad (9)$$

where $1 \le \lambda_1 < \infty$, $-1 \le \lambda_0 \le 1$, $0 \le \varphi_1, \varphi_0 \le 2\pi$, and $\eta_1^*, \eta_1, \eta_2^*, \eta_2$ are Grassmann (anticommuting) variables. According to Zirnbauer's integral theorem,¹⁹ there are two kinds of contributions to $\langle Z(P) \rangle$ in these coordinates, so that we may write $\langle Z(P) \rangle = \langle Z(P) \rangle_s + \langle Z(P) \rangle_{max}$. The first term is due to an anomaly of the Berezin integral in Efetov's coordinates and the second term is a contribution from the coefficient of the term with a maximum number of Grassmann variables. Inserting this result into Eq. (7) we get

$$h(z) = h_s(z) - \int_1^\infty d\lambda_1 \int_{-1}^1 d\lambda_0 \frac{k(\lambda_1, \lambda_0; z)}{(\lambda_1 - \lambda_0)^2}, \quad (10)$$

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where $h_s(z) = \sum_{n=1}^{N_1} T_n^{(1)} / (1 - zT_n^{(1)})$ and

$$k(\lambda_1, \lambda_0; z) = g(\lambda_1, \lambda_0; z) \prod_{n=1}^{N_2} \frac{\gamma_n^{(2)} + \lambda_0}{\gamma_n^{(2)} + \lambda_1}$$
(11)

in which $\gamma_n^{(j)} \equiv 2/T_n^{(j)} - 1$ (j=1,2). It remains to specify $g(\lambda_1, \lambda_0; z)$, which is in fact the hardest part of the calculations in this approach. The technical procedure is straightforward, albeit quite cumbersome. It consists of unwrapping the Grassmann structure of $Z_P(Q)$ and collecting the term containing the maximum number of anticommuting variables, i.e., the one proportional to $\eta_1^* \eta_1 \eta_2^* \eta_2$. The huge amount of terms makes analytical progress only possible with computer algebra. The computer program we used for this purpose has been written in the MapleV language with the help of some optimized routines²⁰ for Grassmann variables manipulations.

Although the formulas obtained thus far are exact and completely general, we shall hereafter give explicit expressions only in the extreme quantum limit, which means that we assume N_1 and N_2 to be small integers. The physical meaning of this limit can be easily understood by considering the time scales of the problem: the ergodic time τ_{erg} for a wavepacket to become uniformly spread throughout the available phase space, the decay time au_d for emission of electrons from the dot, and the Heisenberg time τ_H . Quantum dots that in the classical limit have nonintegrable chaotic dynamics satisfy the condition $\tau_{erg} \ll \tau_d, \tau_H$. The dimensionless conductance of the dot, $g \sim \tau_H^2 / \tau_d$, can be used to define some regimes of interest: (i) the semiclassical limit $(g \ge 1)$; (ii) the extreme quantum limit $(g \ge 1)$, which is considered in this work, and (iii) the Coulomb blockade regime (g≪1).

We remark that while the semiclassical and the Coulomb blockade regimes have been studied in a great number of theoretical works and an essentially complete understanding has emerged, much less is known about the extreme quantum limit.

For the sake of simplicity, we shall present explicit results only for some interesting particular values of the coupling parameters.

(i) We consider first a quantum dot with ballistic point contacts, which means that the transmission coefficients have maximum value, i.e., $T_n^{(1)} = 1 = T_n^{(2)}$. We get $h_s(z) = N_1/(1 - z)$ and

$$\frac{k(\lambda_1,\lambda_0;z)}{(\lambda_1-\lambda_0)} = \frac{2N_1^2(1+\lambda_0)^{N_2}F_{N_1-1}(\lambda_0;z)F_{N_1}(\lambda_1;z)}{(1+\lambda_1)^{N_2}(1-2z+\lambda_1)^{2N_1+1}},$$

where

$$F_{n}(\lambda;z) = \sum_{m=0}^{n} C_{m}^{(n)} P_{m}(\lambda) P_{m}(1-2z),$$

 $P_m(x)$ are the Legendre polynomials and the numerical coefficients $C_m^{(n)}$ are determined by the binomial expansion $(1+x)^n = \sum_{m=0}^n C_m^{(n)} P_m(x)$. The above formula has been obtained for N_2 arbitrary and for $1 \le N_1 \le 7$, which is sufficient for our purpose since it covers well the extreme quantum limit. We have found strong evidence (but no formal proof) that this formula for h(z) is, in fact, valid for arbitrary N_1 and N_2 . One such evidence is the exact relation between the average conductance and h(z): $\langle G \rangle = G_0 h(0)$ $= G_0 N_1 N_2 / (N_1 + N_2)$, which is correct for all N_1 and N_2 . Other evidence comes from results of similar general validity that can be obtained from the coefficients of the Taylor expansion of h(z) about z=0.

The density of transmission eigenvalue can be obtained by using Eq. (6). We find for $1 \le N_1$, $N_2 \le 11$ the remarkably compact result

$$\rho(\tau) = \tau^r \sum_{n=0}^{s-1} (2n+r+1) \{ P_n^{(r,0)}(1-2\tau) \}^2, \qquad (12)$$

where $r = |N_1 - N_2|$, $s = \min\{N_1, N_2\}$, and $P_n^{(\alpha, \beta)}(x)$ is the Jacobi polynomial. Just as before, we believe (although we have no formal proof) that Eq. (12) is valid for arbitrary N_1 and N_2 . This result is consistent with the random-matrix approach of Ref. 13, which predicts for the same system a joint distribution of transmission eigenvalues given by the Jacobi ensemble, from which Eq. (12) can be derived. We have thus found independent evidence for the application of the Jacobi ensemble in this problem.

Using Eq. (12) we can calculate the average of several useful observables, such as the conductance

$$\langle G/G_0 \rangle = \int_0^1 \rho(\tau) \tau d\tau = \frac{N_1 N_2}{N},$$

where $N \equiv N_1 + N_2$ and the shot noise power

$$\langle P/P_0 \rangle = \int_0^1 \rho(\tau) \tau(1-\tau) d\tau = \frac{(N_1 N_2)^2}{N(N^2-1)},$$

in which $P_0 = 2e|V|G_0$ (V is the applied voltage).

This simple example illustrates the power of our approach to get exact and explicit results for quantities that so far have only been accessible by combined maximum entropyorthogonal polynomials methods. We shall next consider systems for which such methods may prove inadequate.

(ii) Let us assume that there is a tunnel barrier in one of the contacts between the quantum dot and the leads. For simplicity we set $T_n^{(1)}=1$ and $T_n^{(2)}=2/(1+\gamma)$. We still get $h_s(z)=N_1/(1-z)$, but

$$\frac{k(\lambda_1,\lambda_0;z)}{(\lambda_1-\lambda_0)} = \frac{2N_1^2(\gamma+\lambda_0)^{N_2}F_{N_1-1}(\lambda_0;z)F_{N_1}(\lambda_1;z)}{(\gamma+\lambda_1)^{N_2}(1-2z+\lambda_1)^{2N_1+1}},$$

with $F_n(\lambda, z)$ defined as before.

Since the explicit expressions for $\rho(\tau)$ become very clumsy as N_1 and N_2 increase, we shall present here only two particular cases. First, we set $N_1 = 1 = N_2$ and find

$$\rho_1(\tau) = 4 \frac{2\gamma + (1-\gamma)\tau}{[(2+(\gamma-1)\tau)]^3}$$

It is interesting to note that for one scattering channel the conductance distribution can be obtained by using the identity $\mathcal{P}(G) = \rho_1(G/G_0)/G_0$. Considering $N_1 = 2 = N_2$, we get

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$$\rho_2(\tau) = 64 \frac{a_0 + a_1\tau + a_2\tau^2 + a_3\tau^3 + a_4\tau^4}{[2 + (\gamma - 1)\tau]^6},$$

where $a_0 = 4\gamma$, $a_1 = 2 - 8\gamma - 6\gamma^2$, $a_2 = 3(2\gamma - 1)(\gamma + 1)^2$, $a_3 = (1 - \gamma)(2\gamma + 1)(3\gamma + 1)$, and $a_4 = \gamma(\gamma - 1)^2$.

As a nontrivial check of our results, we change the roles of the contacts by setting $T_n^{(1)} = 2/(1 + \gamma)$ and $T_n^{(2)} = 1$. On physical grounds, one would expect to get the same answers, and indeed we recover this by performing very different and apparently unrelated calculations.

(iii) As a final example, consider a quantum dot connected to the leads via two tunnel barriers, so that $T_n^{(1)} = 1/(1 + \gamma) = T_n^{(2)}$. Just as before we shall concentrate on small particular values of N_1 and N_2 . For $N_1 = 1 = N_2$ we find

$$\rho_1(\tau) = \frac{(\gamma^2 - 1)^2 \tau^2 + (\gamma^4 - 1)\tau + 4\gamma^2}{4[1 + (\gamma^2 - 1)\tau]^{5/2}},$$

which is in agreement with the random S-matrix approach of Ref. 21. For $N_1 = 2 = N_2$ we get

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$$\rho_{2}(\tau) = \frac{a_{0} + a_{1}\tau + a_{2}\tau^{2} + a_{3}\tau^{3} + a_{4}\tau^{4} + a_{5}\tau^{5}}{16[1 + (\gamma^{2} - 1)\tau]^{9/2}},$$

in which $a_0 = 64\gamma^2$, $a_1 = -16(1+8\gamma^2+3\gamma^4)$, $a_2 = 24(2 + 3\gamma^2+3\gamma^6)$, $a_3 = (\gamma^2-1)(51+43\gamma^2-7\gamma^4+9\gamma^6)$, $a_4 = 2(\gamma^2-1)^2(\gamma^2+1)(3\gamma^2+11)$, and $a_5 = 3(\gamma^2-1)^3(3\gamma^2+1)$.

In summary, we have proposed a powerful method based on supersymmetry for calculating exactly the transmission eigenvalue density of quantum dots in the nonperturbative, and experimentally relevant, limit of small number of scattering channels. As a by-product we establish a direct link between the zero-dimensional nonlinear σ model and the maximum entropy *S*-matrix theory. Extensions of our method to other symmetry classes and higher order correlation functions are straightforward (albeit much more laborious) and will be the subject of future works.

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