Scattering Approach to Quantum Transport: Toward a Consistent Physical Picture

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Quantum transport in disordered systems can be studied via the transfer matrix M. In a previous paper, the statistical distribution of M at the mesoscopic level was constructed from single-scattering units. The assumption of "isotropy," that restricted the model to certain observables for quasi-1D systems, is relaxed in this Letter. The new limiting distribution satisfies a diffusion equation, is universal, specified by the mean free paths between all pairs of channels, and is insensitive to other microscopic details. Results for the ballistic, metallic, and localized regimes are promising.

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The scattering approach to quantum transport, initiated by Landauer [1], has been applied by a number of authors to discuss the problem of disordered conductors [2–4] (for a review, see Ref. [2] and references contained therein). For instance, Ref. [3] relies on a maximum-entropy criterion to find the statistical distribution of the transfer matrix. Reference [4] shows that the result of Ref. [3] is the consequence of a *central-limit theorem (CLT)* of a novel kind, thus representing a universal limiting distribution. For quasi-one-dimensional (quasi-1D) systems the model of Refs. [3] and [4] gives excellent results [5–7], in agreement with perturbative calculations [8,9] and consistent with experiments [10], for the weak-localization correction to the conductance, universal conductance fluctuations, the backscattering enhancement, long-range correlations between pairs of transmission or reflection coefficients, and time-reversal-symmetry breaking by a magnetic field. This model, despite its successes, suffers from the rather unphysical "isotropy assumption," a generalization of the random-phase hypothesis [11] in 1D. In the *isotropic model (IM)* there are N channels, each one being mixed randomly with all the others. This implies that diffusion in the transverse direction occurs instantaneously and the dimensionality can enter only through the number of channels $N\sim(k_F W)^{d-1}$, where W denotes the width: The physics of the transverse direction is thrown out by construction. Our aim here is, first, to present a more general approach not incorporating isotropy—again leading to universal limiting distributions—and, second, to discuss some of the predictions.

In the scattering approach, the system is placed between two perfect leads, where the scattering states at the Fermi energy define N channels. The $2N\times 2N$ *transfer matrix* [2,3] M relates the $2N$-component wave function (N waves travel in either direction) on the right of the system to that on the left. Time-reversal (T) symmetry implies $M^*=\Sigma_x M\Sigma_x$ and flux conservation (FC) requires $M\Sigma_z M^\dagger=\Sigma_z$; Σ_x,Σ_z are Pauli matrices, with 1 and 0 replaced by the unit and zero matrices. M has $N(2N+1)$ independent parameters and can be represented as [12]

$$M=\begin{pmatrix} u & 0 \\ 0 & u^* \end{pmatrix}\begin{pmatrix} \sqrt{1+\lambda} & \sqrt{\lambda} \\ \sqrt{\lambda} & \sqrt{1+\lambda} \end{pmatrix}\begin{pmatrix} v & 0 \\ 0 & v^* \end{pmatrix}, \tag{1}$$

where u,v are $N\times N$, unitary, and λ is real, diagonal, with positive elements $\lambda_1,\ldots,\lambda_N$. Quantities of interest can be written in terms of u,v,λ; e.g., the total transmission coefficient is $T=\sum_a(1+\lambda_a)^{-1}$ and the conductance measured in a two-probe experiment [13] is $g=2T$.

Let our system consist of n units [4], each being a slice of microscopic thickness with transfer matrix M_1, its probability density being $p_1(M_1)$. For two units in series, independent and identically distributed, the resulting p_2 is the convolution [3,4,14] p_1*p_1, giving the recursion relation $p_{n+1}=p_n*p_1$. In Ref. [4], $p_1(M_1)$ is isotropic, i.e., a function of the $(\lambda_1)_a$ only and independent of u_1,v_1, which are then distributed according to the invariant measure of the unitary group [15]. The *weak-scattering limit (WSL)* is then taken [4]: The density of units, ν, and their number n approach ∞, while the total reflection coefficient of one unit (summed over outgoing and averaged over incoming channels) approaches 0, so that $n/\nu=L$ is the fixed length of the sample and $N^{-1}\nu\times\sum_{ab}\langle(R_1)_{ab}\rangle=l_0^{-1}$ is finite, l_0 being the *overall mean free path (mfp)* for reflection. The probability density $w_L(\lambda)$ then obeys the diffusion equation

$$\frac{\partial w_L(\lambda)}{\partial L}=\frac{1}{l_0}\frac{2}{N+1}\sum_{a=1}^{N}\frac{\partial}{\partial\lambda_a}\left[\lambda_a(1+\lambda_a)J(\lambda)\frac{\partial}{\partial\lambda_a}\frac{w_L(\lambda)}{J(\lambda)}\right], \tag{2}$$

where $J(\lambda)=\prod_{a<b}|\lambda_a-\lambda_b|$; the initial condition is $w_0(\lambda)=\delta(\lambda)$.

In (2), the information about the microscopic distribution enters only via the parameter l_0, other details being irrelevant. Thus, whatever the solution of (2), it is *universal* once l_0 is specified (this constitutes a CLT).

The isotropic distribution of M_1 for an individual scattering slice (the fundamental assumption) was driven by the mathematical convenience of the "polar representation" (1), which automatically satisfies FC and T sym-

metry. However, a more physical interpretation of disorder, through either a model of random δ scatterers or a Born approximation applied to a more general potential, leads, for M_1, to the form

$$M_1=\begin{pmatrix}1+ih & \eta\\ \eta^* & 1-ih^*\end{pmatrix}=I+\epsilon\,, \tag{3}$$

for which we cannot assume an isotropic distribution. In (3), $h=h^\dagger$, $\eta=\eta^T$ are $N\times N$ matrices. In this approach, the "Cartesian representation" (i.e., the actual matrix elements M_{ab}) is the more natural to work with. While (3) satisfies T symmetry, FC is not trivial to impose. To circumvent this problem, we first propose a statistical distribution for h and η, and impose FC *on average*; it can then be shown that, when the WSL described above Eq. (2) is taken, *exact FC is recovered:* Roughly speaking, this is because, in the WSL, FC is violated, for each unit, only to second order in $1/\nu$. Our statistical model consists in assuming that h and η are statistically independent, $\langle\epsilon\rangle=0$,

$$\nu\langle h_{ab}h_{cd}\rangle=\delta_{ad}\delta_{bc}\sigma'_{ab}\,, \tag{4a}$$

$\langle\eta_{ab}\eta_{cd}\rangle=0$, and

$$\nu\langle\eta_{ab}\eta^*_{cd}\rangle=(1+\delta_{ab})^{-1}(\delta_{ac}\delta_{bd}+\delta_{ad}\delta_{bc})\sigma_{ab}\,. \tag{4b}$$

The WSL was taken in Eqs. (4), which define the inverse mfp's from channel b and a for forward and backward scattering ($\sigma'_{ab}=1/l'_{ab}$, $\sigma_{ab}=1/l_{ab}$), respectively. From average FC we find $\sum_b\sigma'_{ab}=\sum_b\sigma_{ab}=1/l_a$. We denote the M matrix elements by $(M^{ab}_{\alpha\beta})^{(i)}$; $a,b=1,2$ label the four $N\times N$ blocks; $\alpha,\beta=1,\ldots,N$ label rows and columns in each block; and $i=1,2$ indicates a matrix element or its complex conjugate. The recursion relation $p_{n+1}=p_n*p_1$ gives, for $p_L(M)$ in the WSL, the diffusion equation

$$\frac{\partial p_L(M)}{\partial L}=\tfrac{1}{2}\,\nu\langle(\epsilon^{1c}_{a\epsilon})^{(i)}(\epsilon^{1c}_{\gamma\zeta})^{(j)}\rangle(M^{ca}_{\epsilon\beta})^{(i)}(M^{cb}_{\zeta\delta})^{(j)}\times\frac{\partial^2 p_L(M)}{\partial(M^{1a}_{\alpha\beta})^{(i)}\partial(M^{1b}_{\gamma\delta})^{(j)}}\,, \tag{5}$$

where a sum over repeated indices is understood.

We again have a CLT: *$p_L(M)$ reaches a universal limiting distribution that satisfies (5); the only microscopic parameters that survive in the limit are the mfp's of (4)*, contained in $\nu\langle\epsilon\epsilon\rangle$. In the IM we had only one overall mfp l_0; now all the mfp's (4) enter and *the structure of the σ matrices depends on the dimensionality d.* Finally, given a function of M, the evolution of $\langle F(M)\rangle_L$ satisfies $\partial_L\langle F\rangle_L=\langle HF\rangle_L$, H being a linear differential operator arising from the right-hand side of (5) after multiplying by F and integrating by parts.

The diffusion equation (5) has a more satisfactory physical basis than Eq. (2) and constitutes the central result of the present Letter. Its most important consequences obtained thus far are discussed below.

1. Traces.—Quantities like T, expressible entirely in terms of the $\{\lambda_a\}$ of Eq. (1), will be called *traces*: Their average depends only on the $\{\sigma_{ab}\}$ and not on the $\{\sigma'_{ab}\}$. In the special case $\sigma_{ab}=\sigma^0_{ab}=(1+\delta_{ab})/(N+1)l_0$ *[the equivalent-channel model (ECM)], the average of a trace is the same as in the IM*, and the distribution of the $\{\lambda_a\}$ of Eq. (1) satisfies the same Eq. (2) as in the IM. σ^0_{ab} is precisely the value of $\nu\langle(R_i)_{ab}\rangle$ of the IM; the derivation of Eq. (2) in the ECM is more satisfactory, though, than in the IM, because it never needs the assumption of isotropy (that involves random phases) for individual scatterers. We conclude that the applications of the IM to traces test the equivalent-channel rather than the isotropy assumption and that, *for traces, any improvement on the IM results must be sought in a nonequivalent-channel model (NECM).*

We discuss some properties of T.

Using the initial condition $\langle T\rangle_{L=0}=N$ one finds, in the general NECM, $(\partial_L\langle T\rangle_L)_0=-\sum_a(1/l_a)=-N/l_0$, which defines an overall mfp l_0, and $(\partial_L^2\langle T\rangle_L)_0=2\sum_a(1/l_a^2)$; these results reduce to those of the ECM when $l_a=l_0$. We see that the curvature of $\langle T\rangle_L$ at $L=0$ is positive and, for a given l_0, larger when the l_a's have a spread around l_0. That a spread in the l_a's "helps conduction" in the ballistic regime can be understood in a two-scatterer problem treated classically (fluxes are added). The description provided by the NECM is thus reasonable in this regime.

In the metallic regime, we first make the ECM approximation, using a "common mfp" l, so that Eq. (2) applies. The results reported elsewhere [5–7] (for $l\ll L\ll Nl\sim\xi_{1D}$) are in remarkable agreement with microscopic Green's-function calculations for quasi-1D systems, indicating that for $L\gg W$ all channels are so thoroughly mixed that replacing all the l_a's by a common l is a good approximation. For instance, one obtains $\langle T\rangle_L=Nl/L-1/3+\cdots$, the first term being Ohm's law and the second one the *weak-localization correction.* For the fluctuation one finds $\mathrm{var}T=2/15+\cdots$, a result independent of L,l,N (*universal conductance fluctuations*).

To go beyond quasi-1D and describe 2D and 3D systems (with $L\sim W$) we need to take into account the spread among the mfp's (NECM) that depends on the system dimensionality. As a first attempt, to see if the NECM corrections go in the right direction, we consider a small departure from the ECM, for a separable $\sigma_{ab}=\tau_a\tau_b$ (attainable, for example, with a δ potential). Let $\tau_a=\tau_0+\epsilon_a$, with $\tau_0=N^{-1}\sum_a\tau_a$. If $|\epsilon_a|\ll\tau_0$, the leading term in $\langle T\rangle_L$ has the same form as above, with $l=l_0(1+\tau_0^{-2}\mathrm{var}\,\tau_a)$ and $l_0^{-1}=N\tau_0^2=\sum_a l_a^{-1}$. We thus have an explicit value for the common mfp l used above that differs from l_0. This is similar to the distinction one makes, in transport theory, between the scattering and the transport mfp's. For a given l_0, departure from ECM helps conduction in this regime. This can be understood in a simple classical model: The Boltzmann equation for

$N=2$ gives $\langle T\rangle_L \approx (\tau_1\tau_2 L)^{-1} \geq 1/\tau_0^2 L$, where $\tau_0=(\tau_1+\tau_2)/2$; if $\tau_1,\tau_2 \approx \tau_0$, we can write $\langle T\rangle_L \approx Nl/L$, with l given as above. This NECM correction is thus satisfactory; we have not calculated yet the NECM modification to the weak-localization correction and to the variance.

2. Quantities other than traces.—These quantities are even more "sensitive" than traces to the relaxation of the isotropy assumption: They usually behave differently in the IM and in the ECM (supplemented with some model for the $\{\sigma'_{ab}\}$), the latter performing better and the NECM being a further improvement.

(a) Individual T_{ab},R_{ab}.—In the ballistic regime one finds

$$\langle T_{aa}\rangle_L = 1 - \left(\sigma'_{aa} + 2\sum_{b(\neq a)} \sigma'_{ab}\right) L + \cdots , \tag{6}$$

while $\langle T_{a\neq b}\rangle_L = \sigma'_{ab} L + \cdots$ and $\langle R_{ab}\rangle_L = \sigma_{ab} L + \cdots$. The reasonable feature that, for $L=0$, $\langle T_{aa}\rangle_0 = 1$, $\langle T_{a\neq b}\rangle_0 = 0$ is realized now *even for the ECM*. In contrast, the IM gives $\langle T_{ab}\rangle_0 = 1/N$, $\forall a,b$. The present model thus provides a more reasonable physical description.

In the metallic regime, the backscattering enhancement and averages and correlations of the T_{ab}'s and R_{ab}'s are reasonably well described by the IM, for quasi-1D systems [6,7]. In Refs. [6] and [7], isotropy plays a central role; since it is also responsible for the missing of the backscattering and correlation "cones," we expect the present model to provide a better description of these phenomena.

(b) The angular and radial parameters u_{ab},λ_b [Eq. (1)].—For the model $\sigma_{ab}=\tau_a\tau_b$ one can estimate that, in the localized regime, $\langle |u_{ab}|^2\rangle$ departs from the IM result $1/N$ as λ_b gets larger. For the largest λ, λ_N, one finds $\langle |u_{aN}|^2\rangle \sim \tau_a$. In particular, for a δ potential and $d=2$, $\tau_n \sim 1/(N^2-n^2)^{1/2}$. We thus find a *correlation* between u and λ, as well as an appreciable *anisotropy* in the u matrix elements, in contrast with the IM, where u,λ are statistically independent and u is isotropically distributed. Numerical evidence has been found [16] that the worst transmitting eigenchannels (largest λ) are preferentially projected on the modes of large transverse kinetic energy, a result consistent with the above estimate.

We see that, as we go from 1 to 2(a) and 2(b) above, more aspects of the present model become relevant for the description of the problem.

(c) The phase of the transmission amplitude t for $N=1$.—One finds

$$\langle t/t^*\rangle = (1+L/l)e^{-3L/l} . \tag{7}$$

In the IM [3,14] this average vanishes by construction $\forall L$; now we find a "randomization length" $\sim l/3$.

(d) Nonlocal quantum-mechanical effects in a three-probe 1D system [17–21].—Classically, a "dangling wire" [19] of length L_3 hanging from a wire of length L_{12} has no effect on the conductance of the latter, whereas quantum mechanically there is an effect, as in wave guides. It is shown in Ref. [20] that one cannot describe this problem in the IM. The present model is thus applied. When the main wire is a perfect conductor, its resulting averaged transmission coefficient is

$$\langle T_{12}\rangle = \tfrac{1}{2}\left[1+e^{-3L_3/l}\cos(2k_F L_3)\right] , \tag{8}$$

showing clearly the nonlocal effect of the dangling wire. For $L_3=0$, $\mathrm{var}T_{12}=0$. For $L_3\to\infty$, $\mathrm{var}T_{12}\to\frac{1}{8}$; disorder thus masks the nonlocal effect for large L_3.

In conclusion, the problem of quantum transport has been formulated in the scattering approach, starting with a more physical description of the individual scatterers than in the IM, and thus providing a more satisfactory physical picture. The results are universal at a macroscopic level, once the various mfp's are specified. It is shown that the successes of the IM for traces, like the two-probe conductance for quasi-1D systems, are to be interpreted as successes of the equivalent-channel approximation rather than of the isotropy assumption: The IM results can thus be improved only in the NECM. Only the correction to the Ohmic term was investigated; other corrections of the NECM will be studied in the future. On the other hand, individual transmission coefficients T_{ab} are not properly described, in the ballistic regime, by the IM, while within the present theory even the ECM gives reasonable results. In the metallic regime, a better description (than in the IM) of backscattering and correlations between T_{ab}'s is also expected, and will be investigated later. Anisotropy of the u_{ab} parameters and correlations with the λ_b's predicted by the present model have been observed in numerical simulations and deserve further attention in the future. For $N=1$, a "randomization length" $\sim l/3$ is found here, instead of the instantaneous randomization of the IM. Finally, the present model, and not the IM, is appropriate for the description of nonlocal quantum effects in multiprobe measurements.

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