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Unified approach to numerical transfer matrix methods for disordered systems : applications to mixed crystals and to elasticity percolation

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Résumé. — Il est démontré que le théorème des valeurs propres négatives et les méthodes de matrice de transfert peuvent être considérés d'un même point de vue unifié pour être ensuite généralisés au calcul des densités d'état projetées, ou plus généralement au calcul de n'importe quelle combinaison linéaire d'éléments de matrice de l'inverse de grandes matrices symétriques aléatoires. Comme exemple d'application on présente les résultats de simulations pour les comportements à un et à deux modes du spectre Raman des cristaux mixtes unidimensionnels ainsi qu'une analyse de taille finie pour les exposants de la classe d'universalité de percolation des forces centrales.

Abstract. — It is shown that the Negative Eigenvalue Theorem and transfer matrix methods may be considered within a unified framework and generalized to compute projected densities of states or, more generally, any linear combination of matrix elements of the inverse of large symmetric random matrices. As examples of applications, extensive simulations for one- and two-mode behaviour in the Raman spectrum of one-dimensional mixed crystals and a finite-size scaling analysis of critical exponents for the central force percolation universality class are presented.

There is a large class of problems in various fields of physics whose solution is in principle obtained by inverting large random matrices. The calculation of densities of states (DOS) (total, local, projected...) for phonons, electrons or spin waves, occupation probabilities in random walks or the conductivity of resistor networks are all examples of linear problems whose solution is in general trivial for ordered systems on regular lattices but extremely difficult in disordered systems because it then requires the inversion of large random matrices.

Nevertheless, it has been realized early [1, 2] that numerical simulations are a very useful tool to understand the behaviour of disordered systems. For the kind of problems discussed above, a numerical simulation means solving exactly the equations of motion for a large (10^4 sites or more) but finite lattice generated by a Monte Carlo procedure. There exists a large number of methods which were developed to handle efficiently the special kind of matrices of interest to physicists. These are in general sparse (many zeros) and of block tridiagonal form. To name only a few methods, there is the Negative Eigenvalue Theorem which has been used to compute total DOS [3], transfer matrix methods [4, 5] which are used for example with finite size scaling to compute the conductivity of random resistors networks, and the Haydock-Lanczos recursion method [6] which is used to compute total, local or projected DOS.

In this paper, we

(a) point out that the Negative Eigenvalue Theorem and transfer matrix techniques may be viewed as special cases of the same general transfer matrix method, which can also be used to compute projected DOS;

(b) show how the above general method can be made more efficient by calculating only the needed matrix elements of the inverse matrix;

(c) give two examples of applications : one to one- and two-mode behaviour in mixed crystals and one to the calculation of exponents of a new percolation universality class. The general method we present is related to the Gaussian elimination method as we further discuss at the end of this paper.

Let us first recall some known analytic results which clearly show that DOS, projected DOS or conductivity problems can be considered from a unified point of view [7]. Let [8]

$$
F(J, E, \eta) = \ln \left\{ \int Du \exp\left[-\frac{1}{2} U^{\mathrm{T}}(E + i\eta - H) U + J^{\mathrm{T}} U \right] \right\}
$$

$$
= \ln \left\{ \int Du \exp(S) \right\} \tag{1}
$$

where the argument of the exponential is written in matrix notation, $U^{\mathrm{T}} = (u_1, u_2, ..., u_N)$ and

$$
\int Du = \int \prod_{i=1}^{N} du_i . \tag{2}
$$

In the electronic tight binding approximation, H is the Hamiltonian, E the energy eigenvalue times the identity matrix with a convergence factor η. A simple redefinition of symbols allows one to make analogous definitions for phonons, random walks, spin waves etc... The Gaussian integral in equation (1) can be performed by standard methods. From this integral, one can derive,

$$
\frac{\partial^2 F}{\partial J_r \partial J_s} = \left[\frac{1}{(E + i\eta - H)} \right]_{rs} \tag{3}
$$

and

$$
\frac{2 \partial F}{\partial E} = \mathrm{Tr} \left[\frac{1}{(E + i\eta - H)} \right] . \tag{4}
$$

The imaginary part of equation (4), in the limit η goes to zero, clearly gives the total DOS. With the proper choice of J, one can compute any projected DOS one wishes. For example, for a lattice with alternating charges on each site,

$$
J^{\mathrm{T}} = x(1, -1, 1, -1, ...) \tag{5}
$$

would allow one to compute the projected DOS relevant for Raman scattering from Im $(\partial^2 F/\partial x^2)$. Also, to compute the bulk modulus, one simply needs to start with $E + i\eta \to -\omega^2 - i\eta = 0$, H equal to the matrix of force constants, and elements of the vector J equal to 0 for sites not on the surface and to x for sites on the surface. The average displacement of surface sites can then be computed from $\partial^2 F/\partial x^2$ and allows one to calculate the bulk modulus. An analogous calculation may be done for the conductivity of a random resistor network.

While much of the above results are familiar, it has apparently not been realized before that the generating function or its derivatives could be computed recursively, providing an efficient numerical scheme to attack any of the above problems. We proceed to show that recursion relations may be obtained which are general but reduced in the appropriate limit to those used in conjunction with the Negative Eigenvalue Theorem or with transfer matrix methods. First, for a problem in arbitrary dimension, we can always single out a direction and write for the argument of the exponential in equation (1) :

$$S = \sum_{i=1}^{N} \left[-\frac{1}{2} U_i^{\mathrm{T}} X_i U_i + U_i^{\mathrm{T}} Y_{i,i+1} U_{i+1} + J_i^{\mathrm{T}} U_i \right] \tag{6}$$

where U_i refers to the n_i sites of the i'th slice of the system, X_i is a $n_i \times n_i$ matrix, $Y_{i,i+1}$ a $n_i \times n_{i+1}$ matrix. In other words, X_i and $Y_{i,i+1}$ are respectively the diagonal and off-diagonal blocks of the block tridiagonal matrix $(E + i\eta - H)$. Performing analytically the Gaussian integral in slice 1 of the system renormalizes the matrix X_2 and the vector J_2 and gives terms which are independent of all the U_i. We call the latter terms C_2. The problem is now the same as the original one with one less slice. That process can be repeated, generating the following recursion formulae,

$$Z_{i+1} = X_{i+1} - Y_{i,i+1}^{\mathrm{T}} Z_i^{-1} Y_{i,i+1} \tag{7}$$

$$L_{i+1} = J_{i+1} + Y_{i,i+1}^{\mathrm{T}} Z_i^{-1} L_i \tag{8}$$

$$C_{i+1} = C_i - \frac{1}{2} \ln (\det Z_i) + \frac{1}{2} L_i^{\mathrm{T}} Z_i^{-1} L_i \tag{9}$$

with initial conditions

$$Z_1 = X_1, \qquad L_1 = J_1, \qquad C_1 = 0 .$$

Equations (7) and (9), the latter with $L_i = 0$, are the Negative Eigenvalue Theorem. Indeed, in the limit $\eta \to 0$, one can show (see Eq. (4)) that the imaginary part of F is simply equal to $\pi/2$ times the total number of states up to energy E. Equations (7) and (9) then simply say that, in the limit η goes to zero, F may be computed from the total number of negative eigenvalues of the smaller matrices Z_i. The detailed proof is slightly more complicated than outlined here and should be given elsewhere. Note in passing that as with the Haydock-Lanczos method, keeping here a finite value of η helps to compare with experiment since the spectra thus obtained are smooth on a scale of η which may correspond to intrinsic linewidth or experimental resolution.

As mentioned earlier, the conductivity of a random resistor network may be obtained from derivatives of the corresponding F with appropriately chosen values of J (as described below Eq. (5)). Recursion formulae for derivatives of F are easily obtained using the chain rule. The resulting set of recursion relations is closely related to the transfer matrix method of Derrida et al. [5] and has the same advantages.

It should now be clear that the Negative Eigenvalue Theorem or transfer matrix methods may be generalized to compute arbitrary projected DOS. For example, in the case of zone centre optic modes, which correspond to J chosen as in equation (5), one would use the chain rule to arrive at the result that one must use equations (7) and (8) with $x = 1$ and $D_{i+1} = D_i + L_i^{\mathrm{T}} Z_i^{-1} L_i$ to compute $\partial^2 F/\partial x^2 = D_N$.

Equation (7) still involves inversion of matrices whose size can also vary as a function of i, as is the case in the percolation problem when sites are completely disconnected. Following a suggestion of Derrida et al. [5], we improve the speed (by a factor of about three) and ease of the calculation of DOS, projected DOS, etc... by deriving an equivalent set of recursion formulae, obtained by eliminating one site at a time instead of a slice at a time. One then does not have to explicitly invert any matrix and the calculation time is reduced because, in a sense, one is concentrating only on the elements of the matrices Z^{-1} one really needs. In the percolation problem, when a site is completely disconnected, one simply « jumps » over it. Note that with this method, one has effectively a one dimensional problem with long range interactions. For example, with a two dimensional system of width n and length N, the longest range interaction is with the n'th neighbour. The range does not increase upon iteration but all possible neighbour interactions between first and n'th are generated by the recursion. Computation time increases, for n and N large, as $n^3 N$. In that limit, storage increases only as $n^2/2$.

The problem of one- and two-mode behaviour in the Raman scattering off mixed crystals is our first example of application. Consider a one dimensional mixed crystal of the type $AB_{1-c} C_c$. Every other atom is an atom of mass M_A. The other sublattice is populated with atoms of mass M_B with probability $1 - c$ and M_C with probability c. Raman scattering from such compounds [9] (or higher dimensional versions [10]) reveals one or two Raman modes depending on the compound and on concentration c. Attempts have been made to explain this behaviour by pure mass disorder (neglect of the force constant disorder) [11]. We have studied such a model. Figure 1 displays a two-mode spectrum obtained in our calculations [12]. Figure 2 gives the parameters for which we have obtained one- or two-mode behaviour. It should be noted that the one- to two-mode transition is not sharp (the approximate width is indicated on the figure) especially in one dimension. Given this uncertainty, the CPA and our results agree equally well with most experiments [10]. We have verified that interchain coupling seems to make the transition region better defined (less structure in the spectrum). Additional results are discussed elsewhere [13].

Our second example of application is with exponents associated with the new percolation universality class found by Feng and Sen [14]. They considered the problem of bond percolation where the bonds have a central force component (Born model). They showed that the exponent f describing the vanishing of the effective force constant at the percolation threshold is different
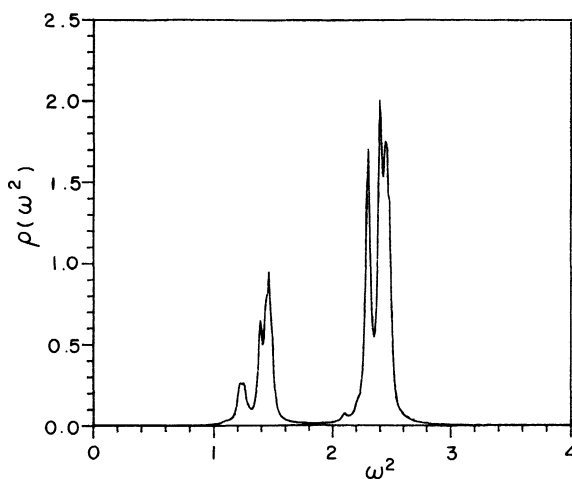

Fig. 1. — Example of projected DOS ρ as a function of ω^2 for two-mode behaviour. $M_A = 4.0$, $M_B = 2.0$, $M_C = 1.0$, concentration $c = 0.5$, $\eta = 0.01$.
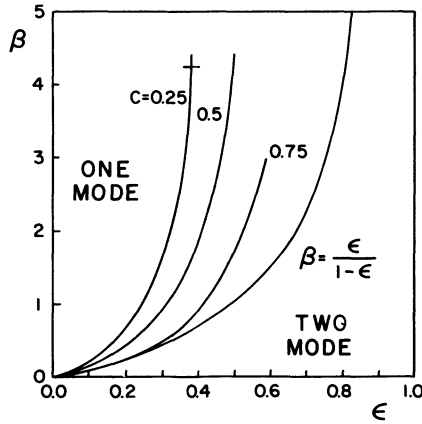
Fig. 2. — $\beta = M_B/M_A$ and $\varepsilon = 1 - (M_C/M_B)$ with $M \propto M_B$. For each value of the concentration c, two-mode behaviour is observed to the right and one-mode behaviour to the left of the line.

from the conductivity exponent t which one finds in the case of isotropic forces. We did a finite size scaling analysis of this problem in the spirit of Derrida *et al.* [5] but with our approach. We considered strips of a triangular lattice in two dimensions of width n, long enough that the effective force constant had very little statistical fluctuations (Typically, $N = 2\,000$ for $n = 3$ to 48 and $N = 460$ for $n = 77$). The top side of the strip is connected to a rigid wall while the sites on the bottom side are attached by a strong isotropic spring (10^3 times the central force strength). This is the analog of the shorts in reference [5]. We then apply a unit force on every site at the bottom and compute the average displacement from a second derivative of the generating function. The large isotropic force constant at the bottom is necessary to avoid pushing on clusters which are disconnected from the wall. The value 10^3 of that force constant is not as critical as if we were pushing on only one end of the spring (cf. Ref. [5]). Note also that we must allow for a small (10^{-5} or smaller) isotropic component to each central force to avoid indeterminacies associated with the lack of restoring force for displacement of clusters in certain directions. The accuracy of our calculation is limited by the value of this small isotropic component when the effective spring constant is too small. Smaller values of the isotropic component lead to numerical errors. From the scaled variable plot of figure 3, we can extract the percolation threshold $p_{cen} = 0.65 \pm 0.005$ for the triangular lattice and the exponents $f = 1.4 \pm 0.2$ and $v_{cen} = 1.05 \pm 0.15$. For isotropic forces, $v = 4/3$, $t = 1.28$ and $p_c = 0.3473$. Our results thus suggest that $f > t$ and $v_{cen} < v$. The above values of p_{cen} and f are appreciably different from the estimates of Feng and Sen, $p_{cen} = 0.58$, $f = 2.4 \pm 0.4$. Our calculation is definitely more extensive. It is also the first time v_{cen} is computed. Our value $f/v_{cen} = 1.35 \pm 0.25$ falls within the upper and lower bounds proposed by Rammal [15].

A few final remarks :

(a) Note that if one writes down recursion relations for $\partial L_r/\partial J_s$ and $\partial^2 F/\partial J_r\, \partial J_s$ for all values of r and s, one can find all the elements of the inverse of an arbitrary symmetric matrix. In our case, one can show that our method is in a sense Gaussian elimination for symmetric matrices. Here, we have improved Gaussian elimination both by specializing it to block tridiagonal matrices and by calculating only one element or linear combination of elements of the inverse matrix.

(b) Even though our method is easily applicable to finite systems of arbitrary spatial dimension, it is especially fast for quasi one dimensional systems. The Haydock-Lanczos recursion method, which differs from ours, is faster for systems of high dimension.
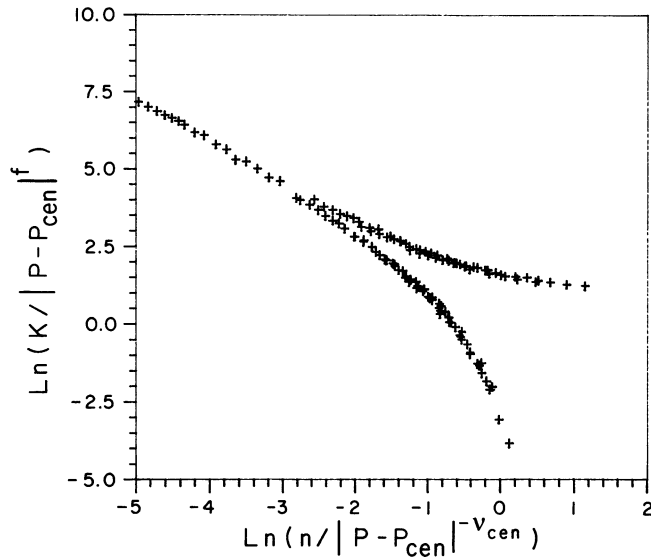
Fig. 3. — Logarithm of the effective scaled shear modulus $(\mathrm{Ln}\ (K/|\,p - p_{cen}\,|^f))$ as a function of log of scaled system size $(\mathrm{Ln}\ (n/|\,p - p_{cen}\,|^{-v_{cen}}))$ for $p_{cen} = 0.649$, $f = 1.4$ and $v_{cen} = 1.0$ and various values of p : 0.60, 0.61, 0.62, 0.63, 0.64, 0.65, 0.66, 0.67, 0.69. The top universal curve is for $p > p_{cen}$, the bottom one for $p < p_{cen}$. The same symbol is used for all values of p to avoid cluttering the figure.

(c) In contrast with the latter method, we do not need to store information about all the lattice to obtain DOS projected on Fourier modes.

Acknowledgments.

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