

# Efficient scheme to calculate Green functions by recursive polynomial expansion

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A general scheme is introduced to evaluate the Green function by recursive polynomial expansion. This scheme has the following advantages: (1) it is possible to calculate both the diagonal and off-diagonal elements of the Green function, and also their products with other quantum operators, (2) energy spectrum can be obtained with any desired resolution by controlling the expansion order, (3) it is applicable to the system with discrete eigenstates, and (4) integrated density of states, eigenvalues, and corresponding eigenvector, can be obtained by the same algorithm. It is also suitable for vector and parallel processing, and required CPU time and memory size are proportional only to the system size (*i.e.* ordered  $N$ ). Applications are made to simple lattice systems for demonstration.

## 1. Introduction

In order to evaluate physical properties of a system described by a large Hamiltonian matrix, several methods have been proposed. It is required for these methods that one can avoid the direct diagonalization of the Hamiltonian, and that the required computer resources are proportional to the system size (*i.e.* ordered  $N$ ). Among these methods, the recursion method<sup>1)</sup> has been most commonly used and found a great variety of applications. The method has however some ambiguity due to the terminator, and suffers from unphysical oscillation in the Green function at high expansion orders.

Recent approaches of the time-dependent method, such as the forced oscillator method (FOM)<sup>2-4)</sup> and the time-dependent Schrödinger equation (TDSE) method,<sup>5-7)</sup> are free from those unphysical features mentioned above, and provide more accurate schemes. They follow the time development of the system numerically, and evaluate several physical properties in the time domain.

On the other hand, recursive approaches based on the Tchebycheff polynomials have been proposed by many researchers.<sup>8)</sup> They expand important functions, such as the delta<sup>9,10)</sup> and Green function,<sup>11)</sup> by the set of the Tchebycheff polynomials, and evaluate physical properties in the energy domain.

In this paper, we extend the Tchebycheff polynomial method, and introduce a general scheme to evaluate the Green function by recursive polynomial expansion. To demonstrate the efficiency of the scheme, we applied it to simple square lattice systems in two dimension. It is shown that the Green functions are evaluated with sufficient accuracy even when the spectrum has a strong discrete nature.

## 2. Calculation scheme

### 2.1 General theory

The basic idea of this method is to expand the Green function by a set of orthogonal polynomials  $\{\phi_n(x)\}$ , which satisfies

the following orthogonality and completeness conditions,

$$\int_{-\infty}^{\infty} W(x)\phi_n^*(x)\phi_m(x)dx = w_n\delta_{nm}, \quad (1)$$

$$\delta(x - x_0) = \sum_{n=0}^{\infty} \frac{W(x)}{w_n} \phi_n^*(x)\phi_n(x_0). \quad (2)$$

There always exists a three-term recurrence formula in the form,

$$\phi_{n+1}(x) = b_n(x - a_n)\phi_n(x) - c_{n-1}\phi_{n-1}(x), \quad (3)$$

for these kind of polynomials. Let us consider to expand the Green function by the set of polynomials  $\{\phi_n(x)\}$  as,

$$\begin{aligned} G(E + i\eta) &= \frac{1}{E + i\eta - H} \\ &= \sum_{n=0}^{\infty} \frac{1}{w_n} C_n(E + i\eta)\phi_n(H). \end{aligned} \quad (4)$$

The expansion coefficient  $C_n(E + i\eta)$  is given by the integration,

$$C_n(E + i\eta) = \int_{-\infty}^{\infty} W(x) \frac{1}{E + i\eta - H} \phi_n^*(x) dx. \quad (5)$$

When using the above set of polynomials, we can separate the integration into the parts with and without singularity, and reduce it elemental one;

$$\begin{aligned} C_n(E + i\eta) &= \left[ \int_{-\infty}^{\infty} \frac{W(x)}{E + i\eta - H} dx \right] \phi_n^*(E + i\eta) \\ &\quad + \psi_n(E + i\eta), \end{aligned} \quad (6)$$

where  $\psi_n(x)$  is the polynomial which satisfies the recurrence formula (3),

$$\psi_{n+1}(x) = b_n(x - a_n)\psi_n(x) - c_{n-1}\psi_{n-1}(x), \quad (7)$$

with  $\psi_0(x) = 0$  and  $\psi_1(x) = 1$ . Then the coefficient  $C_n(x)$  is no more a polynomial, but also satisfies the same recurrence formula,

$$C_{n+1}(x) = b_n(x - a_n)C_n(x) - c_{n-1}C_{n-1}(x). \quad (8)$$

For several orthogonal polynomials, the integration of the first term in Eq. (6) can be done analytically, and we can obtain the expansion coefficients  $C_n(E + i\eta)$  in Eq. (4) in the analytic form. Some examples are shown in the following section.

Note that the Green function is separated into the energy dependent part ( $C_n(E)$ ) and the system dependent part ( $\phi_n(H)$ ) in these equations. For each choice of a polynomial, the coefficient  $C_n(E)$  is a universal function independent of the system, and one needs to calculate it only once and for all.

## 2.2 Relation to time dependent approach

There is a close approach to our method, which evaluates several physical properties by using the time-development operator  $e^{-iHt}$  expanded by a set of polynomials  $\{\phi_n(H)\}$  in the form,<sup>12-14)</sup>

$$e^{-iHt} = \sum_{n=0}^{\infty} C'_n(t) \phi_n(H). \quad (9)$$

Our method is related to it through a Fourier transformation of the expansion coefficients  $C'_n(t)$  and  $C_n(E)$  as,

$$C_n(E) = -i \int_{-\infty}^{\infty} \theta(t) C'_n(t) e^{iEt} dt, \quad (10)$$

where  $\theta(t)$  is the step function. This is trivial from the relation,

$$G(E) = -i \int_{-\infty}^{\infty} \theta(t) e^{-iHt} e^{iEt} dt. \quad (11)$$

## 2.3 Expansion by Hermite polynomials

The Hermite polynomial  $H_n(x)$  is defined in the infinite range  $[-\infty, \infty]$  by Rodrigues' formula,

$$H_n(x) = (-)^n e^{\frac{x^2}{2}} \left( \frac{d}{dx} \right)^n e^{-\frac{x^2}{2}}, \quad (12)$$

and satisfies the orthogonality,

$$\int_{-\infty}^{\infty} e^{-\frac{x^2}{2}} H_n^*(x) H_m(x) dx = n! \sqrt{2\pi} \delta_{nm}. \quad (13)$$

According to Eqs. (4) and (6), the Green function is expanded by the Hermite polynomials into the form,

$$G(E) = \lim_{N \rightarrow \infty} \sum_{n=0}^N C_n^H(E) H_n(H), \quad (14)$$

$$C_n^H(E) = \frac{1}{n! \sqrt{2\pi}} \times \left[ e^{-\frac{x^2}{2}} \left\{ \frac{\pi}{i} \text{Erf} \left( i \frac{E}{\sqrt{2}} \right) - i\pi \right\} H_n(E) - \mathcal{H}_n(E) \right], \quad (15)$$

where  $\text{Erf}(z)$  is the error function and  $\mathcal{H}_n(x)$  is the polynomial obtained from the same recurrence formula that the Hermite polynomial satisfies, with  $\mathcal{H}_0(x) = 0$  and  $\mathcal{H}_1(x) = 1$ .

## 2.4 Expansion by Jacobi polynomials

The Jacobi polynomial  $P_n^{(\alpha, \beta)}(x)$  is defined in the finite range  $[-1, 1]$  by Rodrigues' formula,

$$P_n^{(\alpha, \beta)}(x) = \frac{(-)^n}{2^n n!} (1-x)^{-\alpha} (1+x)^{-\beta}$$

$$\times \left( \frac{d}{dx} \right)^n \left\{ (1-x)^{n+\alpha} (1+x)^{n+\beta} \right\}, \quad (16)$$

and satisfies the orthogonality,

$$\int_{-1}^1 W^{(\alpha, \beta)}(x) P_n^{(\alpha, \beta)*}(x) P_m^{(\alpha, \beta)}(x) dx = w_n^{(\alpha, \beta)} \delta_{nm}, \quad (17)$$

where  $W^{(\alpha, \beta)}(x)$  and  $w_n^{(\alpha, \beta)}$  are the weight function and normalization integral defined as,

$$W^{(\alpha, \beta)}(x) = (1-x)^\alpha (1+x)^\beta, \quad (18)$$

$$w_n^{(\alpha, \beta)} = \frac{2^{\alpha+\beta+1}}{2n+1} \frac{\Gamma(n+\alpha+1)\Gamma(n+\beta+1)}{n!\Gamma(n+\alpha+\beta+1)}. \quad (19)$$

When expanding the Green function by the Jacobi polynomials, we have to use the rescaled energy parameter  $\tilde{E}$  and Hamiltonian matrix  $\tilde{H}$  so that the eigenvalues lie within the range  $[-1, 1]$ , because the Jacobi polynomials are defined in this range. The rescaled energy and Hamiltonian are given by,

$$\tilde{E} = \frac{E-a}{2b}, \quad \tilde{H} = \frac{H-aI}{2b}, \quad (20)$$

where  $I$  is the unit matrix, and the parameters  $a$  and  $4b$  are to be so chosen that they roughly correspond to the band center and the band width, respectively. However these parameters are arbitrary as far as the eigenvalues of the original Hamiltonian  $H$  lie within the range  $[a-2b, a+2b]$ . The result of the calculations is very insensitive to the choice of the parameters. This implies a great advantage over the recursion method that we need not know the positions of the exact band edges prior to the calculation. Hereafter, we use  $E$  and  $H$  instead of  $\tilde{E}$  and  $\tilde{H}$  for convenience.

According to Eqs. (4) and (6), the Green function is expanded by the Jacobi polynomials as,

$$G(E + i\eta) = \sum_{n=0}^{\infty} \frac{1}{w_n^{(\alpha, \beta)}} C_n^{(\alpha, \beta)}(E + i\eta) P_n^{(\alpha, \beta)}(H), \quad (21)$$

$$C_n^{(\alpha, \beta)}(E) = -\frac{2^{\alpha+\beta+1} B(\alpha+1, \beta+1)}{1-E} \times {}_2F_1(1, \beta+1; \alpha+\beta+2; \frac{2}{1-E}) P_n^{(\alpha, \beta)}(E) - Q_n^{(\alpha, \beta)}(E), \quad (22)$$

where  $B(\alpha, \beta)$  and  ${}_2F_1(1, \alpha+1; \alpha+\beta+2; z)$  are the beta function and the hypergeometric function, respectively. The functions  $Q_n^{(\alpha, \beta)}(x)$  are the polynomials obtained from the same recurrence formula that the Jacobi polynomials satisfy, with  $Q_0^{(\alpha, \beta)}(x) = 0$  and  $Q_1^{(\alpha, \beta)}(x) = 1$ .

We introduce two special cases of the Jacobi polynomial for the practical calculation. When choosing  $\alpha = \beta = 0$ , the Jacobi polynomial becomes the Legendre polynomial, and Eqs. (21) and (22) are reduced to

$$G(E) = \lim_{N \rightarrow \infty} \sum_{n=0}^N C_n^L(E) P_n(H), \quad (23)$$

$$C_n^L(E) = \frac{2n+1}{2} \{2\text{Re}Q_n(E+i0) - i\pi P_n(E)\}, \quad (24)$$

where  $Q_n(z)$  is the Legendre function of the second kind. This function appears in relation to  $Q_n^{(\alpha,\beta)}(z)$ , but the definition is different for historical reasons.

On the other hand, when choosing  $\alpha = \beta = -\frac{1}{2}$ , the Jacobi polynomial becomes the Tchebycheff polynomial, and Eqs. (21) and (22) are reduced to

$$G(E) = \lim_{\mathcal{N} \rightarrow \infty} \sum_{n=0}^{\mathcal{N}} C_n^T(E) T_n(H), \quad (25)$$

$$C_n^T(E) = \frac{2 - \delta_{n0}}{\sqrt{1-E^2}} \{-U_n(E) - iT_n(E)\}, \quad (26)$$

where  $U_n(x)$  is the Tchebycheff function of the second kind.

### 3. Practical calculations

#### 3.1 Calculation of matrix elements

In the practical calculation of the Green function matrix elements, we evaluate the state vector

$$G(E)|j\rangle = \lim_{\mathcal{N} \rightarrow \infty} \sum_{n=0}^{\mathcal{N}} \frac{1}{w_n} C_n(E) \phi_n(H)|j\rangle \quad (27)$$

for basis vectors  $|j\rangle$  representing the Hamiltonian. Since the coefficients  $C_n(E)$  are universal functions, the central part of the calculation is the evaluation of the vector  $\phi_n(H)|j\rangle$ . This can be performed by successive operations of the Hamiltonian  $H$  according to the recursive formula (3). It is notable that we obtain not only the diagonal elements, but also the off-diagonal elements of the Green function by this procedure. The infinite summation in Eq. (27) must be truncated at some finite order  $\mathcal{N}$ , and it determines the resolution of the whole energy spectrum through the energy separation of the nodes for  $\phi_{\mathcal{N}}(E)$ . Thus the energy resolution can be controlled explicitly.

In this method, we can also evaluate the product of the Green function and other quantum operator  $A$  such as  $\langle i|\dots G(E)AG(E)|j\rangle$ , by choosing the initial state  $|j\rangle$  in Eq. (27) as  $|j'\rangle = AG(E)|j\rangle$  and repeating the procedure described above. Thus we can extend the present scheme to the calculation of various physical properties.

#### 3.2 DOS and Integrated DOS

The densities of states (DOS) is evaluated by taking the trace of the Green function, and it is given by,

$$n(E) = \sum_{n=0}^{\infty} \frac{W(E)}{w_n} \phi_n(E) \sum_{j=1}^N \langle j|\phi_n(H)|j\rangle, \quad (28)$$

where  $N$  is the total number of basis vectors. The integrated DOS  $N(\tilde{E})$  is obtained by integrating the above equation as,

$$N(E) = \sum_{n=0}^{\infty} \int_{-\infty}^E \frac{W(x)}{w_n} \phi_n(x) dx \times \sum_{j=1}^N \langle j|\phi_n(H)|j\rangle. \quad (29)$$

The integration involved in the above expression is readily performed analytically by using Rodrigues' formula (12) and (16) for the case of the Hermite polynomial,

$$N(E) = N \left[ \frac{1}{2} + \frac{1}{\sqrt{\pi}} \text{Erf} \left( \frac{E}{\sqrt{2\pi}} \right) \right] - \sum_{n=1}^{\infty} \frac{1}{n! \sqrt{2\pi}} e^{-\frac{E^2}{2}} H_{n-1}(E) \sum_{j=1}^N \langle j|H_n(H)|j\rangle, \quad (30)$$

and for that of the Jacobi polynomials,

$$N(E) = N \frac{B_{\frac{1+E}{2}}(\alpha+1, \beta+1)}{B(\alpha+1, \beta+1)} - \sum_{n=1}^{\infty} \frac{1}{2nw_n^{(\alpha,\beta)}} (1-E)^{(\alpha+1)} (1+E)^{(\beta+1)} \times P_{n-1}^{(\alpha+1, \beta+1)}(E) \sum_{j=1}^N \langle j|P_n^{(\alpha,\beta)}(H)|j\rangle, \quad (31)$$

where  $B_x(\alpha+1, \beta+1)$  is the incomplete beta function.

Thus the integrated DOS  $N(E)$  is obtained without further effort in our scheme. Note that it is conserved to the number of eigenvalues at the upper edge of the domain in which polynomials are defined, even though the infinite summation is truncated at any order in Eqs. (30) and (31).

#### 3.3 Eigenvectors

We can also evaluate the eigenvector  $|E_n\rangle$  corresponding to an eigenvalue  $E_n$  in our method. Let us consider a operation,

$$\sum_{n=0}^{\mathcal{N}} \frac{W(E_n)}{w_n} \phi_n(E_n) \phi_n(H)|j\rangle, \quad (32)$$

where  $|j\rangle$  is an arbitrary state vector. The resultant vector becomes proportional to the eigenvector  $|E_n\rangle$ , when the expansion order  $\mathcal{N}$  is taken high enough that each eigenvalue can be resolved.

### 4. Application

To demonstrate the efficiency of the scheme, we apply it to square lattice systems in two dimension. A tight-binding Hamiltonian is employed in which only the nearest neighbor interactions are taken into account with the periodic boundary condition. The Green function is expanded by the Legendre polynomial  $\{P_n(x)\}$ .

Firstly, the method is applied to the  $1000 \times 1000$  square lattice. In order to obtain a smoothed Green function which approximates that for the infinite crystalline system, we truncated the expansion at much lower order ( $\mathcal{N} = 2000$ ) than the number of the system size  $N$ , Figure 1 shows the calculated diagonal element of the Green function (solid line) for the real part (energy is in unit of the nearest neighbor hopping integral). It is compared with the exact solution for the infinite system (dashed line) in the same figure. The calculated result well approximate the exact one, and we can hardly distinguish them.

There the result is also compared with that of the recursion

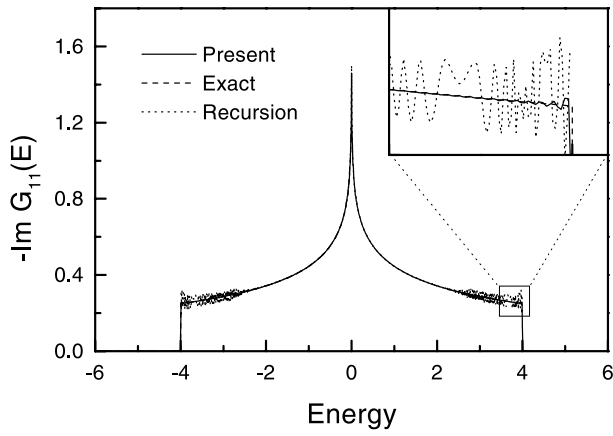


Fig. 1. Imaginary part of the Green function  $G_{ij}(E)$  calculated for the  $1000 \times 1000$  square lattice system in two dimension. The Legendre polynomials are used in the calculation, and the expansion order is 2000. It is compared with the exact solution (dashed line) for the infinite crystalline system, and with the calculated result by the recursion method (dotted line) with the expansion order of 800.

method with the expansion order (*i.e.* the number of recursive steps) of 800 (dotted line). The comparison is limited to the range of  $[-4, 4]$ , because the recursion method does not work outside the energy band. Although the expansion order is much lower than that used in the present scheme, there already appears oscillation around the band edge. As is well known, this spurious oscillation is due to the “over-expansion” of the recursive basis orbitals beyond the cluster boundary, which starts to occur around the expansion order of 500 in the present system.

Also in our method, a very fine oscillation is seen to appear at higher expansion orders. This oscillation, however, is not a spurious one and reflects the discrete nature of the eigenvalues of the finite cluster.

In order to confirm this point, we have calculated the DOS of a much smaller system of  $4 \times 4$  square lattice with the expansion order of 1000. The result is plotted in Fig. 2 and compared to the exact result of

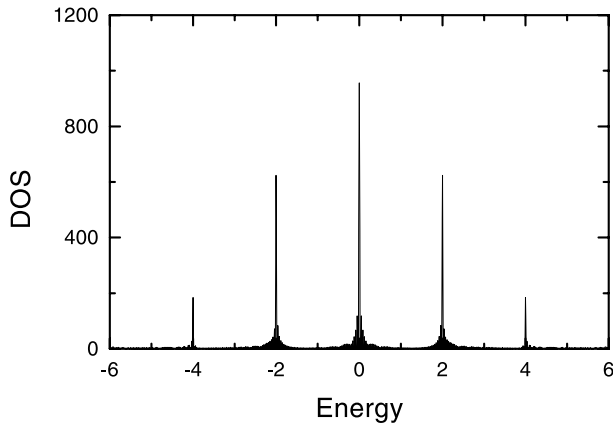


Fig. 2. DOS calculated for the  $4 \times 4$  square lattice system. The Legendre polynomials are used in the calculation, and the expansion order is 1000.

$$n(E) = \delta(E + 4) + 4\delta(E + 2) + 6\delta(E) + 4\delta(E - 2) + \delta(E - 4). \quad (33)$$

The calculated DOS reproduces the discrete structure of the exact one (33) fairly well, and we can even identify each eigenvalue from the position of the peak.

Furthermore, the degeneracy of each eigenstate can be determined by calculating the integrated DOS according to Eq. (31). This is illustrated in Fig. 3, and we clearly see that the integrated DOS consists of step functions and increases discontinuously by integer number corresponding to the degeneracy at each eigenvalue.

The corresponding eigenvector  $|E_n\rangle$  can be also evaluated from Eq. (32). In Fig. 4, we plot the root mean square of error for the calculated eigenvector at  $E = -4$  as a function of expansion order. It decreases monotonically as increasing the expansion order, because the dominant part of the error originates from the contamination of other eigenvectors due to the truncation of the expansion. We can reduce it to a few percent by conducting the summation up to the order of ten times of a system size  $N$ .

These calculations show that the present scheme can be used even when the DOS has discrete spectrum or singular points,

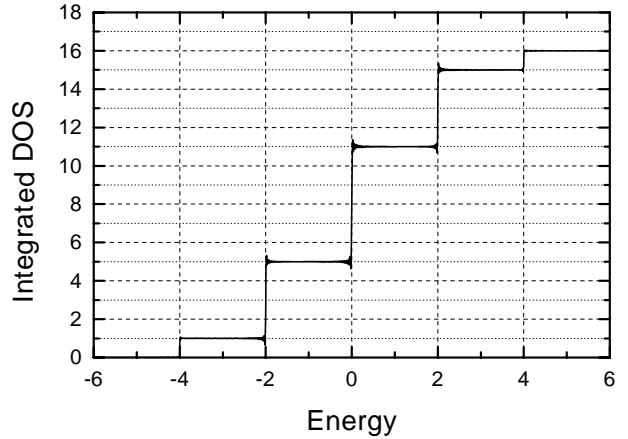


Fig. 3. Integrated DOS calculated for the  $4 \times 4$  square lattice system. The Legendre polynomials are used in the calculation, and the expansion order is 1000.

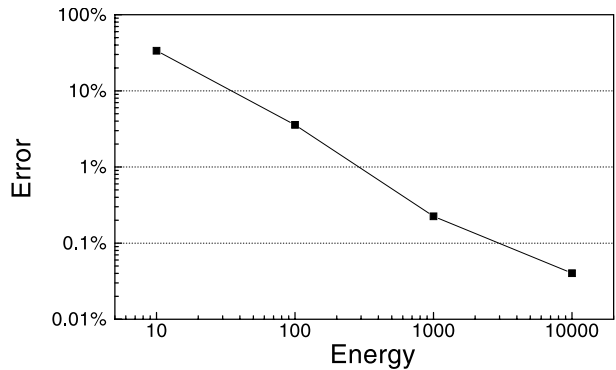


Fig. 4. Root mean square of error for the calculated eigenvector at  $E = -4$  as a function of expansion order.

and will be particularly useful to investigate systems with localized states.

## 5. Summary

In summary, we have introduced a general scheme for calculating the Green function on the basis of polynomial expansion technique. The scheme has several advantages. It is possible to calculate both the diagonal and off-diagonal elements of the Green function, and also their products with other quantum operators. The energy resolution of the spectrum can be controlled explicitly by the expansion order. The integrated density of states, eigenvalues, and eigenvectors can be also obtained in the same algorithm. We applied the scheme to the simple square lattice systems, and showed that it can evaluate the Green function with sufficient accuracy, even though the system has discrete eigenstates.

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