Calculating the linear response functions of noninteracting electrons with a time-dependent Schrödinger equation

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An $O(N)$ algorithm is proposed for calculating linear response functions of noninteracting electrons. This algorithm is simple and suitable to parallel and vector computation. Since it avoids $O(N^3)$ computational effort of matrix diagonalization, it requires only $O(N)$ computational efforts, where N is the dimension of the state vector. The use of this $O(N)$ algorithm is very effective since, otherwise, we have to calculate a large number of eigenstates, i.e., the occupied one-electron states up to the Fermi energy and the unoccupied states with higher energy. The advantage of this method compared to the Chebyshev polynomial method recently developed by Wang and Zunger [L. W. Wang, Phys. Rev. B **49**, 10 154 (1994); L. W. Wang and A. Zunger, Phys. Rev. Lett. **73**, 1039 (1994)] is that our method can calculate linear response functions without any storage of huge state vectors on external storage. [S1063-651X(97)12607-1]

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I. INTRODUCTION

Computing the linear response functions (and the density of states) of large systems with thousands of atoms by using conventional methods requires us to calculate the eigenvalues and eigenvectors of $N \times N$ Hamiltonian matrices ($N \gtrsim 10^6$) from the lowest state to the Fermi energy and beyond it. The standard diagonalization routines are too time consuming in treating these problems because their computing time is proportional to N^3. Therefore, efficient numerical algorithms, such as recursive Green's function methods [1,2], the Lanczos methods [3–6], the Chebyshev polynomial expansion [9–17], and conjugate gradient methods [7,8] have been developed and applied to various problems.

In this paper, we present an efficient method for calculating the linear response functions of large quantum system. We give up the calculation of each exact eigenstates, instead we compute linear response functions by integrating the time-dependent Schrödinger equations for a finite period determined by the required energy resolution. Since it avoids $O(N^3)$ computational efforts of matrix diagonalization, it requires only $O(N)$ computational efforts for sparse Hamiltonian matrices. To realize this scheme, we exploit several numerical techniques such as the Chebyshev polynomial expansion of matrix functions [9–17], the random state vectors [17–19], Hamiltonian matrix discretized in real space [20,21], the time-dependent Schrödinger equation discretized in real time [22–35].

II. TIME-DEPENDENT METHODS

In this section, we describe how we reached the conclusion that we can efficiently calculate the linear response functions of large quantum systems by using the time-dependent homogeneous Schrödinger equations.

A. Diagonalize or not diagonalize?

Let us compare the computational efforts of the conventional diagonalization method and the time-dependent method by counting the number of floating point multiplications as a function of matrix dimension N, and show that the time-dependent method is more efficient when large numbers of eigenstates are involved.

First, we review the relation between the eigenstate representation and the time-dependent representation of linear response functions. The linear response function $\chi_{BA}(\omega + i\eta)$ of an observable B due to a *monochromatic* perturbation $H^{ex} = e^{-i(\omega + i\eta)t}A$ is calculated by the time-dependent perturbation theory [36],

$$\chi_{BA}(\omega + i\eta) = (-i)\int_0^\infty dt\, e^{+i(\omega + i\eta)t}$$
$$\times \{\langle E_g | e^{+iHt}Be^{-iHt}A | E_g\rangle - \text{c.c.}\}, \quad (1)$$

$$\approx 2\int_0^T dt\, e^{+i(\omega + i\eta)t}$$
$$\times \text{Im}\{\langle E_g | Be^{-iHt}A | E_g\rangle e^{+iE_g t}\}, \quad (2)$$

where $|E_g\rangle$ and E_g are the ground state of the many electron system and its energy, respectively; ω and η are the frequency and its resolution, respectively; $T \gg 1/\eta$ is the integration time. We use atomic units (a.u.) and indicate the complex conjugate by c.c. In the numerical calculation of Eq. (2), we have to discretize it in time, e.g.,

$$\chi_{BA}(\omega + i\eta) = 2\sum_{m=0}^M \Delta t\, e^{+i(\omega + i\eta)m\Delta t}$$
$$\times \text{Im}\{\langle E_g | Be^{-iHm\Delta t}A | E_g\rangle e^{+iE_g m\Delta t}\}, \quad (3)$$

where $M = T/\Delta t$ is the number of time steps, T is the integration time in Eq. (2), and Δt is the width of the time step.

TABLE I. Comparison of the diagonalization method and the time-dependent method.

Diagonalization method

$$\chi_{BA}(\omega+i\eta)=\sum_{m=1}^{N}\frac{\langle E_g|B|E_m\rangle\langle E_m|A|E_g\rangle}{(\omega+i\eta)-(E_m-E_g)}-\sum_{m=1}^{N}\frac{\langle E_g|A|E_m\rangle\langle E_m|B|E_g\rangle}{(\omega+i\eta)+(E_m-E_g)}$$

	Dense matrix		Sparse matrix	
Calculation	Computation	Memory	Computation	Memory
$E_m,|E_m\rangle$	N^3	N^2	N^3	N^2
$\langle E_g|A|E_m\rangle$	N^2	N	N	N
Σ_m	N	N	N	N

Time-dependent method

$$\chi_{BA}(\omega+i\eta)=2\sum_{m=0}^{M}\Delta t e^{+i(\omega+E_g+i\eta)m\Delta t}\mathrm{Im}\langle E_g|Be^{-iHm\Delta t}A|E_g\rangle$$

	Dense matrix		Sparse matrix	
Calculation	Computation	Memory	Computation	Memory
$e^{-iHm\Delta t}B|E_g\rangle$	MN^2	N^2	MN	N
$\langle E_g|Ae^{-iHm\Delta t}B|E_g\rangle$	N^2	N	N	N
$\Sigma_{m=0}^M$	M	1	M	1

On the other hand, we obtain the eigenstate representation by inserting $I=\Sigma_{m=1}^{N}|E_m\rangle\langle E_m|$ into Eq. (1),

$$\chi_{BA}(\omega+i\eta)=\sum_{m=1}^{N}\frac{\langle E_g|B|E_m\rangle\langle E_m|A|E_g\rangle}{(\omega+i\eta)-(E_m-E_g)}$$
$$-\sum_{m=1}^{N}\frac{\langle E_g|A|E_m\rangle\langle E_m|B|E_g\rangle}{(\omega+i\eta)+(E_m-E_g)}. \qquad (4)$$

Next, we show the estimated computational efforts in Table I. The diagonalization method for the $N\times N$ Hamiltonian matrix requires the memory space of $O(N^2)$ and the computational effort of $O(N^3)$. On the other hand, the time-dependent method requires the memory space of $O(N^2)$ and the computational effort of $O(MN^2)$, where M is the number of time steps determined by the required energy resolution (see Sec. II C). By choosing an appropriate basis set, we can make the Hamiltonian a sparse matrix having only $O(N)$ nonzero matrix elements [20,25]. This results in the computational effort and the memory space of the time-dependent method being reduced to $O(MN)$ and $O(N)$, respectively. Thus the time-dependent method can be more efficient than the diagonalization method in the large N limit.

B. Newton or Schrödinger?

Table II classifies various time-dependent methods in terms of the kinds of equations and homogeneity. Though the Newton equations of harmonic oscillators [37–41] are mathematically equivalent to the Schrödinger equations in the eigenstate representation, use of the Schrödinger equation [22–35] has the advantage that we can exploit well developed concepts and the formalism of quantum theory. It is especially true when we want to deal with quantum systems. Therefore, in this paper, we only study the Schrödinger equations.

C. Homogeneous or inhomogeneous?

In this subsection we show that inhomogeneous time-dependent equations are more inefficient than homogeneous ones. This conclusion is valid not only for the Schrödinger equation (particle source method [28]) but also for the Newton equation (forced oscillator method [37–41]) because both equations are equivalent in the eigenstate representation.

Let us define the computational effort of the time-dependent method by the number of time steps $M=T/\Delta t$. Then the computational effort M is determined by the integration time T, because the maximum width of the time step is limited by the *sampling theorem* [9] independent of the detail of the method we use. The time step should be much smaller than the inverse of the bandwidth π/E_B to reproduce the correct spectrum since, otherwise, according to Eq. (3) we cannot distinguish the eigenvalues [30]

$$E_k=E+\frac{2\pi k}{\Delta t}\quad(k=1,2,\dots). \qquad (5)$$

TABLE II. Comparison of time-dependent equations.

	Equation	Homogeneous	Inhomogeneous
Classical mechanics	Newton	Harmonic oscillator	Forced oscillator [37–41]
Quantum mechanics	Schrödinger	TDSE [22–27,29,31,32,35]	Particle source [28]

In the following, we evaluate T for homogeneous and inhomogeneous Schrödinger equations to calculate the real-time Green's functions at many frequencies, $\omega_l = l \Delta \omega$, $l = 0, \pm 1, \pm 2, \ldots$, within a required relative accuracy δ. It turns out that T of inhomogeneous equations can be much longer than that of homogeneous equations. This conclusion applies to the calculation of the linear response functions also.

First let us try to calculate the Green's function by solving the homogeneous equation,

$$i \frac{d}{dt} |\phi; t\rangle = H |\phi; t\rangle, \tag{6}$$

with the initial condition $|\phi; t=0\rangle = |j\rangle$. The auxiliary vectors are calculated as

$$|\widetilde{\phi}_l; T\rangle = (-i) \int_0^T dt' |\phi; t'\rangle e^{+i(\omega_l + i\eta)t'}, \tag{7}$$

$$= (-i) \int_0^T dt' e^{-iHt'} |j\rangle e^{+i(\omega_l + i\eta)t'}, \tag{8}$$

$$= \frac{1}{\omega_l + i\eta - H} [1 - e^{i(\omega_l + i\eta - H)T}] |j\rangle, \tag{9}$$

$$\approx \frac{1}{\omega_l + i\eta - H} |j\rangle, \tag{10}$$

$$= G(\omega_l + i\eta) |j\rangle, \tag{11}$$

where we have neglected the second term of Eq. (9) by assuming T is large enough so that $e^{-\eta T} < \delta$. Therefore, we estimate M for the homogeneous equation as

$$M_1 \approx \frac{T}{\Delta t} = \frac{-\ln \delta}{\eta \Delta t}. \tag{}$$

Next let us calculate the Green's function by solving the inhomogeneous Schrödinger equation,

$$i \frac{d}{dt} |\phi; t\rangle = H |\phi; t\rangle + |j\rangle \left(\sum_{l=-L}^{L} e^{-i(\omega_l + i\eta)t} \right) \theta(t), \tag{12}$$

with the initial condition $|\phi; t=0\rangle = 0$. The solution at large T becomes

$$|\phi; T\rangle \approx \sum_l G(\omega_l + i\eta) |j\rangle e^{-i(\omega_l + i\eta)T}, \tag{13}$$

where T satisfies $e^{-\eta T} \ll \delta$. Then the auxiliary vectors $|\widetilde{\phi}_l; T_2\rangle$ are defined as

$$|\widetilde{\phi}_{l'}; T_2\rangle = \frac{1}{T_2} \int_0^{T_2} dt' |\phi; t\rangle e^{+i(\omega_{l'} + i\eta)t'}$$

$$= \frac{1}{T_2} \int_0^{T_2} dt' \sum_l G(\omega_l + i\eta) |j\rangle e^{-i(\omega_l - \omega_{l'})t'}, \tag{14}$$

$$= G(\omega_{l'} + i\eta) |j\rangle$$

$$+ \sum_{l \neq l'} G(\omega_l + i\eta) |j\rangle \frac{i[e^{-i(\omega_l - \omega_{l'})T_2} - 1]}{T_2(\omega_l - \omega_{l'})}, \tag{15}$$

$$\approx G(\omega_{l'} + i\eta) |j\rangle, \tag{16}$$

where we have neglected the second term of Eq. (15) by assuming that T_2 is large enough so that $T_2 \Delta \omega \gg 1/\delta$. Therefore, M becomes

$$M_2 \approx \frac{1}{\Delta \omega \Delta t \delta}, \tag{17}$$

which can be much larger than M_1 when $\Delta \omega$ is small.

III. NONINTERACTING ELECTRONS

In this section, we apply the time-dependent homogeneous Schrödinger equation to efficiently calculate the linear response functions and density of states of noninteracting electron systems, since it is well known that there exist wide and practically important areas in condensed matter physics where noninteracting electron models are useful to predict various physical properties. Hereafter we assume that the system is described by the one-electron Hamiltonian,

$$H = \frac{1}{2} \vec{p}^2 + V(\vec{r}). \tag{18}$$

A. Linear response function

For noninteracting electrons, the linear response function (4) can be rewritten by using the one-particle eigenstates as [36]

$$\chi_{BA}(\omega) = \sum_{E_i \leq E_f, E_j > E_f} \frac{\langle i|B|j\rangle \langle j|A|i\rangle}{(\omega + i\eta) - (E_j - E_i)}$$

$$- \sum_{E_i \leq E_f, E_j > E_f} \frac{\langle i|A|j\rangle \langle j|B|i\rangle}{(\omega + i\eta) + (E_j - E_i)}, \tag{19}$$

where E_f is the Fermi energy, and $|i\rangle$ and $|j\rangle$ are the occupied and empty one-particle states, respectively. This formula can be rewritten again in time-dependent representation as

$$\chi_{BA}(\omega + i\eta) \tag{20}$$

$$= (-i)\int_0^T dt \sum_{\substack{E_i \leqslant E_f \\ E_j > E_f}} e^{+i(\omega + i\eta)t}$$

$$\times \{\langle i|e^{+iHt}Be^{-iHt}|j\rangle\langle j|A|i\rangle - \text{c.c.}\}, \tag{21}$$

$$= (-i)\int_0^T dt \sum_{E_i,E_j} e^{+i(\omega + i\eta)t}$$

$$\times \{\langle i|\theta(E_f - H)e^{+iHt}Be^{-iHt}\theta(H - E_f)|j\rangle$$

$$\times \langle j|A|i\rangle - \text{c.c.}\}, \tag{22}$$

$$= \left\langle\!\!\left\langle \int_0^T dt\, e^{+i(\omega + i\eta)t}K(t) \right\rangle\!\!\right\rangle, \tag{23}$$

where the double brackets indicate the statistical average over random vectors $|\Phi\rangle$ and $K(t)$ is the time correlation function defined by

$$K(t) = 2\ \text{Im}\langle\Phi|\theta(E_f - H)e^{+iHt}Be^{-iHt}\theta(H - E_f)A|\Phi\rangle. \tag{24}$$

Equations (23) and (24) are the main result of this paper. Note that calculating the trace over the initial states $|i\rangle$ by using random vectors reduces the computational effort by a factor of N. As the result, the computational effort still remains $O(N)$ in spite of the double summation in Eq. (19).

In the above equations, we have introduced several numerical techniques. First, the time-dependent state vectors,

$$e^{-iHt}\theta(H - E_f)A|\Phi\rangle$$

$$e^{-iHt}\theta(E_f - H)|\Phi\rangle \tag{25}$$

are calculated by the leap frog method [22–25,28]

$$|\phi;t + \Delta t\rangle = -2i\Delta tH|\phi;t\rangle + |\phi;t - \Delta t\rangle, \tag{26}$$

where the Hamiltonian matrix is discretized by finite difference [20,21]

$$\frac{\partial^2\phi}{\partial x^2} = \sum_{n=-N_{diff}}^{N_{diff}} \frac{1}{\Delta x^2}C_n^{(2)}\phi(x + n\Delta x, y, z) + O(\Delta x^{2N_{diff}}). \tag{27}$$

Due to this discretization, the Hamiltonian matrix becomes sparse and the matrix vector multiplication in Eq. (26) can be done with $O(N)$ computational complexity. We use the $N_{diff} = 4$ formula in this paper.

Second, the matrix step function for a normalized Hermitian matrix X whose eigenvalues X_i are in the range $[-1,1]$ is defined in its eigenstate basis

$$\theta(X) = \sum_{X_i} |X_i\rangle\theta(X_i)\langle X_i|. \tag{28}$$

By using this step function, we can avoid the difficulties in the partial sum in Eq. (20). Operation of this function on an arbitrary vector $|\phi\rangle$ is numerically approximated by the Chebyshev polynomial expansion [9–17],
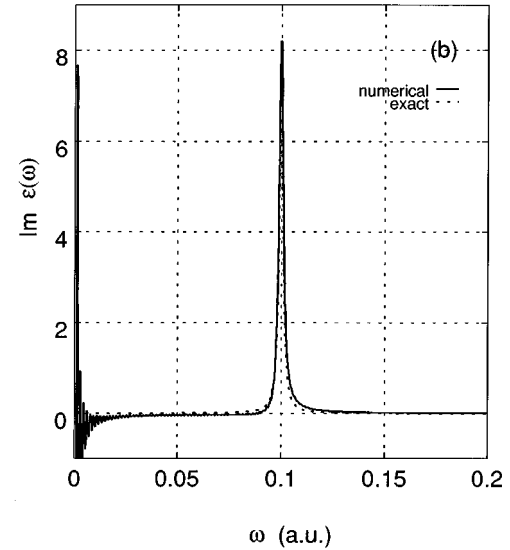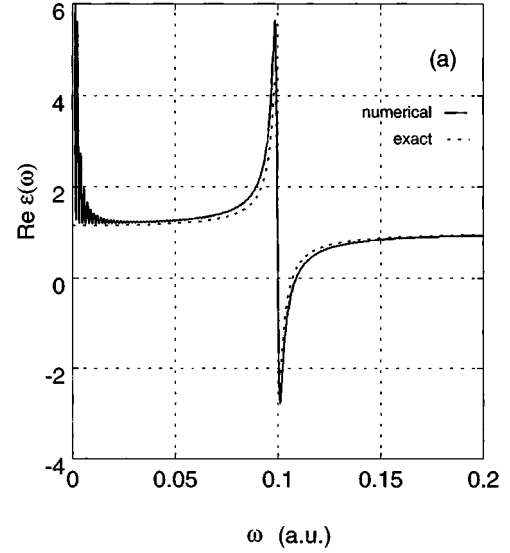

FIG. 1. $\epsilon_{xx}(\omega)$ of four electrons in a three-dimensional harmonic oscillator calculated with 32^3 cubic meshes, $\omega_0 = 0.1$, $\eta = 10^{-4}$; (a) real part, (b) imaginary part.

$$\theta(X)|\phi\rangle \approx \sum_{k=1}^K c_k T_{k-1}(X)|\phi\rangle, \tag{29}$$

where each term on the right-hand side is calculated by vector recursion formulas

$$T_0(X)|\phi\rangle = |\phi\rangle, \tag{30}$$

$$T_1(X)|\phi\rangle = X|\phi\rangle, \tag{31}$$

$$T_{n+1}(X)|\phi\rangle = 2XT_n(X)|\phi\rangle - T_{n-1}(X)|\phi\rangle \quad n \geqslant 1. \tag{32}$$

To use this matrix function in Eq. (25), we should normalize the Hamiltonian matrix so that $X = (H - E_f)/E_{norm}$ has eigenvalues in the range $[-1,1]$.

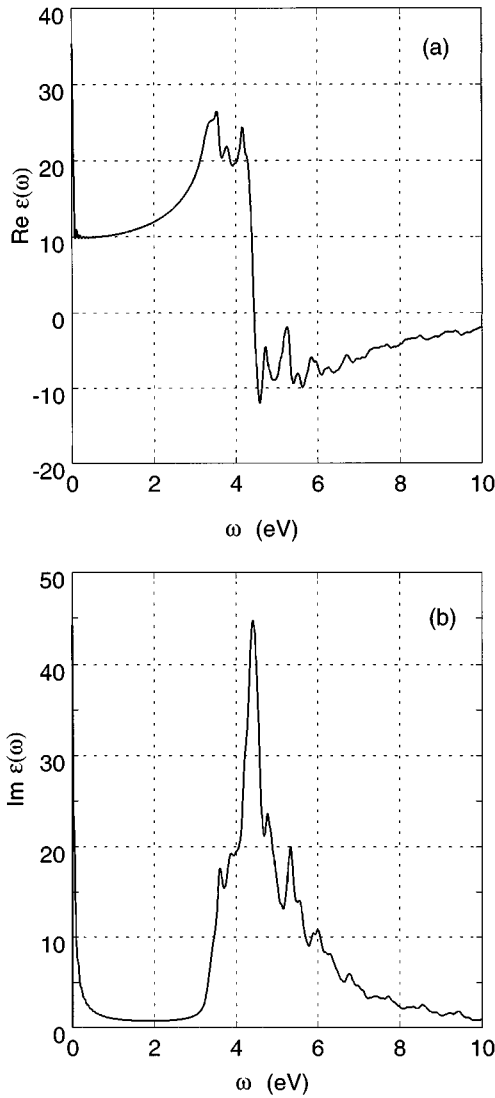Thirdly, we define random vectors with random phase by

FIG. 2. $\epsilon_{xx}(\omega)$ of silicon crystal consisting of 2^{15} Si atoms in a cubic supercell of 16^3 unit cells. Each unit cell is divided into 8^3 cubic meshes. The energy resolution is $\eta = 0.05$ eV. We used the empirical local pseudopotential in Ref. [14]. (a) real part, (b) imaginary part.

$$|\Phi\rangle = \sum_{n=1}^{N} |n\rangle e^{+i\phi_n}, \qquad (33)$$

where $|n\rangle$ are basis vectors and $-\pi < \phi_n \leq \pi$, $(n = 1, \ldots, N)$ are uniform random variables that satisfy $\langle\langle e^{-i\phi_{n'}} e^{i\phi_n}\rangle\rangle = \delta_{n'n}$. Then we can derive various useful identities such as

$$\langle\Phi|\Phi\rangle = \sum_n \langle\Phi|n\rangle\langle n|\Phi\rangle = \sum_n e^{-i\phi_n} e^{i\phi_n} = N, \quad (34)$$

$$\langle\langle|\Phi\rangle\langle\Phi|\rangle\rangle = \sum_{n'n} |n'\rangle\langle\langle e^{-i\phi_{n'}} e^{i\phi_n}\rangle\rangle\langle n|$$

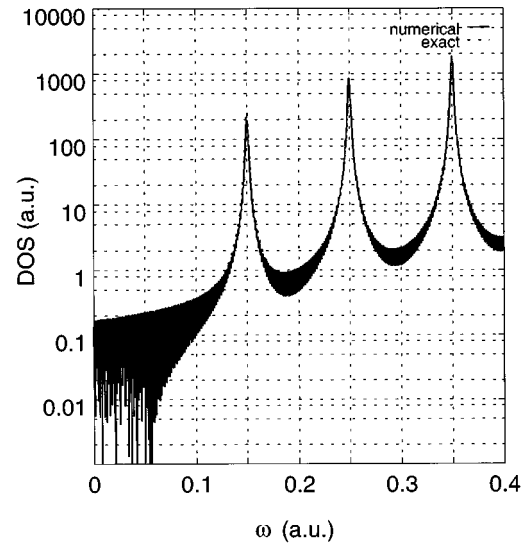$$= \sum_n |n\rangle\langle n| = I, \qquad (35)$$

FIG. 3. Density of states of 3D harmonic oscillator calculated with 32^3 cubic meshes, $\omega_0 = 0.1$, and $\eta = 10^{-4}$, and analytical result.

$$\langle\langle\langle\Phi|A|\Phi\rangle\rangle\rangle = \sum_{n,n'} \langle\langle e^{i(\phi_n - \phi_{n'})}\rangle\rangle\langle n'|A|n\rangle$$

$$= \sum_n \langle n|A|n\rangle = \text{tr}[A] = \sum_{E_m} \langle E_m|A|E_m\rangle. \qquad (36)$$

Equation (34) shows that each random vector is normalized to N, the number of one-particle eigenstates. Equation (35) shows that random vectors have normalized completeness. Equation (36) shows that the expectation value of an operator by random vectors gives the trace of the operator. We used this identity to calculate the trace over $|i\rangle$ in Eqs. (23) and (24). These random vectors with random *phase* are more
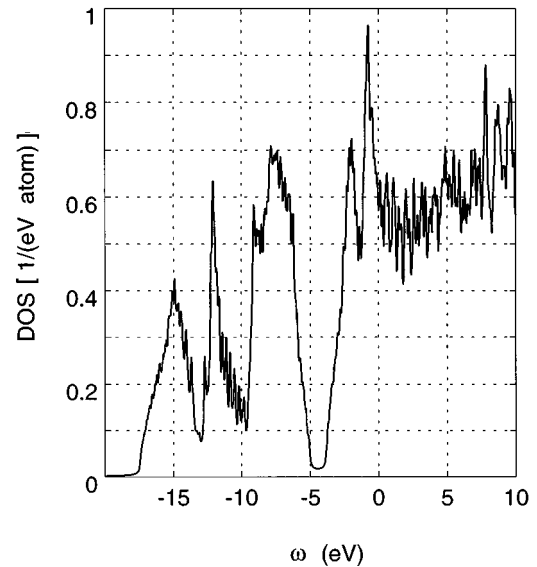

FIG. 4. Density of states of silicon crystal consisting of 2^{15} Si atoms in 16^3 unit cells. Each unit cell is divided into 8^3 cubic meshes. The energy resolution is $\eta = 0.05$ eV.
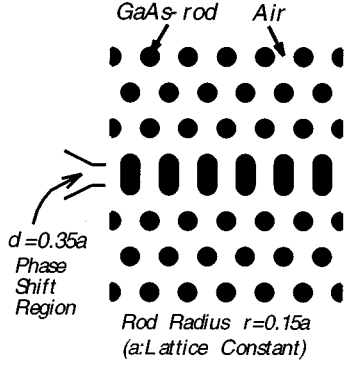
FIG. 5. A typical structure of two-dimensional photonic crystal cavities used in our calculation.

useful in calculating expectation values than random vectors with random *amplitude* since each random vectors are automatically normalized.

Finally the formula for numerical calculation of polarizability function $\chi_{\beta\alpha}(\omega)$ with $\alpha,\beta=x,y,z$ becomes

$$\chi_{\beta\alpha}(\omega)\approx\left\langle\left\langle\int_0^T dt\ e^{-\eta t}(e^{+i\omega t}-\delta_{\beta\alpha})K(t)\right\rangle\right\rangle, \quad (37)$$

$$K(t)=\frac{-2}{V(\omega+i\eta)^2}\mathrm{Im}\langle\Phi|\theta(E_f-H)e^{+iHt}p_\beta e^{-iHt}$$
$$\times\theta(E_{cut}-H)\theta(H-E_f)p_\alpha|\Phi\rangle, \quad (38)$$

where V is the volume of the supercell, and the dipole moment operators

$$\langle j|A|i\rangle=\langle j|x_\alpha|i\rangle, \quad (39)$$

$$\langle i|B|j\rangle=\frac{-1}{V}\langle i|x_\beta|j\rangle, \quad (40)$$

are modified to momentum operators by partial integration. We also inserted a low energy projection operator $\theta(E_{cut}-H)$ into Eq. (38) to eliminate unphysical high energy components of the random vectors. This filter is much more effective than the quadratic filter used in [14]. In calculating very large systems, we need only few random vectors for statistical averaging, since the fluctuation becomes smaller as the system size N becomes larger [28].

Figure 1 shows the dielectric function $\epsilon_{xx}(\omega)=1+4\pi\chi_{xx}(\omega)$ of four electrons in the three-dimensional (3D) harmonic potential

$$V(\vec{r})=\frac{(\omega_0 r)^2}{2} \quad (41)$$

calculated with 32^3 cubic meshes, $\omega_0=0.1$, $\eta=10^{-4}$. Three random vectors are used. The analytical result [42]

$$\epsilon_{xx}(\omega)=1+\frac{4\pi N_e}{V}\frac{1}{\omega_0^2-\omega^2-i\omega\eta} \quad (42)$$

is also shown for comparison, where N_e is the number of electrons in the supercell of volume V. The deviation from
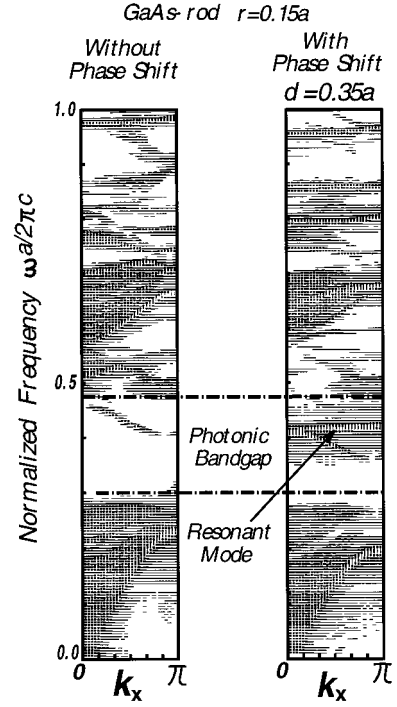

FIG. 6. Calculated density of states as a function of frequency and wave number.

the exact result near $\omega=0$ is due to finite η. The result shows that our method works very well for $\omega\gg\eta$.

Figure 2 shows the dielectric function with energy resolution $\eta=0.05$ eV of silicon crystal consisting of 2^{15} Si atoms in a cubic supercell of 16^3 unit cells. Each unit cell is divided into 8^3 cubic meshes. One random vector is used. We used the empirical local pseudopotential in Ref. [43]. The result agrees with experimental results and other theoretical calculations [44,45].

In some cases we may want to ask which part of the real space the electrons contributing to the linear response function come from. We can answer this question by calculating the linear response function by restricting the range of the trace in Eq. (37) within a real space domain D. This can be done by replacing $|\Phi\rangle$ by $|\Phi'\rangle=P_D|\Phi\rangle$, where $P_D=\Sigma_{n\in D}|n\rangle\langle n|$ is the real space projection operator onto D.

B. Density of states

The density of states of the system can be calculated as [32]

$$\rho(\omega)=\frac{-1}{\pi}\sum_n\mathrm{Im}\ G_{nn}(\omega+i\eta)=\frac{-1}{\pi}\mathrm{Im}\{\mathrm{tr}[G(\omega+i\eta)]\} \quad (43)$$

by combining Eqs. (11) and (36).

Figure 3 shows the numerical and analytical results of the density of states in the 3D harmonic potential with 32^3 cubic meshes, $\omega_0=0.1$, and $\eta=10^{-3}$. Three random vectors are used. Figure 4 shows the density of states of silicon crystal consisting of 2^{15} Si atoms in a cubic supercell of 16^3 unit

cells. Each unit cell is divided into 8^3 cubic meshes. The energy resolution is $\eta = 0.05$ eV. Three random vectors are used.

We can also calculate the *local* density of states integrated in a given domain D by using the real space projection operator P_D to restrict the summation in Eq. (33) within D,

$$\rho_D(\omega) = \frac{-1}{\pi} \sum_{n \in D} \text{Im } G_{nn}(\omega + i\eta)$$

$$= \frac{-1}{\pi} \text{Im} \{ \text{tr} [P_D G(\omega + i\eta)] \}. \qquad (44)$$

Photonic band structures in two-dimensional periodic structure of dielectric material [46–48] can also be calculated by using Eqs. (43) or (44) since the Maxwell equations of this system are reduced to the Schrödinger equation with position dependent mass, i.e.,

$$\mathcal{H} H_z(x,y) = \frac{\omega^2}{c^2} H_z(x,y) = E H_z(x,y), \qquad (45)$$

$$\mathcal{H} = \frac{\partial}{\partial x} \frac{-1}{\epsilon(x,y)} \frac{\partial}{\partial x} + \frac{\partial}{\partial y} \frac{-1}{\epsilon(x,y)} \frac{\partial}{\partial y}, \qquad (46)$$

for H mode, where H_z is the z component of the magnetic field, and

$$\mathcal{H} E_z(x,y) = \frac{\omega^2}{c^2} E_z(x,y) = E E_z(x,y), \qquad (47)$$

$$\mathcal{H} = \frac{-1}{\epsilon(x,y)} \left\{ \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right\} \qquad (48)$$

for E mode, where E_z is the z component of the electric field.

Figure 5 shows a typical structure of two-dimensional photonic crystal cavities used in our calculation, and Fig. 6 shows the calculated density of states as a function of the frequency and wave number.

IV. SUMMARY

In this paper we proposed a numerical method suitable for calculating the linear response functions (and the density of states) of noninteracting electrons, in which the sum over the initial one-particle states is efficiently calculated by using random vectors. The advantage of this method, compared to the Chebyshev polynomial method by Wang and Zunger to calculate optical absorption of noninteracting electrons [14], is that our method can calculate not only the imaginary part but also the real part of the linear response functions at the same time, and that it can calculate them without any input output (I/O) of state vectors on external storage. As a result, our method can calculate much larger systems than Wang's method. The Chebyshev polynomial method of degree M should store $O(M)$ state vectors of size $O(N)$ on external storage to make the table of $O(M^2)$ generalized Chebyshev moments $\Lambda_{m,m'}$ and may take a very long I/O time. The application of this method to photonic band structures, silicon nanocrystallites, and periodic structures of chaotic systems will be presented elsewhere [49–51].

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