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Scattering in the Framework of the Green's Function Monte-Carlo Method

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A method based on the Green's Function Monte-Carlo approach is used to solve the integral equation for the scattering wave function. The algorithm employed is explained for two-body scattering and tested for cases where the exact solution is known.

1. INTRODUCTION

There are hardly any interesting systems for which the wave function is known in analytic form. Therefore one has to resort to approximation schemes in order to obtain solutions of the Schrödinger equation. Many of these algorithms have unknown convergence properties that leave their application open to some reasonable doubt. In contrast, the Green's function Monte-Carlo (GFMC) method is in principle exact; its results are subject to statistical uncertainty only that can be reduced to an arbitrarily small value by increasing the computational effort. Of course, such a powerful method has its own limitations; it is mainly successful in the determination of the ground state of many-boson systems. Another limitation, of a more technical nature, exists; in order to be able to calculate the full Green's function of the system one deals with, the GFMC requires the availability of a good initial approximation to the ground state wave function, called a guidance function, and a reasonable approximation to the Green's function, called a trial Green's function, such that the resolvent equation can be solved exactly.

In this paper we apply the GFMC method in the form that originates with Kalos [1–3] and was later developed by Ceperley [4] and Ceperley and Alder [5]. In a previous paper [6] a modification of their method was introduced that proved effective in those cases where the kernel of the integral equation to be solved turned out to be not strictly positive. Here we propose a technique very similar to that of [6] for solving the integral equations for scattering. As a "proof of principle" of our algorithm, we apply it to several two-body model problems for which the scattering amplitudes and phase shifts are exactly known.

The organisation of this paper is as follows: in Section 2 we describe the algorithm in detail and give the essential differences with the GFMC method for bound states. Section 3 contains the formulae for the scattering amplitudes connected to the model problems we solve. The next section contains the results of our numerical experiments, and in the final section we discuss our results and draw some conclusions.

2. THE MODIFIED GREEN'S FUNCTION MONTE-CARLO METHOD FOR SCATTERING

Let H be the hamiltonian of a quantum system, then the ground state $|\psi_0\rangle$ can be projected out from any initial wave function $|\psi\rangle$ that is not orthogonal to $|\psi_0\rangle$ by the $\beta \to \infty$ limit of the imaginary-time evolution:

$$|\psi_0\rangle \sim \lim_{\beta\to\infty} e^{-\beta H}|\psi\rangle. \tag{1}$$

Equivalently, one may work in the time-independent representation and apply the resolvent $G(E) = (H - E)^{-1}$ many times to the state $|\psi\rangle$. This procedure forms the basis of the standard GFMC method for finding the energy of the bound state of a many-body system.

Our approach to the scattering problem is to calculate the resolvent $G(E)$ by means of the GFMC method, i.e. by performing random walks, and to use it in the standard way in a calculation of the scattering amplitude or T-matrix:

$$T(E) = V + VG(E)V. \tag{2}$$

The operator V is, of course, the potential: $H = H_0 + V$, H_0 being the kinetic energy operator. The resolvent is constructed using the well-known resolvent identities,

$$\begin{aligned} G(E) &= G_{\mathrm{tr}}(E) + G_{\mathrm{tr}}(E)(V_{\mathrm{tr}} - V)G(E) \\ &= G_{\mathrm{tr}}(E) + G(E)(V_{\mathrm{tr}} - V)G_{\mathrm{tr}}(E), \end{aligned} \tag{3}$$

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where V_{tr} is the trial potential for which the corresponding resolvent, $G_{tr}(E) = (H_0 + V_{tr} - E)^{-1}$, is known. The iteration

$$G(E) = \sum_{n=0}^{\infty} G_{tr}(E)K(E)^n, \quad K(E) = (V_{tr} - V)G_{tr}(E), \tag{4}$$

will of course converge only if the norm of the kernel $K(E)$ is less than unity.

The random walks are performed most conveniently in coordinate space, so we describe the procedure in **x**-language for the case of one particle scattered by the local potential $V(\mathbf{x})$. We will work with the Laplace-transformed density matrix

$$\tilde{\rho}(\mathbf{x}, \mathbf{x}') = \frac{1}{\Delta} G(\mathbf{x}, \mathbf{x}'; E). \tag{5}$$

It solves the Bloch equation

$$\tilde{\rho}(\mathbf{x}, \mathbf{x}') = \rho_{tr}(\mathbf{x}, \mathbf{x}') + \Delta \cdot \int d^3x\, \tilde{\rho}(\mathbf{x}, \mathbf{x}'')\tilde{K}(\mathbf{x}'', \mathbf{x}') \tag{6}$$

with the kernel

$$\tilde{K}(\mathbf{x}'', \mathbf{x}') = [V_{tr}(\mathbf{x}'') - V(\mathbf{x}'')]\tilde{\rho}_{tr}(\mathbf{x}'', \mathbf{x}'). \tag{7}$$

(The variable Δ is the parameter of the Monte-Carlo algorithm defined below.)

The scattering amplitude is calculated as the Fourier transform of the expression (2) on the basis of the formula:

$$f(E) = -\frac{m}{2\pi}\left\{\int d^3x'\, e^{-i\mathbf{k}\mathbf{x}'}V(x')e^{ikz'} - \int d^3x\, e^{-i\mathbf{k}\mathbf{x}}V(x)\int d^3x'\, G(\mathbf{x}, \mathbf{x}')V(x')e^{ikz'}\right\}. \tag{8}$$

(The quantity x' is the length of the vector $\mathbf{x}'$, z' is its third component.) Apparently we encounter terms in the integrand that are oscillatory. As the standard way of applying Monte-Carlo techniques relies on the interpretation of (part of) the integrand as a probability distribution, some modification is needed. The modification applied here consists of treating integrals of the form $I = \int dx\, f(x)\psi(x) / \int dx\, f(x)$ such that $|f(x)|$ is interpreted as a probability distribution. Then I is evaluated as

$$I = \int dx |f(x)| e^{i\delta(x)}\psi(x) \Big/ \int dx |f(x)| e^{i\delta(x)} \tag{9}$$

to be estimated in the Monte-Carlo fashion as

$$I \approx \sum_{k=1}^{K} e^{i\delta(x_k)}\psi(x_k) \Big/ \sum_{k=1}^{K} e^{i\delta(x_k)}, \tag{10}$$

where the points x_k are sampled from a population with density $|f(x)|$.

Now we describe the algorithm in some detail (see also [6]):

(a) basic parameters are chosen: the mean imaginary time step Δ and the scattering energy E, from which the momentum $k = \sqrt{2mE}$ can be derived;

(b) In a sphere of radius R_{cut} a set of points is sampled from a distribution $|V(\mathbf{x}')|$ with phases equal to $\delta^{old}(\mathbf{x}') = kx_3' = kz'$ corresponding to the initial state $e^{ikz'}$. All points are assigned a multiplicity. In the initial population it is set equal to unity: $M^{old}(\mathbf{x}') = 1$, $\forall \mathbf{x}'$. (The procedure of cutting the potential is applied for practical reasons. For short-range interactions it leads to an approximation that can be improved at will if sufficient computational effort is spent.)

(c) To each point $\mathbf{x}'$ in the initial population diffusion is applied; i.e., it is subjected to Brownian motion corresponding to the density matrix ρ_D defined as

$$\rho_D(\mathbf{x}, \mathbf{x}'; \beta) = \left(\frac{m}{2\pi\beta}\right)^{3/2} \exp\left(-\frac{m}{2\pi\beta}(\mathbf{x} - \mathbf{x}')^2\right); \tag{11}$$

this diffusion corresponds to the free motion of particles in the imaginary time, $\partial\psi/\partial\beta = \Delta\psi$.

A Laplace transformation is carried out by sampling the imaginary time $\beta = it$ from the distribution $(1/\Delta)\exp(-\beta/\Delta)$. This gives

$$\tilde{\rho}_D(\mathbf{x}, \mathbf{x}') = \int_0^{\infty} \frac{d\beta}{\Delta} e^{-\beta/\Delta}\rho_D(\mathbf{x}, \mathbf{x}'; \beta). \tag{12}$$

By this diffusion a new generation of points $\mathbf{x}$ is produced. In order to construct the new generation, new points $\mathbf{x}$ with multiplicity $M(\mathbf{x}) = M^{old}(\mathbf{x}') \cdot m_D$ are created, according to the rule

$$m_D = \frac{1}{\Delta}\left|\frac{G_{l,tr}(x, x'; E)}{xx'}\right| \Big/ \tilde{\rho}_D(\mathbf{x}, \mathbf{x}'). \tag{13}$$

Here we use for the trial Green function the partial wave decomposition. In our calculations $G_{l,tr}$ is the Green function for the square well; see the Appendix. The new points have phases $\delta(\mathbf{x}) = \delta^{old}(\mathbf{x}') + \delta_G$, with

$$\delta_G = \mathrm{Im}[G_{l,tr}(x, x'; E)]/\mathrm{Re}[G_{l,tr}(x, x'; E)]. \tag{14}$$

The occurrence of $\tilde{\rho}_D$, the Laplace-transformed density matrix given by

$$\tilde{\rho}_D(\mathbf{x}, \mathbf{x}') = \frac{m}{2\pi}\frac{1}{\Delta}\frac{1}{|\mathbf{x} - \mathbf{x}'|}\exp(-\sqrt{2m/\Delta}|\mathbf{x} - \mathbf{x}'|), \tag{15}$$

is required as it must compensate for the diffusion in the first

step from $\{\mathbf{x}'\}$ to $\{\mathbf{x}\}$. The "new" points thus created correspond to the first iteration of Eq. (6). Next "intermediate" points are created with multiplicity m_l given by

$$m_l = \Delta |K_l(x, x')| / \tilde{\rho}_D(\mathbf{x}, \mathbf{x}'), \tag{16}$$

where

$$K_l(x, x') = [V_{tr}(x) - V(x)] \frac{G_{l,tr}(x, x'; E)}{xx'}. \tag{17}$$

If m_l does not vanish, the point $\mathbf{x}$ is added to the initial population with multiplicity $M_{\mathbf{x}} = M_{\mathbf{x}}^{old} \cdot m_l$; the phase of the point $\mathbf{x}$ is equal to

$$\delta_{\mathbf{x}} = \delta_{\mathbf{x}}^{old} + \delta_G + \begin{cases} \pi, & K_l(\mathbf{x}, \mathbf{x}') < 0, \\ 0, & K_l(\mathbf{x}, \mathbf{x}') > 0. \end{cases} \tag{18}$$

Intermediate points correspond to the second integral in Eq. (8). This process is continued until eventually all initial and intermediate points are transferred to the new generation.

(d) In order to achieve good statistics, the whole procedure is repeated a number of times, say N. The full scattering amplitude is estimated by combining the points in the initial generation, corresponding to the distribution $V\psi_0$, and the new generation that corresponds to $GV\psi_0$.

In the case of S-wave scattering this amounts to (see Eq. (8)) the following Monte-Carlo summation

$$f_0^{(n)}(E) = -\frac{m}{2\pi} \frac{1}{N_{x'}} \left\{ \sum_{x'} j_0(kx') e_{x'}^{i\delta^{old}} + \sum_{x} j_0(kx) V(x) M_x e^{i\delta_x} \right\} \tag{19}$$

for the nth estimate. The final result is obtained by averaging:

$$f_0(E) = \frac{1}{N} \sum_{n=1}^{N} f_0^{(n)}(E). \tag{20}$$

A remark about the convergence of the Born series is appropriate here: because the convergence depends crucially on the magnitude of the kernel K_l, the use of a trial potential V_{tr} that is as close as possible to the true potential V, is required to speed up the convergence of the algorithm. In our practical calculations described below, we employed the square well as the trial potential.

3. SOME EXACTLY SOLVABLE CASES

It is obviously very important for a test of the correctness of the algorithm to employ some potentials for which the scattering states are known analytically. Furthermore, we need a suitable trial potential V_{tr}. In this work we use the square well:

$$V_{tr}(\mathbf{x}) = \begin{cases} -V_T, & 0 \le |\mathbf{x}| \le R_T \\ 0, & |\mathbf{x}| > R_T. \end{cases} \tag{21}$$

In our practical calculations we solve the scattering equations for one partial wave at a time, so we consider partial-wave equations. (Note that this is not a limitation or special case; as the centrifugal barrier increases, the scattering amplitude decreases, so in general the lowest partial waves are computed more accurately than the higher ones, if one uses the same statistics for all values of the angular momentum l.)

As it is straightforward to write down Green's function in terms of the regular and irregular solutions of the Schrödinger equation and the latter are well known for all l-values in case of the square well, we give the relevant results in the Appendix.

In order to check our algorithm we employed two interactions for which the S-wave phase shifts are known [7]. These are the exponential potential:

$$V(r) = V_0 e^{-r/d} \tag{22}$$

and the Pöschl–Teller potential:

$$V(r) = W_0 \cosh^{-2}(r/d). \tag{23}$$

If we write V_0 as

$$V_0 = z_0^2/(2m \cdot 4d^2), \tag{24}$$

then the S-wave S-matrix for the exponential potential is

$$S_0(E) = \left(\frac{z_0}{2}\right)^{-4idk} \frac{\Gamma(1 - 2idk) J_{2idk}(z_0)}{\Gamma(1 + 2idk) J_{-2idk}(z_0)}; \tag{25}$$

(J_ν is, of course, the ordinary Bessel function).

If one writes in the case of the Pöschl–Teller potential,

$$W_0 = -\frac{\lambda(\lambda - 1)}{2d^2}, \tag{26}$$

then the S-wave phase shift is given by

$$\delta_0 = \frac{\pi}{2} + \arg \frac{\Gamma(idk) \exp(-idk \log 2)}{\Gamma((\lambda + 1)/2 + idk/2) \Gamma(1 - \lambda/2 + idk/2)}. \tag{27}$$

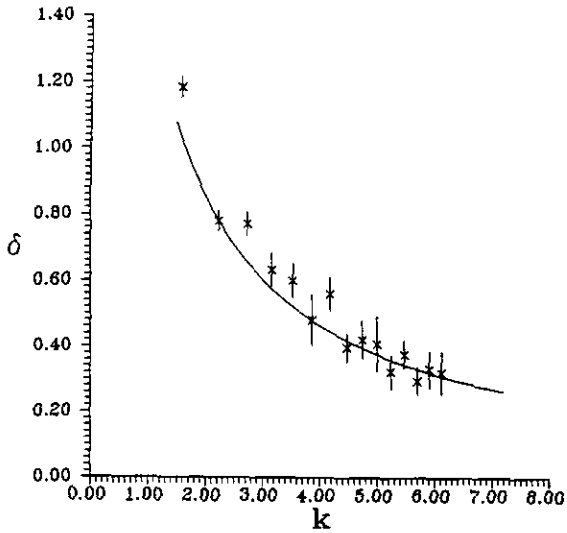

FIG. 1. The phase shifts for the exponential potential. The parameters of the potential are $V_0 = -7$, $d = 1.1$.

Our results are shown in Figs. 1 and 2. The parameters for the cases considered were: in units such that $\hbar = m = 1$ the strength V_0 of the exponential potential is -7 and its range parameter $d = 1.1$; for the Pöschl–Teller potential we took $W_0 = -1$, $d = 4$. The curves in the figures are the exact S-wave phase shifts, the points with error bars are the results of our Monte-Carlo calculation. It is clear that good agreement is obtained, even when the phase shifts are large.

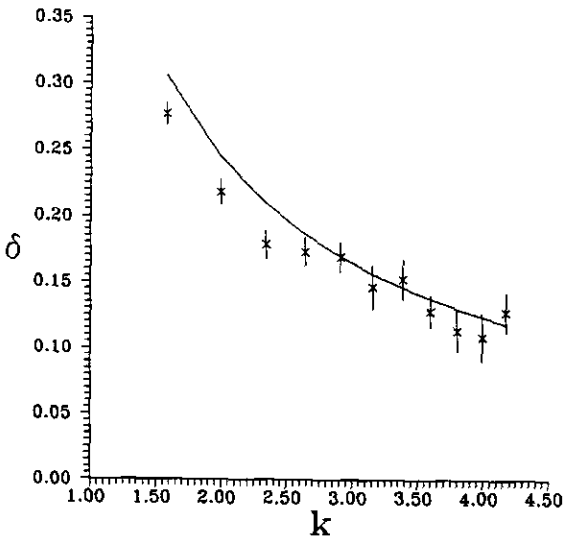

FIG. 2. The phase shifts for the Pöschl–Teller potential. The parameters of the potential are $W_0 = -1$, $d = 4$.

APPENDIX: SQUARE-WELL GREEN'S FUNCTION

Consider a square well with radius R and depth $-V_0$. Let E be the energy of our stationary state and k, the corresponding value of the momentum. The wave number inside the well is denoted by K. We use the notation $h_l^{(\pm)}(kr)$ for the spherical Hankel function that behaves asymptotically as a purely outgoing (incoming) spherical wave.

Then the regular solution for angular momentum l of the square-well Schrödinger equation is denoted by $J_l(r; E)$. Inside the potential it is

$$J_l(r; E) = A_l j_l(Kr), \quad 0 \le r \le R. \tag{28}$$

Outside it is given by

$$J_l(r; E) = -\frac{i}{2}\{h_l^{(-)}(kr) - S_l(E)h_l^{(-)}(kr)\}, \tag{29}$$

where $S_l(E)$ is the S-matrix of the square well. The irregular solution inside the potential,

$$H_l^{(+)}(r; E) = B_l j_l(Kr) + C_l n_l(Kr), \tag{30}$$

is a linear combination of a spherical Bessel and a spherical Neumann function. The coefficients A_l, B_l, and C_l are determined by the requirement that the regular and irregular solutions J_l and H_l, respectively, and their derivatives be continuous at $r = R$. If we denote by $r_<$ ($r_>$) the smaller (larger) of the two variables r and r', then the r-space resolvent of the square well is

$$G_l(r', r; E) = -kJ_l(r_<; E)H_l^{(+)}(r_>; E). \tag{31}$$

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