Monte Carlo method for scattering reactions

Helmut Kröger
Département de Physique, Université Laval, Québec, P.Q., G1K 7P4 Canada
(Received 14 August 1986)

We propose how to rewrite the scattering solution of the Schrödinger equation in terms of positive matrix elements of positive operators. These can be interpreted as probability distributions and we suggest applying a Monte Carlo method for its calculation. We outline the relation between the probability distributions and S-matrix elements for scattering reactions.

I. INTRODUCTION

The Monte Carlo technique has proven very useful in many-body physics or systems with many degrees of freedom. In particular for lattice-gauge theories, using a space-time lattice, one has been able to calculate mass gaps, correlation length, etc.[1,2] In nuclear physics, the Monte Carlo Green's function method has been used to calculate ground-state binding energies of light nuclei.[3] The latter method uses the positivity of the coordinate-space Green's function and the ground-state wave function. It is based on a reformulation of the Schrödinger equation for the ground state in terms of positive probability functions.[4] The Monte Carlo Green's function method has been devised by Kalos and co-workers.[5–11] Other random-number methods have been used to determine properties of the α particle.[12]

In this paper we want to propose a formulation of the scattering problem amenable to the Monte Carlo technique. Our main purpose is the discussion for the case of nonrelativistic potential scattering.

The solution of the bound-state problem can be viewed as the solution of an eigenvalue problem of the Hamiltonian with certain boundary conditions, namely, a rapid fall-off behavior of the wave function at a large distance. On the other hand the scattering problem can be viewed as the solution of an eigenvalue problem with boundary conditions which reflect the asymptotic states.

Let us consider a scattering process, described by the full Hamiltonian H, where the asymptotic incoming and outgoing state is described by $H_\alpha^{\rm as}$ and $H_\beta^{\rm as}$, respectively. Let us consider the potential V to be strong and short ranged. Then the S matrix is given by

$$S_{\beta\alpha}=(\Omega_\beta^{(-)})^\dagger\Omega_\alpha^{(+)}\ , \tag{1.1}$$

where

$$\Omega_\alpha^{(\pm)}=s\lim_{t\to\mp\infty}\exp(iHt)\exp(-iH_\alpha^{\rm as}t)P_\alpha^{\rm as} \tag{1.2}$$

are the corresponding Moller operators and $P_\alpha^{\rm as}$ is the channel projector onto an asymptotic state.[13] There are many different approaches to calculating N-body scattering matrix elements and amplitudes. One of the most widely used methods for the description of stationary scattering theory is the set of Faddeev-Yakubovski integral equations.[14] The latter is a coupled set of nested equations for Green's functions in different subsystems, which incorporate the boundary conditions. Due to its complicated structure it is not useful for our purpose to construct positive probability functions, which determine the solution.

In stationary scattering theory, the resolvent

$$G(z)=(z-H)^{-1},\quad \mathrm{Im}(z)\neq 0 \tag{1.3}$$

plays an important role. It obeys the simple resolvent type of equation

$$G(z)=G^0(z)+G^0(z)VG(z)\ , \tag{1.4}$$

which could be used to calculate $G(z)$.

However, Eq. (1.4) has the decisive drawback that in the scattering region, which requires taking the physical limit $z=E+i\varepsilon$, $\varepsilon\to+0$ the solution is not unique in the case for three or more particles due to the existence of different asymptotic states. This was one of the incentives to construct the more complicated Faddeev-Yakubovski equations.[14] By imposing additional boundary conditions on Eq. (1.4) the ambiguity can be made to vanish.

In this paper we do not want to go the limit $z=E+i\varepsilon$, $\varepsilon\to+0$ because of the boundary-condition problem. We suggest incorporating the physical boundary conditions by using the time-dependent Moller wave operators, given by Eq. (1.2).

We introduce the following approximation:

$$\Omega_\alpha^{(\pm)}\to\Omega_\alpha(\mp T)=\exp(\mp iHT)\exp(\pm iH_\alpha^{\rm as}T)P_\alpha^{\rm as}\ , \tag{1.5}$$

$$S_{\beta\alpha}\to S_{\beta\alpha}(T,-T)=P_\beta^{\rm as}\exp(iH_\beta^{\rm as}T)\exp(-2iHT)\times\exp(iH_\alpha^{\rm as}T)P_\alpha^{\rm as}\ , \tag{1.6}$$

where T denotes a large but finite time parameter.

This approximation has been found useful and the error was found well under control in the numerical experience gained from time-dependent scattering calculations in nonrelativistic few-nucleon reactions[15–19] as well as in relativistic-field-theory applications.[20,21]

Our aim is to relate the S matrix to some positive probability densities. The problem of calculating the S matrix is basically solved, if one knows the time evolution $\exp(iHT)$ corresponding to the full Hamiltonian. But instead of trying to express the time evolution in terms of some positive probability densities, it looks more promising to express the resolvent $G(z)$ in terms of positive probabilities.

Hence we relate the time evolution $\exp(iHT)$ to the

resolvent $G(z)$ via a Cauchy integral

$$\exp(iHT)=\frac{1}{2\pi i}\int_C dz\,\exp(izT)G(z)\ , \tag{1.7}$$

where C is a closed contour which can be chosen to have a finite distance from the real axis. Some care has to be exercised with regard to closing the contour at the high-energy "end."

This "end-point" problem can be resolved in two ways.

(i) From the rigorous point of view Eq. (1.7) has a well-defined meaning, if H is a bounded operator. Thus also its spectrum $\sigma(H)$ is bounded and lies in the interior of and at a finite distance from the closed contour C (see Fig. 1). However, in physical applications the Hamiltonian H is unbounded. It is possible to approximate the unbounded Hamiltonian H by a bounded Hamiltonian $H(u)$, such that $H(u)$ tends to H in the sense of strong resolvent convergence and the time evolution $\exp[iH(u)T]$ tends to $\exp(iHT)$ in the strong sense, when the approximation parameter u tends to its limit. This has been proven for a large class of potentials in Refs. 22 and 23. Then if H is replaced by $H(u)$ in the time evolution and the resolvent, Eq. (1.7) is exactly valid.

(ii) From the practical point of view it seems easier to keep the unbounded Hamiltonian H, but to approximate the contour C by C_Λ which ends at a high-energy cut off Λ (Fig. 2). The physical justification for doing so is the intertwining property of the wave operators and the energy conservation of the S matrix. This property implies that an asymptotic state of a sharp energy E_1 is mapped on a scattering state corresponding to the point E_1 in the spectrum of H and an asymptotic wave packet covering a finite energy interval $[E_1,E_2]$ is mapped on a scattering state corresponding to the same interval in the spectrum of H. Thus changing the contour C to C_Λ at a sufficiently large distance from the interval $[E_1,E_2]$ should have an arbitrarily small effect on the S-matrix element. Hence we write

$$S_{\beta\alpha}(T,-T)=P_\beta^{\rm as}\exp(iH_\beta^{\rm as}T)\frac{1}{2\pi i}\times\int_C dz\,e^{-2izT}G(z)\exp(iH_\alpha^{\rm as}T)P_\alpha^{\rm as}\ , \tag{1.8}$$

which relates the approximate S matrix to the resolvent $G(z)$. Now we want to express $G(z)$ in terms of some positive operators.

We assume that $H=H^0+V$ is self-adjoint and moreover positive. If H is not positive, then it is reasonable to assume that H has a lowest-lying negative eigenvalue and

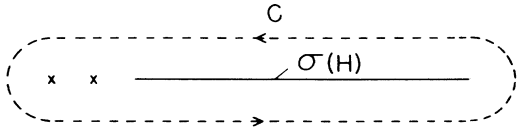

FIG. 1. Schematic plot of spectrum $\sigma(H)$ with a contour curve C.

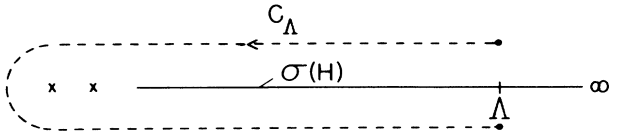

FIG. 2. Schematic plot of a spectrum $\sigma(H)$ which extends to $+\infty$ with a cutoff contour curve C_Λ.

there is a positive constant a such that $H'=H+a$ is positive. Then we continue to work with H'. Then we proceed to calculate the probability functions P^A, Q^A, R^A, P^B, Q^B, R^B, the resolvent G, and the time evolution U corresponding to H'. The time evolution $U_H(T)=\exp(iHT)$ corresponding to the original Hamiltonian H and the time evolution $U_{H'}(T)=\exp(iH'T)$ corresponding to the Hamiltonian H' are simply related by

$$U_H(T)=\exp(-iaT)U_{H'}(T)\ . \tag{1.9}$$

This expression is then substituted in Eqs. (1.5) and (1.6) for the wave operators and S matrix.

In order to express $G(z)$ in terms of positive operators we define

$$A(z)=\{[\mathrm{Re}(z)-H]^2+\mathrm{Im}(z)^2\}^{-1}\ , \tag{1.10a}$$

$$B(z)=H\{[\mathrm{Re}(z)-H]^2+\mathrm{Im}(z)^2\}^{-1}\ , \tag{1.10b}$$

$$\mathrm{Re}[G(z)]=\tfrac{1}{2}[G(z)+G^\dagger(z)]\ , \tag{1.10c}$$

$$\mathrm{Im}[G(z)]=\frac{1}{2i}[G(z)-G^\dagger(z)]\ . \tag{1.10d}$$

Then one has

$$\mathrm{Re}[G(z)]=[\mathrm{Re}(z)-H]\{[\mathrm{Re}(z)-H]^2+\mathrm{Im}(z)^2\}^{-1}=\mathrm{Re}(z)A(z)-B(z)\ , \tag{1.11a}$$

$$\mathrm{Im}[G(z)]=-\mathrm{Im}(z)\{[\mathrm{Re}(z)-H]^2+\mathrm{Im}(z)^2\}^{-1}=-\mathrm{Im}(z)A(z)\ . \tag{1.11b}$$

One can split G

$$G(z)=\mathrm{Re}[G(z)]+i\,\mathrm{Im}[G(z)]=z^*A(z)-B(z)\ . \tag{1.12}$$

One observes that both $A(z)$ and $B(z)$ are positive operators, which is based on the fact that a positive function of a positive self-adjoint operator is positive.

In Sec. V we will exploit this property to construct positive probability distributions and discuss their relation to the S matrix. In Sec. III we briefly review the Monte Carlo method. In Sec. IV we give some concluding remarks. In the Appendix we discuss an approximative representation of the time evolution.

II. PROBABILITY DISTRIBUTIONS FOR A CONTINUOUS HAMILTONIAN

Firstly, we set up equations for the positive operators $A(z)$ and $B(z)$, given by Eq. (1.10a) and (1.10b), which

uniquely determine the resolvent $G(z)$ for any z off the real axis via Eq. (1.12).

The resolvent Eq. (1.4) has an alternate form,

$$G(z)=G^0(z)+G(z)VG^0(z)\ . \tag{2.1}$$

Substituting Eq. (2.1) into Eq. (1.4) one obtains

$$G(z)=G^0(z)+G^0(z)VG^0(z)+G^0(z)VG(z)VG^0(z)\ . \tag{2.2}$$

Using Eqs. (1.10)—(1.12), and assuming that the interaction V is self-adjoint, we split Eq. (2.2) into its real and imaginary parts,

$$\begin{aligned}\mathrm{Re}[G(z)]=&\mathrm{Re}[G^0(z)]+\mathrm{Re}[G^0(z)]V\,\mathrm{Re}[G^0(z)]-\mathrm{Im}[G^0(z)]V\,\mathrm{Im}[G^0(z)]\\&+\mathrm{Re}[G^0(z)]V\,\mathrm{Re}[G(z)]V\mathrm{Re}[G^0(z)]-\mathrm{Re}[G^0(z)]V\,\mathrm{Im}[G(z)]V\,\mathrm{Im}[G^0(z)]\\&-\mathrm{Im}[G^0(z)]V\,\mathrm{Re}[G(z)]V\,\mathrm{Im}[G^0(z)]-\mathrm{Im}[G^0(z)]V\,\mathrm{Im}[G(z)]V\,\mathrm{Re}[G^0(z)]\ ,\end{aligned} \tag{2.3a}$$

$$\begin{aligned}\mathrm{Im}[G(z)]=&\mathrm{Im}[G^0(z)]+\mathrm{Re}[G^0(z)]V\,\mathrm{Im}[G^0(z)]+\mathrm{Im}[G^0(z)]V\,\mathrm{Re}[G^0(z)]\\&+\mathrm{Im}[G^0(z)]V\,\mathrm{Re}[G(z)]V\,\mathrm{Re}[G^0(z)]+\mathrm{Re}[G^0(z)]V\,\mathrm{Im}[G(z)]V\,\mathrm{Re}[G^0(z)]\\&+\mathrm{Re}[G^0(z)]V\,\mathrm{Re}[G(z)]V\,\mathrm{Im}[G^0(z)]-\mathrm{Im}[G^0(z)]V\,\mathrm{Im}[G(z)]V\,\mathrm{Im}[G^0(z)]\ .\end{aligned} \tag{2.3b}$$

This set of coupled equations can be expressed in terms of the positive operators $A(z)$, $B(z)$, defined by Eqs. (1.10a) and (1.10b). In order to do this we rewrite Eq. (1.11a) and (1.11b),

$$A(z)=-\frac{\mathrm{Im}[G(z)]}{\mathrm{Im}(z)}\ , \tag{2.4a}$$

$$B(z)=-\frac{\mathrm{Re}(z)}{\mathrm{Im}(z)}\mathrm{Im}[G(z)]-\mathrm{Re}[G(z)]\ . \tag{2.4b}$$

Substituting Eqs. (2.3a) and (2.3b) into Eqs. (2.4a) and (2.4b) and expressing on the right-hand side (rhs) $\mathrm{Re}[G(z)]$, $\mathrm{Im}[G(z)]$, $\mathrm{Re}[G^0(z)]$, $\mathrm{Im}[G^0(z)]$ by A, B, A^0, B^0 via Eqs. (1.11a) and (1.11b) one obtains

$$\begin{aligned}A(z)=&A^0(z)+2\,\mathrm{Re}(z)A^0(z)VA^0(z)-B^0(z)VA^0(z)-A^0(z)VB^0(z)\\&+[4\,\mathrm{Re}^2(z)-|z|^2]A^0(z)VA(z)VA^0(z)-2\,\mathrm{Re}(z)B^0(z)VA(z)VA^0(z)\\&-2\,\mathrm{Re}(z)A^0(z)VA(z)VB^0(z)+B^0(z)VA(z)VB^0(z)-2\,\mathrm{Re}(z)A^0(z)VB(z)VA^0(z)\\&+B^0(z)VB(z)VA^0(z)+A^0(z)VB(z)VB^0(z)\ ,\end{aligned} \tag{2.5a}$$

$$\begin{aligned}B(z)=&B^0(z)+|z|^2A^0(z)VA^0(z)-B^0(z)VB^0(z)+2\,\mathrm{Re}(z)\,|z|^2A^0(z)VA(z)VA^0(z)\\&-|z|^2B^0(z)VA(z)VA^0(z)-|z|^2A^0(z)VA(z)VB^0(z)-|z|^2A^0(z)VB(z)VA^0(z)+B^0(z)VB(z)VB^0(z)\ .\end{aligned} \tag{2.5b}$$

We define

$$\begin{aligned}I^A(z)=&A^0(z)+2\,\mathrm{Re}(z)A^0(z)VA^0(z)\\&-B^0(z)VA^0(z)-A^0(z)VB^0(z)\ ,\end{aligned} \tag{2.6a}$$

$$X_1^{AA}(z)=[4\,\mathrm{Re}^2(z)-|z|^2]A^0(z)V\ , \tag{2.6b}$$

$$Y_1^{AA}(z)=VA^0(z)\ , \tag{2.6c}$$

$$X_2^{AA}(z)=-2\,\mathrm{Re}(z)B^0(z)V\ , \tag{2.6d}$$

$$Y_2^{AA}(z)=VA^0(z)\ , \tag{2.6e}$$

$$X_3^{AA}(z)=-2\,\mathrm{Re}(z)A^0(z)V\ , \tag{2.6f}$$

$$Y_3^{AA}(z)=VB^0(z)\ , \tag{2.6g}$$

$$X_4^{AA}(z)=B^0(z)V\ , \tag{2.6h}$$

$$Y_4^{AA}(z)=VB^0(z)\ , \tag{2.6i}$$

$$X_1^{AB}(z)=-2\,\mathrm{Re}(z)A^0(z)V\ , \tag{2.6j}$$

$$Y_1^{BA}(z)=VA^0(z)\ , \tag{2.6k}$$

$$X_2^{AB}(z)=B^0(z)V\ , \tag{2.6l}$$

$$Y_2^{BA}(z)=VA^0(z)\ , \tag{2.6m}$$

$$X_3^{AB}(z)=A^0(z)V\ , \tag{2.6n}$$

$$Y_3^{BA}(z)=VB^0(z)\ , \tag{2.6o}$$

$$I^B(z)=B^0(z)+|z|^2A^0(z)VA^0(z)-B^0(z)VB^0(z)\ , \tag{2.6p}$$

$$X_1^{BA}(z)=2\,\mathrm{Re}(z)\,|z|^2A^0(z)V\ , \tag{2.6q}$$

$$Y_1^{AB}(z)=VA^0(z)\ , \tag{2.6r}$$

$$X_2^{BA}(z)=-|z|^2B^0(z)V\ , \tag{2.6s}$$

$$Y_2^{AB}(z)=VA^0(z)\ , \tag{2.6t}$$

$$X_3^{BA}(z)=-|z|^2A^0(z)V\ , \tag{2.6u}$$

$$Y_3^{AB}(z)=VB^0(z)\ , \tag{2.6v}$$

$$X_1^{BB}(z)=-|z|^2A^0(z)V\ , \tag{2.6w}$$

$$Y_1^{BB}(z)=VA^0(z)\ , \tag{2.6x}$$

$$X_2^{BB}(z)=B^0(z)V\ , \tag{2.6y}$$

$$Y_2^{BB}(z)=VB^0(z)\ . \tag{2.6z}$$

Then Eqs. (2.5a) and (2.5b) can be written, by using Eq. (2.6),

$$A(z)=I^A(z)+\sum_\alpha X_\alpha^{AA}(z)A(z)Y_\alpha^{AA}(z)+\sum_\alpha X_\alpha^{AB}(z)B(z)Y_\alpha^{BA}(z)\ , \tag{2.7a}$$

$$B(z)=I^B(z)+\sum_\alpha X_\alpha^{BA}(z)A(z)Y_\alpha^{AB}(z)+\sum_\alpha X_\alpha^{BB}(z)B(z)Y_\alpha^{BB}(z)\ . \tag{2.7b}$$

Now we want to construct positive probability distributions. Let $\{e_j\}_{j=1,2,\ldots}$ denote a complete orthonormal basis of expansion functions. Then Eq. (2.7) can be written in the form (suppressing the summation over α in the notation)

$$\langle e_m\mid A(z)\mid e_n\rangle=\langle e_m\mid I^A(z)\mid e_n\rangle+\sum_{k,l}\langle e_m\mid X^{AA}(z)\mid e_k\rangle\langle e_k\mid A(z)\mid e_l\rangle\langle e_l\mid Y^{AA}(z)\mid e_n\rangle+\sum_{k,l}\langle e_m\mid X^{AB}(z)\mid e_k\rangle\langle e_k\mid B(z)\mid e_l\rangle\langle e_l\mid Y^{BA}(z)\mid e_n\rangle\ , \tag{2.8a}$$

$$\langle e_m\mid B(z)\mid e_n\rangle=\langle e_m\mid I^B(z)\mid e_n\rangle+\sum_{k.l}\langle e_m\mid X^{BA}(z)\mid e_k\rangle\langle e_k\mid A(z)\mid e_l\rangle\langle e_l\mid Y^{AB}(z)\mid e_n\rangle+\sum_{k,l}\langle e_m\mid X^{BB}(z)\mid e_k\rangle\langle e_k\mid B(z)\mid e_l\rangle\langle e_l\mid Y^{BB}(z)\mid e_n\rangle\ . \tag{2.8b}$$

We want to use the property of a positive operator C that an arbitrary matrix element can be expressed in terms of positive matrix elements

$$\langle f_1\mid C\mid f_2\rangle=\tfrac{1}{2}\langle f_1+f_2\mid C\mid f_1+f_2\rangle-\frac{i}{2}\langle f_1+if_2\mid C\mid f_1+if_2\rangle+\frac{i-1}{2}\langle f_1\mid C\mid f_1\rangle+\frac{i-1}{2}\langle f_2\mid C\mid f_2\rangle\ . \tag{2.9}$$

Hence we define the following functions, which are positive for all z, m, n,

$$P_{mn}^A(z)=\langle e_m+e_n\mid A(z)\mid e_m+e_n\rangle\ , \tag{2.10a}$$

$$Q_{mn}^A(z)=\langle e_m+ie_n\mid A(z)\mid e_m+ie_n\rangle\ , \tag{2.10b}$$

$$R_m^A(z)=\langle e_m\mid A(z)\mid e_m\rangle\ , \tag{2.10c}$$

$$P_{mn}^B(z)=\langle e_m+e_n\mid B(z)\mid e_m+e_n\rangle\ , \tag{2.10d}$$

$$Q_{mn}^B(z)=\langle e_m+ie_n\mid B(z)\mid e_m+ie_n\rangle\ , \tag{2.10e}$$

$$R_m^B(z)=\langle e_m\mid B(z)\mid e_m\rangle\ , \tag{2.10f}$$

which will be later interpreted as probability distributions. We denote the matrix elements of the operators I, X, Y by

$$O_{m,n}(z)=\langle e_m\mid O(z)\mid e_n\rangle\ . \tag{2.11}$$

Now we substitute Eq. (2.8) into Eqs. (2.10). Then we express on the rhs the matrix elements of A and B in terms of P^A,Q^A,R^A,P^B,Q^B,R^B by using Eq. (2.9),

$$P_{m,n}^A(z)=I_{m,m}^A(z)+I_{m,n}^A(z)+I_{n,m}^A(z)+I_{n,n}^A(z)+\sum_{k,l}[X_{m,k}^{AA}(z)+X_{n,k}^{AA}(z)]\left[\tfrac{1}{2}P_{k,l}^A(z)-\frac{i}{2}Q_{k,l}^A(z)+\frac{i-1}{2}[R_k^A(z)+R_l^A(z)]\right][Y_{l,m}^{AA}(z)+Y_{l,n}^{AA}(z)]+\sum_{k,l}[X_{m,k}^{AB}(z)+X_{n,k}^{AB}(z)]\left[\tfrac{1}{2}P_{k,l}^B(z)-\frac{i}{2}Q_{k,l}^B(z)+\frac{i-1}{2}[R_k^B(z)+R_l^B(z)]\right][Y_{l,m}^{BA}(z)+Y_{l,n}^{BA}(z)]\ , \tag{2.12a}$$

$$Q_{m,n}^A(z)=I_{m,m}^A(z)+iI_{m,n}^A(z)-iI_{n,m}^A(z)+I_{n,n}^A(z)+\sum_{k,l}[X_{m,k}^{AA}(z)-iX_{n,k}^{AA}(z)]\left[\tfrac{1}{2}P_{k,l}^A(z)-\frac{i}{2}Q_{k,l}^A(z)+\frac{i-1}{2}[R_k^A(z)+R_l^A(z)]\right][Y_{l,m}^{AA}(z)+iY_{l,n}^{AA}(z)]+\sum_{k,l}[X_{m,k}^{AB}(z)-iX_{n,k}^{AB}(z)]\left[\tfrac{1}{2}P_{k,l}^B(z)-\frac{i}{2}Q_{k,l}^B(z)+\frac{i-1}{2}[R_k^B(z)+R_l^B(z)]\right][Y_{l,m}^{BA}(z)+iY_{l,n}^{BA}(z)]\ , \tag{2.12b}$$

$$R_m^A(z)=I_{m,m}^A(z)+\sum_{k,l}X_{m,k}^{AA}(z)\left[\tfrac{1}{2}P_{k,l}^A(z)-\frac{i}{2}Q_{k,l}^A(z)+\frac{i-1}{2}[R_k^A(z)+R_l^A(z)]\right]Y_{l,m}^{AA}(z)$$
$$+\sum_{k,l}X_{m,k}^{AB}(z)\left[\tfrac{1}{2}P_{k,l}^B(z)-\frac{i}{2}Q_{k,l}^B(z)+\frac{i-1}{2}[R_k^B(z)+R_l^B(z)]\right]Y_{l,m}^{BA}(z)\ , \tag{2.12c}$$

$$P_{m,n}^B(z)=I_{m,m}^B(z)+I_{m,n}^B(z)+I_{n,m}^B(z)+I_{n,n}^B(z)$$
$$+\sum_{k,l}[X_{m,k}^{BA}(z)+X_{n,k}^{BA}(z)]\left[\tfrac{1}{2}P_{k,l}^A(z)-\frac{i}{2}Q_{k,l}^A(z)+\frac{i-1}{2}[R_k^A(z)+R_l^A(z)]\right][Y_{l,m}^{AB}(z)+Y_{l,n}^{AB}(z)]$$
$$+\sum_{k,l}[X_{m,k}^{BB}(z)+X_{n,k}^{BB}(z)]\left[\tfrac{1}{2}P_{k,l}^B(z)-\frac{i}{2}Q_{k,l}^B(z)+\frac{i-1}{2}[R_k^B(z)+R_l^B(z)]\right][Y_{l,m}^{BB}(z)+Y_{l,n}^{BB}(z)]\ , \tag{2.12d}$$

$$Q_{m,n}^B(z)=I_{m,m}^B(z)+iI_{m,n}^B(z)-iI_{n,m}^B(z)+I_{n,n}^B(z)$$
$$+\sum_{k,l}[X_{m,k}^{BA}(z)-iX_{n,k}^{BA}(z)]\left[\tfrac{1}{2}P_{k,l}^A(z)-\frac{i}{2}Q_{k,l}^A(z)+\frac{i-1}{2}[R_k^A(z)+R_l^A(z)]\right][Y_{l,m}^{AB}(z)+iY_{l,n}^{AB}(z)]$$
$$+\sum_{k,l}[X_{m,k}^{BB}(z)-iX_{n,k}^{BB}(z)]\left[\tfrac{1}{2}P_{k,l}^B(z)-\frac{i}{2}Q_{k,l}^A(z)+\frac{i-1}{2}[R_k^B(z)+R_l^B(z)]\right][Y_{l,m}^{BB}(z)+iY_{l,n}^{BB}(z)]\ , \tag{2.12e}$$

$$R_m^B(z)=I_{m,m}^B(z)+\sum_{k,l}X_{m,k}^{BA}(z)\left[\tfrac{1}{2}P_{k,l}^A(z)-\frac{i}{2}Q_{k,l}^A(z)+\frac{i-1}{2}[R_k^A(z)+R_l^A(z)]\right]Y_{l,m}^{BA}(z)$$
$$+\sum_{k,l}X_{m,k}^{BB}(z)\left[\tfrac{1}{2}P_{k,l}^B(z)-\frac{i}{2}Q_{k,l}^B(z)+\frac{i-1}{2}[R_k^B(z)+R_l^B(z)]\right]Y_{l,m}^{BB}(z)\ . \tag{2.12f}$$

Equations (2.12) constitute a set of coupled linear equations for the determination of the positive probability distributions P^A,Q^A,R^A,P^B,Q^B,R^B.

There are a number of symmetries and relations among these probability functions. From Eq. (2.10) one obtains the following relations, which holds among the P^A,Q^A,R^A, as well as among the P^B,Q^B,R^B:

$$P_{mn}=P_{nm}\ , \tag{2.13a}$$
$$Q_{mn}+Q_{nm}=2(R_m+R_n)\ , \tag{2.13b}$$
$$P_{mm}=2Q_{mm}=4R_m\ . \tag{2.13c}$$

Using Eqs. (1.10a) and (1.10b) which yields

$$B(z)=HA(z)\ , \tag{2.14a}$$
$$\langle e_m\mid B(z)\mid e_n\rangle=\sum_k\langle e_m\mid H\mid e_k\rangle\langle e_k\mid A(z)\mid e_n\rangle\ , \tag{2.14b}$$

one can express P^B,Q^B,R^B in terms of P^A,Q^A,R^A,

$$P_{mn}^B(z)=\sum_k(H_{mk}+H_{nk})\left[\tfrac{1}{2}[P_{km}^A(z)+P_{kn}^A(z)]-\frac{i}{2}[Q_{km}^A(z)+Q_{kn}^A(z)]+\frac{i-1}{2}[2R_k^A(z)+R_m^A(z)+R_n^A(z)]\right]\ , \tag{2.15a}$$

$$Q_{mn}^B(z)=\sum_k(H_{mk}-iH_{nk})\left[\tfrac{1}{2}[P_{km}^A(z)+iP_{kn}^A(z)]-\frac{i}{2}[Q_{km}^A(z)+iQ_{kn}^A(z)]+\frac{i-1}{2}[(1+i)R_k^A(z)+R_m^A(z)+iR_n^A(z)]\right]\ , \tag{2.15b}$$

$$R_m^B(z)=\sum_k H_{mk}\left[\tfrac{1}{2}P_{km}^A(z)-\frac{i}{2}Q_{km}^A(z)+\frac{i-1}{2}[R_k^A(z)+R_m^A(z)]\right]\ . \tag{2.15c}$$

Finally, one has the following symmetry under reflection of z on the real energy axis. Equations (1.10a) and (1.10b) yields

$$A(z)=A(z^*)\ , \tag{2.16a}$$
$$B(z)=B(z^*)\ . \tag{2.16b}$$

By definition (2.10) this immediately implies for both sets A and B,

$$P(z)=P(z^*)\ , \tag{2.17a}$$
$$Q(z)=Q(z^*)\ , \tag{2.17b}$$
$$R(z)=R(z^*)\ . \tag{2.17c}$$

After having solved Eq. (2.12) for P^A,Q^A,R^A,P^B,Q^B,R^B one can reconstruct an arbitrary resolvent matrix element from the probability distributions by using Eq. (1.12),

$$\langle e_m \mid G(z) \mid e_n \rangle = z^* \left[\tfrac{1}{2} P^A_{mn}(z) - \frac{i}{2} Q^A_{mn}(z) + \frac{i-1}{2} [R^A_m(z) + R^A_n(z)] \right] - \left[\tfrac{1}{2} P^B_{mn}(z) - \frac{i}{2} Q^B_{mn}(z) + \frac{i-1}{2} [R^B_m(z) + R^B_n(z)] \right] . \tag{2.18}$$

From that the S matrix is obtained by Eq. (1.18).

III. MONTE CARLO METHOD

We want to solve Eqs. (2.12) for the unknown functions $P^A, Q^A, R^A, P^B, Q^B, R^B$. Because we would like to be able also to treat a many-body system, we propose to apply a Monte Carlo method. The set of Eqs. (2.12) is a set of coupled linear equations. Monte Carlo solutions of linear operator equations using Markov chains are discussed by Hammersley and Handscomb in Ref. 24. However, those results are given only for cases where the operator of the linear equation is smaller than one in a certain norm. In our case we do not assume such a stringent constraint to hold, because we also want to treat potentials describing strong forces. However, in our case we know that the functions $P^A, Q^A, R^A, P^B, Q^B, R^B$, have in addition the property of being positive. Thus we suggest applying the Monte Carlo technique similarly to the Monte Carlo Green's function method.[5–11] The latter technique aimed to calculate the ground state, and it relies on the fact that the ground-state wave function (for bosons) is a positive quantity and hence can be viewed as a probability in a Monte Carlo computation. The same holds in our case for the functions $P^A, Q^A, R^A, P^B, Q^B, R^B$. We write Eq. (2.12) in abbreviated form as

$$\psi(\nu) = \phi(\nu) + \sum_{\nu'} K(\nu,\nu') \psi(\nu') , \tag{3.1}$$

where ψ stands for $P^A, Q^A, R^A, P^B, Q^B, R^B$ and ϕ stands for the inhomogeneous terms in Eq. (2.12). We define a succession of functions $\psi^{(n)}$ by

$$\psi^{(n+1)}(\nu) = \phi(\nu) + \sum_{\nu'} K(\nu,\nu') \psi^{(n)}(\nu') \tag{3.2}$$

and ψ is the asymptotic $\psi^{(n)}$ for large n. Now the Monte Carlo method is employed to sample sets of "coordinates" at random from a trial function $\psi^{(0)}$. We call a set of "coordinates" ν a configuration. For any configuration ν_n, and given $\psi^{(n)}(\nu_n)$, we obtain ν_{n+1} and $\psi^{(n+1)}(\nu_{n+1})$ by sampling $K(\nu_{n+1},\nu'_n)\psi^{(n)}(\nu'_n)$ and adding $\phi(\nu_{n+1})$, which is considered as a density function for the configuration ν_{n+1}. The population of a configuration for a given value n is denoted as generation.

We want to conclude this section with two remarks. Firstly, one might ask why we have started from the once-iterated resolvent equation (2.2) instead of the simpler original equation (1.4). The answer is that Eq. (2.12) derived from Eq. (2.2) is more suitable for Monte Carlo purposes than an analogous equation derived from Eq. (1.4) would have been. In fact, creating a new configuration ν from an old one ν' by Eq. (3.2) proceeds via calculation of the matrix elements $K(\nu,\nu')$. If we would have used the equation analogous to (2.2) derived from (1.4), the kernel $K(\nu,\nu')$ would have contained δ functions, imposing severe constraints on the new configuration which might lead to conflicts with Monte Carlo sampling.

Secondly, we would like to point out a possible source of error in a numerical calculation. Although the probability distributions P,Q,R are positive by definition via Eq. (2.10), the Monte Carlo solution $\psi^{(n)}(\nu)$ for a finite-dimensional configuration, obtained via Eq. (3.2), is not necessarily positive, because the inhomogeneous term ϕ and the kernel K allow for negative contributions. This should be accounted for, e.g., by choosing a sufficiently large configuration for the trial function or eventually by putting negative values of $\psi^{(n)}(\nu)$ to zero.

IV. CONCLUSION

We have suggested how to solve the Schrödinger equation for scattering reactions of many-body systems or systems with many degrees of freedom. This should be useful in atomic and molecular physics as well as in nuclear physics (heavy-ion reactions). The basic idea is to calculate the resolvent $G(z)$ for energies z off the real axis, by splitting G into in positive functions. A set of linear equations is set up which determines those functions. The positivity of those functions is an essential ingredient to render the scheme suitable for application of the Monte Carlo method, which is an efficient tool to treat many degrees of freedom. Finally, we have proposed how to relate the S matrix of a scattering reaction to the resolvent $G(z)$ (off the energy axis), namely, by incorporating the scattering boundary conditions via finite-time Moller wave operators and constructing the time evolution via a Cauchy-type contour integral of $G(z)$.

ACKNOWLEDGMENT

The author is grateful for support from the Natural Sciences and Engineering Research Council of Canada.

APPENDIX: APPROXIMATION OF THE SPECTRAL REPRESENTATION OF exp(iHT)

In Eq. (1.7) we have related the time evolution exp(iHT) to the resolvent $G(z)$ via a cauchy contour integral which avoids the complications when going to the real energy axis $z = E + i\varepsilon$, $\varepsilon \to +0$. In this appendix we want to present an alternative approximate representation of exp(iHT) via a spectral representation, where $z = E + i\varepsilon$ approaches but does not reach the real axis. We find that the error is small if $\varepsilon T \ll 1$.

The spectral theorem for a self-adjoint Hamiltonian H

$$\exp(iHT)=\int dE\,\exp(iET)P(E)\ . \tag{A1}$$

We write the spectral projector $P(E)$ formally as

$$P(E)=\delta(H-E)\ , \tag{A2}$$

where the δ function of an operator shall be understood in the following sense. Let $|\psi_{E'}\rangle$ denote an eigenstate of H corresponding to the eigenvalue E'. Then

$$\int dE\,\delta(H-E)\,|\psi_{E'}\rangle=\int dE\,\delta(E'-E)\,|\psi_{E'}\rangle=|\psi_{E'}\rangle\ . \tag{A3}$$

We want to approximate the δ function by a regular distribution. We use

$$\delta(x)=\lim_{\varepsilon\to+0}\frac{1}{\pi}\frac{\varepsilon}{x^2+\varepsilon^2}\ . \tag{A4}$$

Substituting Eq. (A4) in (A2), Eq. (A1) reads

$$\begin{aligned}\exp(iHT)&=\lim_{\varepsilon\to+0}\frac{1}{\pi}\int dE\,\exp(iET)\frac{\varepsilon}{(H-E)^2+\varepsilon^2}\\&=\lim_{\varepsilon\to+0}-\frac{1}{\pi}\int dE\,\exp(iET)\mathrm{Im}[G(E+i\varepsilon)\ .\end{aligned} \tag{A5}$$

Compared to the representation via the contour integral [Eq. (1.7)] where $G(z)$ has to be evaluated for all z values of the contour, Eq. (A5) has the advantage that $G(E+i\varepsilon)$ has to be evaluated only at or in the vicinity of the scattering energy E. But like in Faddeev-Yakubovski integral equations of stationary scattering theory one has to take the limit $\varepsilon\to+0$. One might ask the question: How large is the error for $\exp(iHT)$ at a given T if one takes a small but nonzero value of the rhs of Eq. (A5)? It can be written

$$\begin{aligned}&\frac{1}{\pi}\int dE\,\exp(iET)\frac{\varepsilon}{(H-E)^2+\varepsilon^2}\\&\quad=\frac{1}{2\pi i}\left[e^{\varepsilon T}\int_{C^+}dz\frac{e^{izT}}{z-H}+e^{-\epsilon T}\int_{C^-}dz\frac{e^{izT}}{z-H}\right],\end{aligned} \tag{A6}$$

where C^+ denotes the line integral given by $z=E+i\varepsilon$, E: $+\infty\to-\infty$, and C^- corresponds to $z=E-i\varepsilon$, E: $-\infty\to+\infty$. The expression (A6) shows that the error is governed by $\exp(\varepsilon T)$ and $\exp(-\varepsilon T)$, respectively. In other words, for a finite but large scattering time T one has to choose the line integral close to the real energy axis, such that

$$|1-\exp(\pm\varepsilon T)|\ll 1\ . \tag{A7}$$

Taking the limit $\varepsilon\to0$ in (A6) and connecting the curves C^+,C^- at $E=\pm\infty$ by a traverse line yields again the Cauchy contour integral representation [Eq. (1.7)] of $\exp(iHT)$.

[1]K. G. Wilson, Phys. Rev. D **10**, 2445 (1974).

[2]C. Rebbi, *Lattice Gauge Theories and Monte Carlo Simulations* (World Scientific, Singapore, 1983).

[3]J. G. Zabolitzky, in *Proceedings of the Tenth International Conference on Few Body Problems in Physics, Karlsruhe 1983,* edited by B. Zeidnitz (North-Holland, Amsterdam, 1984), Vol. 1, p. 401c.

[4]N. Metropolis and S. Ulam, J. Am. Stat. Assoc. **44**, 335 (1949).

[5]M. H. Kalos, Phys. Rev. **128**, 1891 (1962).

[6]M. H. Kalos, J. Comp. Phys. **1**, 127 (1966).

[7]M. H. Kalos, Nucl. Phys. **A126**, 609 (1969).

[8]M. H. Kalos, Phys. Rev. A **2**, 250 (1970).

[9]M. H. Kalos, D. Levesque, and L. Verlet, Phys. Rev. A **9**, 2178 (1974).

[10]P. A. Whitlock, D. M. Ceperley, G. V. Chester, and M. H. Kalos, Phys. Rev. B **19**, 5589 (1979).

[11]M. H. Kalos, M. A. Lee, P. A. Whitlock, and G. V. Chester, Phys. Rev. B **24**, 115 (1981).

[12]Y. Akaishi, in *Proceedings of the Tenth International Conference on Few Body Problems in Physics, Karlsruhe 1983,* edited by B. Zeidnitz (North-Holland, Amsterdam, 1984), Vol. 1, p. 409c.

[13]This is the general form of a wave opertor in a multichannel system. See, e.g., the textbook by C. J. Joachain, *Quantum Collision Theory* (North-Holland, Amsterdam, 1975), Sec. 14, p. 352, Eq. (14.55).

[14]For a review of Faddeev-Yakubovski theory see W. Glöckle, *The Quantum Mechanical Few-Body Problem* (Springer-Verlag, Berlin, 1983).

[15]H. Kröger, Phys. Lett. B **135**, 1 (1984).

[16]H. Kröger, and R. J. Slobodrian, Phys. Rev. C **30**, 1390 (1984).

[17]H. Kröger, A. M. Nachabe, and R. J. Slobodrian, Phys. Rev. C **32**, 628 (1985).

[18]M. Batinic, Z. Bajzer, and H. Kröger, Phys. Rev. C **33**, 1187 (1986).

[19]H. Kröger, A. M. Nachabe, and R. J. Slobodrian, Phys. Rev. C **33**, 1208 (1986).

[20]R. Girard and H. Kröger, Phys. Lett. B **164**, 117 (1985).

[21]H. Kröger, A. Smailagic, and R. Girard, Phys. Rev. D **32**, 3221 (1985).

[22]H. Kröger, J. Math. Phys. **24**, 1509 (1983).

[23]H. Kröger, J. Math. Phys. **26**, 139 (1985).

[24]J. M. Hammesley and D. C. Handscomb, Monte Carlo Methods (Methuen, London, 1964), Chap. 7 and references therein.