Densities of states, projected densities of states, and transfer-matrix methods from a unified point of view

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It is shown that various numerical methods to compute densities of states, projected densities of states (relevant for light scattering spectra), electrical or elastic properties of disordered media can all be considered as special cases of a general approach to these problems. This approach is based on a recursive evaluation of a generating function which in appropriate limits reduces, for example, to the approach based on the negative-eigenvalue theorem or to Gaussian elimination optimized for symmetric sparse matrices. The approach is simple and systematic. It also leads to an alternate proof of the negative-eigenvalue theorem. The general formalism and various special cases are discussed in detail. Comparisons with other methods such as the transfer-matrix, conjugate-gradient, and Haydock-Lanczos methods are provided.

I. INTRODUCTION

Many problems of current interest are described by a “linear” Hamiltonian. The difficulty of the problem in such cases arises from the lack of symmetry which forces to either devise approximate techniques or to diagonalize large $N \times N$ matrices. Many such problems belong to the physics of “disordered” systems. For example, one may be interested in the density of states (DOS) of elementary excitations (phonons, spin waves, tight-binding free electrons) of a disordered system, or in random walks in disordered media, or in the projected (or partial) density of states which determines the light-scattering spectrum of such systems, or simply in the conductivity of macroscopically inhomogeneous composites.

In this paper, we focus on the numerical solution of problems of the type mentioned above. While all our examples will be drawn from the physics of disordered systems, the general results have a wider range of applicability. Our starting point is the generating function for the physical quantity of interest. While the generating-function approach is a frequent starting point of approximation methods in disordered systems or nonlinear systems (phase transitions, field theory), we do not think that it has been realized before that it could be useful in numerical calculations of “linear” problems.

The generating-function approach has two advantages. First, it shows that various frequently used numerical methods are in fact closely related to each other and in essence do not differ. For example, the fact that the negative-eigenvalue theorem (NET) (or Sturm’s sequence technique) for calculating integrated DOS is closely related to Gaussian elimination is sometimes not evident and it is also sometimes not realized that the NET can easily be generalized to obtain projected DOS. The second advantage of the generating-function approach, is that one almost always obtains the most efficient numerical algorithm using only the most elementary techniques of Gaussian integration and matrix algebra. For example, for DOS calculations of Hamiltonians with finite-range interactions one automatically recovers the NET specialized to band-diagonal matrices, and for the conductivity of random resistor networks, one recovers a technique which is different from, but closely related to, transfer-matrix techniques. For a general symmetric-matrix inversion problem, one recovers the fastest known Gaussian elimination technique (see Appendix B).

Since all the numerical techniques obtained in this paper from the generating-function approach are in some sense a form of Gaussian elimination, they have been widely used in the literature in one form or another. As mentioned above, we feel that it is the simplicity and unifying aspects of the generating-function approach which justify the present exposition. As an added bonus, the approach suggests a proof of the negative-eigenvalue theorem which is simple and, we believe, original (Appendix A).

Elastic constants and density of states of percolating elastic networks, conductivity and noise of random resistor networks and light scattering spectrum (Raman or infrared) of mixed crystals are all examples of problems which have been studied numerically using recurrence relations derived from a generating-function approach. Some of these works are quoted in the present paper as examples of numerical applications of the recurrence relations derived here but the list should...
not be considered exhaustive: The negative-eigenvalue theorem\textsuperscript{2,3} and Gaussian elimination\textsuperscript{15} have been around for a very long time. What we are trying to emphasize here is the relation between the methods. While a short summary of the generating function approach has been published in Ref. 8, no details of the method have appeared in any of the subsequent work.

In Sec. II we first recall how physical quantities of interest can be obtained from the generating function or from its derivatives and then show how these quantities can be evaluated recursively, providing easily implementable numerical algorithms. In Sec. III we show explicitly how to derive recurrence relations to compute integrated DOS, DOS, projected DOS, and conductivity problems for systems in a strip (rectangular) geometry. This geometry corresponds to band-diagonal matrices. Numerical applications of the recurrence relations in Sec. III have already appeared. Section IV contains estimations of the polynomial dependence of computation time on system size for various cases, and comparisons with other methods. Conclusions are given in Sec. V. Appendix A contains a derivation of the negative-eigenvalue theorem and Appendix B the detailed connection to Gaussian elimination techniques in the case of general symmetric matrices.

II. GENERATING FUNCTION AND ITS RECURSIVE EVALUATION

In the first part of this section we recall known properties of the generating function,\textsuperscript{1} in particular how derivatives of this function are related to quantities of physical interest. In the second part, we outline a general recursive way of evaluating the generating function, or its derivatives, which is easily programmable.

A. Generating function

All quantities of interest mentioned in the introduction may be obtained from the following generating function

\[
\mathcal{J}(E,\{J\}) = \ln \left[ \int_{-\infty}^{\infty} \prod_{i=1}^{N} du_i \exp \left[ -\frac{1}{2} U^T \left( [E + i\eta I - H] U + V^T V \right) \right] \right],
\]

where \( U^T = (u_1, u_2, \ldots, u_N) \), \( J^T \) is a row vector of dimension \( N \), \( H \) is an \( N \times N \) symmetric matrix, \( I \) is the identity matrix, and \( \eta \) a small positive number. (Matrix multiplication is implied.) In the electronic tight-binding approximation, for example, \( H \) would be the Hamiltonian matrix, \( E \) the energy, and \( \eta \) a convergence factor which will be discussed in more detail below.

To formally evaluate the multiple integrals in Eq. (1) it suffices to change the integration variable to \( V = \mathcal{T} U \) where \( \mathcal{T} \) is the unimodular orthogonal transformation that diagonalizes \( E I - H \). Then one can perform the Gaussian integrations in the variables \( v_i \) independently of each other. The final result, written in terms of the original variables is,\textsuperscript{16}

\[
\mathcal{J} = \ln \left[ \frac{(2\pi)^N}{\det([E + i\eta I - H])]^{1/2}} \exp \left[ \frac{1}{2} J^T \left( [E + i\eta I - H]^{-1} \right) J \right] \right].
\]

Note that if we let \( J = x (j_1, j_2, \ldots, j_N) \), then

\[
\frac{\partial^2 \mathcal{J}}{\partial x_k \partial x_l} = \sum_{k,l} j_k j_l \left[ [E + i\eta I - H]^{-1} \right]_{kl}.
\]

Clearly then, derivatives of \( \mathcal{J} \) can yield any linear combination of the elements of \( [E + i\eta I - H]^{-1} \), provided that the coefficients of the linear combination are of the form \( c_{kl} = j_k j_l \). Also, by taking cross derivatives such as \( \frac{\partial^2 \mathcal{J}}{\partial j_k \partial j_l} \), one can obtain any specific matrix element.

The case \( J = 0 \) is also of interest. Let \( E_\alpha \) with \( \alpha = 1, 2, \ldots, N \) be the eigenvalues of \( H \). Then, expressing Eq. (2) in the diagonal basis, one obtains,

\[
\frac{2}{\pi} \lim_{\eta \to 0} \text{Im}(\mathcal{J}) = -\frac{1}{\pi} \lim_{\eta \to 0} \sum_{\alpha=1}^{N} \text{Im} \left[ \ln \left( [(E - E_\alpha)^2 + \eta^2]^{1/2} \exp \left[ i \arctan \left( \frac{\eta}{E - E_\alpha} \right) \right] \right) \right]
\]

\[
= \frac{1}{\pi} \sum_{\alpha=1}^{N} \lim_{\eta \to 0} \arctan \left( \frac{\eta}{E - E_\alpha} \right).
\]

In the limit \( \eta \to 0 \) the arctangent is either 0 or \( \pi \) depending on the sign of the denominator. Hence, the above number is equal to the number of eigenvalues of \( H \) smaller than \( E \). Similarly,

\[
\frac{2}{\pi} \lim_{\eta \to 0} \frac{\partial \mathcal{J}}{\partial E} = \frac{1}{\pi} \sum_{\alpha=1}^{N} \lim_{\eta \to 0} \frac{\eta}{(E - E_\alpha)^2 + \eta^2}
\]

\[
= \sum_{\alpha=1}^{N} \delta(E - E_\alpha),
\]

so that this derivative is the so-called density of states (DOS). In principle the limit \( \eta \to 0 \) must be taken, but in practice the calculations are done with a finite \( \eta \). As should be clear from Eq. (5), this means that there is a Lorentzian around each energy level instead of a \( \delta \) function. This "level broadening" may be useful to compare with experiment,\textsuperscript{13,14} where for a variety of reasons, such as anharmonicities in phonon problems, levels are never infinitely sharp. Also, the larger the value of \( \eta \), the faster the DOS converges to the infinite-volume-limit result. In
Sec. III we make extensive use of the above relations to compute integrated DOS, DOS, projected DOS, conductances of random networks, etc.

**B. Recursive evaluation of the generating function**

Many of the above results are familiar. However, it has apparently not been generally recognized that it is possible to evaluate the generating function and its derivatives recursively.

We are especially interested in sparse matrices, but the results are easily generalized. Suppose that \((E+i\eta)L-H\)

is such a matrix, with the numbering of the rows and columns (sites in the physical problem) chosen in such a way that it is a block tridiagonal matrix with the following structure,

\[
\begin{bmatrix}
X_1 & Y_{12} & 0 & 0 & \cdots \\
Y_{12} & X_2 & Y_{23} & 0 & \\
0 & Y_{23} & X_3 & Y_{34} & \\
0 & 0 & Y_{34} & X_4 & \\
\vdots & & & & \\
\end{bmatrix}
\]

The dimensions are \(n_1 \times n_1\) for \(X_1, n_1 \times n_2\), for \(Y_{12}, n_2 \times n_2\) for \(X_2\), etc. The generating function may be written, if there are \(L\) diagonal blocks, as

\[
\mathcal{F} = \ln \left[ \int_{-\infty}^{\infty} \prod_{i=1}^{L} \prod_{\alpha=1}^{n_i} du_{i\alpha} \exp \left( -\frac{1}{2} \mathbf{U}^T \mathbf{X}_i \mathbf{U}_i - \mathbf{U}^T \mathbf{Y}_{i,i+1} \mathbf{U}_{i+1} + \mathbf{J}^T \mathbf{U}_i \right) \right].
\]

Performing the integrals over the variables \(u_{11}, u_{12}, u_{13}, \ldots, u_{n_1}\) which correspond to the block \(X_1\) using the same procedures as in Eq. (2), we are left with

\[
\mathcal{F} = \ln \left[ \int_{-\infty}^{\infty} \prod_{i=2}^{L} \prod_{\alpha=1}^{n_i} du_{i\alpha} \right] \left( \frac{2\pi}{n} \right)^{n_i-1} \left( \det(X_1) \right)^{1/2} \exp \left( \frac{1}{2}( \mathbf{U}_2^T \mathbf{Y}_{12} - \mathbf{J}^T \mathbf{X}_{12} - \mathbf{U}^T \mathbf{Y}_{12} \mathbf{U}_2 - \mathbf{J}^T \mathbf{U}_1 \right)
\]

This may be rearranged to look like Eq. (6):

\[
\mathcal{F} = C_2 + \ln \left[ \int_{-\infty}^{\infty} du_{21} \int_{-\infty}^{\infty} du_{22} \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} du_{n_2} \prod_{i=3}^{L} \prod_{\alpha=1}^{n_i} du_{i\alpha} \exp \left( -\frac{1}{2} \mathbf{U}^T \mathbf{Z}_2 \mathbf{U}_2 - \mathbf{U}^T \mathbf{Y}_{23} \mathbf{U}_3 + \mathbf{L}_2^T \mathbf{U}_2 - \frac{1}{2} \mathbf{U}^T \mathbf{X}_1 \mathbf{U}_1 - \mathbf{U}^T \mathbf{Y}_{i,i+1} \mathbf{U}_{i+1} + \mathbf{J}^T \mathbf{U}_i \right) \right],
\]

\[
C_2 = \frac{1}{2} n_1 \ln(2\pi) - \frac{1}{2} \ln(\det(Z_1)) + \frac{1}{2} \mathbf{L}_2^T \mathbf{Z}_2^{-1} \mathbf{L}_1,
\]

where

\[
Z_1 = X_1, \quad L_1 = J_1, \quad Z_2 = X_2 - Y_{12}^T Z_1^{-1} Y_{12}, \quad L_2 = J_2 - Y_{12}^T Z_1^{-1} L_1.
\]

The problem is now the same as the original one but with a smaller number of variables to integrate over. The steps leading from Eq. (6) to Eq. (8) can thus be repeated so that \(\mathcal{F}\) can be evaluated recursively:

\[
Z_{i+1} = X_{i+1} - Y_{i,i+1}^T Z_i^{-1} Y_{i,i+1}, \quad (9)
\]

\[
L_{i+1} = J_{i+1} - Y_{i,i+1}^T L_i, \quad (10)
\]

\[
C_{i+1} = C_i + \frac{1}{2} n_i \ln(2\pi)
\]

\[
- \frac{1}{2} \ln(\det(Z_i)) + \frac{1}{2} \mathbf{L}_i^T \mathbf{Z}_i^{-1} \mathbf{L}_i, \quad (11)
\]

\[
\mathcal{F} = C_{L+1} + . \quad (12)
\]

For one-dimensional problems the size of the unit cell determines the size of the matrices \(X_i, \mathbf{Y}_{i,i+1}\) in a natural manner. For small unit cells, one can directly use Eqs. (9)–(12) (or their generalizations for derivatives of the generating function).

In general, however, it is possible to improve on Eqs. (9)–(12), saving both computation time and the need to do the matrix inversions which appear explicitly in these equations. To this end, we take advantage of the arbitrariness in the division of the original matrix into blocks. One can take for \(X_1\) the element \((E+i\eta)L-H\) \(11\); then \(Y_{12}\) would be the vector \((E+i\eta)L-H\) \(12\), \((E+i\eta)L-H\) \(13\), \ldots, \((E+i\eta)L-H\) \(1m\), where \(1, m\) labels the last nonzero element of the first row. \(X_2\) would then be an \((m-1) \times (m-1)\) matrix whose first element is \((E+i\eta)L-H\) \(22\). Once the integration over \(u_1\) is done, the process can be repeated to integrate over \(u_2\), etc.

Before writing down the recursion relations specialized to this "element by element" elimination, let us consider, for the sake of concreteness, a specific example. Suppose we are studying an electronic tight-binding Hamiltonian on a finite two-dimensional regular lattice. The use of a regular lattice simplifies the notation without much loss of generality because most irregular lattices can easily be
mapped on regular ones with missing sites or bonds. To simplify the discussion even further, we consider a square lattice. If the sites of that lattice are numbered as illustrated in Fig. 1(a), the problem is equivalent to a one-dimensional problem with long-range interactions, the largest range being equal to \( n \), the width of the original system. This is illustrated in Fig. 1(b). Note that equivalent one-dimensional long-range problems can always be found for finite systems on any lattice in arbitrary dimension. Let \( x \) denote a nonzero element, then the matrix \((E + i\eta)\mathbf{L} - \mathbf{H}\) for the problem just discussed has the following structure:

\[
\begin{bmatrix}
X_1 \\
\vdots \\
X_n \\
\end{bmatrix} = \begin{bmatrix}
0 & X_2 \\
\vdots & \ddots & \ddots \\
X_{n-1} & \cdots & 0
\end{bmatrix} Y_{12}
\]

Let us integrate over \( u_1 \). We call this “elimination of the first site.” \( Y_{12} \) is a vector of length \( n \) (equal to the largest interaction range in units of the lattice spacing). We then write the relation \( \mathbf{Z}_2 = \mathbf{X}_2 - \mathbf{Y}_{12} \mathbf{Z}^{-1} \mathbf{Y}_{12} \) element by element, taking advantage of the symmetric nature of the original matrix. (Or, more simply, one can work directly with the equivalent one-dimensional long-range interaction problem.) Let \( z_i \) denote the diagonal \( (i,i) \) elements of \((E + i\eta)\mathbf{L} - \mathbf{H}\) and \( W_{ij} \) the off-diagonal ones \( (i,j) \), with the indices also corresponding to site numbers as in Fig. 1. The result may be written in the form:

\[
z_i' = z_i - (W_{ii}^2 / z_1), \quad \text{with} \ 2 \leq i \leq n+1 ;
\]

\[
W'_{ij} = W_{ij} - (W_{ii} W_{ij} / z_1),
\]

\[
\text{with} \ 2 \leq i \leq n \ \text{and} \ i < j \leq n+1.
\]

Note that Eqs. (13) and (14) could be combined in a single equation by defining \( W'_{ij} = z_i \) and letting indices run over the appropriate range. We refrain from doing this because of the physical interpretation of the \( z_i \) as “site” quantities and of the \( W_{ij} \) as “interactions.” In some sense, then, in Eqs. (13) and (14) we have renormalized the site energies and the various interactions between sites 2 to \( n+1 \) to take into account the elimination of the first site. We can consider this problem with one less site as a new problem; if the labels of all the sites are now shifted down by one unit, the problem becomes completely analogous to the original one. Note in particular that the largest range of interaction has not increased even though all intermediate range interactions may be generated even if they were absent from the original problem. When the total number of sites is \( N \), this process simply has to be repeated \( N \) times to eliminate all the sites. It should now be clear that the recursion formulae, including renormalization of the elements \( l_i \) of the “source” term \( \mathbf{L} \) in Eq. (10), can be written down as follows:

\[
z_i' = z_i + 1 - (W_{i,i+1}^2 / z_1), \quad \text{with} \ 1 \leq i \leq n ;
\]

\[
W'_{ij} = W_{i+1,j+1} - (W_{i,j+1} W_{i+1,j+1} / z_1),
\]

\[
\text{with} \ 1 \leq i < n \ \text{and} \ i < j \leq n ;
\]

\[
l'_i = l_i + 1 - (W_{i,i+1} l_i / z_1), \quad \text{with} \ 1 \leq i \leq n ;
\]

\[
C' = C + \frac{1}{2} \ln(2\pi) - \frac{1}{2} \ln z_1 + \frac{1}{2} l'_i / z_1 .
\]

At the end of the process

\[
\mathcal{F} = C .
\]

Initially \( z_i \) and \( W_{ij} \) are equal, respectively, to \( [(E + i\eta)\mathbf{L} - \mathbf{H}]_{ii} \ (1 \leq i \leq n+1) \) and to \( [(E + i\eta)\mathbf{L} - \mathbf{H}]_{ij} \ (1 \leq i < n \ \text{and} \ i < j \leq n+1) \); then, at each iteration, one only needs to introduce the new quantities \( z_{i+1} \) and \( W_{i,i+1} \ (1 \leq i \leq n) \) which are not yet renormalized and which correspond, with \( k \) the number of iterations performed \( [k=1 \ \text{after one has gone through Eqs. (15) and (18) once}], to elements

\[
[(E + i\eta)\mathbf{L} - \mathbf{H}]_{k,i+1} = 0
\]

and

\[
[(E + i\eta)\mathbf{L} - \mathbf{H}]_{k,i,k+n+1}
\]

of the original matrix. Analogous considerations hold for the quantities \( l_i \) whose initialization, however, depends on the final linear combination of the inverse matrix one is interested in.

This elimination of one site at a time is clearly the best strategy in terms of computation time because one then avoids useless manipulations of zeros. Indeed, if we were instead eliminating one block at a time [Eqs. (9)–(12)], then we would be dealing with the many null elements in the upper right-hand part of \( \mathbf{Y}_{i,i+1} \).
III. A FEW EXPLICIT EXAMPLES

In this section we give explicit examples of the use of the above recursion relations to compute quantities of physical interest. Depending on the quantity of interest, one needs, in general, additional recursion relations for various derivatives of the generating function. These recursion relations can be derived easily from those above using the chain rule. We will give the results derived only from the scalar form of the recursion relations [Eqs. (15)–(19)], but it should be clear that a similar analysis can be done directly on the matrix form [Eqs. (9)–(12)] of the recursion relations. We also restrict ourselves to "strip" geometries such as those illustrated in Fig. 1: In general there will be nonvanishing matrix elements at most $n$ columns away from the diagonal of the corresponding $N \times N$ Hamiltonian matrix, and the total number of degrees of freedom will be $N = nL$. $n$ then corresponds to the range of the interaction in one dimension, or to the width of the strip in a nearest-neighbor two-dimensional problem, or to the number of sites on the surface of the "bar" in three-dimensional nearest-neighbor problems. Note also that on both ends of the long direction, free or fixed boundary conditions are allowed but not periodic or antiperiodic boundary conditions, since in the latter cases the corresponding matrices cannot be written in the form preceding Eq. (6).

A. Densities of states (DOS's)

In many cases of physical interest, it is not necessary to know exactly all eigenvalues of a given problem. Their density in any particular energy interval often suffices. This is the so-called density of states (DOS). For example, we may want to evaluate the DOS of an electron whose Hamiltonian has the following tight-binding form

$$\[ -(K_{12} + K_{1, n+1})/M_1 + (\omega^2 + i\eta), \ K_{12}/(M_1M_2)^{1/2}, 0, \ldots, 0, K_{1,n+1}/(M_1M_{n+1})^{1/2}, 0, \ldots. \]$$

Again if we can compute the number of eigenvalues of $M^{-1/2}K M^{-1/2}$ which are smaller than $\omega^2$, we know the integrated DOS as a function of $\omega^2$.

1. Integrated DOS

We have already shown that the number of eigenvalues of $H(M^{-1/2}K M^{-1/2})$ smaller than $E(\omega^2)$ is given by [Eq. (4)]

$$\frac{2}{\pi} \lim_{\eta \to 0} \text{Im}(\mathcal{F})(l_i = 0).$$

Hence, iterating with a particular value of $E(\omega^2)$ the recursion relations [Eqs. (15) and (16)]

$$z'_i = z_{i+1} - (W_{i+1}^2/z_1), \quad \text{with} \ 1 \leq i \leq n;$$

$$W'_i = W_{i+1} + 1 - (W_{i+1}^2/z_1),$$

with $1 \leq i < n$ and $i < j \leq n$; the integrated DOS for that particular value of $E(\omega^2)$ can be obtained at the end of the recursive process by evaluating $C/N$ (where $N$ is the total number of degrees of freedom). $z_i$ and $W_{ij}$ are initialized as described below Eq. (19).

In practice, real numbers can be used instead of complex numbers because it can be shown that the relation (26) is equivalent, in the limit $\eta \to 0$, to counting the number of times $z_1$ takes a given sign. In other words, we have recovered the well-known negative-eigenvalue theorem. The details of the proof can be found in Appendix A. Note, however, that when using real numbers it is important to choose a value of $E(\omega^2)$ which is not an eigenvalue of $H(M^{-1/2}K M^{-1/2})$; otherwise the recursion relations become singular.

From the integrated DOS, one can obtain the DOS by numerical differentiation. As we now proceed to show,
it is also possible and it might even be desirable to com-
pute directly the DOS.

2. DOS

The DOS (Ref. 8) of $H$ can be obtained from Eq. (5)

$$
\lim_{\eta \to 0} \frac{\partial F}{\partial E} = \frac{1}{\pi} \sum_{\alpha} \lim_{\eta \to 0} \eta \delta(E - E_{\alpha}) = \sum_{\alpha} \delta(E - E_{\alpha}).
$$

This derivative can be evaluated directly by applying the chain rule to the recursion relations. Taking the derivative of Eqs. (18) and (19), it is clear that we need $\partial E_{\alpha}/\partial E$. By differentiating Eq. (15) we see that $\partial W_{ij}/\partial E$ is also needed. Defining $y_j = \partial E_{\alpha}/\partial E$ and $v_{ij} = \partial W_{ij}/\partial E$, the complete formulas become Eqs. (24), (25), and the following three equations:

$$
\begin{align*}
y_{j+1} &= y_{j+1} - 2W_{l,i+1}v_{l,i+1}/z_l + W_{l,i+1}v_{l,i+1}/z_l, \\
v_{i,j+1} &= v_{i,j+1} - (W_{l,i+1}v_{l,i+1} + W_{l,i+1}v_{l,i+1})/z_l + W_{l,i+1}v_{l,i+1}/z_l,
\end{align*}
$$

with $1 \leq i \leq n$ and $1 \leq j \leq n$.

$$
C' = C - \frac{1}{\pi} \text{Im}(y_{1}/z_1).
$$

Initially, $y_j = \partial E_{\alpha}/\partial E = 1$, $v_{ij} = 0$. The normalized DOS, at a particular value of energy $E$, is given by $C/N$, where $N$ is as usual the number of degrees of freedom. Equations (27)–(29) remain valid if $(\omega^2 + i\eta)I - M^{-1/2}K M^{-1/2}$ is substituted for $[(E + i\eta)I - H]$ and $\partial /\partial \omega$ for $\partial /\partial E$.

Since we now have four times as many recursion relations as before, and because we must work with complex numbers, the DOS at one value of the energy ($E$ or $\omega^2$) can become too large to compute on the integrated DOS by a factor of order 10. The DOS must be obtained by numerical differentiation of the integrated DOS but the derivative of that function is in reality a set of $\delta$ functions so that appropriate coarse graining (corresponding to finite $\eta$) or histogram displays must then be used.

B. Projected DOS

It is sometimes necessary to weigh each $\delta$ function in the DOS by the square of some transition-matrix elements. This type of quantity, which we call a projected DOS, arises, for example, in scattering problems such as Raman, infrared, or neutron scattering.

To illustrate $4,13,14$ with a very simple-minded argument how projected DOS arise, consider a square lattice of damped harmonic oscillators with isotropic force constants $20$ of the type already discussed. Suppose that each atom has a unit electric charge whose sign alternates in a chessboard configuration. If we apply a uniform electric field whose amplitude varies sinusoidally with time, then the power absorbed by the lattice is proportional to the projected DOS. The demonstration follows.

The equation of motion in matrix form is

$$
(K - M\omega^2)U = F,
$$

where the symbols have the same meanings as in Eq. (23). Normalizing to unity the force exerted by the electric field on each atom, the force vector in Eq. (30) becomes,

$$
F^T = \left\{ (-1,1,-1,1,\ldots)_{n}, (-1,1,-1,1,\ldots)_{n}, \ldots \right\},
$$

where $n$ is the width of the lattice, and there are $n$ elements in each subgroup. The power $P$ absorbed by the system while it is driven by the external force field is proportional to $\text{Re}(i\omega U^T F^*)$. Using Eq. (30), and the fact that $F$ is real, the power is proportional to

$$
P \approx \omega \text{Im}[(K - M(\omega^2 + i\eta))^{-1}F].
$$

Let $\rho(\omega^2)$ be the projected DOS,

$$
\rho(\omega^2) \approx \text{Im}[(K - M(\omega^2 + i\eta))^{-1}F] / N.
$$

To evaluate $F^T[K - M(\omega^2 + i\eta)]^{-1}F$ we use Eq. (3),

$$
\text{Im} \left[ \frac{\partial^2 F}{\partial x^2} \right] = -\text{Im} \left[ F^T[K - M(\omega^2 + i\eta)]^{-1}F \right].
$$

While the derivation leading to Eq. (35) is oversimplified, more rigorous approaches to scattering problems in general lead to formulas for the spectra which have the same functional form but with $F$ replaced by a vector of transition matrix elements $4,13,21$

To compute $\partial^2 F /\partial x^2$ recursively, we use again the chain rule. Applying $\partial^2 /\partial x^2$ to Eq. (18), one sees that $\partial l_i /\partial x$ is needed (note that $\partial^2 l_i /\partial x^2 = 0$). Let $y_j = \partial l_i /\partial x$, then the full recursion relations are Eqs. (24), (25), and

$$
y_{j+1} = y_{j+1} - (W_{l,i+1}v_{l,i+1} + W_{l,i+1}v_{l,i+1})/z_l + W_{l,i+1}v_{l,i+1}/z_l,
$$

$$
C' = C + \text{Im}(y_{1}/z_1).
$$

The recursion relations are initialized this time with $J = xF$ (hence, $y_j = F_j$) and with $M(\omega^2 + i\eta) - K$ instead of $[(E + i\eta)I - H]$. When all sites are eliminated, the projected DOS is equal to $C/N$.

C. Conductance of a resistor network

The present method is akin to transfer matrix methods which are widely used $4,5$ in the context of calculations of conductivities of random resistor networks and related problems $11,12$. As an example then, we show how to compute the conductance of a two-dimensional square lattice of length $L$ and width $W$. Lattice bonds are occupied by a unit resistance with probability $p$ or unoccupied with probability $1 - p$. The boundary conditions, illustrated in Fig. 2, are that the top end of each of the uppermost resistors is held at zero voltage (no site to eliminate there) while the bottom side is connected by a bus bar of infinite conductivity. A current of magnitude $J = L$ is fed in the bottom bus bar. The conductance of the system follows from the potential on that bar: Since the conductivity of
DENSITIES

FIG. 2. Strip geometry and site labeling for the conductivity problem. The bonds drawn with a thick line have as large a conductivity as possible (in practice, for IBM double precision calculations, about \(10^7\) when the conductivity of the other bonds is 1). Because the conductivity of the thick bonds is not strictly infinite, the external current leads are placed symmetrically. The top sites are connected to ground by a unit conductance.

the system is \(n/L\) times the conductance, which in turn equals \(I/(\sum_j V_j/L)\), where the prime sum is over the potentials \(V_j\) at the sites \(j\) that belong to the bus bar, the conductivity \(\sigma\) is

\[
\sigma = \frac{nL}{\sum_j V_j}.
\]

Note that we took the precaution to define the potential of the bus bar as \(\sum_j V_j/L\) because the conductivity of the last row of resistors in practice is not infinity; hence, the bus bar is not strictly an equipotential. We also minimize the artificial effects of this "machine infinity" by feeding a unit current to every node of the bus bar instead of a current \(L\) at one end only (see Fig. 2).

Using Ohm's law and Kirchhoff's laws, the exterior current \(I\) leaving (or entering depending on sign convention) the system at site \(j\) is equal to

\[
i_j = g_{j,l} V_j - 1 + g_{j,l} V_j - 2 + \ldots + g_{j,l} V_j - n + g_{j,l} V_j + 1 + \ldots + g_{j,l} V_j + n
\]

(39)

where \(g_{jk}\) is the conductance between sites \(j\) and \(k\) (\(g_{jk} = g_{kj}\)). This set of equations can be expressed in matrix notation as

\[
G V = I,
\]

(40)

where, with the labels of Fig. 2, \(V^T = (V_1, V_2, \ldots, V_{nL})\), \(I^T = (i_1, i_2, \ldots, i_{nL})\), and \(G\) is a \(nL \times nL\) matrix whose first row is equal to

\[
(\ldots, g_{1} + g_{1,2} + g_{1,3} + \ldots, g_{1,n} + 0, \ldots, 0, g_{1,n} + 1, 0, \ldots)
\]

(41)

where \(g_1\) is the conductance of the bond linking site 1 to the ground.

Since the input current is equal to \(L\), we set \(i_1 = 1\), \(i_{2n} = 1\), \(\ldots\), \(i_{n-1} = 1\). All other \(i_j\) are equal to zero. We can thus write

\[
\sum_j V_j = I^T V = I^T G^{-1} I,
\]

(42)

and the conductivity is obtained from the following formula:

\[
\sigma = \frac{nL}{I^T G^{-1} I},
\]

(43)

whose denominator can be computed like in Eq. (35) with the substitution \([M(\omega^2 + i\eta) - K] \rightarrow G\) and \(F \rightarrow I\). The appropriate set of recursion relations is given by Eqs. (24), (25), (36), and the following equation [instead of Eq. (37)]

\[
C^* = C + (y^2/z_1^2).
\]

(44)

Initially, \(z_1 = G_{11}\) \((1 \leq i \leq n+1)\), \(W_{ii} = G_{ii}\) \((1 \leq i \leq n)\), \((i < j \leq n + 1)\), and \(y_1 = i_1 = 0\), \(y_2 = i_2 = 0\), \(y_n = i_n = 1\). At the end of the iterations, the conductivity is \(\sigma = nL/C\).

Obviously this time only real numbers are used in the calculation but if capacitors or inductors are added in the circuit, it suffices to work with complex numbers to generalize the above results.

It is important to note that, when our method is applied to percolation problems, it may happen that a site is completely disconnected. In this case there is no degree of freedom associated with the site so one simply "jumps" over it by decreasing the various indices by unity without applying the recursion formulas. In the language of the generating function, we must not perform the integral over a noninteracting variable: It leads to divisions by zero which simply mean that the potential at that site is arbitrary since it is completely disconnected from the rest of the network.

One advantage of the method is that we are not limited to the computation of the conductance. We can, if necessary, compute the voltages at each site. This is important because in certain cases, such as for the calculation of resistance noise, one needs the current in each individual resistor. To obtain the voltage \(V_k\) at a particular node, one defines \(J = J_1 + J_2\) with \(J_1 = x_1 U\) and \(J_2 = x_2 I\) with \(I\) as already defined and with \(u_i = 0\) for all \(i\) except \(i = k\).

Since \(V_k = U^T V = U^T G^{-1} I = U^T G^{-1} U\), we have

\[
V_k = \frac{\alpha^2}{\alpha x_1} \frac{\partial}{\partial x_1} \frac{\partial}{\partial x_2}
\]

(45a)

with

\[
\mathcal{F} = \ln \left[ \frac{(2\pi)^n}{(\det G)^{1/2}} \exp \left\{ \frac{1}{2} (Ux_1 + x_2)^T G^{-1} (Ux_1 + x_2) \right\} \right].
\]

(45b)

Results for resistance noise in percolating networks have already appeared.12 Explicit recursion formulas can be found in Ref. 22.

Note that elastic moduli for a two-dimensional central force network have also been calculated with the above method.8 One then associates two degrees of freedom (in two dimensions) with each mass (site). More complicated elastic models can also be studied.

### D. Miscellaneous

It is natural to ask what kind of recursion relations are obtained if we want to compute all elements of the inverse
of a general symmetric matrix using our method. It is not difficult to show (Appendix B) that we obtain the standard Gaussian elimination technique \( \text{15} \) specialized to symmetric matrices. (We went from Gaussian integration to Gaussian elimination.) In a sense then, the method presented here is a generalization of the negative-eigenvalue theorem (since we can also obtain projected DOS, etc.) and a systematic way to specialize Gaussian elimination to the band-diagonal matrices which generally arise in problems of physical interest.

Finally, we may ask about the calculation of quantum transport properties. Recalling that \( \left[ (E+i\eta)I-H \right]^{-1} \) is the Green's function for a given realization of the disorder, even quantum transport properties can be obtained from this function if appropriate products of various matrix elements are taken before averaging over disorder. One can proceed as in Ref. 23, for example. (We describe in the following section how to obtain the necessary Green's functions.) Alternatively, a generating function for the Kubo formula can be written down \( \text{24} \) and recursion formulas can be obtained from it.

IV. ADVANTAGES, DISADVANTAGES, AND COMPARISONS WITH OTHER METHODS

The number of operations necessary to perform the various types of calculations described in the previous section is given in Table I. In the following, we outline the comparative advantages and disadvantages of various numerical techniques, starting with the methods which are most similar to those of this paper.

A. Green's functions approaches and Gaussian elimination

Tight-binding electronic models in the strip geometry have been studied, for example, in Ref. 23. Equation (5) of this paper is equivalent to Eq. (9) of the present paper.

In Ref. 23 Eq. (6) also allows one to compute a specific matrix element of the Green's functions. This approach, which was also used in Ref. 25, is also known \( \text{26} \) as "double-sided Gaussian elimination." It can be obtained from the generating function point of view by using appropriate source terms, as described in Sec. III C and by integrating out variables starting from both the first and last site.

B. Transfer-matrix method

The Gaussian elimination algorithm obtained from the generating-function approach shares many of the advantages and disadvantages of the transfer-matrix method \( \text{7} \) that Derrida and Vannimenus \( \text{6} \) developed for the conductivity problem. This method is advantageous mostly when long, quasi-one-dimensional strips are appropriate. This may occur when one simulates properties of a material which actually has such a structure or when one wishes to have self-averaging samples in percolation problems, i.e., when one wants to avoid averaging over various realizations of the disorder. \( \text{27} \) It also seems appropriate to work in such a geometry when one is interested in the DOS projected on a plane wave (Sec. III B). Then it is natural to take the long direction along the direction of propagation of the plane wave.

While the algorithm of Derrida and Vannimenus \( \text{6} \) differs from Gaussian elimination, the leading polynomial dependence \( (n^3L/2) \) on size of the number of multiplications or additions in the scalar program code \( \text{28} \) is identical to that of the method of Sec. III C; in other words, they should take the same amount of time for large system sizes. Both methods share the advantage that in a random medium problem, the lattice is generated as the calculation goes on, and the amount of storage necessary for the calculations depends only on the width of the transverse direction, and not on the length of the system. This

<table>
<thead>
<tr>
<th>Calculated quantity</th>
<th>Number of additions and subtractions</th>
<th>Number of multiplications and divisions</th>
</tr>
</thead>
<tbody>
<tr>
<td>Integrated DOS (Sec. III A 1)</td>
<td>( \frac{n^3}{2} + \frac{n^2}{2} + n ) ( L )</td>
<td>( \frac{n^3}{2} + \frac{3n^2}{2} ) ( L )</td>
</tr>
<tr>
<td>DOS (Sec. III A 2)</td>
<td>( 2n^3 + 2n^2 + n ) ( L )</td>
<td>( 2n^3 + 2n^2 + n ) ( L )</td>
</tr>
<tr>
<td>(Partial) projected DOS (Sec. III B)</td>
<td>( \frac{n^3}{2} + \frac{3n^2}{2} + n ) ( L )</td>
<td>( \frac{n^3}{2} + \frac{5n^2}{2} + 2n ) ( L )</td>
</tr>
<tr>
<td>Conductivity (Sec. III C)</td>
<td>( \frac{n^3}{2} + \frac{3n^2}{2} + n ) ( L )</td>
<td>( \frac{n^3}{2} + \frac{5n^2}{2} + 2n ) ( L )</td>
</tr>
</tbody>
</table>
translates into smaller memory requirements. Also, when either method is applied to random medium calculations, unoccupied sites can be simply “skipped” as they arise. On the other hand, the algorithm of Sec. III C is a little bit more complicated to program and is probably not as efficient in “skipping” sites as that of Refs. 6 and 7. The latter algorithm also generates less numerical errors in the way it handles infinite conductivity bus bars in the percolation conductivity problem. Nevertheless, the algorithm of Sec. III C has the advantage that it is applicable to any lattice, while the Derrida-Vannimenus algorithm does not appear generalizable, for example, to the central force problem on a triangular lattice.

C. Iterative methods
(Haydock-Lanczos, conjugate gradient)

The Haydock-Lanczos\textsuperscript{29} and conjugate gradient\textsuperscript{30–32} techniques are two popular examples of iterative methods for matrix inversion. In such “iterative” methods, the calculation may be stopped at any stage to obtain an approximate solution to the matrix inversion problem. For finite matrices, both methods obtain the exact solution after a finite number of iterations, but for general matrices, the number of operations required is larger than either Gaussian elimination techniques. The great advantage of such methods lie in the fact that for sparse matrices the number of operations\textsuperscript{29} is in general smaller than Gaussian elimination, and, furthermore, it is in practice rarely necessary to iterate the algorithms to their theoretical maximum to obtain an acceptable approximation to the solution.\textsuperscript{29–32} The conjugate gradient technique solves for the vector $x$ in matrix equations of the type $Ax = b$, while the Haydock-Lanczos method yields $F^T A^{-1} F$, where $F$ is a vector that one can choose. Clearly, then, both methods are suited for either projected densities of states or conductivity calculations of the type described above.\textsuperscript{24} Total densities of states are obtained by a somewhat more cumbersome but workable procedure. For total DOS, one must compute the trace of $A^{-1}$. In the Haydock-Lanczos technique this is achieved by adding up the values of $F^T A^{-1} F$ for several random\textsuperscript{35} starting vectors $F$. A similar approach could be applied to the conjugate gradient technique by choosing $b = F$ random.

For “strip” or “bar” geometries, the approach of Sec. III has smaller memory requirements and even does better on time when compared with the theoretical maximum number of iterations of either the Haydock-Lanczos or conjugate-gradient techniques. Nevertheless, whenever the long strip geometries $(L \rightarrow \infty)$ can be avoided,\textsuperscript{37} the iterative techniques will always be more advantageous as far as time is concerned because a few iterations usually suffice to obtain “machine precision.”\textsuperscript{36} The advantage of iterative techniques for short-range interaction problems in hypercubic geometries in higher dimensions is even more pronounced since, in these cases, even the theoretical maximum number of operations\textsuperscript{35} is smaller than that of Sec. III.

V. CONCLUSION

To summarize, we have shown that a recursive evaluation of the generating function leads to the familiar algorithm based on the “negative-eigenvalue theorem.” Other special problems, such as partial (or projected) DOS, conductivities, or even matrix inversion through Gaussian elimination, can be done by a recursive evaluation of the derivatives of the generating function and are thus seen as closely related to the popular negative-eigenvalue theorem for integrated densities of states. The method is simple and directly leads to the most efficient Gaussian-elimination-type approach for either full symmetric matrices or for band-diagonal symmetric matrices (without pivoting\textsuperscript{35,32,37}). While the algorithms are not for the most part new, this method also shows relations between different approaches and allows the simplest derivation of the negative-eigenvalue theorem that we know of.

The method is especially suited for one-dimensional problems or for strip (in two dimensions) or bar (in three dimensions) geometries. Its leading polynomial dependence on time in this case is comparable to that of transfer-matrix methods,\textsuperscript{6,7} and it has the same advantages of being storage concerning the lattice can be generated by section as the calculation proceeds. To calculate the conductivity in two dimensions, for “square geometries,” iterative methods (Haydock-Lanczos,\textsuperscript{29} conjugate gradient\textsuperscript{30–32}), when iterated to their theoretical maximum for exact matrix inversion, have the same polynomial dependence on system size as the methods of Sec. III but with a larger prefactor. In practice, however, they may converge before this theoretical maximum and hence be more efficient (see Ref. 36 for the case of the conductivity). In higher dimensions, iterative methods are always more efficient for nearest-neighbor problems in hypercubic geometries. To compute the full current distribution, they are also more efficient even in two-dimensional square geometries.

ACKNOWLEDGMENTS

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APPENDIX A: PROOF OF THE NEGATIVE-EIGENVALUE THEOREM

We want to prove that taking the limit

$$\lim_{\eta \to 0} \frac{1}{\pi} \text{Im}(\ln z)$$

in Eq. (26) is equivalent to checking the sign of $z_1$, evaluated with $\eta = 0$.

Let us suppose that this $z_1$ is associated with site number $l$. The $l-1$ first sites have thus been eliminated. The
The best way to eliminate those sites, in terms of computing time, is to eliminate them site by site, but we could as well eliminate them altogether with the help of Eq. (9). This procedure gives the same value for the elements of the matrix which is left and eases the demonstration. Let us then take \( X_1 \) to be an \((l-1)\times(l-1)\) matrix and \( Y_{12} \) to be an \((l-1)\times m\) matrix with \( m \) large enough so that all matrix elements vanish if they are in the first \( l-1 \) rows of \((E+i\eta)I-H\) and if their column index is larger than \( l-1+m \). \( X_2 \) is then an \( m\times m \) matrix.

The elimination of the \((l-1)\) first sites therefore gives,

\[
Z_2=X_2-\frac{X_1}{E} X_1^{-1} Y_{12} .
\] (A2)

Clearly, \( z_1 = (Z_2)_{11} \). To study this element, let us recall that we can write \( X_1 \) in the form \((E+i\eta)I-H\). Let \( T \) be the transformation which diagonalizes \( H \)

\[
TX_1T^T=(E+i\eta)I-D.
\] (A3)

Then, Eq. (A2) may be rewritten,

\[
Z_2=X_2-Y_1 T^T [(E+i\eta)I-D]^{-1} T Y_{12} .
\] (A4)

Defining \( B=TX_{12} \) (which is exclusively composed of real numbers) then,

\[
(Z_2)_{11}=E+i\eta-(H_2)_{11}+\sum_k \frac{B_{tk} B_{kj}}{E-d_k+i\eta} ,
\]

\[
\text{Im}(z_1)=\eta \left[ 1 + \sum_k \frac{(B_k)^2}{(E-d_k+i\eta)^2} \right] = \eta \theta, \quad \text{with } \theta > 0 .
\]

Thus,

\[
\lim_{\eta \to 0} \text{Im} (\ln z_1) = \lim_{\eta \to 0} \pi \left[ \frac{\eta \theta}{(-\text{Re} z_1)} \right] = \begin{cases} 1 & \text{if } \text{Re} z_1 > 0 , \\ 0 & \text{if } \text{Re} z_1 < 0 . \end{cases}
\]

The proof can be repeated for all \( z_1 \). Since it has already been proven that the number of eigenvalues of \( H \) smaller than \( E \) is given by the sum over all \( z_1 \)'s of 

\[
-\pi \lim_{\eta \to 0} \pi \text{Im} (\ln z_1) \]

[Eq. (9)] and [Eq. (26)], then it is also given by the number of positive \( z_1 \)'s computed with \( \eta = 0 \) [since \( \lim_{\eta \to 0} \text{Re} z_1(\eta) = z_1(\eta = 0) \)].

Note that if we start from \( H-(E+i\eta)I \) instead of \((E+i\eta)I-H\), then to obtain the number of eigenvalues of \( H \) smaller than \( E \) we have to count the number of negative \( z_1 \)'s \( (\eta = 0) \) instead of the positive ones. The negative-eigenvalue theorem (NET) is usually presented with this choice of convention.

To summarize, the use of Eqs. (24) and (25) with the real matrix \( H-E \) together with the counting of the negative \( z_1 \)'s allows one to compute the number of eigenvalues of \( H \) smaller than \( E \). This is exactly the NET (Refs. 2 and 3) (specialized to site elimination, which is the way to use it in practice).

**APPENDIX B: EQUIVALENCE WITH THE GAUSSIAN ELIMINATION TECHNIQUE**

Let \( A \) be a complex nonsingular \( N \times N \) symmetric matrix. If we let

\[
\mathcal{F}=\ln \left[ \int_{-\infty}^{\infty} \prod_{i=1}^{N} du_i \exp\left( -\frac{1}{2} U^T A U + J^T U \right) \right],
\] (B1)

then, as can be seen from Eq. (2),

\[
(A^{-1})_{ij} = \frac{\partial^2 \mathcal{F}}{\partial J_i \partial J_j} .
\] (B2)

Let us write Eqs. (15)–(19) in a new notation. This time, diagonal and off-diagonal elements are not denoted by a different letter, so \( z \) and \( W \) become \( a \), elements of the matrix \( A \). Furthermore, we do not decrease all indices by 1 at each recursive step. Instead, we introduce a new index \( k \) that increases by 1 at each iteration. The generating function can then be obtained from,

\[
a^{(k)}_{ij} = a_{ij} - \frac{a^{(k-1)}_{ii} a^{(k-1)}_{jj}}{a^{(k-1)}_{kk}} , \quad \text{with } 1 \leq k < N, \ k < i \leq N, \ \text{and } i \leq j \leq N ;
\] (B3)

\[
l^{(k)}_{ij} = l^{(k-1)}_{ij} - \frac{a^{(k-1)}_{ii} l^{(k-1)}_{ij}}{a^{(k-1)}_{kk}} , \quad \text{with } 1 \leq k < N \ \text{and } k < i \leq N ;
\] (B4)

\[
\mathcal{F} = \frac{N}{2} \ln(2\pi) + \sum_{k=1}^{N} \left[ -\frac{1}{2} \ln a^{(k)}_{kk} + \frac{1}{2} \frac{l^{(k-1)}_{kk}^2}{a^{(k-1)}_{kk}} \right] .
\] (B5)

Note that \( k \) takes the value 1, then \( i \) takes its first permitted value 2, then \( j \) runs in its allowed range. In other words, the outermost loop index is \( k \), and the innermost one is \( j \). Initially, \( a^{(0)}_{ij} = a_{ij} \) and \( l^{(0)}_{ij} = J_i \). Thus, since by Eq. (B4) \( l^{(k)}_{ij} \) remains linear in \( J_j \), we have,

\[
\frac{\partial^2 \mathcal{F}}{\partial J_j \partial J_j} = \sum_{k=1}^{N} \left[ \frac{\partial l^{(k-1)}_{ij}}{\partial J_j} \right] \frac{\partial l^{(k-1)}_{ij}}{\partial J_i} \left[ \frac{1}{a^{(k-1)}_{kk}} \right] .
\] (B6)

Applying \( \partial / \partial J_j \) to \( l^{(k)}_{ij} \), we find recursion relations for \( v^{(k)}_{ij} = \partial l^{(k)}_{ij} / \partial J_j \) so that the inverse matrix can be calculated from

\[
\frac{\partial^2 \mathcal{F}}{\partial J_j \partial J_j} = \frac{v^{(k-1)}_{ij} a^{(k)}_{ij}}{a^{(k-1)}_{kk}} , \quad \text{with } 1 \leq k < N, \ k < i \leq N, \ \text{and } i \leq j \leq N ;
\] (B7)
\begin{align}
\psi^{(k)}_{ij} &= \psi^{(k-1)}_{ij} - \frac{a^{(k-1)}_{ij}}{a^{(k-1)}_{kk}} \psi^{(k-1)}_{kj}, \quad \text{with } 1 \leq k < N, k < i \leq N, \text{ and } 1 \leq j < i; \\
\psi^{(k-1)}_{ij} &= \sum_{k=1}^{N} \psi^{(k-1)}_{ki} \psi^{(k-1)}_{kj} a^{(k-1)}_{kk}, \quad \psi^{(k-1)}_{ij} = 0 \quad \text{for } j > k.
\end{align}

Initially, \(\psi^{(0)}_{ij} = \partial l^{(0)}_{ij}/\partial J_f = \delta_{ij}\). The above algorithm is equivalent to Gaussian elimination for symmetric matrices. This can be recognized by going mechanically through the operations. In particular, the denominator \(a^{(k-1)}_{kk}\) is the so-called "pivot."

More formally though, we recognize first that the complete set of recursions in Eq. (B7) defines an upper triangular matrix \(U\) through a series of operations which can be represented formally by an operator \(Q\):

\[ Q A = U. \]  \hfill (B10)

The set of operations \(Q\) leading to \(U\) can in turn be represented in matrix form by applying these same operations to the identity matrix \(\psi^{(0)}_{ij} = \delta_{ij}\),

\[ Q I = L^{-1}. \]  \hfill (B11)

We have denoted the lower triangular matrix on the right-hand side as \(L^{-1}\). (The inverse of a lower triangular matrix is lower triangular.) The matrix element \(m, i\) of \(L^{-1}\) is \(\psi_{mi}^{(N-1)}\) for \(i < m\) [which in turn, given the index inequalities of Eqs. (B8), is equal to \(v_{mi}^{(m-1)}\)], and is equal to 1 for \(m = i\). Hence, Eq. (B9) states that

\[ A^{-1} = (L^{-1})^T D^{-1} L^{-1}. \]  \hfill (B12)

Inverting, we obtain,

\[ A = L D L^T \]  \hfill (B13)

where, noting the indexing in Eq. (B7), we see that the diagonal matrix is precisely the diagonal of \(U\) in Eq. (B10). Such identities are used [e.g., Eq. (2.32), Ref. 15] in Gaussian elimination to simplify the calculations. Note that our procedure has lead directly to the most efficient algorithm: The leading term in the number of operations to perform scales as \(N^3/6\) for both multiplications and additions.\(^{15,16}\) To leading order then, the number of operations is the same as in the Cholesky factorization method.\(^{15,30,32}\)

\(^{1}\)Present address.

\(^{2}\)Permanent address.

\(^{3}\)For a review, see P. Dean, Rev. Mod. Phys. 44, 127 (1972).


\(^{16}\)Recall that the determinant in Eq. (2) equals the product of the eigenvalues of \((E + i \gamma H)\).

\(^{17}\)See, among others, Refs. 8 and 18.


\(^{20}\)Such interactions are not rotationally invariant and should be handled with care when applied to real systems. See P. N. Keating, Phys. Rev. 145, 637 (1966).


\(^{27}\)To date, there is no significant difference between percolation exponents obtained by averaging square samples over disorder or by working in strip geometries.

\(^{28}\)The version of the program in Ref. 7 has twice as many operations as necessary in a scalar code because it is written in a form which is automatically vectorizable by supercomputer compilers.


\(^{30}\)W. H. Press, B. P. Flannery, S. A. Teukolsky, and W. T. Vetterling, Numerical Recipes (Cambridge University Press,
London, 1986). See also D. M. Wood and A. Zunger, J.
Phys. A 18, 1343 (1985) for a summary of other iterative tech-
niques.

31 M. R. Hestenes, Conjugate direction methods in optimization
(Springer-Verlag, New York, 1980).

32 P. G. Ciarlet, Introduction à l'analyse numérique matricielle et
da l'optimization (Masson, Paris, 1982).

33 For $N$ sites, each with $z$ nearest neighbors, in arbitrary dimen-
sion, the number of multiplications for both the Lanczos and
conjugate-gradient techniques scales as $Nl(z+4)$, where $l$ is
the number of iterations. $l$ is at most equal to $N$. ($l$ may
exceed $N$ in problems where numerical errors accumulate. See
Ref. 32, p. 200.)

34 For conductivity calculations with the Haydock-Lanczos ap-
proach, it is preferable to inject or extract the current on only
one site of the bus bar in Fig. 2 instead of uniformly at each
site of the bus bar, because in the uniform case this avoids
unwanted degeneracies.

35 J. Hafner, Phys. Rev. B 27, 678 (1983), contains an example of
such an approach.

36 Ghassan George Batrouni, Alex Hansen, and Mark Nelkin,


38 J. R. Bunch, thesis, University of California Berkeley, Report