Direct calculation of the S matrix for scattering of charged particles

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(Received 22 July 1985)

A recently proposed method for the direct calculation of the S matrix is tested on proton-proton scattering. The agreement with the S matrix calculated from a standard approach is satisfactory. Optimal conditions of the method are thoroughly investigated. Special attention is paid to criteria on the efficiency of the numerical approximation for a limited number of expansion functions. Two criteria are proposed which are based on exact relations in scattering theory: the intertwining property of the wave operators and the commutation property of the S matrix and the free Hamiltonian. As a result of this study we are able to give recommendations for a successful application of the method.

I. INTRODUCTION

Few-body scattering processes in nuclear and atomic physics very often involve charged particles. The interaction between charged particles at nonrelativistic energies is described by Coulomb-type potentials involving the long-range Coulomb potential and short-range potentials. Multichannel scattering theory for short-range potentials is well established and there is a variety of applicable methods for the calculation of scattering or breakup amplitudes.[1,2] This is not the case when the Coulomb potential and more than two particles are involved. Although one can formally establish a rigorous multichannel scattering theory for Coulomb-type potentials[3–10] its application to few-body problems becomes often very difficult or impossible.[11–18] Recently Kröger proposed[19,20] a straightforward and theoretically transparent approach for the calculation of scattering (or breakup) amplitudes for few-body processes involving Coulomb-type potentials. The main characteristics of this approach are its rigorous mathematical background[21] and its orientation to numerical rather than analytical methods. Such an orientation is motivated by the complexity of an analytical analysis on one side, and by everyday enhancement of computing capabilities on the other side.

Let us briefly describe the method. The S matrix is composed from Møller wave operators which contain all the scattering information. The wave operators are approximated by exponentials of an approximated finite rank Hamiltonian operator using a large but finite time. That applies to the standard Møller wave operator as well as to the Dollard modified wave operator if Coulomb potentials are involved.[3] The finite rank Hamiltonian is obtained from the original Hamiltonian by projecting onto the space of expansion functions. That enables one to calculate the exponential in the eigenrepresentation of the finite rank Hamiltonian matrix. As expansion functions we chose step functions like in Ref. 20. The advantage of those functions is based on the fact that the asymptotic channel Hamiltonian is diagonal in that basis and matrix elements of the two-body Coulomb potential and the kinetic energy can be calculated analytically.

First numerical tests of the proposed method for a two-body system are encouraging.[20,21] Also the calculation of a $p+d$ breakup amplitude at low energies has been performed.[20,21] While in the two-body case one can obtain very good agreement with the exact S matrix, in the three-body case the results are not as good in comparison with experimental data.[21] One of the reasons is probably a too small number of expansion functions in the three-body case which cannot be enlarged substantially without enlarging the available computer memory.

In the present study we investigate the proposed method in more detail searching for an optimal choice of approximation parameters of the method. Numerical tests are performed in the two-body case using more realistic nucleon-nucleon potentials than in Ref. 20. Our choice of a short-range potential is guided by three requirements: (i) the potential should allow an exact calculation of the S matrix via a standard approach, (ii) it should describe realistic scattering experiments, and (iii) it should not be too complicated in order that many different numerical tests can be performed easily. According to these requirements, we have chosen the Graz potential[22] (s wave) and the Yamaguchi potential (s wave; the parameters were chosen to reproduce the experimental values for pp scattering length and effective range).

The main objective of the present study is to find optimal conditions to minimize the error of the method in realistic two-body cases with special attention to criteria on the efficiency of the numerical approximation for a given number of expansion functions. This investigation is certainly required as the first step in order to perform precise three-body calculations with this method. In fact one can always consider a two-body calculation as a special case of a three-body calculation and fix certain conditions of the method on the two-body level where exact results are known. In Sec. II of this study we present the

proposed direct method for the calculation of the S matrix in some detail. Two criteria for efficiency of the numerical approximation are established on the basis of the intertwining property of wave operators and the commutation property of the free Hamiltonian with the S-matrix operator. Section III is devoted to numerical tests in order to find optimal conditions to minimize the error. In the concluding Sec. IV these conditions are summarized. Some explicit formulae for the calculation of the S matrix involving Coulomb-type potentials in the standard approach are quoted in the Appendix.

II. S MATRIX FOR TWO-BODY SCATTERING

In the following we consider the two-body quantum mechanical scattering problem in the center of mass system. Natural units $\hbar=c=1$ are chosen for simplicity. $H=H^0+V$ is the total Hamiltonian of the system with H^0 denoting the kinetic energy operator of the free relative motion and V denoting the two-body Coulomb-type potential:

$$V=V^s+V^C .$$

V^s denotes the short-range potential and V^C the Coulomb potential given in coordinate space by $V^C(r)=e_1e_2/r$, where e_1 and e_2 are the charges of the two particles. Their reduced mass is denoted by μ. A two-body scattering process is described by the S matrix which in the case of Coulomb-type potentials can be written as follows:[11,23,24]

$$\langle\phi\,|\,S\,|\,\psi\rangle=-2\pi i\int d^3\mathbf{q}\int d^3\mathbf{q}'\phi^*(\mathbf{q}')\delta(E_q-E_{q'})\mathscr{T}(\mathbf{q}',\mathbf{q};E_q)\psi(\mathbf{q}) , \tag{2.1}$$

$$\mathscr{T}(\mathbf{q}',\mathbf{q};E_q)=\lim_{\epsilon\to+0}[(E_q-E_{q'}+i\epsilon)^{-i\eta(q')}\langle\mathbf{q}'\,|\,T(E_q+i\epsilon)\,|\,\mathbf{q}\rangle(i\epsilon)^{-i\eta(q)}]C(q)C(q') , \tag{2.2}$$

$$C(q)=(2q^2/\mu)^{i\eta}e^{-(\pi/2)\eta}/\Gamma(1-i\eta),\quad \eta=\frac{e_1e_2\mu}{q},\quad E_q=q^2/2\mu . \tag{2.3}$$

$\phi(\mathbf{q})=\langle\mathbf{q}\,|\,\phi\rangle$ and $\psi(\mathbf{q})=\langle\mathbf{q}\,|\,\psi\rangle$ are ingoing and outgoing wave packets, respectively, in momentum space representation. $T(z)$ is the T-matrix operator satisfying the Lippmann-Schwinger equation:

$$T(z)=V+VG^0(z)T(z),\quad G^0(z)=(z-H^0)^{-1} ,$$
$$\mathrm{Im}z\neq0 .$$

The standard approach to calculate $\langle\phi\,|\,S\,|\,\psi\rangle$ is based, generally speaking, on solving an integral equation of Lippmann-Schwinger–type for the T matrix and performing the on-shell limit in an appropriate way.[9,11,16,23–26] For a certain class of Coulomb-type potentials with a separable short-range part, $\mathscr{T}(\mathbf{q},\mathbf{q}';z)$ can be calculated analytically and expressed in terms of special functions.[22,23,27,28] In this work we shall use an explicit analytical formula for $\mathscr{T}$ when the short-range potential is a s-wave rational separable potential[23] (see the Appendix).

The new direct approach to calculate $\langle\phi\,|\,S\,|\,\psi\rangle$ is based on the definition of time dependent scattering theory and a strong approximation of wave operators.[21] The following relations hold:[20,21]

$$\langle\phi\,|\,S\,|\,\psi\rangle=\lim_{T\to\infty}\lim_{N\to\infty}\langle\phi\,|\,S(T,N)\,|\,\psi\rangle , \tag{2.4}$$

$$S(T,N)=\Omega^\dagger(T,N)\Omega(-T,N) ,$$
$$\Omega(T,N)=e^{iH_NT}e^{-iH_N^{0C}(T)} . \tag{2.5}$$

H_N and H_N^{0C} are finite rank approximations of H and the asymptotic Hamiltonian of Dollard,[3] respectively:

$$H_N=P_NHP_N , \tag{2.6}$$

$$H_N^{0C}(t)=P_N\left[H^0t+\mathrm{sgn}(t)\left[\frac{\mu}{2H^0}\right]^{1/2}e_1e_2\times\ln(4H^0\,|\,t\,|\,)\right]P_N . \tag{2.7}$$

P_N is the projector given by

$$P_N=\sum_{i=1}^{N}\sum_{l=0}^{L}\sum_{m=-l}^{l}|\,h_ilm\,\rangle\langle\,h_ilm\,|\,,\langle h_i\,|\,h_j\rangle=\delta_{ij} , \tag{2.8}$$

$$\langle\,\mathbf{q}\,|\,h_ilm\,\rangle=h_i(q)Y_{lm}(\hat{\mathbf{q}}) , \tag{2.9}$$

where $h_i(q)$ is the step function normalized to unity, corresponding to the interval $[q_i,q_{i+1}]$ given by

$$h_i(q)=\begin{cases}\alpha_i \text{ if } q_i<q<q_{i+1},\ \alpha_i=[\frac{1}{3}(q_{i+1}^3-q_i^3)]^{-1/2},\\ 0 \text{ elsewhere},\end{cases} \tag{2.10}$$

and

$$0=q_1<q_2<\cdots<q_N<q_{N+1}=q_{\mathrm{cut}}^{(N)}$$

denotes a finite partition $D^{(N)}$ of the interval $I^{(N)}=[0,q_{\mathrm{cut}}^{(N)}]$ such that for increasing N

$$q_{\text{cut}}^{(N)} \to \infty, \quad \max_{i \in \{1,\ldots,N\}} |q_{i+1}-q_i| \to 0 . \tag{2.11}$$

The whole calculation of the S matrix according to (2.4) is performed numerically. It has two parts conceptually: (a) the calculation of $\langle \phi | S(T,N) \psi \rangle$ for a given T and N and (b) the numerical determination of the limits.

A. Calculation of $\langle \phi | S(T,N) | \psi \rangle$

First we observe that H^0 and $H^{0C}(t)$ are diagonal in the basis vectors $|h_i lm\rangle$. Using successively Eqs. (2.4)–(2.10) we obtain the following expression for the S matrix:

$$\langle \phi | S(T,N) | \psi \rangle = \sum_{klm} \sum_{k'l'm'} \langle \phi | h_k lm \rangle e^{i\epsilon_k^C(T)} M_{klm,k'l'm'}(T) e^{i\epsilon_{k'}^C(T)} \langle h_{k'} l'm' | \psi \rangle , \tag{2.12}$$

$$\epsilon_k^C(t) = \langle h_k lm | H^{0C}(t) | h_k lm \rangle = \epsilon_k t + 4\pi \operatorname{sgn}(t) \alpha_k^2 e_1 e_2 \mu \left[\tfrac{1}{2}(q_{k+1}^2 - q_k^2) \left(\ln \frac{2|t|}{\mu} - 1 \right) + q_{k+1}^2 \ln q_{k+1} - q_k^2 \ln q_k \right] ,$$

$$k = 1, \ldots, N , \tag{2.13}$$

$$\epsilon_k = \langle h_k lm | H^0 | h_k lm \rangle = \frac{2\pi}{5\mu} \alpha_k^2 (q_{k+1}^5 - q_k^5) , \tag{2.14}$$

$$M_{klm,k'l'm'}(T) = \langle h_k lm | e^{-2iH_N T} | h_{k'} l'm' \rangle . \tag{2.15}$$

The problem therefore rests on the calculation of $M_{klm,k'l'm'}(T)$. As already suggested[19,21] the most promising way is to diagonalize H_N. In this work we are performing the diagonalization using Jacobi's method.

B. Numerical determination of the limits

The diagonalization of H_N for large N can, generally speaking, be performed only numerically. This is the main reason why the determination of the limits in Eq. (2.4) has to be performed by a numerical procedure. According to the definition of the S matrix as a time limit and a discussion in Refs. 20 and 21, it is clear that the limes $N \to \infty$ should be performed first. It depends on the choice of interval $I^{(N)}$ and on the parameter T. Also, in principle, the choice of the partition $D^{(N)}$ could influence the convergence. We shall investigate in detail all these dependencies of the method in Sec. III.

Now let us discuss some criteria for the accuracy of the method. There are some properties of the S matrix and wave operators which are exactly valid and in principle can be used to estimate the accuracy of the numerical approximation. Firstly, we quote the following property of Dollard's wave operators:[29]

$$e^{iHt}\Omega_{\pm} = \Omega_{\pm} e^{iH^0 t}, \quad \Omega_{\pm} = \underset{t \to \mp\infty}{s\text{-lim}} e^{iHt} e^{-iH^{0C}(t)} . \tag{2.16}$$

By differentiation of (2.16) with respect to t and setting $t=0$, one obtains the well-known intertwining property:

$$H^n \Omega_{\pm} = \Omega_{\pm} (H^0)^n, \quad n = 0,1,2,\ldots , \tag{2.17}$$

which together with the isometry property of the wave operators leads to the equality

$$\langle \phi | \Omega_{\pm}^{\dagger} H^n \Omega_{\pm} | \psi \rangle = \langle \phi | (H^0)^n | \psi \rangle . \tag{2.18}$$

The right-hand side of this equation can be calculated exactly and the left-hand side approximately using $\Omega(T,N)$ [as shown in Ref. 21 $\Omega(\mp T,N)$ strongly converges to $\Omega_{\pm}$]. Thus the quantity

$$\Delta_n = \left| \frac{\langle \phi | \Omega^{\dagger}(T,N) (H_N)^n \Omega(T,N) | \psi \rangle}{\langle \phi | (H^0)^n | \psi \rangle} - 1 \right| \tag{2.19}$$

gives some estimate of the accuracy of the numerical approximation.

Another criterion is based on the conservation of energy in scattering experiments which can be expressed through the commutation property of S and H^0,[30]

$$SH^0 = H^0 S, \quad H^0 = S^{\dagger} H^0 S . \tag{2.20}$$

Thus the quantity

$$\Delta_s = \left| \frac{\langle \phi | S^{\dagger}(T,N) H_N^0 S(T,N) | \psi \rangle}{\langle \phi | H^0 | \psi \rangle} - 1 \right| \tag{2.21}$$

may also be used to estimate the quality of our approximation.

An important feature of the method considered here lies in fact that the S matrix is calculated for wave packets of finite width. Scattering experiments are usually performed with very narrow wave packets. On the other hand, the calculation of the differential cross section is usually performed for a sharp state of well-defined wave number; i.e., $d\sigma/d\Omega$ is proportional to the absolute square of the on-shell T matrix: $|\mathcal{T}(\mathbf{q},\mathbf{q}';E_q)|^2, q=q'$. The result of such a calculation should be the same as the result of a calculation with a wave packet in the limit of an infinitely narrow wave packet.[31,32] This means that in calculating $\langle \phi | S | \psi \rangle$ we have to choose narrow wave packets and investigate the sensitivity of the result on the variation of the width.

III. NUMERICAL CALCULATION FOR REALISTIC s-WAVE POTENTIALS

In this section we shall numerically investigate stability properties and error estimates which are important in applying the direct method for a calculation of the S matrix. As mentioned in the Introduction we perform our investigation using realistic short-range s-wave potentials. Thus we choose the Graz potential[22] which reproduces s-wave phase shifts up to 500 MeV and the Yamaguchi potential which fairly reproduces s-wave phase shifts up to 100 MeV. The form and the parameters of these potentials are presented in the Appendix.

Concerning the form of the wave packets we adopted the suggestion already given in Ref. 20:

$$\Phi(q_M,w)\equiv\langle \mathbf{q}\mid\phi\rangle=\begin{cases}\kappa\left[1-\cos\left[2\pi\dfrac{k_2-q}{k_2-k_1}\right]\right], & k_1<q<k_2\ ,\\ 0, \text{ elsewhere.}\end{cases}\tag{3.1}$$

The parameter κ is fixed by the requirement of normalization to unity. This bell-shaped wave packet is symmetrical having a peak at $q_M=(k_1+k_2)/2$ and a half-width $w=(k_2-k_1)/2$. In most of the following numerical investigations we shall use the wave packet $\Phi(0.2\ \text{fm}^{-1}, 0.02\ \text{fm}^{-1})$ as the standard wave packet (SWP) ($\hbar=c=1$ units are assumed). It is narrow enough to cause a deviation of $\langle\phi\mid S\mid\phi\rangle$ from the corresponding S-matrix element in the sharp momentum limit which is smaller than 0.1% for all potentials considered (as illustrated in Table I).

In order to investigate the influence of the partition set $D^{(N)}$ on the convergence we have chosen several different types:

$$D_2^{(N)}=\{q_i\mid q_i=(i-1)^2q_{\text{cut}}^{(N)}/N^2,\ i=1,\ldots,N+1\}-\text{quadratic}\ ;\tag{3.2}$$

$$\begin{aligned}D^{(N)}(N_1,N_2;\epsilon_1,\epsilon_2,\epsilon_3)=\{q_i\mid\ & q_{i+1}-q_i=\epsilon(i)(q_i-q_{i-1}),\ i=2,\ldots,N\ ;\\ & q_1=0,\ q_{N_1+1}=k_1,\ q_{N_1+N_2+1}=k_2,\ q_{N+1}=q_{\text{cut}}^{(N)};\ \epsilon(i)=\epsilon_1,\ 2\le i\le N_1\ ;\\ & \epsilon(i)=\epsilon_2,\ N_1+2\le i\le N_1+N_2;\ \epsilon(i)=\epsilon_3,\ N_1+N_2+2\le i\le N\}\ ,\end{aligned}\tag{3.3}$$

geometrical progression by part

$$D_f^{(N)}=\left\{q_i\ \middle|\ \int_{q_i}^{q_{i+1}}f(q)dq=1,\ \int_0^{q_{N+1}}f(q)dq=N;f(q)\ge 0\right\}-\text{general}\ .\tag{3.4}$$

TABLE I. Exact value of S matrix for different wave packets and different potentials. For definitions k_1, k_2, and q_M see Eq. (3.1). The values for infinitely narrow wave packets are presented in the rows where only q_M is indicated.

k_1 (fm^{-1})	q_M (fm^{-1})	k_2 (fm^{-1})	$\langle\phi\mid S\mid\phi\rangle$ Coulomb potential	$\langle\phi\mid S\mid\phi\rangle$ Yamaguchi potential	$\langle\phi\mid S\mid\phi\rangle$ Coulomb + Yamaguchi potential
0.00		0.10	$0.940\,381-0.332\,377i$	$0.044\,700+0.978\,277i$	$0.069\,721-0.023\,069i$
0.03		0.07	$0.933\,919-0.355\,856i$	$0.119\,421+0.988\,268i$	$0.989\,741-0.095\,554i$
0.045		0.055	$0.932\,760-0.360\,394i$	$0.124\,464+0.990\,616i$	$0.992\,496-0.119\,249i$
	0.05		$0.932\,683-0.360\,698i$	$0.135\,553+0.990\,770i$	$0.992\,671-0.120\,860i$
0.10		0.20	$0.991\,344-0.130\,730i$	$-0.506\,114+0.862\,224i$	$0.146\,844+0.982\,234i$
0.13		0.17	$0.991\,276-0.131\,717i$	$-0.506\,862+0.861\,990i$	$0.155\,871+0.986\,630i$
0.145		0.155	$0.991\,263-0.131\,895i$	$-0.506\,995+0.861\,946i$	$0.157\,462+0.987\,453i$
	0.15		$0.991\,262-0.131\,906i$	$-0.506\,971+0.861\,962i$	$0.157\,603+0.987\,499i$
0.20		0.30	$0.996\,819-0.079\,506i$	$-0.501\,085+0.865\,295i$	$-0.243\,619+0.969\,703i$
0.23		0.27	$0.996\,817-0.079\,721i$	$-0.502\,986+0.864\,278i$	$-0.244\,774+0.969\,553i$
0.245		0.255	$0.996\,814-0.079\,760i$	$-0.503\,327+0.864\,095i$	$-0.244\,982+0.969\,526i$
	0.25		$0.996\,814-0.079\,762i$	$-0.503\,328+0.864\,095i$	$-0.244\,971+0.969\,529i$

The last type is the most general one allowing an arbitrary density of the nodes according to some distribution function $f(q)$. It is, for instance, possible to choose for $f(q)$ the form factor of a separable potential or its derivative which could lead to a better approximation.

Firstly, we illustrate the convergence of the direct method in the case of the Coulomb + Graz (CG) s-wave potential. Figure 1 shows globally the convergence to the reference value $\langle\phi|S|\phi\rangle$ (calculated with a standard method) depending on the time parameter T and the number of nodes N. The deviation from the reference value is measured by

$$\Delta(T,N)=\left|\frac{\langle\phi|S(T,N)|\phi\rangle}{\langle\phi|S|\phi\rangle}-1\right| . \tag{3.5}$$

For a given T, Δ is typically smaller for larger N and by increasing T the limiting values of Δ, $N>70$ are also smaller. This is not generally the case, however, as can be better seen from Fig. 2. Δ oscillates slowly as a function of N about its limiting value which is obtained for $N>150$. By increasing T, the limit in N approaches to $\Delta\approx 0.5\%$, which can be considered as the result of a finite $q_{\rm cut}^{(N)}$. By increasing $q_{\rm cut}^{(N)}$ and performing the limit in N and T, one expects an improved result.

The typical behavior of Δ as a function of T is shown in Fig. 3. It decreases rapidly until a certain value T_0 (which negligibly varies with N) and then becomes relatively stable up to a certain T_1 after which it increases rapidly. In the case of a short-range potential the region of stability is very emphasized while after including the

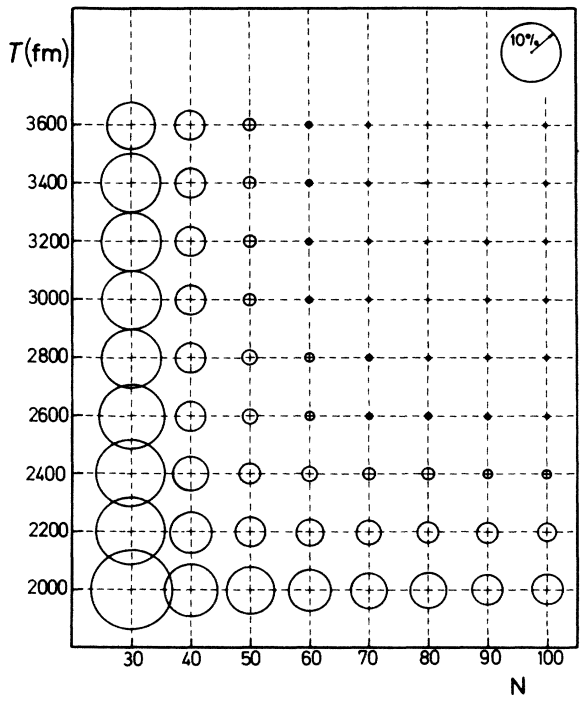

FIG. 1. The convergence of $\langle\phi|S(T,N)|\phi\rangle$ for the CG potential. The radius of the circles $r=\Delta(T,N)$ [see Eq. (3.5)] represents the deviation from the reference value $\langle\phi|S|\phi\rangle=-0.141\,668+0.989\,694i$; the standard wave packet (SWP) $\Phi(0.2\ \text{fm}^{-1}, 0.02\ \text{fm}^{-1})$ and $q_{\rm cut}^{(N)}=40\ \text{fm}^{-1}$ was used.

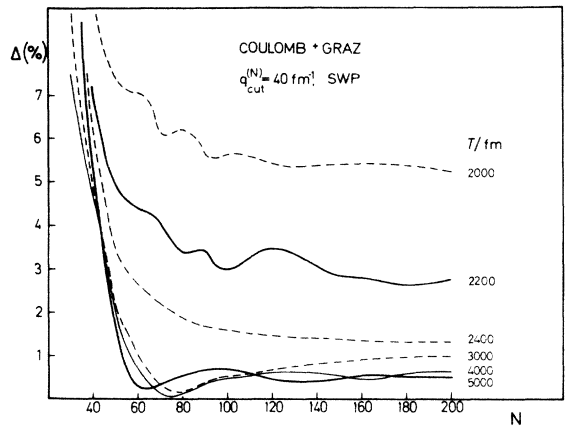

FIG. 2. Deviation $\Delta(T,N)$ as a function of the number of nodal points N for different times T. The convergence for large N and T is clearly seen.

Coulomb potential oscillations may occur within this region (Fig. 4). The region of stability (i.e., T_1) is increasing with N (Fig. 5). We found that the time T_0 is about inversely proportional to the energy width of the wave packet:

$$w_E=(q_M+w/2)^2/(2\mu)-(q_M-w/2)^2/(2\mu)$$
$$=q_M w/\mu .$$

The described typical behavior of Δ may be a useful guideline for the limiting procedure when the exact solution is not known. It is important to note that the main computational effort of the method considered here lies in the diagonalization of H_N. Once this is done the calculation of $\langle\phi|S(T,N)|\phi\rangle$ for different values of T is easy to perform. Thus from the practical point of view we can easily calculate the T dependence of the S matrix for a given N and than proceed with the calculation for larger N bearing in mind that limit $N\to\infty$ should be performed firstly. In fact we can search for the limit $N\to\infty$ of $\langle\phi|S(T,N)|\phi\rangle$ being relatively stable with respect to T. The stability region is obtained simultaneously for the real and the imaginary part of $\langle\phi|S(T,N)|\phi\rangle$ (Fig. 6).

The number N of nodal points is practically limited by the available computer storage. It is therefore worthwhile

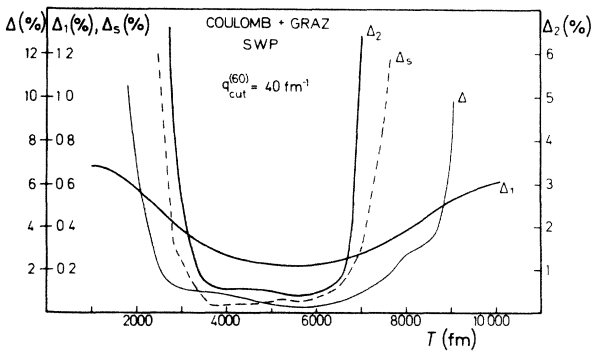

FIG. 3. Deviation $\Delta(T,60)$, $\Delta_1(T,60)$, $\Delta_2(T,60)$, and $\Delta_S(T,60)$ as a function of T [see Eqs. (2.19), (2.21), and (3.5)].

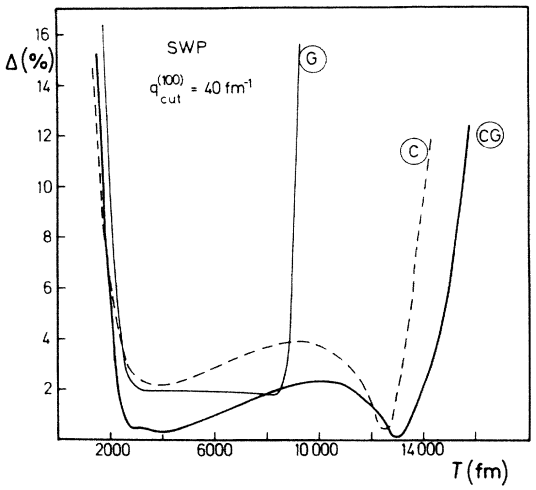

FIG. 4. Deviation $\Delta(T,100)$ as a function of T for different potentials: G represents Graz, C represents Coulomb, CG represents Coulomb + Graz.

to investigate whether for a given N the choice of the interval $[0,q_{\rm cut}^{(N)}]$ and the partition set $D^{(N)}$ has some importance. We found that by increasing $q_{\rm cut}^{(N)}$ (while keeping N fixed) the result achieved is better up to a certain value of $q_{\rm cut}^{(N)}$ (see Fig. 7). For larger $q_{\rm cut}^{(N)}$ one cannot obtain any substantial improvement which is in accordance with the requirement (2.11). The choice of the optimal value for $q_{\rm cut}^{(N)}$ depends on the behavior of the potential in momentum space. Thus in the case of the Graz potential the optimal $q_{\rm cut}^{(N)}$ is about 40 fm^{-1} and for the Yamaguchi potential it is 20 fm^{-1}. Concerning the choice of the partition set $D^{(N)}$ we found that for an equidistant and a quadratic distribution of nodes one needs a much larger N to obtain convergence, than for the other two types (3.3) and (3.4). The sensitivity of the method on the choice of the partition set is illustrated in Fig. 8, where we used three different sets of $D^{(60)}$ $(N_1,N_2,1,1,\epsilon_3)$. For the same case using a quadratic nodal distribution $D_2^{(60)}$, the best value obtained for Δ is 17%. The main reason for such a result is the fact that the interval (0.18 fm^{-1}, 0.22 fm^{-1}) where the wave packet Φ(0.2 fm^{-1}, 0.02 fm^{-1}) is nonvanishing,

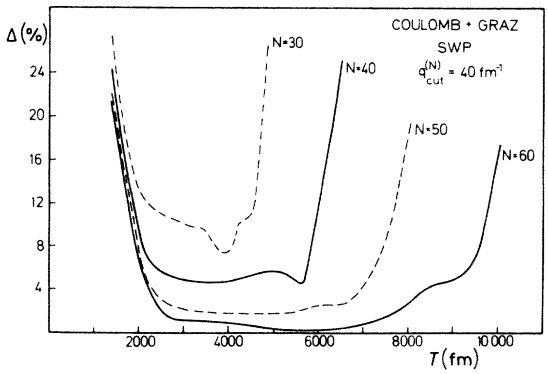

FIG. 5. Deviation $\Delta(T,N)$ as a function of T for different N. By increasing N the region of stability is increased.

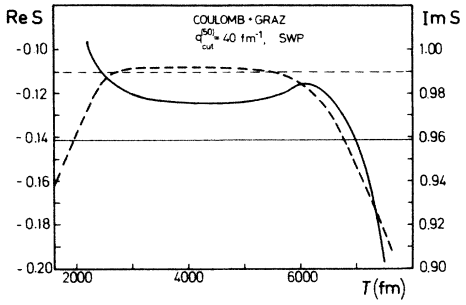

FIG. 6. Real (full line) and imaginary (dashed line) part of $\langle\phi|S(T,50)|\phi\rangle$ as a function of T. The straight lines represent the real (full line) and the imaginary part (dashed line) of the exact S matrix $\langle\phi|S|\phi\rangle$.

covers only two successive nodal points. We found that it is important to have several nodal points in the interval of the wave packet.

To fix somehow the partition set we propose to relate it to the potential using the most general type of partition (3.4). Thus, for instance, in the case of the pure Yamaguchi potential we use the functions

$$\text{(a) } f_1(q)=a_1(\beta^2+q^2)^{-1}+be^{-c(q-q_M)^2},$$

$$\text{(b) } f_2(q)=a_2\frac{d}{dq}(\beta^2+q^2)^{-1}+be^{-c(q-q_M)^2}.$$

The second term of Gaussian shape is included to generate a higher density of nodal points in the interval of the wave packet. The case (b) is chosen in order to distribute the nodal points according to the rate of change of the form factor as a function of q. In both cases similar results are obtained and these partitions do not show any advantage compared with those given by (3.3) except that they are related to the potential. However, such a relation cannot be established in the case of Coulomb-type potentials.

Let us now discuss the proposed criteria (2.19) and (2.21). Our numerical investigations led us to the conclusion that there is no simple correlation between Δ and Δ_s or Δ_n. Particularly for different pairs (T_1,N_1) and (T_2,N_2), the relation $\Delta_s(T_1,N_1)<\Delta_s(T_2,N_2)$ does not necessarily imply $\Delta(T_1,N_1)<\Delta(T_2,N_2)$. The same ap-

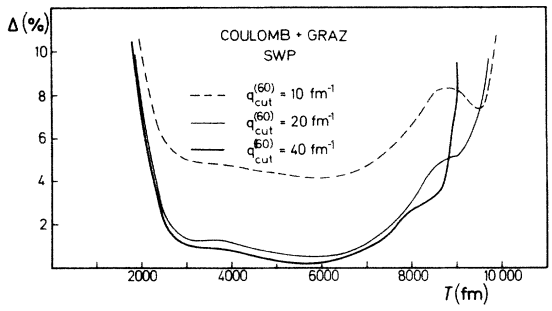

FIG. 7. Deviation $\Delta(T,60)$ as a function of T for different $q_{\rm cut}^{(60)}$.

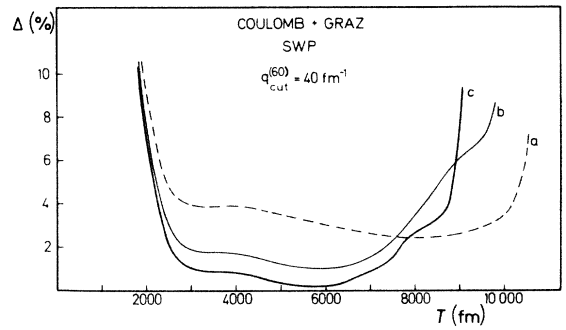

FIG. 8. Deviation $\Delta(T,60)$ as a function of T for different partitions: (a) $D^{(60)}(20,8;1,1,1.218)$; (b) $D^{(60)}(18,6;1,1,1.205)$; (c) $D^{(60)}(15,6;1,1,1.178)$.

plies to Δ_n. However, the behavior of Δ_s and Δ_n as a function of T for fixed N is similar to the behavior of Δ (Fig. 3). In certain cases a minimum of Δ_1 corresponds to the minimum of Δ but that cannot be considered as a rule. The stability region for Δ_2 and Δ_s is more emphasized than for Δ_1. We found that Δ_1 for a given N is approximately a periodical function of T with a period $2\pi\mu n[q_M(k_2-k_1)]^{-1}$ (n is the number of nodal points in the region of the wave packet). This property holds in the case of an equidistant partition in the region of the wave packet [e.g., $D^{(N)}(N_1,N_2,1,1,\epsilon_3)$].

What is the conclusion on the usefulness of the proposed criteria for the quality of the approximation? From the above discussion it follows that the most important feature of Δ_s and Δ_2 is the existence of a stability region which corresponds to the stability region of Δ when considered as a function of T for fixed N. The first local minimum of Δ_1 falls within the same stability region. Thus using criteria Δ_1, Δ_2, and Δ_s we can determine the time interval in which the S matrix is stable with respect to T and close to its exact value. The question now arises what is the best value of T, while keeping N fixed, which one would choose within the region of stability. A well-defined choice would be $T^1_{\min}$ which is the time for which Δ_1 achieves its first minimum. However, this is not the best choice as can be seen from Table II. In fact $\langle\phi|S(T^1_{\min},N)|\phi\rangle$ does not converge properly with N. A much better choice is the value of T which falls in the first region where the S matrix is most stable when T is increasing, that is T' which is the smallest value of T for which $|(\partial/\partial T)\langle\phi|S(T,N)\phi\rangle|$ is minimal. The convergence of $\langle\phi|S(T',N)|\phi\rangle$ with respect to N is in most cases better than for an arbitrarily chosen fixed T (see Table II). Furthermore, $\langle\phi|S(T',N)|\phi\rangle$ seems to be correlated with the first minimum of Δ for a given N (last column in Table II).

IV. CONCLUSION

We have shown that the method of the direct calculation of the S matrix can be successfully applied to proton-proton s-wave scattering using a realistic interaction. We investigated in detail conditions of stability and error estimates of the method and proposed criteria on the efficiency of the numerical approximation. As a result of these investigations we can give the following recipe for an application of the method:

(i) Use the partition $D^{(N)}(N_1,N_2,1,1,\epsilon_3)$ which is flexible and simple enough to perform different tests. It is important to distribute enough nodel points in the region of the wave packet.

(ii) For a given N and $q^{(N)}_{\text{cut}}$ calculate the S matrix, Δ_1, Δ_2, and Δ_S as a function of the time T, and find the region of stability which should appear in the real and imaginary part of the S matrix in Δ_2 and Δ_S, while Δ_1 exhibits a well-defined minimum in this region.

(iii) By increasing $q^{(N)}_{\text{cut}}$ gradually find its minimal value such that the S matrix does not change substantially for greater $q^{(N)}_{\text{cut}}$.

(iv) For a given N and $q^{(N)}_{\text{cut}}$ consider the S matrix as a function of T and choose as the best approximation the value for which the absolute value of the S matrix is most stable.

(v) If possible, increase the number N of nodal points leaving $q^{(N)}_{\text{cut}}$ constant and perform again the steps (ii)—(iv). This leads to a better limiting value of the S matrix.

The experience gained from the two-body calculations reported here should be of considerable importance in an application of the method to the three-body problem.

TABLE II. Deviation $\Delta(T,N)$ from the exact value of the S matrix for increasing N and different T: $T^1_{\min}$ is the time for which $\Delta_1(T,N)$ achieves for given N the first minimum; T' is the smallest value of T for which $|\partial/\partial T\langle\phi|S(T,N)|\Phi\rangle|$ is minimal; $T_{\min}$ is the time for which $\Delta(T,N)$ achieves for given N the first minimum in the region of stable $\Delta(T,N)$.

N	$\Delta(T=3000,N)$	$\Delta(T=500,N)$	$T^1_{\min}$	$\Delta(T^1_{\min},N)$	T'	$\Delta(T',N)$	$T_{\min}$	$\Delta_{\min}$
30	10.124	32.558	2800	10.582	3000	10.124	4000	7.554
40	4.870	6.516	3800	4.861	3200	4.769	3400	4.733
50	2.236	1.777	4600	1.748	3400	2.045	4800	1.744
60	1.168	0.410	5600	0.250	3400	1.047	5800	0.238
70	0.416	0.241	6500	0.827	3400	0.345	4600	0.037
80	0.161	0.426	7500	1.457	3400	0.045	3800	0.034
90	0.354	0.558	8500	1.963	3600	0.235	3800	0.226
100	0.465	0.549	9500	2.259	3800	0.309	3800	0.309
120	0.706	0.565	11 000	2.631	4000	0.444	4200	0.442
150	0.889	0.527	14 000	3.020	4400	0.496	4400	0.496
200	1.034	0.481	$>15\,000$	>2.581	5200	0.479	5200	0.479

ACKNOWLEDGMENTS

One of the authors (H.K.) is grateful for the warm hospitality during his stay at Ruder Bošković Institute when part of this work was done. This work has been supported in part by the Natural Science and Engineering Research Council of Canada and in part by SIZ 1 SRH (Yugoslavia) under project No. 7 and contract N5F.

APPENDIX

Here we present explicit analytical formulae for $\mathcal{T}(\mathbf{q},\mathbf{q}';E_q)$, given by Eq. (2.2), for the case when the separable potential belongs to the class of rational separable s-wave potentials:

$$\langle \mathbf{q}' \mid V^s \mid \mathbf{q} \rangle = \sum_{i,j=1}^{N} \langle \mathbf{q}' \mid g_i \rangle \lambda_{ij} \langle g_j \mid \mathbf{q} \rangle ,$$
$$\langle \mathbf{q} \mid g_j \rangle = \langle g_j \mid \mathbf{q} \rangle = P_j(q^2) \prod_{\rho=1}^{\nu_j} (q^2+\beta_{j\rho}^2)^{-\mu_{j\rho}} . \tag{A1}$$

P_j are real polynomials of a degree smaller than $\sum_{\rho=1}^{\nu_j} \mu_{j\rho}$. The parameters $\{\beta_{j1} \cdots \beta_{j\nu_j}\} \equiv \{\beta_j\}$, $j=1,\ldots,N$ are complex numbers with $\mathrm{Re}\,\beta_{j\rho} > 0$ for all j and ρ. According to Ref. 23, $\mathcal{T}(\mathbf{q},\mathbf{q}';E_q)$ is given by

$$\mathcal{T}(\mathbf{q}',\mathbf{q};E_q) = T_C(\mathbf{q}',\mathbf{q};E_q) + T_{Cs}(\mathbf{q}',\mathbf{q};E_q) , \tag{A2}$$

where the first term corresponds to pure Coulomb scattering;

$$T_C(\mathbf{q}',\mathbf{q};E_q) = \langle \mathbf{q}' \mid V^C \mid \mathbf{q} \rangle (q/\mu)^{-2i\eta} \mid \mathbf{q}'-\mathbf{q} \mid^{-2-2i\eta} \times e^{\pi\eta} \mid \Gamma(1+i\eta) \mid^2 , \tag{A3}$$

and the second one includes nuclear and Coulomb effects.

$$T_{Cs}(\mathbf{q}',\mathbf{q};E_q) = \sum_{i,j=1}^{N} h_i(E_q,\mathbf{q}') \tau_{ij}(E_q) h_j(E_q,\mathbf{q}) , \tag{A4}$$

$$h_j(E_q,\mathbf{q}') = (q/q')(q+q')^{-2i\eta} \mid \Gamma(1+i\eta) \mid^2 \sum_{\rho=1}^{\nu_j} \Delta_{j\rho} \left[R_{j\rho}(-iq,\{\beta_j\}) \left[\frac{q-i\beta_{j\rho}}{q+i\beta_{j\rho}} \right]^{-1-i\eta} \right] , \tag{A5}$$

$$R_{j\rho}(p,\{\beta_j\}) = \frac{P(-\beta_{j\rho}^2)}{(-2)^{\mu_{j\rho}-1}(\mu_{j\rho}-1)!(p+\beta_{j\rho})^2} \prod_{\substack{\sigma=1 \\ \sigma\neq\rho}}^{\nu_j} (\beta_{j\sigma}^2-\beta_{j\rho}^2)^{-\mu_{j\sigma}} , \tag{A6}$$

$$\Delta_{j\rho} \equiv \left[\frac{1}{\beta_{j\rho}} \frac{d}{d\beta_{j\rho}} \right]^{\mu_{j\rho}-1} . \tag{A7}$$

The formulae for $R_{j\rho}$ and the operator $\Delta_{j\rho}$ as stated in Ref. 23, Eq. (42), are incorrect. Here we present the correct expressions. The energy dependent term τ_{ij} can be explicitly expressed as follows:[23]

$$\tau_{ij}(E_q) = \{[\Lambda^{-1}-M(E_q)]^{-1}\}_{ij} , \tag{A8}$$
$$(\Lambda)_{ij} = \lambda_{ij} ,$$
$$[M(E_q)]_{ij} = 8\pi^2\mu i \sum_{\sigma=1}^{\nu_i} \sum_{\rho=1}^{\nu_j} [\tilde{\Delta}_{i\sigma} \Delta_{j\rho}^{*} H_{\sigma\rho}^{ij}(E_q) F(i\eta;B_{\sigma\rho}^{ij})]_{\tilde{\beta}_{i\sigma}=\beta_{i\sigma}} , \tag{A9}$$

$$H_{\sigma\rho}^{ij}(E_q) = R_{i\sigma}(-iq,\{\tilde{\beta}_i\}) R_{j\rho}(-iq,\{\beta_j^{*}\}) (1-B_{\sigma\rho}^{ij})^{-1} , \tag{A10}$$

$$B_{\sigma\rho}^{ij} = \frac{(\tilde{\beta}_{i\sigma}+iq)(\beta_{j\rho}^{*}+iq)}{(\tilde{\beta}_{i\sigma}-iq)(\beta_{j\rho}^{*}-iq)} , \tag{A11}$$

$$F(x,y) = (1+x)^{-1} {}_2F_1(1,x;2+x;y) , \tag{A12}$$

Equations (A1)—(A12) determine $\mathcal{T}(\mathbf{q},\mathbf{q}';E_q)$ explicitly.

The s-wave Graz potential[22] belongs to the class of rational separable potentials as given by (A1). It can be obtained by the following specifications:[22]

$N=2$, $\lambda_{11}=4\pi\times(-0.0072069)\ \mathrm{fm}^{-2}$, $\lambda_{22}=4\pi\times 33.35516\ \mathrm{fm}^{-2}$,
$\lambda_{12}=\lambda_{21}=0$,
$P_1(q^2)=\sum_{k=0}^{2} a_{1k}q^{2k}$, $P_2=\sum_{k=1}^{4} a_{2k}q^{2k}$,
$a_{10}=2.756054\ \mathrm{fm}^{-4}$, $a_{11}=5.104415\ \mathrm{fm}^{-2}$, $a_{12}=3.698168$,
$a_{21}=21.02945\ \mathrm{fm}^{-6}$, $a_{22}=1055.773\ \mathrm{fm}^{-4}$, $a_{23}=45.04107\ \mathrm{fm}^{-2}$,
$a_{24}=1.327066$,

$\nu_1=2,\ \mu_{11}=1,\ \mu_{12}=2,\ \beta_{11}=0.813\,167\,8\ \text{fm}^{-1},\ \beta_{12}=1.288\,463\ \text{fm}^{-1}$,

$\nu_2=2,\ \mu_{21}=2,\ \mu_{22}=3,\ \beta_{21}=7.496\,476\ \text{fm}^{-1},\ \beta_{22}=1.661\,389\ \text{fm}^{-1}$.

The numerical calculation of the S matrix for the Graz + Coulomb potential is now straightforward although it requires a lot of work. It is therefore worth noting that our calculation of the $^1S_0$ phase shift is in agreement with that obtained in Ref. 22, where different analytical formulae were used.

The Yamaguchi potential also belongs to the class of rational separable s-wave potentials and is obtained with the following specifications:

$N=1,\ P_1(q^2)=1,\ \nu_1=1,\ \mu_{11}=1$,

$\lambda_{11}=-0.027\,881\,1\ \text{fm}^{-2},\ \beta_{11}=1.127\,47\ \text{fm}^{-1}$.

[1]R. Newton, *Scattering Theory of Waves and Particles,* 2nd ed. (Springer, New York, 1982).

[2]W. Glöckle, *The Quantum Mechanical Few-Body Problem* (Springer, Berlin, 1983).

[3]J. D. Dollard, J. Math. Phys. **5**, 729 (1964).

[4]J. V. Noble, Phys. Rev. **161**, 945 (1967).

[5]C. Chandler and A. G. Gibson, J. Math. Phys. **15**, 291 (1974).

[6]A. G. Gibson and C. Chandler, J. Math. Phys. **15**, 1366 (1974).

[7]E. Prugovečki, J. Math. Phys. **14**, 957 (1973); Phys. Lett. **49B**, 305 (1974).

[8]E. Prugovečki and J. Zorbas, Nucl. Phys. **A213**, 541 (1973).

[9]J. Zorbas, Lett. Nuovo Cimento **10**, 121 (1974); Rep. Math. Phys. **9**, 309 (1976); J. Math. Phys. **18**, 1112 (1977); **19**, 177 (1978); **20**, 6 (1979).

[10]G. Bencze and H. Zankel, Phys. Lett. **82B**, 316 (1979).

[11]A. M. Vesselova, Teor. Mat. Fiz. **3**, 326 (1970); **13**, 368 (1972); **35**, 180 (1978).

[12]G. Bencze, Nucl. Phys. **A196**, 135 (1972).

[13]S. Oryu, Prog. Theor. Phys. **44**, 1208 (1970).

[14]E. O. Alt, W. Sandhas, H. Zankel, and H. Ziegelmann, Phys. Rev. Lett. **37**, 1537 (1976).

[15]E. O. Alt, W. Sandhas, and H. Ziegelmann, Phys. Rev. C **17**, 1981 (1978).

[16]E. O. Alt and W. Sandhas, Phys. Rev. C **21**, 1733 (1980).

[17]C. Chandler, *The Few Body Problem,* edited by F. S. Levin (North-Holland, Amsterdam, 1981), p. 129c.

[18]S. P. Merkuriev, Acta Phys. Austriaca, Suppl. XXIII, **65**, (1981).

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

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

[21]H. Kröger, J. Math. Phys. **24**, 1509 (1983); **25**, 1875 (1984).

[22]W. Schweiger, W. Plessas, L. P. Kok, and H. van Haeringen, Phys. Rev. C **27**, 515 (1983).

[23]Ž. Bajzer, Z. Phys. A **278**, 97 (1976).

[24]Ž. Bajzer, *Proceedings of the Workshop on Few-Body Problems in Nuclear Physics, Trieste, 1978* (IAEA, Vienna, 1978), p. 365.

[25]H. van Haeringen, J. Math. Phys. **17**, 995 (1976).

[26]A. Gersten, Nucl. Phys. **B103**, 465 (1976).

[27]H. van Haeringen and R. van Wageningen, J. Math. Phys. **16**, 1441 (1975).

[28]W. Plessas and W. Schweiger, J. Phys. G **7**, 1019 (1981).

[29]B. Simon, *Quantum Mechanics for Hamiltonians Defined as Quadratic Forms* (Princeton University Press, Princeton, 1971), p. 111.

[30]This property is formally the consequence of the intertwining property; see for example, J. R. Taylor, *Scattering Theory* (Wiley, New York, 1972), p. 40.

[31]K. Gottfried, *Quantum Mechanics* (Benjamin, New York, 1966).

[32]C. J. Goebel and K. W. McVoy, Ann. Phys. (N.Y.) **37**, 62 (1966).