Generalization of the DMPK equation beyond quasi one dimension

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Electronic transport properties in a disordered quantum wire are very well described by the Dorokhov-Mello-Pereyra-Kumar (DMPK) equation, which describes the evolution of the transmission eigenvalues as a function of the length of a multichannel conductor. However, the DMPK equation is restricted to quasi-one-dimensional systems only. We derive a generalized DMPK equation for higher dimensions, containing dependence on the dimensionality through the properties of the transmission eigenvectors, by making certain statistical assumptions about the transfer matrix. An earlier phenomenological generalization is obtained as a special case.

The Dorokhov-Mello-Pereyra-Kumar (DMPK) equation[1,2] has been enormously successful in describing the electron transport properties of a quasi-one-dimensional disordered conductor.[3] The equation describes the evolution of the joint probability distribution of the transmission eigenvalues with increasing length of the system and has been shown to be equivalent[4] to the description in terms of a nonlinear σ model[5] obtained from the microscopic tight-binding Anderson Hamiltonian. The advantage of the DMPK approach over the nonlinear σ model is that one can consider the full distribution of transport quantities rather than the mean and variance alone. Recent analytical as well as numerical results show that the distribution of conductances[6] has many surprises, including very sharp features at (dimensionless) conductance $g = 1$ which could not be anticipated from studies of the moments of the distribution and which should have important consequences for the Anderson transition. One major disadvantage of the DMPK equation, however, is that it does not contain information about the spatial structure of the sample in directions perpendicular to the direction of the current flow, limiting its applicability to quasi one dimension (Q1D) only. Since at present there is no other analytic approach available to study the full distribution of transport properties, it is clear that a generalization of the DMPK equation valid in higher dimensions is of fundamental importance. A phenomenological generalization, with an *ad hoc* constraint to conserve probability, was recently proposed[7] which seems to agree with numerical results[8] in systems beyond Q1D in some restricted regimes. In the present paper we derive a further generalization that contains a dependence on the dimensionality through the properties of the transmission eigenvectors and contains the earlier model as a special case. No additional constraint is needed to conserve probability in the present approach. Moreover, the approach reproduces the expression for Lyapunov exponents in higher dimensions obtained in Ref. 9. Known properties of these exponents provide useful constraints on the phenomenological parameters in the current model.

In the transfer matrix approach, a conductor of length L is placed between two perfect leads of finite width. The scattering states at the Fermi energy define N channels. The $2N \times 2N$ transfer matrix M relates the flux amplitudes on the right of the system to that on the left.[11] Flux conservation and time reversal symmetry (we consider the case of unbroken time reversal symmetry only) restricts the number of independent parameters of M to $N(2N+1)$ and can be written in general as[2]

$$M = \begin{pmatrix} u & 0 \\ 0 & u* \end{pmatrix} \begin{pmatrix} \sqrt{1+\lambda} & \sqrt{\lambda} \\ \sqrt{\lambda} & \sqrt{1+\lambda} \end{pmatrix} \begin{pmatrix} v & 0 \\ 0 & v* \end{pmatrix} \equiv U\Gamma V, \quad (1)$$

where u, v are $N \times N$ unitary matrices and λ is a diagonal matrix with positive elements λ_i, $i = 1, 2, \ldots, N$. An ensemble of random conductors of length L, all with the same macroscopic disorder characterized by the same mean free path l, but different microscopic realizations of the randomness, is described by an ensemble of random transfer matrices M, whose differential probability depends parametrically on L and can be written as $dp_L(M) = p_L(M) d\mu(M) = p_L(\Gamma, U, V) d\mu(\Gamma) d\mu(U) d\mu(V)$. Here $d\mu(M)$ is the invariant Haar measure of the group, given in terms of the parameters in Eq. (1) by $d\mu(M) = J(\lambda) [\Pi_i^N d\lambda_i] d\mu(u) d\mu(v)$, where $J(\lambda) = \Pi_{i<j} |\lambda_i - \lambda_j|^\beta$ with the "symmetry exponent" $\beta = 1$ in our case, and $d\mu(u)$ and $d\mu(v)$ are the invariant measures of the unitary group $U(N)$.

We now take two conductors, with lengths L and δL, to make a conductor of length $L + \delta L$ (Fig. 1). Denoting the corresponding transfer matrices by M'', M', and $M = M''M'$ with probability densities $p_L(M'' = MM'^{-1})$, $p_{\delta L}(M')$, and $p_{L+\delta L}(M)$, respectively, we have the relation[2]

$$p_{L+\delta L}(M) = \int p_L(MM'^{-1}) p_{\delta L}(M') d\mu(M'). \quad (2)$$

The restriction of the DMPK equation to Q1D arises from the "isotropy" approximation, that the distribution $p_L(M)$ is independent of the matrices u and v. Several attempts have been made in order to relax the isotropy approximation.[7,9,10]

FIG. 1. A small wire with length δL, "the building block," is attached to a long one with length L ($\delta L \ll L$). The total transfer matrix M is given by $M = M''M'$.

We will avoid writing a set of coupled evolution equations for λ, u, and v by considering the marginal distribution

$$\bar{p}_L(\lambda) = \int p_L(\Gamma, U, V) d\mu(U) d\mu(V). \quad (3)$$

We first show that the U integration can be done exactly and then we make statistical assumptions about certain products of the matrix elements of V.

Consider the combination $H = MM^\dagger = U\Gamma^2 U^\dagger$. At length L, we get $H'' = M''M''^\dagger = U\Gamma V M'^{-1}(M'^{-1})^\dagger V^\dagger \Gamma U^\dagger \equiv U''\Gamma''^2 U''^\dagger$. It then follows that we can write $U'' = U \cdot U'''(\Gamma, V, M')$. Similarly, by considering the combination $Q = M^\dagger M = V^\dagger \Gamma^2 V$, we get $Q'' = M''^\dagger M'' = (M'^{-1})^\dagger V^\dagger \Gamma^2 V M'^{-1} \equiv V''^\dagger \Gamma''^2 V''$, which implies that we can write $\Gamma'' = \Gamma''(\Gamma, V, M')$ and $V'' = V''(\Gamma, V, M')$. Equation (2) can then be rewritten as

$$p_{L+\delta L}(U, \Gamma, V) = \int p_L(U \cdot U'''(\Gamma, V, M'), \Gamma''(\Gamma, V, M'), V''(\Gamma, V, M')) p_{\delta L}(M') d\mu(U') d\mu(\Gamma') d\mu(V'). \quad (4)$$

We now integrate both sides of Eq. (4) over the invariant measure $d\mu(U)$. The left-hand side defines a marginal distribution $q_{L+\delta L}(\Gamma, V)$. On the right side, since the measure is invariant, $d\mu(U) = d\mu(U \cdot U''')$ for U''' fixed. Therefore $d\mu(U) = d\mu(U'')$, and integrating over $d\mu(U'')$ gives the marginal distribution $q_L(\Gamma'', V'')$ with the following convolution equation:

$$q_{L+\delta L}(\lambda, v) = \int q_L(\lambda'', v'') p_{\delta L}(\lambda', u', v') d\mu(M'), \quad (5)$$

where we have used Eq. (1) to introduce the matrix elements λ, v, λ', v', etc.

Writing $\lambda'' = \lambda + \delta\lambda$ and $v'' = v + \delta v$, Eq. (5) can be rewritten as

$$q_{L+\delta L}(\lambda, v) = \langle q_L(\lambda + \delta\lambda(\lambda, v), v + \delta v(\lambda, v)) \rangle_{\delta L}, \quad (6)$$

where $\langle \cdots \rangle_{\delta L}$ denotes an average over the ensemble of M'. In order to obtain $\delta\lambda$ and δv within a perturbation theory, we search for a matrix constructed from M whose eigenvalues and eigenvectors are given by λ and columns of v, respectively. Consider the matrix $Q = M^\dagger M = V^\dagger \Gamma^2 V$. Flux conservation implies $Q^{-1} = \Sigma_z Q \Sigma_z$, where Σ_z is the $2N \times 2N$ generalization of the Pauli matrix σ_z. It then follows that the matrix $X = [Q + Q^{-1} - 2I]/4$, where I is the identity matrix, is block diagonal. It has been shown that V diagonalizes X,[11] leading to N doubly degenerate eigenvalues λ. We can therefore obtain $\delta\lambda$ and δv by considering the change $\delta X = X'' - X$ due to change in M arising from M'. Writing $\delta Q = Q'' - Q$, it is easy to see that δX is also block diagonal, with $\delta X_{11} = \frac{1}{2}\delta Q_{11}$ and $\delta X_{22} = \frac{1}{2}\delta Q_{11}^*$. Since both X and δX are block diagonal, the perturbation can be treated as acting separately on the two subblocks of X, and one can use ordinary, as opposed to degenerate, perturbation theory to obtain $\delta\lambda$ and δv by considering one subblock only.

Denoting the perturbation by $\tilde{w} = v(\delta X_{11})v^\dagger = \frac{1}{2}v(\delta Q_{11})v^\dagger$ we get

$$\begin{aligned}\tilde{w} = &-\lambda + v u'[\lambda' + \sqrt{1+\lambda'} v' v^\dagger \lambda v v'^\dagger \sqrt{1+\lambda'} \\ &+ \sqrt{\lambda'} v'^* v^{*\dagger} \lambda v^* v'^{*\dagger} \sqrt{\lambda'}] u'^\dagger v^\dagger \\ &- v u'[\sqrt{1+\lambda'} v' v^\dagger \sqrt{\lambda(1+\lambda)} v^* v'^{*\dagger} \sqrt{\lambda'} \\ &+ \sqrt{\lambda'} v'^* v^{*\dagger} \sqrt{\lambda(1+\lambda)} v v'^\dagger \sqrt{1+\lambda'}] u'^\dagger v^\dagger. \quad (7)\end{aligned}$$

We expect $\lambda' \propto \delta L/l \ll 1$. Since $\tilde{w}$ contains terms proportional to $\sqrt{\lambda'}$, we need to consider corrections to both λ and v up to second order in $\tilde{w}$ in order to keep terms up to $O(\lambda')$. Standard perturbation theory[12] gives $\delta\lambda_a = \delta\lambda_a^{(1)} + \delta\lambda_a^{(2)}$ and $\delta v_{an}^\dagger = \delta v_{an}^{\dagger(1)} + \delta v_{an}^{\dagger(2)}$ with

$$\delta\lambda_a^{(1)} = \tilde{w}_{aa}, \quad \delta\lambda_a^{(2)} = \sum_{b(\neq a)} \frac{\tilde{w}_{ab}\tilde{w}_{ba}}{\lambda_a - \lambda_b}, \quad (8)$$

$$\delta v_{an}^{\dagger(1)} = \sum_{m(\neq n)} \frac{\tilde{w}_{mn}}{\lambda_n - \lambda_m} v_{am}^\dagger, \quad (9)$$

and similarly for $\delta v_{an}^{\dagger(2)}$. Note that $v + \delta v$ has to remain unitary, which imposes an additional constraint.

The averages over the "building block" M' appearing in Eq. (6) involve averages over combinations of λ', u', and v' which appear in $\tilde{w}$. Note that the building block is highly anisotropic; in the limit $\delta L \to 0$, the transfer matrix $M' \to I$. This condition will be implemented by assuming $u'v' = I$. In addition, instead of modeling the full $p_{\delta L}(\lambda', v')$, we use the following averages over M':

$$\left\langle \sum_a \lambda_a' v_{a\alpha}'^* v_{a\gamma}' \right\rangle_{\delta L} = \kappa \delta_{\alpha\gamma}, \quad (10)$$

$$\left\langle \sum_{ab} \sqrt{\lambda_a' \lambda_b'} v_{a\alpha}'^* v_{a\beta}'^* v_{b\delta}' v_{b\gamma}' \right\rangle_{\delta L} = \kappa \delta_{\alpha\gamma} \delta_{\beta\delta} \delta_{\alpha\beta}, \quad (11)$$

where $\kappa = \delta L/l$. The first average is used in Ref. 2, the second one in Ref. 9; the latter incorporates the fact that the thin slice allows backward scattering without changes in the

channel indices and is highly anisotropic. Equations (10) and (11), with the conditions $u'v'=I$ and $\kappa \ll 1$, define the model of our building block.

Using the above model and the expansion $\sqrt{1+\lambda'}=1+\lambda'/2+O(\lambda'^2)$, we average $\delta\lambda$, Eq. (8), over M':

$$\langle \delta\lambda_a \rangle_{\delta L} = \kappa(1+2\lambda_a)$$
$$+ \kappa \sum_{b(\neq a)} \frac{\lambda_a+\lambda_b+2\lambda_a\lambda_b}{\lambda_a-\lambda_b} \sum_\alpha |v_{a\alpha}|^2 |v_{b\alpha}|^2, \tag{12}$$

$$\langle \delta\lambda_a \delta\lambda_b \rangle_{\delta L} = \delta_{ab} 2\kappa\lambda_a(1+\lambda_a)\sum_\alpha |v_{a\alpha}|^4. \tag{13}$$

Similar calculations can be done to obtain the corresponding averages for δv.

We should now, in principle, expand Eq. (6) in a Taylor series around both λ and v and evaluate the average over M'. However, for weak disorder, it is known that the isotropy approximation is very good, which means $\partial q_L/\partial v_{ab} \rightarrow 0$. In the strong-disorder limit, the eigenvectors are localized, so that in the nth row v_{na} has only one element equal to unity, all other elements being zero. Since different rows are orthogonal to each other, we can see from Eq. (9) that in this limit $\delta v \rightarrow 0$ because of the restricted sum $m \neq n$. So in both these limits, the product $(\partial q_L/\partial v_{ab})\langle \delta v_{ab} \rangle_{\delta L} \rightarrow 0$. To a good approximation, in these limits, we can therefore treat v at the macroscopic L as a parameter that depends on disorder but for a given strength of disorder does not change any further with δL. In general, a conductor has a fraction (depending on the disorder) of its channels closed;[13] i.e., the corresponding eigenvectors are localized, while the others are open, the corresponding eigenvectors being extended. We expect the isotropy approximation to remain good for the open channels and the closed channels to contribute $\delta v \rightarrow 0$ since they are localized. In other words, the product $(\partial q_L/\partial v_{ab})\langle \delta v_{ab} \rangle_{\delta L}$ can be assumed to be small [compared to the contribution from $(\partial q_L/\partial\lambda)\langle \delta\lambda \rangle_{\delta L}$] for all channels for a wide range of intermediate disorder as well. Physically, since the eigenvalues depend on the length exponentially, $\delta\lambda(\lambda,v)$ remains important for all lengths at any disorder. On the other hand, we expect that at a macroscopic length L, the eigenvectors already evolve to either metallic (isotropic) or insulating (localized) structures for a given macroscopic disorder, and any further change due to δL (as opposed to change in disorder) is likely to be negligible. We will therefore expand the ensemble-averaged marginal probability density $q_L(\lambda,v)$ within the approximation

$$\langle q_L(\lambda+\delta\lambda(\lambda,v), v+\delta v(\lambda,v)) \rangle_{\delta L}$$
$$\approx \langle q_L(\lambda+\delta\lambda(\lambda,v), v) \rangle_{\delta L}. \tag{14}$$

We show below that this approximation retains the dominant eigenvector correlations [via $\delta\lambda(\lambda,v)$] needed to reproduce the Lyapunov exponents in arbitrary dimensions as obtained in Ref. 9. The price we pay for not including δv in our calculation is that we will not be able to evaluate the eigen-

vector correlations self-consistently, but will have to use them as phenomenological parameters.

Using Eq. (14), we expand Eq. (6) in a Taylor series about λ,

$$q_{L+\delta L}(\lambda,v) \approx q_L(\lambda,v) + \sum_a \frac{\partial q_L(\lambda,v)}{\partial\lambda_a} \langle \delta\lambda_a \rangle_{\delta L}$$
$$+ \frac{1}{2} \sum_{ab} \frac{\partial^2 q_L(\lambda,v)}{\partial\lambda_a \partial\lambda_b} \langle \delta\lambda_a \delta\lambda_b \rangle_{\delta L} + \cdots, \tag{15}$$

where the ellipsis includes terms containing higher-order derivatives of λ. We choose $\kappa = \delta L/l \ll 1$, which allows us to truncate the Taylor series at the third term, neglecting terms of $O(\kappa^2)$ and higher. Using Eqs. (12) and (13), the reduced distribution $\bar{p}_L(\lambda) = \int q_L(\lambda,v)d\mu(v)$ can then be written as

$$\bar{p}_{L+\delta L}(\lambda) \approx \bar{p}_L(\lambda) + \kappa \sum_a (1+2\lambda_a)\frac{\partial \bar{p}_L(\lambda)}{\partial\lambda_a}$$
$$+ \kappa \sum_{b \neq a} \frac{\lambda_a+\lambda_b+2\lambda_a\lambda_b}{\lambda_a-\lambda_b}$$
$$\times \int \sum_\alpha |v_{a\alpha}|^2 |v_{b\alpha}|^2 \frac{\partial q_L(\lambda,v)}{\partial\lambda_a}d\mu(v)$$
$$+ \frac{\kappa}{2} \sum_a 2\lambda_a(1+\lambda_a)$$
$$\times \int \sum_\alpha |v_{a\alpha}|^4 \frac{\partial^2 q_L(\lambda,v)}{\partial\lambda_a^2}d\mu(v). \tag{16}$$

In order to make further progress, we will now make a *mean-field* approximation, where the products of four v's that appear inside the integrals in Eq. (16) are replaced by their mean values which can be taken out of the integrals. This is equivalent to the assumption that for a given disorder, fluctuations in such quantities are small compared to their averages. In the weak-disorder regime, each matrix element is of order $1/\sqrt{N}$, differing mostly in their phases; once the phases cancel, the fluctuations are negligible for homogeneous disorder. In the strong-disorder regime, each eigenvector has one element which is unity representing a localized site and the rest are zero, but different samples will have different localized sites, leading to large sample-to-sample fluctuations for individual elements. However, it is expected that the fluctuations in the sum over the elements of any eigenvector for a given disorder will remain negligible. Therefore the mean-field approximation is reasonable in these two limits. As argued before, we will assume that the assumption remains valid in the intermediate region of disorder as well, based on the picture of open and closed channels. Within this approximation and expanding the left-hand side of Eq. (16) in powers of $\delta L/l$, we get

$$\frac{\partial \bar{p}_L(\lambda)}{\partial (L/l)} \approx \sum_a (1+2\lambda_a) \frac{\partial \bar{p}_L(\lambda)}{\partial \lambda_a}$$

$$+ \sum_{a \neq b} \frac{\lambda_a + \lambda_b + 2\lambda_a \lambda_b}{\lambda_a - \lambda_b} K_{ab} \frac{\partial \bar{p}_L(\lambda)}{\partial \lambda_a}$$

$$+ \sum_a \lambda_a (1+\lambda_a) K_{aa} \frac{\partial^2 \bar{p}_L(\lambda)}{\partial \lambda_a^2}. \quad (17)$$

Here we have defined

$$\sum_\alpha \langle |v_{a\alpha}|^2 |v_{b\alpha}|^2 \rangle_L \equiv \sum_\alpha \int |v_{a\alpha}|^2 |v_{b\alpha}|^2 q_L(\lambda,v) d\mu(\lambda)$$

$$\times d\mu(v) \equiv K_{ab}. \quad (18)$$

Since v is unitary, K_{ab} satisfies the sum rule $\Sigma_b K_{ab} = 1$. This allows us to rewrite Eq. (17), following Ref. 7, as

$$\frac{\partial \bar{p}_L(\lambda)}{\partial (L/l)} = \frac{1}{\bar{J}} \sum_a \frac{\partial}{\partial \lambda_a} \left[\lambda_a (1+\lambda_a) K_{aa} \bar{J} \frac{\partial \bar{p}}{\partial \lambda_a} \right], \quad (19)$$

with

$$\bar{J} = \prod_{a<b} |\lambda_a - \lambda_b|^{\gamma_{ab}}, \quad \gamma_{ab} = \frac{2K_{ab}}{K_{aa}}. \quad (20)$$

Equation (19), with the definition (20), is our generalization of the DMPK equation. Note that in the DMPK equation, time reversal symmetry fixes the exponent in the Jacobian J to be $\beta=1$. In our case, as the eigenvectors v are integrated over, the coupling between the eigenvalues and eigenvectors adds an effective matrix exponent to the existing symmetry exponent, resulting in an effective $\bar{J}$ in Eq. (19).

Under isotropy condition $K_{ab} = (1+\delta_{ab})/(N+1)$, we recover the DMPK equation ($\gamma_{ab}=1$). If we choose $K_{ab} = \mu_1/(N+1)$ and $K_{aa} = 2\mu_2/(N+1)$, we obtain the generalization of Ref. 7, where an extra condition was needed between μ_1 and μ_2 in order to satisfy the conservation of probability. In our current framework, that condition is identical to the sum rule $\Sigma_b K_{ab}=1$.

As a check of our model, we evaluate the Liapunov exponents $\nu_a = (l/2\delta L)\ln(1+\delta\lambda_a/\lambda_a)$ in the limit $\lambda_1 \gg \lambda_2 \gg \cdots \gg \lambda_N \gg 1$ and compare with Ref. 9. Expanding in powers of $\delta\lambda_a/\lambda_a$, averaging over v, and using the results for $\langle \delta\lambda \rangle$, Eqs. (12) and (13), we obtain

$$2\nu_a \frac{\delta L}{l} \approx 2\kappa + 2\kappa \sum_{b(\neq a)} \frac{\lambda_b}{\lambda_a - \lambda_b} \left\langle \sum_\alpha |v_{a\alpha}|^2 |v_{b\alpha}|^2 \right\rangle_L$$

$$- \kappa \left\langle \sum_\alpha |v_{a\alpha}|^4 \right\rangle_L. \quad (21)$$

Separating the sum over b into a term less than a and another greater than a and using the unitarity of v, ν_a can be rewritten in the form

$$\nu_a \approx \frac{1}{2} K_{aa} + \sum_{b=a+1}^N K_{ab}, \quad (22)$$

which coincides with that of Ref. 9. Note that the isotropy approximation gives the smallest Liapunov exponent to be $\nu_N = 1/(N+1)$. While this is the correct form in the metallic regime ($\lambda_i \ll 1$), the approximation fails to reproduce the expected behavior in the insulating regime, $\nu_N \sim O(1)$, independent of N. Our approach incorporates the necessary eigenvector correlations to describe the Liapunov exponents at weak- as well as strong-disorder limits. Known properties of these exponents should provide a guide for constructing a model of K.

It is important to note that while Eq. (19) is of the same form as the DMPK equation, the pressure of the matrix K might not allow a solution of Eq. (19) in the same generic form as that of the DMPK equation.[3]

In summary, the DMPK equation for the distribution $p_L(\lambda)$ was obtained by adding a thin slice of length δL to a conductor of macroscopic length L. The assumption that p_L depends only on λ and not on (u,v) limited the equation to Q1D only. We consider the marginal distribution where the u and v are integrated over. The u integration is done exactly. We then assume that while the changes in λ due to the added slice depend crucially on the eigenvectors v, the eigenvectors themselves do not change much with length; i.e., they remain either metallic or insulating as already determined at length L. This implies that our equation is valid only beyond the relaxation length of the parameters K_{ab}. We also assume that the eigenvector correlations $\Sigma_\alpha |v_{aa}|^2 |v_{ba}|^2$ have sharp distributions. While these assumptions were made to obtain the simplest generalization that captures the essentials of dimensionality dependence and need to be verified independently (e.g., numerically), we show that our approach keeps the dominant eigenvector correlations that reproduce the Liapunov exponents in higher dimensions at both weak and strong disorder. The fact that the parameters K_{ab} may incorporate proper dimensionality dependence has already been shown in Ref. 9. Finally, Eq. (19) reduces to the DMPK equation as well as to an earlier generalization[7] in appropriate limits.

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