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Density of states for energy-dependent effective Hamiltonians

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We provide two analytic expressions particularly useful for the evaluation of the density of states of multichannel interacting structures described by effective energy-dependent Hamiltonians. We show that the knowledge of the off-diagonal matrix elements of a properly defined Green's function, between the terminal sites of the system, is the main ingredient to obtain the total density of states. We have used our expressions to calculate the densities of states of ladder chains where each site of the chains may be connected to an external system. A couple of significant examples clarify the feasibility of these expressions.

I. INTRODUCTION

The study of the electronic properties of multichannel quantum wires is very often performed by describing[1-6] these systems in terms of m interacting chains, of length N, whose tight-binding Hamiltonian matrix can be written as

$$H = \begin{pmatrix} \mathcal{E}_1 & \mathcal{T}_{1,2} & & & & \\ \mathcal{T}_{2,1} & \mathcal{E}_2 & \mathcal{T}_{2,3} & & & \\ & \mathcal{T}_{3,2} & \ddots & \ddots & & \\ & & \ddots & \ddots & \ddots & \\ & & & \ddots & \ddots & \mathcal{T}_{N-1,N} \\ & & & & \mathcal{T}_{N,N-1} & \mathcal{E}_N \end{pmatrix}, \quad (1)$$

where $\mathcal{E}_i$ and $\mathcal{T}_{i,i+1}$ are $m \times m$ matrices. In a previous paper[7] we have provided an analytic expression for the evaluation of the density of states of a multichannel system. Generalizing a result by Kirkman and Pendry,[8] we have shown that for the system described by the matrix Hamiltonian (1) the total density of states $N(E)$ can be calculated by means of the following expression:

$$N(E) = \frac{1}{\pi} \operatorname{Im}\left(\frac{\partial}{\partial E}[\ln \det G_{1,N}(E)]\right), \quad (2)$$

where $G_{1,N}(E)$ is the resolvent of the Hamiltonian (1), evaluated only between the first and the last sites of the m chains.

The proof of expression (2) requires that $\det \mathcal{T}_{i,i+1} \neq 0 \ \forall i$ and that both $\mathcal{T}_{i,i+1}$ and the eigenvalues λ_i of H are *independent of energy E*. Often we are faced with situations where the quantities appearing in expression (1) and thus also the eigenvalues λ_i *do depend on energy*. This may happen, for instance, when the system that we are considering (system A) is part of a larger system (system B) with which it interacts, and by means of standard decimation-renormalization procedure[10,11] we resort to describe system A by an effective energy-dependent Hamiltonian $H_{eff}^{AA}(E)$. The usual definition of the total density of states projected on system A is

$$N_{AA} = -\frac{1}{\pi} \operatorname{Im} \operatorname{Tr} G_{AA}(E), \quad (3)$$

where $G_{AA}(E) = 1/[E - H_{eff}^{AA}(E)]$. In this paper we show that also in the case where the system Hamiltonian is energy dependent, we can provide an analytic expression for the total density of states similar to Eq. (2); eventually we shall evaluate $N_{AA}(E)$, without performing the trace of $G_{AA}(E)$, considering only the off-diagonal elements of the Green's function between the terminal sites of the chains. This can be done as follows.

Let us define the Green's function

$$\mathcal{G}(\delta, E) = \frac{1}{E + \delta - H_{eff}^{AA}(E)}, \quad (4)$$

FIG. 1. (a) Two interacting chains of N atoms with side chains with random length between 0 and M atoms; each atom has site energy E_0 and hopping interaction t. (b) Equivalent effective system.

where δ is an auxiliary continuous, energy-independent variable and the identity operator multiplying $E+\delta$ is understood. We have

$$\lim_{\delta \to 0} \mathcal{G}(\delta, E) = G_{AA}(E). \qquad (5)$$

An expression for $\mathrm{Tr}\, G_{AA}(E)$ is obtained from $\mathcal{G}_{1,N}(\delta, E)$ exploiting the relations indicated below:

$$\lim_{\delta \to 0} \frac{\partial}{\partial \delta} \ln \det[\mathcal{G}_{1,N}(\delta, E)]$$

$$= \lim_{\delta \to 0} \frac{\partial}{\partial \delta} \ln \frac{\prod_{i=1}^{N-1} \det \mathcal{T}_{i,i+1}(E)}{\det[E+\delta - H_{eff}^{AA}(E)]}$$

$$= \lim_{\delta \to 0} \frac{\partial}{\partial \delta} \ln \frac{\prod_{i=1}^{N-1} \det \mathcal{T}_{i,i+1}(E)}{\prod_{i=1}^{mN} [E+\delta - \lambda_i(E)]}$$

$$= \lim_{\delta \to 0} \frac{\partial}{\partial \delta} \ln \prod_{i=1}^{mN} \frac{1}{E+\delta - \lambda_i(E)}$$

$$= \lim_{\delta \to 0} \sum_{i=1}^{mN} \frac{-1}{E+\delta - \lambda_i(E)} = -\mathrm{Tr}\, G_{AA}(E). \qquad (6)$$

As in the relation (2) $\mathcal{G}_{1,N}(\delta, E)$ indicates the Green's-function matrix elements between sites at the terminals (1 and N) of the system. Thus from the relation (3) we have

$$N_{AA}(E) = \frac{1}{\pi} \mathrm{Im} \left[\frac{\partial}{\partial \delta} \ln \det[\mathcal{G}_{1,N}(\delta, E)] \right]_{\delta=0}, \qquad (7)$$

which generalizes expression (2) in the case of energy-dependent tridiagonal matrices (1).
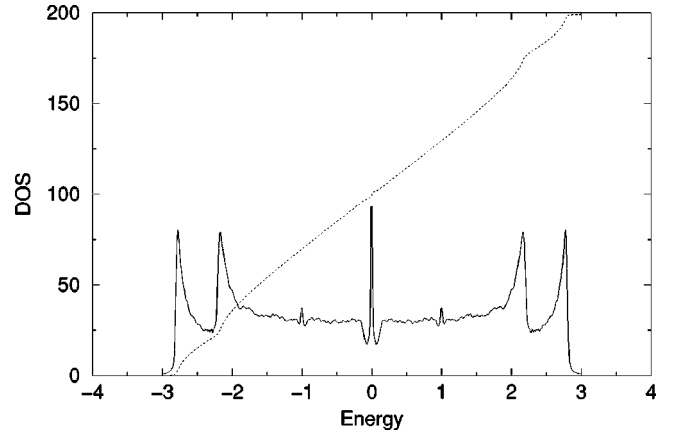
FIG. 2. Integrated (dotted line) and total (continuous line) density of states of the effective system of Fig. 1(b), with $N=100$, $M=10$, $E_0=0$, and $t=-1$. Energies are given in units of $|t|$.

II. A NUMERICAL EXAMPLE ON THE USE OF EQ. (7)

In order to illustrate an application of Eq. (7) we consider the system depicted in Fig. 1(a). It consists in two interacting chains with a random distribution of side chains. This structure can be useful to treat systems with topological disorder such as fractals, percolation clusters, and branched polymers.[9] The two chains have N atoms, each one interacting with a side chain of random length m with $0 \leq m \leq M$; the site energies E_0 and the hopping nearest-neighbor interactions t are assumed constant.

By the renormalization procedure one can decimate the side chains and reduce the system of Fig. 1(a) to the effective system of Fig. 1(b) where the energies of the sites, which were in correspondence with a side chain of m atoms, are given by $E_0 + \Sigma_m(E)$, with

$$\Sigma_m(E) = \frac{t^2}{[E - E_0 - \Sigma_{m-1}(E)]} \quad \text{with} \quad \Sigma_0(E) = 0. \quad (8)$$

In a single stroke the density of states of the Hamiltonian of Fig. 1(b) can be evaluated by means of the relation (7). To obtain $\det[\mathcal{G}_{1,N}(\delta, E)]$ we have made use of the same recursion procedure illustrated in Ref. 7 to obtain $\det[G_{1,N}(E)]$.

In Fig. 2 it is reported the average over 100 configurations of the total density of states of the system of Fig. 1(b) with $N=100$, $M=10$, $E_0=0$, and $t=-1$. The peak at $E=0$ is due to the fact that the effective energy Σ_m, for odd m, diverges; analogously the peaks $E=\pm 1$ are due to the two poles of Σ_m for $m=2$. Generalizing, Σ_m has m poles where the density of states should increase but peaks corresponding to higher values of m are smeared out because their weight decreases with m. The peaks at $E=\pm 2$ are due to the nature itself of the two interacting chains, and their separation depends on the interchain hopping.[7]

III. THE CASE $\det(\mathcal{T}_{i,i+1}) = 0$

Let us now consider the case where the matrix elements of the Hamiltonian (1) can depend on energy, with the further condition that some or all the values of $\det(\mathcal{T}_{i,i+1})$ [and thus also $\det(\mathcal{G}_{1,N})$] vanish.

In this case Eq. (7) is useless for the evaluation of $N(E)$

and a different approach has to be followed; we resort to the definition (4),

$$N(E) = -\frac{1}{\pi}\left[\text{Im Tr}\frac{1}{E+\delta-H}\right]_{\delta=0}$$

$$\equiv -\frac{1}{\pi}\text{Im}\left[\frac{\partial}{\partial\delta}\ln\det(E+\delta-H)\right]_{\delta=0}, \quad (9)$$

and look for a recursive method to calculate the determinant of $(E+\delta-H)$. One can write

$$E+\delta-H=\begin{vmatrix} A_1 & B_{1,2} & & & & \\ B_{2,1} & A_2 & B_{2,3} & & & \\ & B_{3,2} & \ddots & \ddots & & \\ & & \ddots & \ddots & \ddots & \\ & & & \ddots & \ddots & B_{N-1,N} \\ & & & & B_{N,N-1} & A_N \end{vmatrix}$$

$$= K_N, \quad (10)$$

where $A_i = E+\delta-\mathcal{E}_i$ and $B_{i,i+1} = -\mathcal{T}_{i,i+1}$; $\mathcal{E}_i$ and $\mathcal{T}_{i,i+1}$ are defined in expression (1). One can partition the matrix K_N into four blocks

$$K_N = \begin{pmatrix} K_{N-1} & \tilde{B}_{N-1,N} \\ \tilde{B}_{N,N-1} & A_N \end{pmatrix}, \quad (11)$$

where K_{N-1} is the minor of the matrix K_N made with the first $m\cdot(N-1)$ columns and rows and $\tilde{B}_{N-1,N}$ is the $m\cdot(N-1)\times m$ matrix made as follows:

$$\tilde{B}_{N-1,N} = \begin{pmatrix} \varnothing_{1,N} \\ \varnothing_{2,N} \\ \vdots \\ \varnothing_{N-2,N} \\ B_{N-1,N} \end{pmatrix} \quad (12)$$

with $\varnothing_{i,j}$ the null $m\times m$ matrix. $\tilde{B}_{N,N-1}$ is the transpose of $\tilde{B}_{N-1,N}$.

Let us consider the following matrix:

$$M = \begin{pmatrix} \mathbb{I}_{N-1} & \varnothing \\ -\tilde{B}_{N,N-1}(K_{N-1})^{-1} & \mathbb{I}_1 \end{pmatrix}. \quad (13)$$

By construction $\det M = 1$ so we have that $\det K_N = \det(M\cdot K_N)$. The matrix $M\cdot K_N$ is given by

$$M\cdot K_N = \begin{pmatrix} \mathbb{I}_{N-1} & \varnothing \\ -\tilde{B}_{N,N-1}(K_{N-1})^{-1} & \mathbb{I}_1 \end{pmatrix} \cdot \begin{pmatrix} K_{N-1} & \tilde{B}_{N-1,N} \\ \tilde{B}_{N,N-1} & A_N \end{pmatrix}$$

$$= \begin{pmatrix} K_{N-1} & \tilde{B}_{N-1,N} \\ \varnothing & A_N - \tilde{B}_{N,N-1}(K_{N-1})^{-1}\tilde{B}_{N-1,N} \end{pmatrix}. \quad (14)$$

Thus we have

FIG. 3. (a) Chain of vertical dimers. Site energies are all equal to E_0, interactions internal to the dimers and between adjacent dimers are equal to t. (b) As system (a), decorated by side chains of random length; each atom has site energy E_0, the hopping interaction between adjacent sites is t_0. (c) Effective system, with energy dependent site energies, equivalent to the system (b).

$$\det K_N = \det(M\cdot K_N)$$

$$= \det K_{N-1}\cdot\det[A_N - \tilde{B}_{N,N-1}(K_{N-1})^{-1}\tilde{B}_{N-1,N}]. \quad (15)$$

We can iterate the procedure to obtain $\det K_{N-1}$ as function of $\det K_{N-2}$ and so on; finally we obtain

$$\det K_N = \det A_1 \cdot \prod_{j=2}^{N}\det[A_j - \tilde{B}_{j,j-1}(K_{j-1})^{-1}\tilde{B}_{j-1,j}], \quad (16)$$

FIG. 4. Integrated and total density of states of the effective system of Fig. 3(b), with $N=500$, $E_0=0$, and $t=-1$. The dotted line corresponds to $M=0$ [undecorated lattice of Fig. 3(a)], the continuous line corresponds to $M=10$ (decorated lattice) averaged over 100 configurations. Energies are expressed in units of $|t|$. The dashed-dotted and dashed curves represent the integrated density of states for the systems 3(a) and 3(b), respectively.

where $(K_{j-1})^{-1}|_{\delta=0} = \mathcal{G}_{j-1}$ is the Green's function of the effective (or real) system built with the first $m \cdot (j-1)$ states.

It is worthwhile to notice that expression (16) is particularly convenient for block tridiagonal matrices but can be used as well as for any kind of matrix K_N; in fact, in the proof we have never used the special form of the matrices $\tilde{B}_{j-1,j}$; moreover, when we iterate the procedure we can choose at each step a different partition of the matrix K_j so that the blocks A_j can have different dimensions. For almost one-dimensional systems, when the matrices $\tilde{B}_{j-1,j}$ have few nonvanishing elements, only few terms of the Green's function $\mathcal{G}_{j-1}$ have to be evaluated to obtain the determinant of K_N.

To test the usefulness of Eq. (16) let us evaluate the electronic density of states of the decorated one-dimensional system shown in Fig. 3 without [Fig. 3(a)] and with [Fig. 3(b)] random distribution of side chains of length m ($0 \leqslant m \leqslant M$). The bare system is composed by two sublattices, A and B, without interactions within the sublattice B [see Fig. 3(a)]. This geometry has been used in the study of the localization of the electronic states in the presence of disorder in the site energies of the two sublattices[12] and it has been proposed also in the study of strongly correlated systems.[13]

For simplicity we assign the same energy E_0 to each site and the same value t to the intersite interactions. Thus in the matrix (1) representing the system of Fig. 3(a), the submatrices $\mathcal{E}_i$ and $\mathcal{T}_{i,i+1}$ are given by

$$\mathcal{E}_i = \begin{pmatrix} E_0 & t \\ t & E_0 \end{pmatrix} \quad \text{and} \quad \mathcal{T}_{i,i+1} = \begin{pmatrix} t & 0 \\ t & 0 \end{pmatrix}.$$

The determinants of $\mathcal{T}_{i,i+1}$ vanish and thus the density of states of the system of Figs. 3(a) and 3(b) are obtained through Eq. (9) by means of the recursive relation (16). The results are reported in Fig. 4 for the bare lattice [Fig. 3(a)] and for the renormalized decorated lattice [Fig. 3(c)].

In Fig. 4, the dotted line shows the density of states of the system in Fig. 3(a) (without side chains): two bands are present for energies $-3.2 \leqslant E \leqslant 0$ and $1.1 \leqslant E \leqslant 2$, and a "surface state" at $E = 1$. The effect of the side chains [system 3(b)] is to fill the forbidden gaps and to add a peak at $E = 0$ which is due, as in the case of Fig. 2, to the poles of Σ_m at $E = 0$ for odd m; the density of states for the system 3(b) is given in Fig. 4 (continuous line); it has been obtained averaging 100 configurations with side chains of random length m ($0 \leqslant m \leqslant 10$).

As a final check we have verified that the integrated density of states exactly sums to the total number of states; this is shown in Fig. 4 for the systems of Figs. 3(a) and 3(b), by the dashed-dotted and dashed curves, respectively.

IV. CONCLUSIONS

We have presented in this paper two analytic expressions which prove very convenient in the evaluation of total and integrated densities of states of multichannel systems described by energy dependent Hamiltonians. Such a situation always appears, for instance, when we deal a part of a given system and describe by the decimation-renormalization method the effect of all the remaining system on the chosen part, by appropriate self-energy corrections.

We have shown that even in this case we can obtain the total density of states from the knowledge of few off-diagonal matrix elements $\mathcal{G}_{1,N}$ of a suitably adapted Green's function, only between the terminal sites of the system. A few applications on representative model systems highlight the shortcut provided by our expressions.

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