Determinant approach to the scattering matrix elements in quasi-one-dimensional and two-dimensional disordered systems

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We have developed an approach based on the characteristic determinant (the Green function poles) to solve the Dyson equation in quasi-one-dimensional (Q1D) and two-dimensional disordered systems without any restriction on the numbers of impurities and modes. We consider two different models for a disordered Q1D wire: a set of two-dimensional δ potentials with signs and strengths determined randomly, and a tight-binding Hamiltonian with several modes and on-site disorder. We calculate analytically the scattering matrix elements for particles coming both from the left and from the right without actually determining the eigenfunctions of the electrons. It is shown that the poles of the Green functions for these models can be deduced from a determinant of rank $N \times N$ (N is the number of scatterers) instead of the rank $NM \times NM$ (M is the number of modes). We calculate the inverse localization lengths for the two models. They are exactly on the order of w^2 for the weak disorder regime and are valid for an arbitrary number of channels, M.

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The quantum transport of electrons in quasi-onedimensional (Q1D) and two-dimensional (2D) disordered systems has been studied extensively over the past decades both theoretically and experimentally.1-7 In particular, research interest was connected with the fact that electron transmission caused by elastic scattering with impurities in such size-quantized systems changes the shape of the conductance quantization due to the presence of evanescent modes. In most of the theoretical work where quantuminterference effects are important, the Anderson tight-binding model (see, e.g., Refs. 5, 8, and 9) has been used. A different model of the 2D disordered system, where the motion of electrons is modeled as regions of free propagation with occasional elastic scattering by a random array of scatterers was discussed in Ref. 1, based on the technique of combining scattering matrices. Another approach was proposed in Ref. 2: current transmission amplitudes in a Q1D wire with a single δ potential impurity were obtained by taking into account both propagating and evanescent modes based on a single-electron Green function (GF) method. However, to our knowledge, the methods available at present to obtain analytical results for the density of states, conductance, etc, in multichannel systems permit us to study only a limited number of defects, because in more complex cases, i.e., when the number of defects increases, such methods are much too tedious.

In this Brief Report we develop, closely following Refs. 10-12, an approach based on the characteristic determinant or the poles of the GF to solve the Dyson equation in Q1D and 2D disordered systems without any restriction on the numbers of impurities and modes. The characteristic determinant is built up from the reflection amplitude of the individual scatterer and the phase accumulated during multiple reflections. We consider two different models for the disordered system: a set of two-dimensional N scatterers of δ potentials with arbitrary signs and strengths placed randomly in the (x,y) plane,

$$V(x,y) = \sum_{l=1}^{N} V_l \delta(x - x_l) \delta(y - y_l), \qquad (1)$$

and a tight-binding Hamiltonian with several modes M and on-site disorder, described by the standard Hamiltonian with nearest-neighbor interaction

$$H = \sum_{i} \epsilon_{i} |r_{i}\rangle\langle r_{i}| + t \sum_{i,j} |r_{i}\rangle\langle r_{j}|, \qquad (2)$$

where ϵ_i is the energy of the site *i* chosen randomly in the range $\left(-\frac{w}{2}, \frac{w}{2}\right)$ with uniform probability, and *t* is the hopping matrix element. The double sum runs over nearest neighbors.

We calculate the transmission and reflection amplitudes for particles coming both from the left and from the right without actually determining the eigenfunctions of the electrons. We show that the Q1D problem can be mapped onto the 1D problem and that the poles of the Green function matrix elements give a determinant of rank $N \times N$, where N is the number of scatterers. The elements of reflection and transmission amplitudes, calculated on the base of the GF, may be presented in the form of a ratio of two determinants where both the numerator and the denominator are polynomials of the Nth degree. We have calculated the localization length of an electron in Q1D and 2D systems in the weak disorder regime for both models and for an arbitrary number of modes M.

The multichannel scattering problem is generally treated by solving the Schrödinger equation in configuration space with appropriate boundary conditions. In the case of a Q1D wire, where the electron is confined in the y direction but is free to propagate in the x direction, we choose an infinite-square-well confining potential in the y direction. We can similarly treat the case of a 2D disordered system by setting the other choice of confinement potential, where electrons can also propagate in the y direction. Thus, two systems will be discussed within the framework of the same approach. We assume the existence of a confining potential in the y direction leading to a set of transverse modes. For definiteness we

choose for $V_c(y)$ the model of an infinite square well where $V_c(y)$ is zero for $0 \le y \le W$ (W is the width of the system in the y direction) and infinite elsewhere, because none of the main results of the paper depend fundamentally on the confinement potential $V_c(y)$. Then the orthonormalized eigenfunction, satisfying a one-dimensional Schrödinger equation with a square-well potential, is $(2m_0 = \hbar = 1) \chi_n(y_l) = \sqrt{\frac{2}{W}} \sin k_n y_l$ with $k_n = \sqrt{E_F - (\frac{n\pi}{W})^2}$, where E_F is the Fermi energy and n is the subband index.

The Dyson equation for a Q1D wire can be written in the form (see, e.g., Refs. 2 and 13)

$$\begin{split} G_{nm}^{(N)}(x,x') &= G_n^{(0)}(x,x') \, \delta_{nm} \\ &+ \sum_{k,q} \int G_n^{(0)}(x,x'') \, \delta_{nk} V_{kq}(x'') G_{qm}^{(N)}(x'',x') dx'' \, . \end{split}$$

This equation is a set of infinitely coupled algebraic equations but in actual calculations we truncate the infinite set of coupled channels to a finite value M, including effects from both the open and closed modes. The upper index (l) of $G_{nm}^{(l)}(x;x')$ indicates the number of δ potentials considered in the calculation of a given GF. The matrix elements $V_{nm}(x) = \int \chi_n^*(y) V(x,y) \chi_m(y) dy$ of the defect potential (1), after performing the integration over y, become

$$V_{nm}(x) = \sum_{l=1}^{N} V_{nm}^{(l)} \delta(x - x_l),$$
 (3)

with $V_{nm}^{(l)} = \frac{2V_l}{W} \sin(\frac{n\pi y_l}{W}) \sin(\frac{m\pi y_l}{W})$ the coupling constant. $G_n^{(0)}(x,x') = -i \exp(ik_n|x-x'|)/2k_n$ is the GF of a propagating mode in the absence of the defect potential V(x,y). If the mode n is an evanescent mode, then one must take an analytical continuation of $k_n = i\kappa_n$.

We assume that a plane wave is incident from the left onto the system. To calculate the whole GF of the Dyson equation and take into account multiple reflections consistently and exactly without use of perturbation theory, we first isolate in the matrix elements of the defect potential $V_{nm}(x)$ the term corresponding to the first potential at x_N :

$$V_{nm}(x) = V_{nm}^{(N)} \delta(x - x_N) + \sum_{l=1}^{N-1} V_{nm}^{(l)} \delta(x - x_l),$$
 (4)

and evaluate the GF for a single δ . The case of two δ potentials, when we separate the next (N-1)th potential from the second term in the expression (4), is solved using the GF for a single δ . Therefore we solve the problem iteratively with N δ potentials, considering the solution with (N-1) δ 's to be known. Thus we obtain the GF elements in an arbitrary interval $[x_n, x_{n+1}]$ $(n=1, \dots, N-1)$ of the disordered system. Here we write out only the explicit form of the GF for $x, x' \leq x_1$,

$$G_{nm}^{(N)}(x,x') = G_n^{(0)}(x,x')\,\delta_{nm} + R_{nmL}^{(N)} \frac{G_n^0(x,x_1)G_m^0(x_1,x')}{\sqrt{G_n^0(x_1,x_1)G_m^0(x_1,x_1)}},$$
(5)

where $R_{nmL}^{(N)}$ are the matrix elements of reflection from the whole system with N δ potentials and may be written as the ratio of two determinants

$$R_{nmL}^{(N)} = \frac{\begin{vmatrix} 0 & r_{nm}^{(1)} & \cdots & r_{nm}^{(N)} e^{ik_n|x_N - x_1|} \\ 1 & \cdots & \cdots & \cdots \\ \vdots & \vdots & (D_{n,l})_{N,M,m} \\ e^{ik_m|x_N - x_1|} & \vdots & \\ \det(D_{n,l})_{N,M,m} & \vdots & \\ \det(D_{n,l})_{N,M,m} & \vdots & \\ \end{pmatrix}}{\det(D_{n,l})_{N,M,m}}.$$
 (6)

 $r_{nm}^{(l)}$ is the complex amplitude of the reflection of an electron from the isolated potential V_l in the absence of the remaining (N-1) potentials,²

$$r_{nm}^{(l)} = \frac{V_{nm}^{(l)} \sqrt{G_n^{(0)}(x_l, x_l) G_m^{(0)}(x_l, x_l)}}{M} \cdot \frac{1 - \sum_{p} V_{pp}^{(l)} G_p^{(0)}(x_l, x_l)}{1 - \sum_{p} V_{pp}^{(l)} G_p^{(0)}(x_l, x_l)}$$
(7)

The numerator of $R_{nmL}^{(N)}$ is obtained from the most significant quantity $\det(D_{n,l})_{N,M,m}$, which is the pole of the GF [see Eq. (9)], by augmenting it on the left and on the top. This determinant in the case of N arbitrary δ potentials and M channels can be written as the determinant of the partitioned matrix $NM \times NM$ in the form

$$D_{N,M} = \det[-I\delta_{nl} + [\lambda_{nl}][r^{(l)}](1 - \delta_{nl})], \tag{8}$$

where I is the unit matrix of rank $M \times M$. $[r^{(l)}]$ is the lth scattering matrix $(r_{nm}^{(l)})$ of rank $M \times M$ and is entirely determined by M(M+1)/2 parameters, because $\det[r^{(l)}]=0$. This can be checked by directly making use of the identity $r_{nm}^{(l)}r_{nm}^{(l)}-r_{nm}^{(l)}r_{nm}^{(l)}=0$. $[\lambda_{nl}]=\dim(e^{ik_1|x_n-x_l|},e^{ik_2|x_n-x_l|},\ldots,e^{ik_M|x_n-x_l|})$ is the square $M \times M$ matrix, which characterizes the phase shift of an electron that propagates freely between the nth and lth δ potentials, and it has nonvanishing elements only on the diagonal.

By a sequence of elementary row and column transformations, we can readily reduce the order of the determinant $NM \times NM$, Eq. (8), and obtain the desired $N \times N$ determinant with the following matrix elements, which now contain information about the number of modes M ($1 \le n, l \le N$; $1 \le m \le M$):

$$(D_{n,l})_{N,M,m} = -\delta_{nl} + (1 - \delta_{nl}) \sum_{p=1}^{M} \frac{r_{1p}^{(n)} r_{pm}^{(l)} \lambda_{nl}^{(p)}}{r_{1m}^{(n)}}.$$
 (9)

The quasibound states of an electron in the disordered Q1D or in a 2D system can be found from the condition $\det(D_{n,l})_{N,M,1}=0$. Note that Eq. (9) reduces to the characteristic derivation of a purely 1D system (see Refs. 11, 12, and 14) if there is no coupling to the second, third, etc., mode, i.e., $r_{pl}^{(p)} = r_{lp}^{(p)} = 0$.

Inserting the appropriate GF matrix elements, Eq. (5),

Inserting the appropriate GF matrix elements, Eq. (5), x=1 and $x'=x_N$, one can calculate the transmission amplitude $T_{nmL}^{(N)}$ of an electron through the system with $N \delta$ poten-

tials. Similarly to $R_{nmL}^{(N)}$, we can write the explicit form of $T_{nmL}^{(N)}$ as a ratio of two determinants,

$$T_{nmL}^{(N)} = \frac{\begin{vmatrix} \delta_{nm} & r_{nm}^{(1)} & \cdots & r_{nm}^{(N)} e^{ik_n |x_N - x_1|} \\ 1 & \cdots & \cdots & \cdots \\ \vdots & \vdots & (D_{n,l})_{N,M,m} \\ e^{-ik_m |x_N - x_1|} & \vdots & \\ \det(D_{n,l})_{N,M,1} & , & (10) \end{vmatrix}}{\det(D_{n,l})_{N,M,1}},$$

where the numerator of $T_{nmR}^{(N)}$ is obtained from the same determinant (9) by augmenting it on the left and on the top.

Note that by employing Eqs. (6) and (10) it is straightforward to check by mathematical induction that, for scattering matrix elements, current conservation takes place:

$$\sum_{m=1}^{M} \left(T_{nmL}^{(N)} T_{nmL}^{(N)^*} + R_{nmL}^{(N)} R_{nmL}^{(N)^*} \right) = 1, \tag{11}$$

where the summation is carried out over only the propagating modes of the wire.

Proceeding along the same lines as before, we can similarly derive the expressions for the reflection and transmission amplitudes for the electrons incident from the right. The only difference now is that we isolate in Eq. (3) the term corresponding to the points on the left-hand edge, x_1 , x_2 , etc. The structures of the expressions of the scattering matrix elements from the right will be very similar to Eqs. (6) and (10). The essential difference is that the numerators of $R_{nmR}^{(N)}$ and $T_{nmR}^{(N)}$ now are obtained from the same determinant (9) by augmenting it on the right and on the bottom. The expression, e.g., for $T_{nmR}^{(N)}$ reads

Our task is now to calculate the electron localization length in a multichannel disordered system for the weak disordered case using the explicit form of $T_{nmL}^{(N)}$, (10). The localization length ξ is obtained from the decay of the average of the logarithm of the conductance, $\ln g$, as a function of the lateral system size L,

$$\xi^{-1} = -\lim_{L \to \infty} \frac{1}{2L} \langle \ln g \rangle, \tag{13}$$

where g is given by the Landauer two-probe formula^{15,16} and $\langle \cdots \rangle$ denotes averaging over the disorder V_l in the interval (-w/2, w/2) with given probability:

$$g = \frac{2e^2}{h} \sum_{n,m} T_{nm}^{(N)} T_{nm}^{(N)^*}.$$
 (14)

In the expressions for $T_{nmL}^{(N)}$ in the limit of weak disorder we are going to keep only the terms that are in the linear order of the strength V_l of the δ potentials. In this regime we have the following approximate expressions for the main quantities:

$$T_{mm}^{(N)} \approx e^{ik_{m}(x_{N}-x_{1})} \prod_{l=1}^{N} \left(1 + r_{mm}^{(l)}\right)$$

$$\approx e^{ik_{m}(x_{N}-x_{1})} \frac{1 + i\sum_{l=1}^{N} V_{l} \left(A_{l} - \frac{\sin^{2}(m\pi y_{l}/W)}{k_{m}W}\right)}{1 + i\sum_{l=1}^{N} V_{l}A_{l}}$$
(15)

and

$$T_{nm}^{(N)} = e^{ik_{m}(x_{N}-x_{1})} \sum_{l=1}^{N} r_{nm}^{(l)} e^{i\phi_{mn}^{(l)}}$$

$$\approx -\frac{ie^{ik_{m}(x_{N}-x_{1})} \sum_{l=1}^{N} V_{l} \frac{\sin(n\pi y_{l}/W)\sin(m\pi y_{l}/W)}{W\sqrt{k_{n}k_{m}}} e^{i\phi_{mn}^{(l)}}}{\left(1 + i\sum_{l=1}^{N} V_{l}A_{l}\right)}$$
(16)

with $A_l = \sum_{n=1}^M \sin^2(n\pi y_l/W)/Wk_n$.

The explicit form of the phase ϕ_{mn} is irrelevant for further calculation and we are not going to write it down. By expanding (13) to lowest order in the amplitudes of the δ potentials using Eqs. (14)–(16) and, after averaging over the realization, we obtain the inverse localization length for the weak disordered case,

$$\frac{1}{\xi_M} = \frac{\alpha}{2NMW^2} \sum_{l=1}^{N} \left(\sum_{m=1}^{M} \frac{\sin^2(m\pi y_l/W)}{k_m} \right)^2.$$
 (17)

Here $\alpha = \langle V_l^2 \rangle = \frac{1}{w} \int_{-w/2}^{w/2} f(V_l) V_l^2 dV_l$ with the distribution function $f(V_l)$ an arbitrary even function of V_l . In particular, for a uniform distribution, i.e., $f(v_l) = 1$, this yields $\alpha = w^2/12$.

uniform distribution, i.e., $f(v_1)=1$, this yields $\alpha=w^2/12$. The above expression ξ_M^{-1} is exact to order w^2 for the weak disorder regime. It is valid also for an arbitrary number of channels M and for two different models for disordered Q1D and 2D systems. To verify the validity of the expression ξ_M^{-1} for the case of the tight-binding model let us discuss the case of few-channel wires for which the localization length was calculated in Ref. 5, using the tight-binding Anderson model. Indeed, for M=1 Eq. (17) yields

$$\frac{1}{\xi_1} = \frac{\alpha}{2Nk_1^2 W^2} \sum_{l=1}^{N} \sin^4 \left(\frac{\pi y_l}{W}\right),\tag{18}$$

which can be related to the standard expression for the localization length in a 1D chain tight-binding model with diagonal disorder of ϵ_i if the ϵ_i are independent Gaussian random variables with zero mean values and with correlation function $\langle \epsilon_{in} \epsilon_{jm} \rangle = \alpha \delta_{i,j} \delta_{m,n}$. To this end, in Eq. (18) we take W=2 (for a tight-binding model the number of modes coincides with the number of sites in the transverse direction with spacing a=1) and $y_i=1$ and replace $k_1 \rightarrow \sin k_1$. After summation over N, Eq. (18) reduces exactly to the well-known formula $\xi_1^{\text{TB}} = 8 \sin^2 k_1 / \alpha$ (see, e.g., Ref. 16) with dispersion relation $E=2 \cos k_1$. At $k_1 \rightarrow 0$ we get $\xi_1^{\text{TB}} = 8k_1^2 / \alpha$, which is the well-known localization length for the white noise model. Reasoning along the same line as in deriving

 $\xi_1^{\rm TB}$, we can show that $1/\xi_M^{\rm TB}$, in the case of M channels and weak disorder, can be written in the compact form $(W{\to}M{+}1)$

$$\frac{1}{\xi_M^{\text{TB}}} = \frac{\alpha}{2M(M+1)^2} \sum_{m=1}^{M} \left[\sum_{n=1}^{M} \frac{\sin^2(\frac{mn\pi}{M+1})}{\sin k_n} \right]^2$$

$$= \frac{\alpha}{16M(M+1)} \left[\sum_{n=1}^{M} \frac{3 + \delta_{2n,M+1}}{\sin^2 k_n} + 2 \sum_{n \neq p}^{M} \frac{2 + \delta_{n+p,M+1}}{\sin k_n \sin k_p} \right], \tag{19}$$

where n < p and the wave vector k_n must be found from the dispersion relation $E=2 \cos k_n + 2t \cos n\pi/(M+1)$ (see, e.g., Refs. 5, 17, and 18). The general expression for $1/\xi_M^{\rm TB}$ is valid also for an $M \times M$ system and together with Eq. (17) represents the central results of this Brief Report. It is readily verified that for M=2,3 the above expression $1/\xi_M^{TB}$ reduces to the analogous expressions for the two- and three-channel wire localization lengths, obtained in Ref. 5 by S-matrix construction from transfer matrices. For $M\gg 1$, as one must expect according to Ref. 19, $\xi_M^{\rm TB}$ is proportional to M. Finally, in the absence of interchan hopping (t=0), it reduces to the localization length $1/\xi_1^{\rm TB}$ for a 1D chain, if formally we take all the k_n to be equal and make a double summation which is equal $M(M+1)^2/4$. Making use of Eqs. (14) and (16) and averaging the dimensionless conductance g (in units of $2e^2/h$) over the disorder in the same regime, we obtain $\langle g \rangle \approx M - 2MN/\xi_M^{\text{TB}}$. The latter coincides with the asymptotic expression of the average conductance obtained in Ref. 6 on the basis of a numerical calculation. Using Eq. (19) and the above expression for $\langle g \rangle$, one can check directly that in the

weak disorder limit the well-known relation $2\langle \ln g \rangle = \ln \langle g \rangle$ between the various localization lengths for a 1D system (see, e.g., Refs. 20 and 21) holds also for multichannel systems, reflecting the fact that conductance is not a self-averaging quantity. Finally, by averaging the inverse localization length (17) over the realizations of random y_l using a uniform distribution and recalling that the number of open modes $M = \operatorname{Int}(k_F W / \pi)$, we get $\langle \xi_M^{-1} \rangle \approx 3k_F^2 \alpha / 16M^3 \pi^2 (\sum_{n=1}^M 1/k_n^2 + \frac{2}{3} \sum_{n \neq m}^M 1/k_n k_m)$.

In summary, we have developed an approach based on the characteristic determinant (poles of the GF) to solve the Dyson equation in Q1D and 2D disordered systems without any restriction on the numbers of impurities and modes. We consider two different models for a disordered Q1D wire: a set of two-dimensional δ potentials with signs and strengths determined randomly, and a tight-binding Hamiltonian with several modes and on-site disorder. We analytically calculated the transmission and reflection amplitudes for particles coming both from the left and from the right without actually determining the eigenfunctions of the electron. Our results for the inverse localization lengths, Eqs. (17) and (19), are exact to order w^2 for the weak disorder regime and are valid for an arbitrary number of channels, M.

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