Scattering of charged particles in a time-dependent approach

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(Received 27 May 1988)

We test a new time-dependent method to compute proton-proton scattering using the Graz plus Coulomb potential.

In Ref. 1 we have shown that the S matrix for proton-proton scattering can be computed with good accuracy using a time-dependent approach. In that work we have used a realistic short-range force, namely the Graz potential, plus the long-range Coulomb potential. The time evolution $\exp(iHt)$ has been computed by approximating the full Hamiltonian H by a finite dimensional $H(N)$ using a momentum-space lattice, then diagonalizing $H(N)$ and finally evaluating $\exp[iH(N)t]$ in its eigenrepresentation. The usefulness of a coordinate-space lattice for local short-range potentials within the time-dependent framework has been discussed in Ref. 2.

In Ref. 3 we have discussed an alternative to compute the time evolution $\exp(iHt)$, which can be briefly described as follows: Firstly one computes $\exp(iH\tau)$ for a small value of τ, using the Taylor expansion or Padé approximation, and then generates $\exp(iHt)$ $(t \gg \tau)$ by iterative squaring of $\exp(iH\tau)$. We have suggested this alternative because we think that for large matrices $H(N)$ it has more advantages than the former way: It allows us to use easily out-of-core computer memory, it is appropriate for vector computing, and we believe it is also more suitable for statistical methods (Monte Carlo) than the first alternative. In Ref. 3 we have applied it to a simple NN short-range interaction, the separable Yamaguchi potential. In the numerical results for the S matrix, we found agreement with the first alternative to a very high accuracy. In this context we would like to mention also the work of Carlson,[4] using small slices of the time evolution within the Green's-function Monte Carlo method.

The purpose of this note is to show that the second alternative time-dependent method also works for p-p scattering, in particular when the Graz-plus Coulomb potential is employed.

The Graz-plus Coulomb potential is given in Ref. 5 (for more details on the following, the reader is referred to Refs. 1, 3, and 5). We have computed s-wave scattering of an asymptotic wave-packet state Φ, which is bell shaped (cosine), has a peak at $q_{\text{peak}}=0.20$ fm^{-1} and a half-width of $q_{\text{width}}=0.02$ fm^{-1}. A momentum-space lattice has been used to describe the $|q|$ dependence of the wave functions. The lattice discretizes the interval $[0,q_{\text{cut}}]$ with $q_{\text{cut}}=40$ fm^{-1} using 30 lattice nodes distributed in a geometric progression [according to Eq. (3.3)

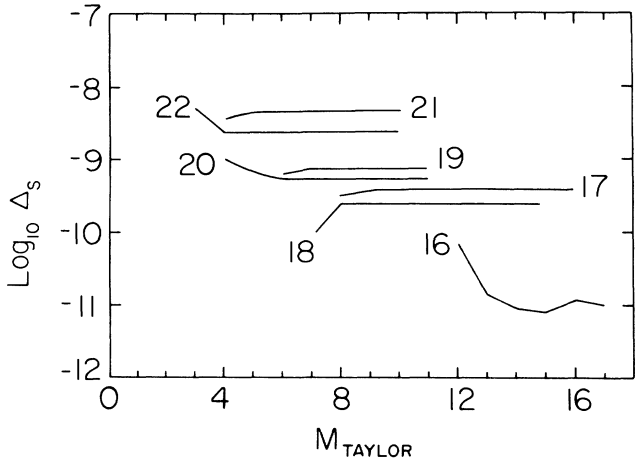

FIG. 1. Deviation in the S matrix Δ_S computed in the second alternative method (Taylor expansion and squaring) as a function of M_{Ta}, the number of Taylor terms, and n_{sq} (indicated in the figure), the number of squaring operations. The reference values have been computed from the first alternative (diagonalization). The scattering time is $T=3000$ fm^{-1}.

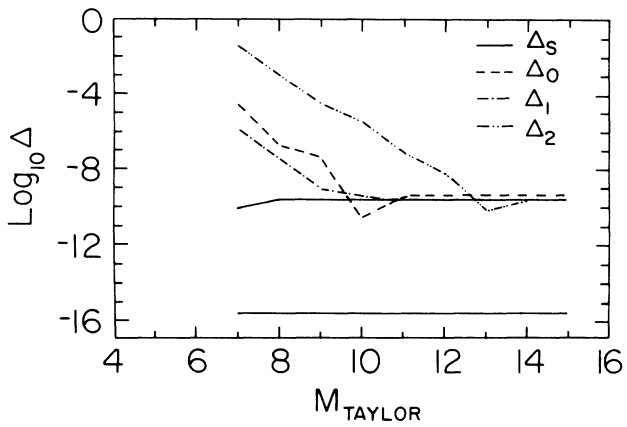

FIG. 2. Deviation in the S matrix Δ_S and in the expectation values of the energy Δ_0, Δ_1, and of energy^2 Δ_2 as a function of M_{Ta}. $n_{\text{sq}}=18$, $T=3000$ fm^{-1}. The reference values have been computed from the first alternative. The straight line at the bottom gives the internal machine precision.

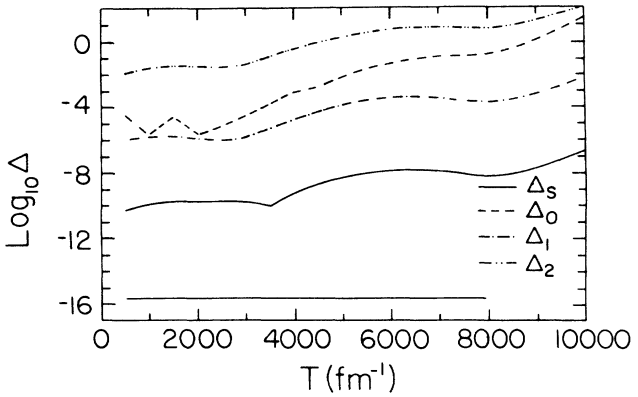

FIG. 3. Deviation in the S matrix Δ_S and in the expectation values of the energy Δ_0, Δ_1, and of energy^2 Δ_2 as a function of the scattering time T. $n_{\mathrm{sq}}=18$, $M_{\mathrm{Ta}}=7$. The reference values have been computed from the first alternative. The straight line at the bottom gives the internal machine precision.

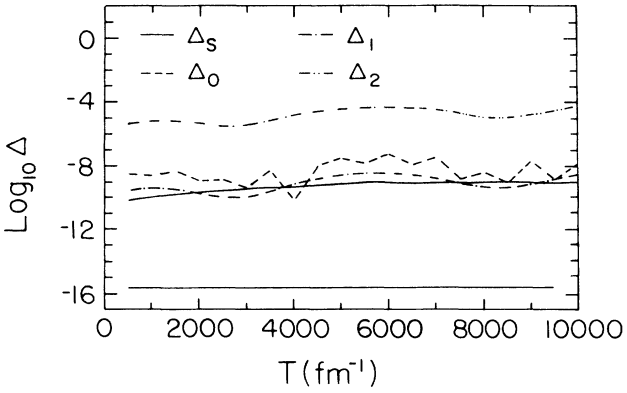

FIG. 4. Same as Fig. 3, but for $M_{\mathrm{Ta}}=10$.

of Ref. 1 with $\epsilon_1=\epsilon_2=1$]. That defines the finite dimensional Hamiltonian $H(N)$ (in the s-wave channel). We denote by

$$U(N,T)=\exp[iH(N)T] , \tag{1}$$

$$U^{0c}(N,T)=\exp[iH^{0c}(N,T)] , \tag{2}$$

$$\Omega^c(N,T)=U(N,-T)U^{0c}(N,T) , \tag{3}$$

$$S^c(N,T)=\Omega^c(N,-T)^\dagger\Omega^c(N,T) , \tag{4}$$

the full time evolution, the asymptotic time evolution including Dollard's anomalous term, the wave operator in Dollard's form, and the S matrix, respectively. We compute the following matrix elements:

$$\langle\Phi|S^c(N,T)|\Phi\rangle , \tag{5}$$

$$\langle\Phi|S^c(N,T)^\dagger H^0(N)S^c(N,T)|\Phi\rangle , \tag{6}$$

$$\langle\Phi|\Omega^c(N,T)^\dagger H(N)\Omega^c(N,T)|\Phi\rangle , \tag{7}$$

$$\langle\Phi|\Omega^c(N,T)^\dagger H(N)^2\Omega^c(N,T)|\Phi\rangle . \tag{8}$$

The second and third one give the expectation value of the energy (note: $[H^0,S^c]=0$, $H\Omega^c=\Omega^cH^0$ in the continuum limit), while the last one gives the expectation value of the square of the energy.

In order to compute all these quantities, one has to compute $U(N,T)$. This can be done by diagonalization of $H(N)$ (first alternative). The new alternative goes as follows: The exponential function has the scaling property

$$\exp[iH(N)T]=\{\exp[iH(N)T/m]\}^m . \tag{9}$$

Choosing $m=2^{n_{\mathrm{sq}}}$, such that $\tau=T/m$ is small, one firstly computes $\exp[iH(N)\tau]$ via Taylor expansion in τ and then obtains $\exp[iH(N)T]$ by squaring $\exp[iH(N)\tau]$ iteratively n_{sq} times. We have computed the matrix elements given by Eqs. (5)–(8) using both alternatives, i.e., where $U(N,T)$ hence $\Omega^c(N,T)$ and $S^c(N,T)$ have been computed in both ways. The relative deviations are denoted $\Delta_S,\Delta_0,\Delta_1,\Delta_2$ corresponding to the matrix elements equations (5)–(8). The numerical results are displayed in Figs. 1–4. Figure 1 shows the deviation for the S matrix as a function of M_{Ta}, the number of Taylor terms and n_{sq}, the number of squaring operations. One obtains numerical agreement in the order of 10^{-10} with a relative small number of squaring operations (~ 18). Note that the scattering time $T=3000$ fm^{-1} is *not* small. These calculations have been performed on an IBM/PC with an internal machine precision of 15 digits. The results are quite stable, when M_{Ta} and n_{sq} is increased.

One should note that Δ_S, which is in the order of between 10^{-8} and 10^{-11}, is very small and we are displaying the region in the parameter space of M_{Ta} and n_{sq}, where Δ_S takes its smallest values. If one increases M_{Ta} or n_{sq} further for a given T value, then more matrix multiplications are involved, which enhances numerical round-off errors thus leading to increased Δ_S and hence produces the pattern in Fig. 1. This type of behavior has also been verified numerically for $\exp(x)$ as a function of an ordinary number x.

For this set of parameters, we have obtained in Ref. 1 an error in the S matrix in the order of a few percent when comparing the first alternative time-dependent method with an "exact" analytical solution as reference. That means that the two alternatives are equivalent when computing the S matrix. Figure 2 shows the deviation in the S matrix and in the expectation values of the energy for $n_{\mathrm{sq}}=18$. One obtains for all functions agreement in the order of 10^{-10} for 12 Taylor terms and stability for larger M_{Ta}. Figures 3 and 4 display the deviations as a function of the scattering time T for $M_{\mathrm{Ta}}=7$ and $M_{\mathrm{Ta}}=10$, respectively. A good numerical agreement is obtained over a wide range of T values.

In conclusion, we find the same kind of behavior for the Graz-plus Coulomb potential, as we found for the Yamaguchi potential in Ref. 3, namely that the two alternative time-dependent methods give equivalent numerical results. The results of this note also suggest that it is sufficient to use the Taylor expansion of the evolution operator, instead of constructing Padé approximants (which would require more computer time and memory).

One of the authors (H.K.) is grateful for support from the Natural Sciences and Engineering Research Council of Canada.

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