Computing the Kubo formula for large systems

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(Received 20 February 1998)

A computational method, in which a system is mapped to the time-dependent Schrödinger equation driven by a periodic external force, is formulated for computing linear response functions of quantum systems. This method, which scales linearly with the system size N, includes computing the Kubo-Greenwood formula for the dynamic conductivities of systems described by large-scale Hamiltonian matrices. In addition, a scaling approach, derived from this algorithm, is presented to determine the exponent of the conductivity $\sigma(\omega) \propto \omega^{\delta}$ near the metal-insulator quantum transition with high speed and accuracy. [S1063-651X(98)10709-2]

PACS number(s): 02.70.−c, 71.10.Fd, 85.30.Vw, 72.15.−v

I. INTRODUCTION

Numerical approaches for large-scale systems not accessible by analytic methods have become very useful in recent years as the performance of vector and parallel supercomputers has improved. The calculations of linear response functions are especially important to gain insight into the dynamic properties of large-scale systems. Calculations of linear response functions for quantum systems described by $N \times N$ Hamiltonian matrices normally require the evaluation of all eigenvalues and corresponding eigenvectors. As the sizes of matrices become large, standard diagonalization routines require a large amount of the CPU time proportional to $O(N^3)$ as well as memory space proportional to $O(N^2)$. They remain limited to systems of modest size because of the high computational cost.

So far, many efficient algorithms suitable for the calculation of linear response functions, such as the Kubo-Greenwood formula for the ac conductivity, have been developed to overcome these difficulties. These include methods based on the continued fraction technique [1], the recursion method [2], the full-diagonalization technique using the Lanczos method [3], the Chebyshev polynomial expansion [4], the conjugated gradient method [5], and the method for direct integration of the time-dependent Schrödinger equation [6]. These are powerful for computing linear response functions of large systems and have been applied to various problems.

Recently, a method often called the forced oscillator method (FOM), addressing classical systems, has been developed to efficiently compute spectral densities of states, eigenvalues, and their eigenvectors of systems described by very large matrices [7,8]. The method is based on the principle that a linear mechanical system, when driven by a periodic external force of frequency Ω, will respond with large amplitude in those eigenmodes close to this frequency. The characteristics of the method are its simplicity, speed, and memory efficiency. The advantages compared to existing methods are that (i) it requires memory space of the order of N for sparse matrices, (ii) it is possible to compute the spectral density of states within an arbitrary range of eigenvalues and with a given resolution, (iii) one can calculate quite accurately the selected eigenvalue and its eigenvector and judge the accuracy, and (iv) the CPU time is linearly proportional to the system size N for calculating the density of states (DOS) and to N^2 for extracting eigenvalues and their eigenvectors. The particular advantages of the FOM lie in its being easily vectorized and parallelized for implementation in an array-processing modern supercomputer. This is due to the fact that the time-consuming part in computations is to solve equations of motion and the program is easily optimized. It is possible to treat matrices by this method having a degree $N \approx 10^7$ or more by using supercomputers with 1-Gbyte memory space [9].

The algorithm has been extended to calculate the response functions [10] and successfully applied to the analysis of $S(q,\omega)$ or the Raman scattering intensity $I(\omega)$ of large-scale *classical* systems [11–13]. In this paper we develop the algorithm to calculate the linear response functions of *quantum* systems described by large-scale Hamiltonian matrices. The method is broadly applicable and may be of interest in a variety of physical systems.

The outline of this paper is as follows. Section II describes the mapping of quantum systems to first-order differential equations driven by a periodic external force. The corresponding relationship is given between the imaginary part of the generalized susceptibility and the ''resonance'' function gained by a periodic external force with the frequency Ω. In Sec. III we show that the Kubo-Greenwood formula for the dynamic (ac) conductivity is related to the resonance function introduced in Sec. II. It will be emphasized that the method is valid for computing not only the longitudinal conductivity but also the transverse one. Section IV demonstrates the efficiency of the method by comparing the calculated results with the analytic solution for the system described by large-scale Hamiltonian matrices in addition to the calculations of ac conductivities of the three-dimensional (3D) Anderson model close to the metal-insulator quantum transition. Section V presents the finite-time scaling approach, derived from this method, to determine the exponent of the ac conductivity $\sigma(\omega) \propto \omega^{\delta}$ at the metal-insulator transition. This approach is especially powerful to obtain the precise value of the exponent δ with high speed and accuracy. A summary and discussion are given in Sec. VI.

II. LINEAR RESPONSE FUNCTION AND RESONANCE FUNCTION

Consider a quantum system described by a set of matrix elements $\{K_{ij}\}$, whose general Hamiltonian is given by

$$\hat{H}=\sum_{i,j} K_{ij}|i\rangle\langle j| \quad (i,j=1,2,\ldots,N), \tag{1}$$

where $\langle j|$ is the bra vector in the *site* notation given by $\langle j|=(0,0,...,1,...,0)$. The ket vector is defined as well. Since the set $\{|i\rangle\}$ satisfies the closure relation $\Sigma_i|i\rangle\langle i|=1$, an arbitrary state is expanded as

$$|\Psi(t)\rangle=\sum_i a_i(t)|i\rangle. \tag{2}$$

We impose a small perturbation $\hat{V}$ to the system expressed by

$$\hat{V}=-\tfrac{1}{2}\sum_\alpha \hat{x}_\alpha(f_0^\alpha e^{-i\omega t}+\text{c.c.}), \tag{3}$$

where $\hat{x}_\alpha$ is the α component of the *generalized* displacement and f_0^α is the corresponding generalized force. c.c. indicates a complex conjugate. In the spectral representation, this is written in the form

$$\hat{V}=\sum_\alpha \sum_{i,j} |i\rangle V_{ij}^\alpha(t)\langle j|$$

$$=-\tfrac{1}{2}\sum_\alpha \sum_{i,j} (|i\rangle x_{ij}^\alpha\langle j|)(f_0^\alpha e^{-i\omega t}+\text{c.c.}). \tag{4}$$

Here we have defined $V_{ij}^\alpha(t)=\langle i|\hat{V}_\alpha|j\rangle$ and $x_{ij}^\alpha=\langle i|\hat{x}_\alpha|j\rangle$. Substituting Eqs. (1) and (3) into the Schrödinger equation for $|\Psi(t)\rangle$ and multiplying by $\langle k|$ from the left, one has the inhomogeneous coupled linear differential equation

$$i\hbar\frac{da_i(t)}{dt}-\sum_j K_{ij}a_j(t)=\sum_\alpha\sum_j V_{ij}^\alpha(t)a_j(t). \tag{5}$$

For a small perturbation, the time-dependent first-order perturbation theory is applicable by putting $a_i(t)=a_i^{(0)}(t)+\Sigma_\alpha a_{i\alpha}^{(1)}(t)$ into Eq. (5). The zeroth-order equation becomes

$$i\hbar\frac{da_i^{(0)}(t)}{dt}-\sum_j K_{ij}a_j^{(0)}(t)=0, \tag{6}$$

while the first-order term yields

$$i\hbar\frac{da_{i\alpha}^{(1)}(t)}{dt}-\sum_j K_{ij}a_{j\alpha}^{(1)}(t)=\sum_j V_{ij}^\alpha a_j^{(0)}(t). \tag{7}$$

By substituting Eq. (4) into Eq. (7), one has the first-order linear differential equation with the periodic external force

$$i\hbar\frac{da_{i\alpha}^{(1)}(t)}{dt}-\sum_j K_{ij}a_{j\alpha}^{(1)}(t)$$

$$=-\frac{\hbar}{2}(F_{i\alpha}e^{-i\omega t}+F_{i\alpha}^*e^{i\omega t})e^{-i\omega_{\lambda 0}t}. \tag{8}$$

Here

$$F_{i\alpha}=\sum_j \frac{f_0^\alpha}{\hbar}x_{ij}^\alpha e_j(\omega_{\lambda 0}), \quad F_{i\alpha}^*=\sum_j \frac{f_0^{\alpha *}}{\hbar}x_{ij}^\alpha e_j(\omega_{\lambda 0}), \tag{9}$$

where $e_j(\omega_{\lambda 0})\equiv\langle j|\omega_{\lambda 0}\rangle$ is the jth element of the initial eigenvector belonging to the eigenvalue $\omega_{\lambda 0}$ of the matrix $\{K_{ij}\}$ [see Eq. (6)]. We have used in Eq. (7) the definition given by

$$a_j^{(0)}(t)=e_j(\omega_{\lambda 0})e^{-i\omega_{\lambda 0}t}.$$

The function $a_{i\alpha}^{(1)}(t)$ is expanded by a set of eigenvectors $\{e_i(\omega_\lambda)\}$ as

$$a_{i\alpha}^{(1)}(t)=\sum_\lambda \xi_\lambda^\alpha(t)e_i(\omega_\lambda), \tag{10}$$

where $\xi_\lambda^\alpha(t)$ is the amplitude of the mode λ. From Eq. (8) and using the orthogonal condition for eigenvectors $\{e_i(\omega_\lambda)\}$, one has the equation for $\xi_\lambda^\alpha(t)$,

$$i\frac{d\xi_\lambda^\alpha(t)}{dt}-\omega_\lambda\xi_\lambda^\alpha(t)=-\frac{1}{2}\left\{\sum_j e_j^*(\omega_\lambda)[F_{j\alpha}e^{-i(\omega_{\lambda 0}+\omega)t}+F_{j\alpha}^*e^{-i(\omega_{\lambda 0}-\omega)t}]\right\}, \tag{11}$$

where the closure relation $\Sigma_j e_j(\omega_\lambda)e_j^*(\omega_{\lambda'})=\delta_{\lambda\lambda'}$ is used. Imposing the initial condition $\xi_\lambda^\alpha(0)=0$, the solution of Eq. (11) yields

$$\xi_\lambda^\alpha(t)=-\frac{e^{-i\omega_\lambda t}}{2}\left\{\sum_j e_j^*(\omega_\lambda)\times\left[F_{j\alpha}\frac{e^{i(\omega_\lambda-\omega_{\lambda 0}-\omega)t}-1}{\omega_\lambda-\omega_{\lambda 0}-\omega}+F_{j\alpha}^*\frac{e^{i(\omega_\lambda-\omega_{\lambda 0}+\omega)t}-1}{\omega_\lambda-\omega_{\lambda 0}+\omega}\right]\right\}. \tag{12}$$

The second term in the square brackets is negligible since we consider the case of zero temperature and treat the Fermi distribution function with the Fermi frequency $\omega_F=E_F/\hbar$ as a step function. This implies that $\omega_\lambda>\omega_F\geqslant\omega_{\lambda 0}$, namely, $\omega_\lambda-\omega_{\lambda 0}>0$, implying that the contribution from the first term close to $\Omega=\omega_{\lambda 0}+\omega\approx\omega_\lambda$ is dominant.

Let us introduce the ''resonance'' function defined by

$$E_{\alpha\beta}(\Omega,t)=\sum_i a_{i\alpha}^{(1)}(t)^*a_{i\beta}^{(1)}(t)=\sum_\lambda \xi_\lambda^\alpha(t)^*\xi_\lambda^\beta(t). \tag{13}$$

By substituting Eq. (12) into Eq. (13), one has

$$E_{\alpha\beta}(\Omega,t)=\sum_\lambda\left\{\sum_i F_{i\alpha}e_i^*(\omega_\lambda)\right\}^*\left\{\sum_j F_{j\beta}e_j^*(\omega_\lambda)\right\}\times\frac{\sin^2\{(\omega_\lambda-\Omega)t/2\}}{(\omega_\lambda-\Omega)^2}, \tag{14}$$

where $\Omega=\omega_{\lambda 0}+\omega$. The orthogonality condition for eigenvectors $\{e_i(\omega_\lambda)\}$ is used to derive Eq. (14). The eigenvectors contributing to the sum in Eq. (14) are those whose frequen-

cies lie within about $\pm(2\pi/t)$ of Ω, where t is the time interval. Suppose that the following conditions are satisfied according to Ref. [7]:

$$\Omega t \gg 1, \tag{15}$$

$$\frac{4\pi}{t\Delta\omega} \gg 1, \tag{16}$$

where $\Delta\omega$ is the average spacing between the frequencies of adjacent eigenmodes. The first condition (15) means that only eigenmodes in a narrow band of frequencies on the scale of Ω contribute to the sum on λ in Eq. (14). The second one (16) ensures that the number of such eigenmodes is much larger than unity. Namely, the number of modes per frequency internal $\Delta\omega$ is of the order of $1/\Delta\omega$ and so the number of modes that are within $\pm 2\pi/t$ of Ω is $4\pi/t\Delta\omega$ [7]. The condition (16), which implies that the resonance width $\Delta\Omega_R = 4\pi/t$ should be much larger than the average level spacing $\Delta\omega$, is easily achieved for a system with a sufficiently large size N because $\Delta\omega$ for such a system becomes very small. For a large N, namely, with a small $\Delta\omega$, the conditions (15) and (16) are unified into the relation

$$\frac{1}{\Omega} \ll t \ll \frac{4\pi}{\Delta\omega}. \tag{17}$$

This condition requires that there should exist a sufficient number of eigenstates within the frequency range Ω to $\Omega + \Delta\Omega_R$. We should note that, for the condition $t \gg 4\pi/\Delta\omega$, the resonance factor in Eq. (14) is so sharp that the resonance width $\Delta\Omega_R$ is less than the spacing $\Delta\omega$. This condition for t is used to extract the pure eigenmode of the initial state expressed by $e_i(\omega_{\lambda 0})$ in Eq. (9) in addition to the optimization condition [8] (see Appendix A).

Taking a proper time interval t satisfying the condition (17), Eq. (14) gives

$$E_{\alpha\beta}(\Omega,t) = \frac{\pi t}{2} \sum_{\lambda} \left\{ \sum_i F_{i\alpha} e_i^*(\omega_\lambda) \right\}^* \times \left\{ \sum_j F_{j\beta} e_j^*(\omega_\lambda) \right\} \delta(\omega_\lambda - \Omega). \tag{18}$$

A straightforward calculation leads to the following representation, using the expression for $F_{i\alpha}$ introduced in Eq. (9):

$$\begin{aligned} \sum_i F_{i\alpha} e_i^*(\omega_\lambda) &= \frac{f_0^\alpha}{\hbar} \sum_{i,j} x_{ij}^\alpha e_j(\omega_{\lambda 0}) e_i^*(\omega_\lambda) \\ &= \frac{f_0^\alpha}{\hbar} \sum_{i,j} \langle \omega_\lambda | i \rangle \langle i | \hat{x}_\alpha | j \rangle \langle j | \omega_{\lambda 0} \rangle \\ &= \frac{f_0^\alpha}{\hbar} \langle \omega_\lambda | \hat{x}_\alpha | \omega_{\lambda 0} \rangle. \end{aligned} \tag{19}$$

Substituting Eq. (19) into Eq. (18) leads to

$$E_{\alpha\beta}(\Omega,t) = \frac{\pi t f_0^{\alpha *} f_0^\beta}{2\hbar^2} \sum_\lambda \langle \omega_{\lambda 0} | \hat{x}_\alpha | \omega_\lambda \rangle \times \langle \omega_\lambda | \hat{x}_\beta | \omega_{\lambda 0} \rangle \delta(\omega_\lambda - \Omega). \tag{20}$$

The generalized susceptibility $\chi_{\alpha\beta}(\omega)$ is given by the Kubo formula [14] under the generalized external force defined in Eq. (3),

$$\chi_{\alpha\beta}(\omega) = \frac{i}{\hbar} \int_0^\infty e^{i\omega t} \langle [\hat{x}_\alpha(t), \hat{x}_\beta(0)] \rangle dt, \tag{21}$$

where angular brackets denote the thermal average. The imaginary part of the generalized susceptibility for the *fixed* initial state $|\omega_{\lambda 0}\rangle$ is expressed by

$$\chi''_{\alpha\beta}(\omega) = \frac{\pi}{\hbar} \sum_\lambda [\langle \omega_{\lambda 0} | \hat{x}_\alpha | \omega_\lambda \rangle \langle \omega_\lambda | \hat{x}_\beta | \omega_{\lambda 0} \rangle \delta(\omega_{\lambda\lambda 0} - \omega) - \langle \omega_{\lambda 0} | \hat{x}_\beta | \omega_\lambda \rangle \langle \omega_\lambda | \hat{x}_\alpha | \omega_{\lambda 0} \rangle \delta(\omega_{\lambda\lambda 0} + \omega)], \tag{22}$$

where the definition is $\omega_{\lambda\lambda 0} = \omega_\lambda - \omega_{\lambda 0}$. The second term in the square brackets obviously makes no contribution because $\omega_{\lambda\lambda 0} > 0$. By comparing Eq. (22) with the resonance function $E_{\alpha\beta}(\Omega,t)$ given in Eq. (20), one has the relation, by setting $f_0^\alpha = f_0^\beta = 1$ without loss of generality,

$$\chi''_{\alpha\beta}(\omega) = \frac{2\hbar E_{\alpha\beta}(\Omega,t)}{t}. \tag{23}$$

This relation is the key equation that relates the resonance function $E_{\alpha\beta}(\Omega,t)$ [Eq. (13)] to the imaginary part of the generalized susceptibility $\chi''_{\alpha\beta}(\omega)$.

III. COMPUTING THE KUBO-GREENWOOD FORMULA

A. Longitudinal dynamic conductivity

This section describes the relationship between the Kubo-Greenwood formula for the ac conductivity and the resonance function defined in Eq. (13) via the imaginary part of the generalized susceptibility $\chi''_{\alpha\beta}(\omega)$. A small perturbation due to the vector potential $\mathbf{A}(t)$ to a electronic system is expressed as $\hat{H}' = -\hat{\mathbf{J}} \cdot \mathbf{A}(t)$, where $\hat{\mathbf{J}}$ is the current operator. Since the conductivity is defined as the response to the electric field $\mathbf{E}(t)$, the generalized conductivity $\Sigma_{\alpha\beta}(\omega)$ is related to the generalized susceptibility $\chi_{\alpha\beta}(\omega)$ by the relation $\Sigma_{\alpha\beta}(\omega) = \chi_{\alpha\beta}(\omega)/i\omega L^d$, where L is the linear size of a d-dimensional system.

The generalized conductivity is expressed as [14]

$$\Sigma_{\alpha\beta}(\omega) = \frac{ine^2}{m\omega} \delta_{\alpha\beta} + \frac{1}{\hbar\omega L^d} \times \lim_{\varepsilon \to 0} \int_0^\infty e^{i\omega t - \varepsilon t} \langle [\hat{J}_\alpha(t), \hat{J}_\beta(0)] \rangle dt, \tag{24}$$

where $\hat{J}_\alpha(t)$ is the α component of the current operator and the angular brackets mean the thermal average. The first term represents the conductivity of a system of free electrons. From this one can derive the *longitudinal* component of the ac conductivity $\sigma(\omega) \equiv \mathrm{Re}[\Sigma_{\alpha\alpha}(\omega)]$ by setting $\alpha = \beta$ and $\hat{x}_\alpha$

$=\hat{J}_\alpha$ in Eq. (22). Taking account of the Fermi distribution function $f(\omega)$, the longitudinal ac conductivity $\sigma(\omega)$ is expressed by the imaginary part of the generalized susceptibility $\chi''(\omega)$ as

$$\sigma(\omega)=\frac{2}{\omega L^d}\sum_{\omega_{\lambda 0}}\chi''(\omega)[f(\omega_{\lambda 0})-f(\omega_{\lambda 0}+\omega)]$$
$$=\frac{2}{\omega L^d}\sum_{\omega_{\lambda 0}=\omega_F-\omega}^{\omega_F}\chi''(\omega), \tag{25}$$

where the spin freedom is taken into account and the definition of the Fermi frequency is $\omega_F=E_F/\hbar$. The meaning of $\Sigma_{\omega_{\lambda 0}=\omega_F-\omega}^{\omega_F}$ is the sum on the initial state $|\omega_{\lambda 0}\rangle$ at zero temperature. Equation (25) can be shown to be equivalent to the Kubo-Greenwood formula [14,16] (see Appendix B).

The explicit form of the longitudinal ac conductivity, expressed by the resonance function given by Eq. (13), becomes

$$\sigma(\omega)=\frac{4\hbar}{\omega t L^d}\sum_{\omega_{\lambda 0}=\omega_F-\omega}^{\omega_F}E(\Omega,t), \tag{26}$$

where the time t satisfies the condition $1/\Omega \ll t \ll 4\pi/\Delta\omega$. This is the key relation for evaluating the ac conductivity from the resonance function $E(\Omega,t)$. We should emphasize that the accuracy of the calculated results becomes better on increasing the system size N since the average level spacing $\Delta\omega$ becomes smaller than the resonance width $\Delta\Omega_R$.

B. Transverse dynamic conductivity

It is straightforward to generalize the formula for the longitudinal conductivity [Eq. (26)] to the transverse ac conductivity $\sigma_{\alpha\beta}(\omega)$. The resonance function $E_{\alpha\beta}(\Omega,t)$ is related to the imaginary part of the generalized susceptibility $\chi''_{\alpha\beta}(\omega)$ via Eq. (23). The use of Eqs. (23) and (25) gives the expression for the transverse ac conductivity

$$\sigma_{\alpha\beta}(\omega)=\frac{2}{\omega L^d}\sum_{\omega_{\lambda 0}=\omega_F-\omega}^{\omega_F}\chi''_{\alpha\beta}(\omega)$$
$$=\frac{4\hbar}{\omega t L^d}\sum_{\omega_{\lambda 0}=\omega_F-\omega}^{\omega_F}E_{\alpha\beta}(\Omega,t). \tag{27}$$

The Onsager reciprocal relation $\sigma_{\alpha\beta}(\omega)=-\sigma_{\beta\alpha}(\omega)$ should be satisfied in Eq. (27) by letting $\omega\to-\omega$ and $i\to-i$. This comes from the relation for the generalized susceptibility $\chi_{\alpha\beta}(\omega)=\chi_{\beta\alpha}(\omega)$ [15].

We have described in this section the method of computing the longitudinal and the transverse ac conductivities for systems described by large-scale Hamiltonian matrices. This algorithm enables us to directly calculate conductivities without making the temporal Fourier transform of the response function or calculating all of the intermediate states $\{e_i(\omega_\lambda)\}$ relevant to the formula (22). This allows the calculation of the ac conductivities with $O(N)$ computational steps.

IV. IMPLEMENTATION OF THE ALGORITHM

A. Time development of the resonance function

The problem of calculating the resonance function in Eq. (23) is reduced to the numerical solution of the first-order coupled linear differential equations under a periodic external force expressed by Eq. (8). By dividing the function $a_{i\alpha}^{(1)}(t)$ in Eq. (8) into a real part $x_i(t)$ and an imaginary part $y_i(t)$, one has, in units of $\hbar=1$,

$$\frac{dx_i(t)}{dt}-\sum_j K_{ij}y_j(t)=\frac{1}{2}F_i\sin(\Omega t), \tag{28}$$

$$\frac{dy_i(t)}{dt}+\sum_j K_{ij}x_j(t)=\frac{1}{2}F_i\cos(\Omega t). \tag{29}$$

Here we have assumed, for simplicity, that the elements $\{K_{ij}\}$ and $\{F_i\}$ are real numbers. By discretizing time t with a step τ, these equations become

$$x_i(n+1)=x_i(n)+\sum_j \tau K_{ij}y_j(n)+\frac{\tau}{2}F_i\sin(\Omega n\tau), \tag{30}$$

$$y_i(n+1)=y_i(n)-\sum_j \tau K_{ij}x_j(n+1)$$
$$+\frac{\tau}{2}F_i\cos[(\Omega(n+1)\tau], \tag{31}$$

where $x_i(t)$ and $y_i(t)$ are the real and the imaginary parts of the ith element $a_{i\alpha}^{(1)}(t)$ at time $t=n\tau$, in which the integer n represents the number of time steps.

It should be noted that the second and third terms on the right-hand side of Eq. (31) depend on the number $n+1$ of time steps, namely, defined by the *retarded* finite-difference form, which is different from the standard Euler method defined by the advanced finite-difference method as used for Eq. (30). The choice in Eq. (31) makes the calculation, by taking the time step τ satisfying the condition $\omega_{\max}\tau<2$, very efficient and accurate, as discovered by Williams and Maris [7].

We chose t as $t=4\pi/\Delta\Omega_R$, where $\Delta\Omega_R$ is a given resolution. This ensures that the number of modes within the range Ω to $\Omega+\Delta\Omega_R$ is much larger than unity. The details of the implementation of our algorithm are as follows. (i) The initial set of vectors $\{x_i(0)\}$ and $\{y_i(0)\}$ to iterate Eqs. (30) and (31) is set to be zero. (ii) We prepare the initial states $\{e_i(\omega_{\lambda 0})\}$ belonging to the eigenfrequency $\omega_{\lambda 0}$ by applying the FOM described in Ref. [8], taking a large time interval satisfying the condition $t\gg 4\pi/\Delta\omega$ or, equivalently, $\Delta\omega\gg\Delta\Omega_R$ for Eqs. (30) and (31) (see Appendix A). (iii) By taking the time interval t as $t=4\pi/\Delta\Omega_R$ ($\Delta\Omega_R\gg\Delta\omega$), we calculate the amplitude $a_{i\alpha}^{(1)}(t)$ under the periodic external force with the frequency Ω. We can finally obtain the resonance function using Eq. (13). Note that the frequency resolution can be determined and controlled by the time interval t.

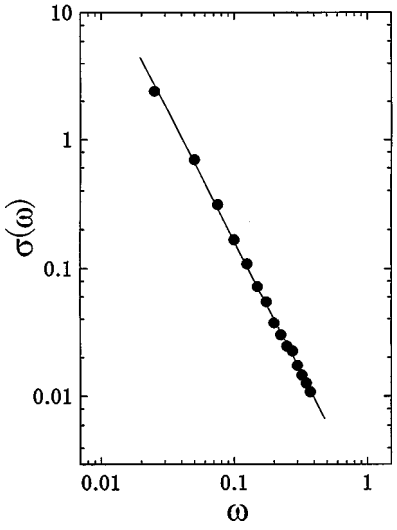

FIG. 1. ac conductivities $\sigma(\omega)$ of the 1D tight-binding chain with the system size $N=10\,000$. The resonance width $\Delta\Omega_R$ is taken to be $\Delta\Omega_R=0.01$ in the frequency range $\omega=0.02-0.4$ in the system of units given in the text. The solid line indicates the analytic solution showing the ω^{-2} dependence.

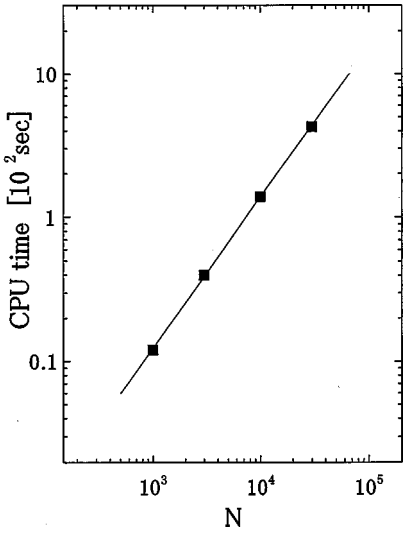

FIG. 2. CPU times on the Ultra-SPARC for various system sizes N. Calculations on ac conductivities have been performed for tight-binding chains with the resonance width $\Delta\Omega_R=0.01$ at the fixed frequency $\omega=0.2$ in the system of units given in the text.

B. Tight-binding chain

In order to assess the efficiency of the algorithm following the procedure described in the preceding subsection, we consider a 1D tight-binding Hamiltonian with N sites given by

$$\hat{H}=\sum_i \epsilon_i|i\rangle\langle i|-\sum_{i,j} t_{ij}|i\rangle\langle j|, \tag{32}$$

where we set $\epsilon_i=2$ and $t_{i,i\pm1}=1$ for hopping terms between nearest neighbors. The matrix elements for the current operator $\hat{J}=e\hat{v}$ are obtained from the Heisenberg equation of motion as $J_{j,j\pm1}=\langle j|\hat{J}|j+1\rangle=\mp ie/\hbar$ by taking a lattice spacing $a=1$. We have calculated the resonance function defined by Eq. (13) for this system by setting $\alpha=\beta$ under the fixed boundary condition. We note that for the system consisting of a regular chain without scattering of waves, the Kubo formula is not applicable because the system cannot reach thermal equilibrium. However, though rather artificial, it is possible to calculate, in a very formal manner, the dynamic conductivity of the system both analytically and numerically in order to test the efficiency of the algorithm.

Figure 1 represents the comparison of numerical results (solid circles) with the analytic solution (solid line) for a 1D chain with $N=10\,000$ on a double logarithmic scale. The system of units used is $e=\hbar=1$. For these calculations, we have chosen the time step as $\tau=2\pi/20\Omega$ and the resonance width in Eq. (14) as $\Delta\Omega_R=4\pi/t$ with $t=4\pi\times100$. This means that there are about 25 modes within the resonance width $\Delta\Omega_R$. In order to prepare the initial eigenfunction $\{e_i(\omega_{\lambda0})\}$ we have performed calculations under the condition $\Delta\omega\approx\Delta\Omega_R$ and taken the number of iterations $p\approx10$. This choice of parameters makes the deviation δ defined in Appendix A take the value $\delta\approx10^{-7}$. The analytic solution for this system is given by the solid line, whose explicit form is omitted here. We see from Fig. 1 that the calculated results agree fairly well with the analytic result over one order of magnitude in frequency. The ω^{-2} frequency dependence is the conventional Drude-like behavior. We emphasize again that the local equilibrium is achieved by sufficiently large scattering rates due to randomness and excitations such as phonons in metals, namely, the assumption that local equilibrium is valid outside the mean scattering length l_s. In the case of perfect metals, the scattering length becomes larger than the system size L, resulting in the inapplicability of the Kubo-Greenwood formula.

In order to demonstrate the $O(N)$ scaling of our method, ac conductivities have been computed by varying the system size N for the tight-binding chain given by Eq. (32). In these calculations, we have taken the same resonance width $\Delta\Omega_R=0.01$ for the fixed frequency $\omega=0.2$. Figure 2 shows the scaling of CPU times with the system sizes N of 1000, 3000, 10 000, and 30 000, respectively. The linear scaling to N is evident from these calculated data.

C. Three-dimensional disordered system

We apply the algorithm to the calculation of the ac conductivities of the 3D Anderson model of noninteracting electrons in a random potential, in which the on-site potential $\{\epsilon_i\}$ in Eq. (32) is distributed uniformly between $-W/2$ and $W/2$. The critical width W is known to be $W_C=16.5$ [17–19]. The $\omega^{1/3}$ dependence of $\sigma(\omega)$ at the metal-insulator transition was predicted by Wegner [20] using the single-parameter scaling hypothesis, but this dependence was not verified numerically until the work by Lambrianides and Shore [21]. They evaluated the Kubo-Greenwood formula by directly calculating eigenvectors of the order of 10^5 for system sizes $L=6-14$ and by pulling out of the integral the densities of states $D(\omega_{\lambda0})$ and $D(\omega_{\lambda0}+\omega)$. We do not need to do so to calculate the ac conductivities since the information on the DOS is automatically involved in our algorithm through Eq. (14). We plot the calculated DOS for the system size $N=30^3$ in Fig. 3. These data are obtained by setting $F_i=e^{i\phi_i}$ in Eq. (8), where ϕ_i is a random quantity. This is

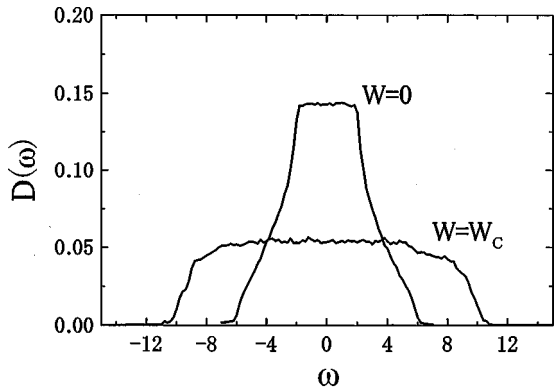

FIG. 3. Spectral density of states for the 3D Anderson model of noninteracting electrons in a uniformly distributed random potential with $W=W_c$ in addition to the regular case $W=0$. The resonance width is taken as $\Omega_R=0.2$ for the system size $N=30^3$. The data are averaged over 10 samples.

the same scheme presented by Williams and Maris [7] to calculate the DOS, which is particularly effective when one needs the DOS at an arbitrary frequency range for systems described by large-scale Hamiltonian matrices in an $O(N)$ fashion. We consider the case of the critical width W_C and choose the Fermi energy $E_F=\hbar\omega_F$ in the center of the flat band (see Fig. 3), for which the mobility edge $\omega_0=\omega_F$. Figure 4 shows the calculated results for 3D systems with $N=30^3$ on 20 samples with various distributions of random potential $\{\epsilon_i\}$. The parameters taken are $t=4\pi\times100$ and $\tau=2\pi/20\Omega$ (or $1.9/\omega_{\max}$). From Fig. 4 the exponent δ is estimated to be $\delta=0.33\pm0.04$ by averaging over 20 samples. The error is within 12%.

V. FINITE-TIME SCALING OF THE ac CONDUCTIVITY NEAR THE QUANTUM PHASE TRANSITION

We consider the frequency dependence of the ac conductivity near the mobility edge ω_0, in particular, the case in which the ac conductivity $\sigma(\omega)$ follows the power-law dependence ω^δ, where the frequency ω is measured from ω_0.

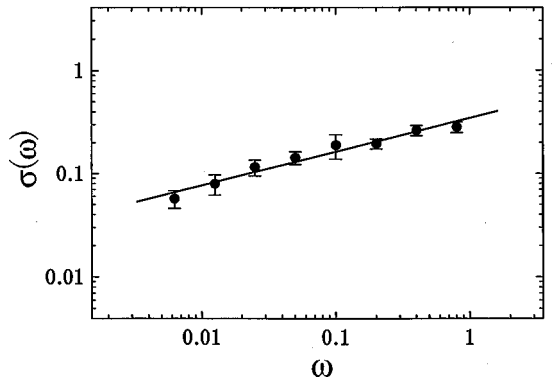

FIG. 4. ac conductivities $\sigma(\omega)$ for the 3D Anderson model of interacting electrons in a uniformly distributed random potential. The system size is $N=30^3$, for which the resonance width is taken as $\Delta\Omega_R=0.01$ in the system of units given in the text. The data are averaged over 20 samples. The solid line is drawn by a least-squares fit and each of the error bars is defined as a standard deviation.

These problems appear in the investigation of quantum phase transitions, where the problem is how to obtain the precise value of the exponent δ. We provide in this section an efficient method based on the finite-time scaling approach to determine the exponent δ.

The explicit form of the resonance function $E(\Omega,t)$ with the definition $\Omega=\omega_{\lambda0}+\omega$ is given by Eq. (14) as

$$E(\Omega,t)=\frac{1}{\hbar}\int d\omega_\lambda D(\omega_\lambda)|\langle\omega_\lambda|\hat{x}|\omega_{\lambda0}\rangle|^2\,\frac{\sin^2\{(\omega_\lambda-\Omega)t/2\}}{(\omega_\lambda-\Omega)^2}, \tag{33}$$

where the density of states $D(\omega_\lambda)$ is introduced by the definition $\Sigma_{\omega_\lambda}=L^d\int d(\hbar\omega_\lambda)D(\omega_\lambda)$. We assume that the longitudinal ac conductivity $\sigma(\omega)$ obeys the power law close to the mobility edge ω_0 as

$$\sigma(\omega)\propto\omega^\delta \tag{34}$$

for $0<\omega\ll\omega_F$ and that the DOS close to ω_0 is nearly constant in the center of the band as shown in Fig. 3. Note that $\omega_0=\omega_F$ for the critical distribution $W_C=16.5$ [17–19]. Under these conditions, Eq. (33) should be, for a sufficiently large time interval t,

$$E(\Omega,t)/t\propto\int d\omega_\lambda(\omega_\lambda-\omega_{\lambda0})^\delta\delta(\omega_\lambda-\Omega)\propto\omega^\delta, \tag{35}$$

where the definition $\Omega=\omega_{\lambda0}+\omega$ is used. For a short time interval $(\Omega-\omega_\lambda)t\ll1$, the sinclike function in Eq. (33) becomes wider than the bandwidth. This yields

$$E(\Omega,t)/t\propto t^{-\delta}.$$

From these two extreme cases, the scaling form of the resonance function or, equivalently, the ac conductivity becomes, as in the case of obtaining the exponent of the spectral DOS at the band edge of the $\pm J$ Ising spin-glass model proposed by Hukushima and Nemoto [22],

$$E(\omega,t)/t\propto t^{-\delta}G(\omega t), \tag{36}$$

where the asymptotic form of $G(z)$ should be

$$G(z)=\begin{cases}z^\delta, & z\gg1\\ \text{const}, & 0<z\ll1.\end{cases} \tag{37}$$

We apply this scheme to the 3D Anderson model of noninteracting electrons in a uniformly distributed random potential studied in Sec. IV. Figure 5 presents the results for $\sigma(\omega)$ for the system $W=W_C$ with $N=20^3$, taking the time interval $t=4\pi\times4n$ $(n=1-8)$. The corresponding resonance widths become $\Delta\Omega_R=1/4n$, where n ranges from 1 to 8. We see from Fig. 5 that the calculated results approach an $\omega^{1/3}$ dependence with increasing the time interval t. Figure 6 plots the scaling function $G(z)$ $(z\gg1)$ defined in Eq. (36). The ordinate represents the quantity $G(z)$ and the abscissa depends on the variable z. The data for $n=6-8$ collapse

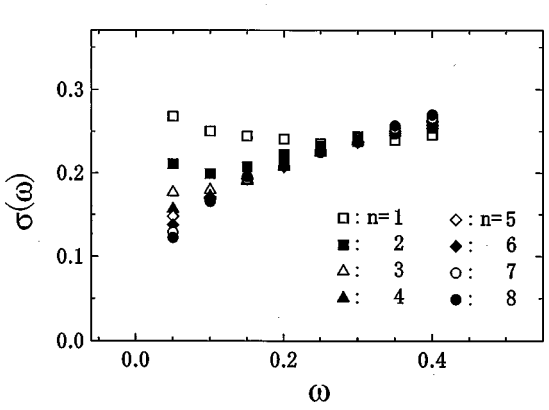

FIG. 5. Calculated ac conductivities taking various time intervals $t=4\pi\times 4n$, for which n ranges from $n=1$ to 8. These choices make the resonance widths range from $\Delta\Omega_R=0.25$ to 0.031 25. The system size is $N=20^3$.

onto a single line over one order of frequency variation. From Fig. 5 the exponent δ is estimated as $\delta=0.337\pm 0.013$, namely, the error is within 4%. We emphasize that the scaling approach presented here has been performed by taking a limited number of initial eigenvectors $\{e_j(\omega_{\lambda 0})\}$ and by varying the time interval t. This enables the computation of the precise exponent δ with significantly less computational effort, in fact, several times faster compared to the effort for evaluating the exponent δ in Fig. 4. The straight line is for $\omega^{1/3}$, indicating fairly good agreement with the calculated results. We have demonstrated in this section that the accuracy has been significantly improved by the use of the finite-time scaling approach.

VI. CONCLUSIONS

We have proposed a method for computing linear response functions for quantum systems described by large-scale Hamiltonian matrices. The method is based on solving the Schrödinger equation numerically in the presence of a generalized external force. This method enables the efficient computation of linear response functions with $O(N)$ computational steps. Simple examples have been considered to confirm the reliability of the method. We have furthermore presented the finite-time scaling method for computing the exponent of the frequency dependence $\sigma(\omega)\propto\omega^{\delta}$ near the metal-insulator Anderson transition. This method is especially powerful for evaluating the precise value of the exponent δ with high speed and accuracy. Although we have examined only conductivity problems, the present method is rather general, so it should be applicable for calculating various types of linear response functions. This issue is especially relevant in quantum systems in a variety of physical contexts.

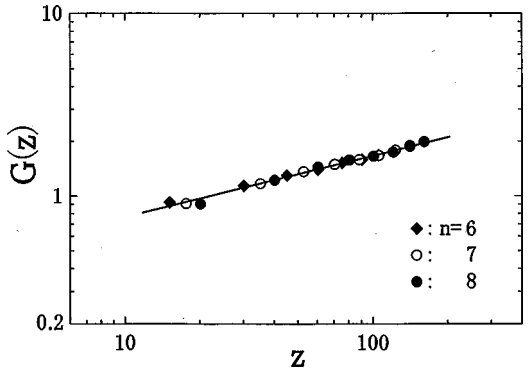

FIG. 6. Finite-time scaling function $G(z)$ introduced in Eq. (36). The data for $n=6-8$ presented in Fig. 5 ($z\gg 1$) are plotted. The straight line showing the $\omega^{1/3}$ dependence is only a guide to the eye.

ACKNOWLEDGMENTS

We thank Hideo Aoki and Kousuke Yakubo for useful suggestions on the present work. This work was supported in part by a Grant-in-Aid from the Japan Ministry of Education, Science, and Culture for Scientific Research. Numerical calculations were partially performed on the FACOM VPP 500 of the Supercomputer Center, Institute of Solid State Physics, University of Tokyo.

APPENDIX A

This appendix presents the procedure to extract the initial eigenfunction $\{e_i(\omega_{\lambda 0})\}$ of the unperturbed system belonging to the eigenfrequency $\omega_{\lambda 0}$, necessary to give the external force defined in Eq. (9) following the FOM [7,8]. A quantum system described by a Hermitian matrix $\{K_{ij}\}$ has a set of eigenfunctions $\{e_i(\omega_\lambda)\}$ defined by

$$\omega_\lambda e_i(\omega_\lambda)=\sum_j K_{ij}e_j(\omega_\lambda), \tag{A1}$$

where we use a system of units of $\hbar=1$. Hereafter we assume all matrix elements described by $\{K_{ij}\}$ to be real and symmetric, or, equivalently, all eigenvalues and their eigenfunctions $\{e_i(\omega_\lambda)\}$ to be real numbers. The extension to the case of complex numbers is straightforward.

The eigenfunction $\{e_i(\omega_\lambda)\}$ of the unperturbed system is obtained by numerically solving the Schrödinger equation given in Eq. (6) by the following procedure. We impose the external force $F_i\exp(-i\Omega t)$ on each site i in Eq. (6). Here F_i should be chosen as

$$F_i=F_0\cos(\phi_i), \tag{A2}$$

where ϕ_i is a random quantity taking a value within the range $0\leqslant\phi_i\leqslant 2\pi$ and F_0 is a constant. Note that this definition of F_i is different from that in Eq. (9) for the perturbed system. We first drive the system for a time interval T, under the initial condition $\{a_i^{(0)}(t=0)=0\}$, after which the amplitude at the site i becomes $a_i^{(0,1)}(t)$. One sees, using Eq. (6), that this amplitude can be written as the sum of normal modes $\{e_i(\omega_\lambda)\}$ after the time interval T,

$$a_i^{(0,1)}(T)=-2i\sum_\lambda F_\lambda h(\Omega,\omega_\lambda,T)e_i(\omega_\lambda)\times\exp\left(-i\,\frac{\Omega+\omega_\lambda}{2}\,T\right), \tag{A3}$$

where

$$F_\lambda = \sum_j F_j e_j(\omega_\lambda) \tag{A4}$$

$$h(\Omega, \omega_\lambda, T) = \frac{\sin\{(\Omega - \omega_\lambda)T/2\}}{\Omega - \omega_\lambda}. \tag{A4}$$

As a next step, the amplitude of the external force in Eq. (A2) applied to the site i is replaced by the new external force $F_i^{(1)} \exp(-i\Omega t)$ with $F_i^{(1)} = a_i^{(0,1)}(T)$. We drive again the system for the time interval T under the new external force starting with all zero amplitudes. After p iterations of this process we have

$$a_i^{(0,p)}(T) = (-2i)^p \sum_\lambda F_\lambda h^p(\Omega, \omega_\lambda, T) e_i(\omega_\lambda) \times \exp\left(-i\,\frac{\Omega + \omega_\lambda}{2}\,pT\right). \tag{A5}$$

This equation indicates that one mode λ_1 close to Ω is dominantly excited after a sufficient number of iterations. This is the mode for which the absolute magnitude of the h function in Eq. (A4) has the largest value. Thus, for a sufficiently large p of around 10, we obtain

$$a_i^{(0,p)}(T) \cong C e_i(\omega_{\lambda_1}) \exp(-ip\omega_{\lambda_1} T), \tag{A6}$$

where C is a constant. In actual calculations, we discretize time t with a step $n\tau$ and drive Eqs. (30) and (31) with the external force $F_i^{(p)} \exp(-i\Omega t)$. Note that we use the modified Euler method defined by the retarded finite-difference form in Eq. (31), which makes the calculations very efficient and accurate, as found by Williams and Maris [7].

In order to estimate the monochromaticity of the exited mode in Eq. (A6) we introduce the quantity δ_i [8] defined by

$$\delta_i = b_i - \tilde{\omega} c_i, \tag{A7}$$

where i denotes the site and

$$b_i = \sum_j K_{ij} a_j^{(0,p)}(T), \quad c_i = a_i^{(0,p)}(T). \tag{A8}$$

We see from Eq. (A7) that if $a_i^{(0,p)}(T)$ is equal to the eigenfunction $e_i(\omega_\lambda)$ and $\tilde{\omega} = \omega_\lambda$, δ_i vanishes for any i. When the excited pattern $\{a_i^{(0,p)}(T)\}$ consists of a few modes with eigenfrequencies close to the external frequency Ω, δ_i becomes small but finite.

The normalized sum of the deviation δ^2 defined below expresses the degree of convergence [8]

$$\delta^2 = \frac{\Sigma_i |\delta_i|^2}{\Sigma_i |b_i|^2}. \tag{A9}$$

We choose the quantity $\tilde{\omega}$ as the deviation δ^2 to be minimized. By differentiating Eq. (A9) with respect to $\tilde{\omega}$, the minimum value of the deviation δ^2 becomes

$$\delta^2 = 1 - \frac{(\Sigma_i b_i c_i^*)^2}{\Sigma_i |b_i|^2 \Sigma_i |c_i|^2} \tag{A10}$$

for

$$\tilde{\omega} = \frac{\Sigma_i b_i c_i^*}{\Sigma_i |c_i|^2}, \tag{A11}$$

which is the expectation value of the frequency for $a_i^{(0,p)}(T)$. If the quantity δ is very small, $\tilde{\omega}$ becomes quite close to the true eigenfrequency. Provided $\{a_i^{(0,p)}(T)\}$ converges to the eigenfunction $\{e_i(\omega_\lambda)\}$, δ approaches zero, indicating that δ^2 is an index for the degree of accuracy. Thus one can judge the convergence of the eigenvector from the magnitude of δ. We emphasize that the value of $\tilde{\omega}$ corresponding to the required eigenvalue, say, $\omega_{\lambda 0}$, is calculated after obtaining the eigenfunction $\{a_i^{(0,p)}(T)\}$, which should be a true eigenvector when $\delta = 0$. This point is different from the procedure of conventional methods such as the Lanczos one, in which the eigenvector is calculated after diagonalizing the matrix. The algorithm mentioned above involves two parameters, the time interval T over which the quantum system is driven and the number of repetitions times of the iteration process p, which can be freely chosen. We need to take a large time interval T with increasing system size N due to the condition $T \approx 4\pi/\Delta\Omega_R$. The details of the optimum choice of these parameters to achieve efficient calculations is given in Ref. [8]. Usually, it is sufficient to take p around 10 as well as $\Delta\omega \approx \Delta\Omega_R = 4\pi/T$.

The method mentioned above is especially useful for calculating eigenvalues and their corresponding eigenfrequencies within a selected range of eigenfrequency distribution. This is definitely required when computing ac conductivities for electron systems treated in Sec. IV. The Lanczos method is widely used for the diagonalization of large matrices. However, this is usually useful for computing only extremely few eigenvalues and their eigenvectors, and is not suitable to calculate those within a selected range of eigenfrequency distribution and their eigenvectors. We note that eigenfunctions belonging to very large systems such as aperiodic waveguides [23], fractal networks [24], and electronic systems [25] have been accurately and efficiently calculated by the present algorithm.

APPENDIX B

We show that Eq. (25) is equivalent to the Kubo-Greenwood formula for the longitudinal conductivity. The explicit form of Eq. (25) is expressed as,

$$\sigma(\omega) = \frac{2}{\omega L^d} \sum_{\omega_{\lambda 0} = \omega_F - \omega}^{\omega_F} \chi''(\omega) = \frac{2}{\omega} \int_{E_F - \hbar\omega}^{E_F} dE_{\lambda 0} D(E_{\lambda 0}) \chi''(\omega), \tag{B1}$$

where $D(E_{\lambda 0})$ means the spectral DOS at the eigenenergy $E_{\lambda 0}=\hbar\omega_{\lambda 0}$. Substituting Eq. (22) into Eq. (B1), one has, taking account of $\omega_\lambda-\omega_{\lambda 0}>0$ as explained in the paragraph below Eq. (12),

$$\sigma(\omega)=\frac{2\pi e^2}{\hbar\omega}\sum_{\omega_\lambda}\left\{\int_{E_F-\hbar\omega}^{E_F}dE_{\lambda 0}|\langle\omega_\lambda|\hat{v}|\omega_{\lambda 0}\rangle|^2 \times D(E_{\lambda 0})\delta(\omega_{\lambda 0}+\omega-\omega_\lambda)\right\}, \tag{B2}$$

where $\hat{v}$ is the velocity operator. The use of the relation $\Sigma_\lambda=L^d\int D(E_\lambda)dE_\lambda$ in Eq. (B2) yields

$$\begin{aligned}\sigma(\omega)&=\frac{2\pi e^2L^d}{\omega}\int dE_\lambda\int_{E_F-\hbar\omega}^{E_F}dE_{\lambda 0}|\langle\omega_\lambda|\hat{v}|\omega_{\lambda 0}\rangle|^2 \times D(E_{\lambda 0})D(E_\lambda)\delta(E_{\lambda 0}+\hbar\omega-E_\lambda)\\ &=2\pi e^2\hbar L^d\int_{E_F-\hbar\omega}^{E_F}dE_{\lambda 0}\frac{|\langle\omega_{\lambda 0}+\omega|\hat{v}|\omega_{\lambda 0}\rangle|^2}{\hbar\omega} \times D(E_{\lambda 0})D(E_{\lambda 0}+\hbar\omega).\end{aligned} \tag{B3}$$

This is the Kubo-Greenwood formula [14,16].

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