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Numerical Solution Methods for Green Function and Solving the Time Independent Schroedinger Equation

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Abstract: The performances of several methods used for the computation of the free space Green's function for doubly periodic arrays are investigated. Green functions, being the basic entities of a great part of electromagnetic theory.We consider the numerical solutions of Schrodinger equation in quantum physics eigen problems with using of numerical method that exhibit Hamiltonian symmetry. The paper provides an introduction and survey of conservative discretization methods for Green function equations. We make a careful study of these methods, based on accuracy and computing time criteria. We show that none of them is able to fulfil both criteria for a large range of parameters.

Key words: Periodic Hamiltonian, numerical computing, large matrices, green function.

INTRODUCTION

Three-dimensional electromagnetic problems require huge computing resources. One way to go through is to consider periodic structures in order to reduce the investigation domain to one cell of the structure. Many numerical methods, such as integral methods, require the computation of a Green's function. Unfortunately, the more straightforward expressions of periodic Green's functions lead to very slow converging seriesNumerical simulation using computers has increasingly become a very important approach for solving problems in engineering and science. It plays a valuable role in providing tests and examinations for theories, offering insights to complex physics, and assisting in the interpretation and even the discovery of new phenomena.Hamiltonian PDEs arise as models in nuclear physics,meteorology and weather prediction, nonlinear optics, solid mechanics and elastodynamics, oceanography, electromagnetism, cosmology and quantum field theory, for example.

From the physical phenomena observed, mathematical models are established with some possible simplifications and assumptions. These mathematical models are enerally expressed in the form of governing equations with proper boundary conditions (BC) and/or initial conditions (IC). The governing equations may be a set of ordinary differential equations (ODE), partial differential equations (PDE), integration equations or equations in any other possible forms of physical laws. Boundary and/or initial conditions are necessary for determining the field variables in space and/or time.

Numerical Methods:

The Monte Carlo method is a numerical solution to a problem that models objects interacting with other objects or their environment based upon simple object-object or objectenvironment relationships. It represents an attempt to model nature through direct simulation of the essential dynamics of the system in question. In this sense the Monte Carlo method is essentially simple in its approach|a solution to a macroscopic system through simulation of its microscopic interactions (Heikkinen *et al.*, 2008). There are many examples of the use of the Monte Carlo method that can be drawn from social science, trafic flow, population growth, finance, genetics, quantum chemistry, radiation sciences, radiotherapy, and radiation dosimetry but our discussion will concentrate on the simulation of neutrons, photons and electrons being transported in condensed materials, gases and vacuum. We will make brief excursions into other kinds of Monte Carlo methods when they they serve to elucidate some point or when there may be a deeper connection to particle-matter interactions or radiation transport in general (Signell, 2008).

Quantum Monte Carlo methods, which generate the imaginary-time Green's functions, have been successfully used for evaluating thermodynamic quantities of relatively large systems (Ogando *et al.*, 2008). For evaluating dynamic quantities such as conductivity, however, one has to rely on numerical analytic continuation (e.g., maximum ntropy method) from the imaginary-time Green's functions to the real-time ones. This procedure is, however, not unambiguous due to two reasons: one is the statistical errors originating from Monte Carlo sampling, which are amplified by numerical analytical continuation, and the other is the bias introduced by the default model in the maximum entropy method (Suzuki *et al.*, 1977).

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Lanczos Method:

The Lanczos methods have been one of few reliable techniques for evaluating dynamical responses of moderate-size Hamiltonian matrices (Silver *et al.*, 1990). The Lanczos methods use a linear transformation to a new basis in which the Hamiltonian matrix has a tridiagonal form, and lead to a continued fraction representation of the diagonal matrix elements of the Green's function. The drawback of these methods is the numerical instability which may lead to spurious eigenstates. Recently, the Lanczos method has been extended to the finite temperature case by introducing random sampling over the ground and excited states (Bullet, 1994).

In this article we use a fast algorithm for the Green's functions called Particle Source Method and applied it in nuclear fusion potential barrier. The *Particle Source Method* has been established by Toshiaki Iitaka and successfully applied to large disordered systems (Yakubo *et al.*, 1991). this methods is based on the numerical solution of the time-dependent Schrödinger equation, use random vectors for calculating the trace and have advantages in implementing on vector-parallel supercomputers. Since this method do not rely on the locality of the wave functions in contrast to many other fast methods, it has been successfully applied to the phenomena originating from the global coherency of the wave function such as the size effects of nanostructures (Yakubo *et al.*, 1991).

Particle Source Method:

In many fields of quantum physics, evaluation of the Green's functions constitutes the most important and demanding part of numerical treatment. Therefore efficient numerical algorithms, such as recursive Green's function methods, quantum Monte Carlo methods, the Lanczos methods, and Forced Oscillator Method (FOM) have been developed and applied to various problems. In this section we introduce another algorithm (the Particle Source Method; PSM) for calculating the Green's functions that uses numerical solutions of the time-dependent Schrödinger equation with a source term. The PSM can be regarded as a quantum version of the FOM, and is expected to play an important role in computational physics by complementing the quantum Monte Carlo methods and Lanczos methods (Jaklic and Prelovsek, 1994).

Expression of the Green's Function"

The doubly periodic Green's function G(x,y,z) under investigation is the solution verifying an outgoing wave condition of the inhomogeneous Helmholtz equation:

$$(\Delta + k^2)\, G(x,y,z) = \delta(z) \sum_{n=-\infty}^{+\infty} \sum_{m=-\infty}^{+\infty} \delta(x - n\, d_x)\, \delta(y - m\, d_y) \exp(i\ \alpha_0\, n\, d_x + i\ \beta_0\, m\, d_y) \tag{1}$$

Where k is the wave number ($k^2 \in \square$), d_x and d_y are the periods on the x and y axes, α_0 and β_0 are the pseudo-periodicity coefficients. In all the paper, we use an orthogonal coordinate system (O,x,y,z). Note that in the underlying electromagnetic problem, the harmonic fields are represented using a time dependence in $\exp(-i\,\omega t)$. This remark is important for the expression of the outgoing wave condition. The spatial form of G(x,y,z) is obtained directly from the elementary solution of $(\Delta + k^2)\, g(x,y,z) = \delta(x,y,z)$, i.e. the free-space $-\exp(ikr)/(4\pi r)$ Green's function , and writes:

$$G(x,y,z) = -\frac{1}{4\pi} \sum_{n=-\infty}^{+\infty} \sum_{m=-\infty}^{+\infty} \frac{\exp(ikr_{nm})}{r_{nm}} \exp(i\,\alpha_0 n\, d_x + i\,\beta_0 m\, d_y) \tag{2}$$

Where r_{nm} is the distance from the "source" located at point (nd_x ,md_y ,0) to the observation point (x,y,z):

Let us introduce the time-dependent Schroedinger equation with a time-dependent source term:

$$i\frac{d}{dt}|\phi;t\rangle = H|\phi;t\rangle + |j\rangle e^{-i(\omega + i\eta)t}\theta(t) \tag{3}$$

Where the wave function $|\phi;t\rangle$ and an arbitrary source $|j\rangle$ are **N**-component complex vectors, the Hamiltonian **H** is an $N \times N$ Hermitian matrix, ω is the frequency of the source, and η is a small positive imaginary part of the frequency, which determines the resolution of frequency. Note that this source term grows up exponentially as a function of time due to this small positive number, which simulates *adiabatic switching on* of the particle source.

This adiabatic switching on, which has been absent in the preceding works, is essential to calculate the exact shape of the Green's function as a function of energy. (Jaklic and Prelovsek, 1994).

The solution of this equation with the initial $|\phi; t = 0\rangle = 0$ condition becomes (Williams and Maris, 1985).

$$|\phi;t\rangle$$

$$= (-i)\int_0^t dt' e^{-iH(t-t')}|j\rangle e^{-i(\omega+i\eta)t'} \tag{4}$$

$$= G(\omega+i\eta)e^{-i(\omega+i\eta)t}|j\rangle \tag{5}$$

Where we have neglected the second term in the parentheses of (3). This approximation is justified by using sufficiently long time t_1 satisfying the condition:

$$e^{-\eta t_1} \langle \delta \tag{6}$$

Where δ is the required relative accuracy of the Green's function.

Then, from the Fourier transformation of (5), the Green's function operated on the ket $|j\rangle$ is obtained as:

$$\frac{1}{t_1}\int_0^{t_1} dt' |\phi;t\rangle e^{i(\omega+i\eta)t} \tag{7}$$

$$= \frac{1}{t_1}\int_0^{t_1} dt' G(\omega+i\eta)|j\rangle \tag{8}$$

$$= G(\omega+i\eta)|j\rangle \cdot \tag{9}$$

If only one or few matrix elements are necessary, we can calculate only these matrix elements as:

$$\frac{1}{t_1}\int_0^{t_1} dt' \langle i|\phi;t\rangle e^{i(\omega+i\eta)t'} \tag{10}$$

$$= \frac{1}{t_1}\int_0^{t_1} dt' \langle i|G(\omega+i\eta)|j\rangle \tag{11}$$

$$= \langle i|G(\omega+i\eta)|j\rangle = G_{ij}(\omega+i\eta) \tag{12}$$

where $\langle i|$ is an arbitrary bra.

Since the numerical error due to the finite timestep is proportional to $(\omega\Delta t)^3$, the best choice of ω is $\omega = 0$ (Toshiaki Iitaka, 1996). The matrix elements with energy $\omega \neq 0$ can be obtained by calculating the shifted green's function at $\omega = 0$:

$$G'(\omega = 0;\eta) = \frac{1}{0 + i\eta - H'} \tag{13}$$

With the shifted Hamiltonian

$$H' = H - \omega I \tag{14}$$

Where **I** is the unit matrix.

Solving the Schroedinger Equation:

To solve the time-dependent Schroedinger equation (3) numerically, we discretize it by using the leap frog method (Toshiaki Iitaka, 1996),

$$|\phi;t+\Delta t\rangle = -2i\Delta t H|\phi;t\rangle + |\phi;t-\Delta t\rangle - 2i\Delta t|j\rangle e^{-i(\omega+i\eta)t}\theta(t). \tag{15}$$

Where Δt is the time step. The time step is set as:

$$\Delta t = \alpha / E_{\max} \tag{16}$$

Where $E_{\max}$ is the absolute value of the extreme eigenvalue. We usually use the parameter α between 10^{-1} and 10^{-2}.

Another method for the time-dependent Schroedinger equation is the Suzuki-Trotter decomposition of the time-evolution operator. Though the Suzuki-Trotter decomposition can be applied effectively only to a special class of Hamiltonian, it might have the advantage of the leap frog method. First it allows larger time step. Second it can be used with non-Hermitian Hamiltonian, such as the Hamiltonian with absorbing boundary condition.

Product of the Green's Functions:

Since $|j\rangle$ in (3) is an arbitrary ket, we can repeat the calculation of the Green's function by using a new source term:

$$|j_2\rangle e^{-i(\omega_2+i\eta_2)t}\theta(t) = A_1 G(\omega_1 + i\eta_1)|j\rangle e^{-i(\omega_2+i\eta_2)t}\theta(t) \tag{17}$$

Where A_1 is an arbitrary operator whose matrix elements are known. In general, we can calculate the matrix elements of a product involving several Green's functions and other operators as:

$$\langle i|A_n G(\omega_n \pm i\eta_n)...A_1 G(\omega_1 \pm i\eta_1)A_0|j\rangle \tag{18}$$

Applying to Periodic Potential:

Let us study the Hamiltonian of an electron in one dimensional space with periodic potential,

$$H = \frac{p^2}{2m_e} + V(x) \tag{19}$$

Where m_e is mass of electron and $V(x)$ is the potential.

In general, the barriers that occur in physical phenomena are not square, and to discuss some applications, we must first obtain and approximate expression for the transmission coefficient $|T^2|$ through an irregularly shaped barrier. The most potentials is through the Wentzel-Kramers-Brillouin (WKB) approximation technique (Economou, 1983).

We observe that consist of a product of two terms, the second of which is by far the more important one. If we write,

$$\log|T^2| \approx -2\kappa(2a) + 2\log\frac{2(\kappa a)(\kappa a)}{(\kappa a)^2 + (\kappa a)^2} \tag{20}$$

We see that under most circumstance the first term dominates the second for any reasonable size of κa. The procedure we adopt is to treat a smooth, curved barrier as a juxtaposition of square barriers (Fig.1). Since transmission coefficients are multiplicative when they re small (in effect, with most of the flux event), we may write approximately

$$\log|T^2| \approx \sum_{\substack{partial\\ barriers}} \log\left|T_{\substack{partial\\ barrier}}\right|^2 \approx -2\sum \Delta x\langle\kappa\rangle$$
$$\approx -2\int_{barrier} dx\sqrt{(2m/\hbar)[V(x)-E]} \tag{21}$$

In the partial barriers, Δx is the width and $\langle\kappa\rangle$ the average value of κ for that barrier. In the last step a limit of infinitely narrow barriers was taken. It is clear from the expression that the approximation is least accurate near the " turning points " where the energy and potential are nearly equal. It is also important that $V(x)$ be a slowly varying function of x, since otherwise the approximation of carved barrier by a stack of square ones is only possible if the latter are narrow and there again Δx is a poor approximation.

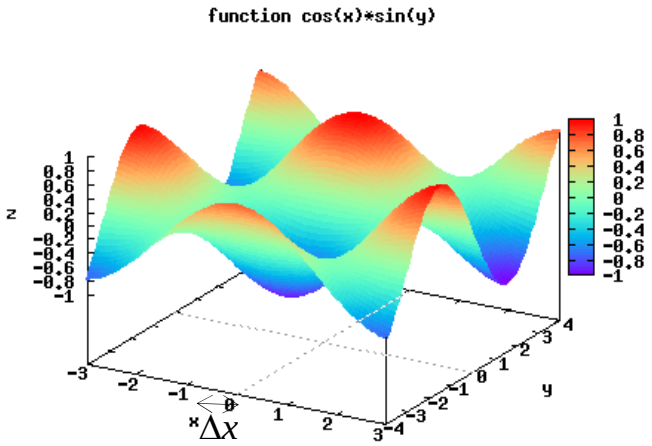

Fig. 1: Approximation of periodic potential by juxtaposition of square potential barriers.

One particular example of such symmetric potential can be found in sinusoidal-form potential:

$V = Cos(x)\ \mathrm{Sin(y)}$ (22)

That $V(x,y) = V(-x,y)$, $x \to \pm\infty$, $V(x) \to 0$

After discretizing in space with the lattice size ΔX, the Hamiltonian is pproximated by a tight binding form,

$$H = \frac{-\hbar^2}{2m_e\Delta x^2}\sum_{n=1}^{N}(c_n^t c_{n+1} + c_n c_{n+1}^t) + \sum_{n=1}^{N}(\varepsilon_n + \frac{\hbar^2}{m_e\Delta x^2})c_n^t c_n \quad (23)$$

where $\varepsilon_n = V(x_n)$ and c_n^t and c_n are the creation and annihilation operator of electron at the site $x_n = n\times\Delta x$ (n=0,1,…,N). The periodic boundary condition is set as:

$$\langle n=0|\phi\rangle = \langle n=N|\phi\rangle \quad (24)$$

Where $|n\rangle$ is the electron state at the n-th site.

When V (x) = 0, the exact analytical eigenstates and eigenvalues of the Hamiltonian (23) with the boundary condition (24) are well known,

$$|E_m\rangle = A\sum_{n=1}^{N}\exp(ik_m n\Delta x)|i\rangle \quad (25)$$

$$E_m = \frac{\hbar^2}{m_e\Delta x^2}[1-\cos(k_m\Delta x)] \quad (26)$$

$$k_m = \frac{m\pi}{N\Delta x} \quad (27)$$

Where A is a normalizing constant and m is an integer $m = 0,\pm1,\pm2,...,\pm(N-2)/2, N/2$ for even N and for odd N. Note that (26) approximates well the parabolic dispersion relation (19) of the continuum model, if $m\langle\langle N$ or $E\langle\langle 1$. In the following, we set $\hbar = m_e = \Delta x = 1$ for simplicity.

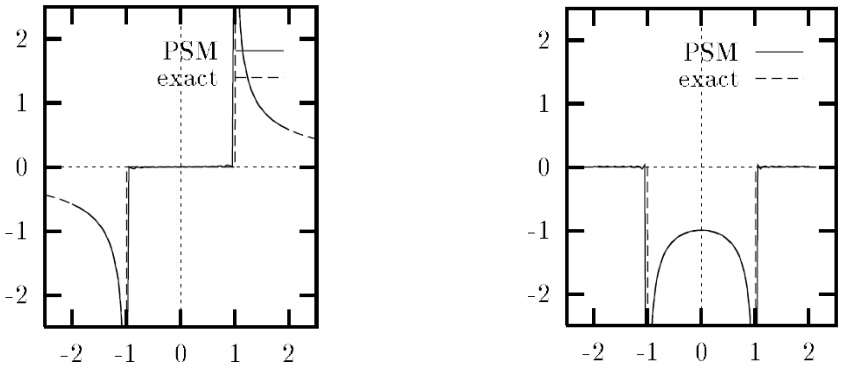

Fig. 2: (a) real part and (b) imaginary part of $G(\omega + i\eta)$.

Figure 2b. shows the imaginary part of the Green's function $G(\omega + i\eta)$ for N = 10 and $\eta = 0.1$, where $\omega = E - 1$ is the energy measured from the band center. The numerical result reproduces faithfully the exact spectrum (26) of the Hamiltonian (19).

Figure 2a,2b. compares the Green's function $G_{nn}(\omega + i\eta)$ of a long perfect lattice calculated by the multiple frequency method to the exact analytical result. For the numerical calculation, we used parameters, $\alpha = 0.1, \eta = 10^{-3}, \delta = 10^{-2}$ and $\Delta\omega = 5 \times 10^{-2}$ and $N = 10^6$.. The exact result in the limit $N \to \infty$ and $\eta \to +0$ is calculated by using the analytical expression (Hong and Li, 2006),

$$G_{nn}(\omega + i\eta) = \frac{-i}{\sqrt{1-\omega^2}} \text{ for } (|\omega| < 1) \tag{28}$$

And

$$G_{nn}(\omega + i\eta) = \frac{\operatorname{sgn}\omega}{\sqrt{\omega^2 - 1}} \text{ for } (|\omega| > 1) \tag{29}$$

Conclusion:

In this paper, we have discussed a techniques for numerical solving Green Function. We derived the appropriate Green function, and we found a numerically stable transformation of the Green function. We also used Monte Carlo method, Lanczos method and Particle source method to calculate the Green function efficiently. This approach has been applied to some examples, and parameters have been calculated over a broad range of frequencies.

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