# Computation of a long-time evolution in a Schrödinger system

Ralph Girard,* Helmut Kröger, and Patrick Labelle
*Département de Physique, Université Laval, Québec, Canada G1K 7P4*

Željko Bajzer†
*Ruder Bošković Institute, University of Zagreb, YU-41001 Zagreb, Croatia, Yugoslavia*
(Received 3 September 1987)

We compare different techniques for the computation of a long-time evolution and the $S$ matrix in a Schrödinger system. As an application we consider a two-nucleon system interacting via the Yamaguchi potential. We suggest computation of the time evolution for a very short time using Padé approximants, the long-time evolution being obtained by iterative squaring. Within the technique of strong approximation of Moller wave operators (SAM) we compare our calculation with computation of the time evolution in the eigenrepresentation of the Hamiltonian and with the standard Lippmann-Schwinger solution for the $S$ matrix. We find numerical agreement between these alternative methods for time-evolution computation up to half the number of digits of internal machine precision, and fairly rapid convergence of both techniques towards the Lippmann-Schwinger solution.

## I. INTRODUCTION

When describing the dynamics of a system governed by the Schrödinger equation, a quantity of central importance is the propagator. Given a Hamiltonian $H$, the propagation in time is determined by the relation $U(t)=\exp(iHt)$, also called the time-evolution operator. We have used here and use throughout the units $\hbar=c=1$. The time-evolution operator enters in a physically measurable quantity, the $S$ matrix

$$S=\lim_{t\to\infty}[U^0(t)U(-2t)U^0(t)]\ , \tag{1.1}$$

where $U^0(t)=\exp(iH^0t)$ is the time-evolution operator corresponding to the asymptotic Hamiltonian $H^0$, which we take for the sake of simplicity to be the same in the asymptotic incoming and outgoing channels. When trying to calculate the time-evolution operator and hence the $S$ matrix directly, one is faced with mathematical problems due to the following two properties: $U(t)$ is a nonlinear function and $H$ is an unbounded operator. On the other hand, $U(t)$ has two simplifying features: It is unitary for all real times $t$ and it is an analytic function for all finite complex $t$. Of course, the same properties hold for the asymptotic time-evolution operator. It has turned out[1] that one can introduce a perturbation to the generator of the time evolution such that on the one hand, the error in the $S$ matrix for a given scattering reaction (i.e., given quantum numbers, momentum, and energy) is small, and on the other hand, one has simpler mathematical properties. In particular, the Hamiltonian $H$ can be perturbed to a bounded and finite-dimensional Hamiltonian $H(N)$. Note that the word "perturbed" does not mean that $H-H(N)$ is everywhere small; it means that $H-H(N)$ is small on that part of the spectrum which is relevant for the scattering process. Corresponding to the perturbed generator $H(N)$, the perturbed time-evolution operator is $U(N,t)=\exp[iH(N)t]$. If one makes sure that $H(N)$ is a self-adjoint operator, then the unitarity and analyticity of $U(t)$ carry over to $U(N,t)$ also. Because $H(N)$ is essentially a finite-dimensional Hermitian matrix, $U(N,t)$ can be computed numerically (see, e.g., Ref. 2). Numerical studies on the two-nucleon system have shown[3] that for a given scattering process and a given finite-dimensional Hamiltonian $H(N)$ there is a finite "scattering time" $T$, for which the error due to the perturbed $S$ matrix,

$$S(N,T)=U^0(N,T)U(N,-2T)U^0(N,T)\ , \tag{1.2}$$

becomes a minimum. Besides, in an experiment, the scattering time is always finite. When we talk of a long-time evolution this is what we mean: The time $T$ is the finite scattering time corresponding to a specific scattering reaction, which is an approximation parameter depending on the perturbed Hamiltonian $H(N)$ and being determined from the minimum of the relative error of the $S$ matrix. The term "long" means that $\langle E\rangle T\gg\hbar=1$, where $\langle E\rangle$ is the scattering energy of a monochromatic beam or the expectation value of the asymptotic Hamiltonian in the case of a wave packet. A very crude estimate of $T$ can be obtained classically: Assuming that the interaction has a finite range $R_{\rm int}$, a lower limit of $T$ is the time needed for the projectile flying with a velocity $v$ to traverse the interaction region $2R_{\rm int}$. Numerical calculations in two- and three-nucleon systems in the low-energy domain show[3,4] that the scattering time $T$ is long in most cases. This fact immediately rules out the idea of computing the perturbed time-evolution operator $U(N,T)$ via a Taylor expansion. Also, more sophisticated techniques giving a larger convergence region, such as, e.g., the Padé technique, turned out to fail numerically. Moler and Van Loan[2] have compared 19 "dubious" ways to compute the exponential of a matrix. According to them, a suitable way to compute the exponential of a matrix, when the ex-

 

ponent is Hermitian or anti-Hermitian as in our case, is via diagonalization,

$$H(N)=\sum_{\alpha} |\psi_\alpha\rangle E_\alpha \langle\psi_\alpha| \ , \tag{1.3}$$

$$U(N,T)=\sum_{\alpha} |\psi_\alpha\rangle \exp(iE_\alpha T)\langle\psi_\alpha| \ . \tag{1.4}$$

As has been shown in Refs. 3 and 4, this is a feasible and numerically accurate way, applicable for long times $T$, which are needed for scattering calculations.

In this paper we want to suggest an alternative route to compute a long-time evolution. Again we start from a finite-dimensional Hermitian approximation $H(N)$ of the generator $H$. We want to compute $U(N,T) = \exp[iH(N)T]$. Because $U(N,T)$ is exactly an exponential, we can take advantage of the following property of the exponential function:

$$\exp(x)=\exp(x/m)^m \ , \tag{1.5}$$

which is valid for every $m$. In particular, one can choose $m$ such that $y=x/m \ll 1$. For convenience, we take $m=2^n$ with some positive integer $n$. Now the idea is first to compute $\exp(y)$ for a small $y$ using a Taylor expansion or the Padé approximation and then compute $\exp(x)$ by squaring $\exp(y)$ $n$ times. That means the following: Take $z_0=\exp(y)$ and square it, giving $z_1$, take $z_1$ and square it, giving $z_2$, and so on, until $z_n=\exp(x)$. This way of computing the exponential $\exp(x)$ with a large exponent $x$ is far superior to a naive direct application of the Taylor or Padé approximation to $\exp(x)$. Let us consider an example; $x=1000$. In order to compute $\exp(x)$ via a Taylor expansion one would need more than 1000 terms, as can be seen from the large-order behavior using Stirling's formula for the error term $x^k/k!$. On the other hand, choosing $m=2^{13}=8192$, $n=13$ and $y=0.1220$, then, $\exp(0.1220)$ can be computed from a few Taylor terms and then the result has to be squared 13 times. This way of computing an exponential with a large exponent can be applied as well when the exponent is a matrix; i.e., in our case, for the purpose of computing the time evolution we write

$$U(N,T)=\exp(iH(N)T/m)^m \ . \tag{1.6}$$

We choose $m=2^n$ appropriately, such that $\|H(N)\tau\| \ll 1$, where $\tau=T/m$. We compute $U(N,\tau)$ using Padé approximants for each matrix element. The method to compute the exponential of a matrix via Padé approximants and squaring has been discussed by several authors and has been reviewed by Moler and Van Loan in Ref. 2. However, in Ref. 2 the technique is discussed using matrix operator Padé approximants, which involve inversion of matrices. Sometimes the denominator matrix of matrix Padé approximants can be very poorly conditioned, with respect to inversion. To avoid this numerical problem, we apply Padé approximation on each matrix element, which leads us to a stable and simple algorithm.

In this paper we will demonstrate numerically that for the computation of the time evolution there are two equivalent ways: One is the diagonalize $H(N)$ and compute $U(N,T)$ in the eigenrepresentation of $H(N)$, and the other one is first to compute $U(N,\tau)$ for small $\tau$ using Padé approximants and then to repeatedly square the result. In particular, we want to demonstrate that, for long times $T$ needed to compute a scattering process, the results of both methods differ very little in the time evolution and in the $S$ matrix. In this paper we have studied the two methods applied to two-nucleon scattering in the low-energy domain. As nucleon-nucleon interaction we have used a short-range separable $s$-wave potential of the Yamaguchi type.

Before going into some detail and discussing numerical results, let us briefly touch upon two questions one might ask. First, what is the deeper reason that these methods work well? Second, what is the need for the second alternative way if the first one works? Concerning the first question, one can establish for the first alternative mathematically rigorous proofs showing convergence of the approximate time evolution and hence of the approximate $S$ matrix.[1] However, the deeper reason for the working of the method, in our opinion, is based on the following fact. Assuming that the generator of the time evolution, the Hamiltonian $H$ is self-adjoint, then the time evolution $U(t)$ belongs to a continuous one-parameter unitary group and vice versa (Stone's theorem, see, e.g., Ref. 5). Our perturbed generator $H(N)$ is also self-adjoint, hence also the perturbed time evolution $U(N,t)$ belongs to a continuous one-parameter unitary group and vice versa. In other words, our approximation does not violate the dynamical-group properties. Here it is worthwhile to draw a parallel to classical mechanics, where the underlying group is the symplectic group. For the purpose of computing the classical trajectories of particles in an accelerator for many orbits. Dragt and his collaborators have formulated classical dynamics in the language of the Lie algebra of the symplectic group.[6] The important feature is that the conservation of the dynamical group under perturbation of the generator of the time evolution, i.e., the introduction of an approximation to the original Hamiltonian, given, e.g., by a magnet in the accelerator ring, still yields an exactly symplectic Hamiltonian flow. This approach has worked very well for calculating particle orbits and is used in the design of new machines.[7]

While in our second alternative the unitary group structure is not exactly conserved (it is violated by the Taylor or Padé approximation), the error is small for small times, and the computation for long times is still reminiscent via Eq. (1.6) of the exponential structure of an element of the unitary group.

The answer to the second question has to do with the problem of how to deal with many degrees of freedom. This does not apply in the case of two nucleons treated as elementary particles, but it applies to light heavy ions treated as a Schrödinger system, and it applies to elementary particles treated in the language of field theory. Then, the dimension of matrices becomes very large and the second alternative gives us more advantages. It allows procedures which are easily adaptable to use out-of-core computer memory. Furthermore, involving only mutually independent operations on matrix elements and

the computation of matrix powers, it is appropriate for vector computing. In our opinion, the second alternative is also more suitable to the application of statistical methods (Monte Carlo) than the first alternative. Suggestions have been made as to how to apply the Monte Carlo technique to scattering reactions.[8] However, this is not the subject of this paper and hence we do not further elaborate on it here.

## II. HAMILTONIAN AND WAVE PACKET

We consider a two-nucleon system in the center-of-mass frame. We take the nucleon mass to be $m=938.259\ \mathrm{MeV/c^2}$. For sake of simplicity we drop the spin. For the nucleon-nucleon interaction we take a phenomenological potential. It is the separable Yamaguchi potential fitted to the effective range parameters in the singlet channel. The potential, being of rank 1 with an $s$-wave form factor, is given by

$$V=|\chi\rangle\lambda\langle\chi|\ , \tag{2.1a}$$

$$\langle\mathbf{q}|\chi\rangle=1/(q^2+\beta^2)\ , \tag{2.1b}$$

$$\lambda=-0.027\,881\,1\ \mathrm{fm}^{-2}\ , \tag{2.1c}$$

$$\beta=1.127\,47\ \mathrm{fm}^{-1}\ . \tag{2.1d}$$

This potential has been taken from Ref. 3. We denote the asymptotic Hamiltonian, describing the free motion, by $H^0$ and the full Hamiltonian by $H=H^0+V$. We will only briefly discuss the construction of the finite-dimensional approximate Hamiltonian $H(N)$, which has been described in Ref. 3. We introduce a basis set of expansion functions in Hilbert space. Our basis set is characterized by the orbital angular momentum quantum numbers $l$ and $m$ and two approximation parameters, $\Lambda$ and $N$. $\Lambda$ denotes a cutoff in momentum space and $N$ denotes an equidistant partition of the interval $[0,\Lambda]$ into $N$ subintervals. The expansion function has a $|\mathbf{q}|$ dependence given by the characteristic functions of the subintervals and a $\hat{q}$ dependence given by the spherical harmonics. Because the potential contributes only in the $s$ wave, we compute only $s$-wave scattering, hence $N$ is the dimension of the set of expansion functions. Let $P(N)$ denote the orthogonal projector onto this basis. Then we define $H(N)=P(N)HP(N)$ and analogously $H^0(N)$, the approximate asymptotic Hamiltonian. We want to compute the approximate time evolution $U(N,T)$ and the approximate $S$ matrix $S(N,T)$; in particular, we want to compute an $S$ matrix element between asymptotically incoming and outgoing states given by wave packets. We have chosen a wave packet given by

$$\phi^{\mathrm{as}}(\mathbf{q})=\phi^{\mathrm{as}}(q)Y_{00}(\hat{q})\ , \tag{2.2a}$$

$$\phi^{\mathrm{as}}(q)=\kappa\sin^2\left[\pi\frac{q_{\mathrm{up}}-q}{q_{\mathrm{up}}-q_{low}}\right]\times\theta(q_{\mathrm{up}}-q)\theta(q-q_{\mathrm{low}})\ , \tag{2.2b}$$

where $\kappa$ is such that $\phi^{\mathrm{as}}$ is normalized to unity. This is a bell-shaped wave packet with a maximum at $q_{\mathrm{max}}=\frac{1}{2}(q_{\mathrm{up}}+q_{\mathrm{low}})$ and a width of $q_{\mathrm{wid}}=\frac{1}{2}(q_{\mathrm{up}}-q_{\mathrm{low}})$, nonvanishing only between $q_{\mathrm{low}}$ and $q_{\mathrm{up}}$. We have chosen the following wave packet parameters: $q_{\mathrm{low}}=1.0\ \mathrm{fm}^{-1}$, $q_{\mathrm{up}}=4.0\ \mathrm{fm}^{-1}$, i.e., $q_{\mathrm{max}}=2.5\ \mathrm{fm}^{-1}$, $q_{\mathrm{wid}}=1.5\ \mathrm{fm}^{-1}$. The corresponding expectation value of the energy is $\langle E\rangle=296.231$ MeV. The wave packet has contributions between the energy $E_{\mathrm{low}}=41.4885$ MeV and the energy $E_{\mathrm{up}}=663.976$ MeV. The wave packet has been chosen to cover a wide range of energies. Although the potential is valid only up to about 100 MeV; this is of minor importance here because we want only to compare two methods, and we are not interested in comparison with experimental data.

Now let us discuss the computation of $U(N,T)$ using Eq. (1.6), the value of the parameter $T$, the scattering time, plays here a numerically important role. As has been mentioned in Sec. I, for each scattering reaction there is an optimal value of $T$ such that the relative error in the $S$ matrix,

$$\Delta_s(N,T)=\left|\frac{\langle\phi^{\mathrm{as}}|S(N,T)-S|\phi^{\mathrm{as}}\rangle}{\langle\phi^{\mathrm{as}}|S|\phi^{\mathrm{as}}\rangle}\right|\ , \tag{2.3}$$

becomes a minimum. Because this function can be computed only when $S$, the exact $S$ matrix, is known, auxiliary functions have been suggested,[3,9] which determine a value of $T$ in the neighborhood of the optimal value of $T$,

$$\Delta_{\langle\ \rangle}=\left|\frac{\langle\Omega(N,T)\phi^{\mathrm{as}}|H(N)|\Omega(N,T)\phi^{\mathrm{as}}\rangle-\langle\phi^{\mathrm{as}}|H^0(N)|\phi^{\mathrm{as}}\rangle}{\langle\phi^{\mathrm{as}}|H^0(N)|\phi^{\mathrm{as}}\rangle}\right|\ , \tag{2.4}$$

where $\Omega(N,T)=U(N,T)U^0(N,-T)$ is the approximate Moller wave operator and

$$\Delta_0(N,T)=\left|\frac{\langle\phi^{\mathrm{as}}|S(N,T)-H^0(N)S(N,T)[H^0(N)]^{-1}|\phi^{\mathrm{as}}\rangle}{\langle\phi^{\mathrm{as}}|S(N,T)|\phi^{\mathrm{as}}\rangle}\right|\ . \tag{2.5}$$

Neither of the functions requires the knowledge of the exact $S$ matrix. Both functions measure the violation of energy conservation of the approximate $S$ matrix. It has been observed that the minima (as a function of $T$) of $\Delta_S(N,T)$, $\Delta_{\langle\rangle}(N,T)$, and $\Delta_0(N,T)$ lie close together.[3] Hence in cases where the exact $S$ matrix is unknown, we use as a working prescription the scattering time $T$ defined as the first minimum of $\Delta\langle\ \rangle$ or $\Delta_0$ (note that due

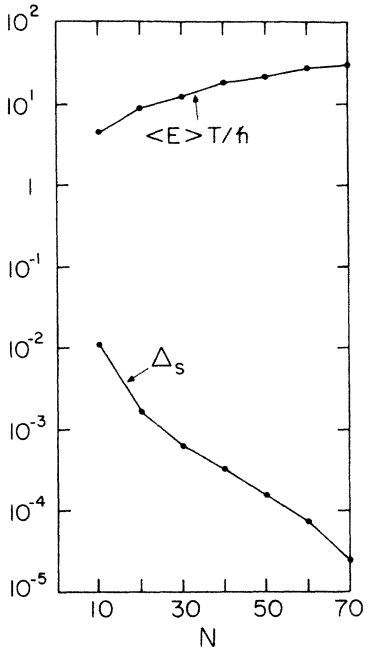


FIG. 1. Dependence of the action $\langle E \rangle T$ and the relative error $\Delta_S(N,T)$, given by Eq. (2.3), of the $S$ matrix $S(N,T)$, computed in the SAM approach, on the dimension $N$. The wave-packet parameters are $q_{\text{low}}=1.0\ \text{fm}^{-1}$, $q_{\text{up}}=4.0\ \text{fm}^{-1}$; the cutoff is $\Lambda=10.0\ \text{fm}^{-1}$. The value of the scattering time $T$ has been chosen as the first minimum of $\Delta\langle\ \rangle(N,T)$.

to the finite-dimensional exponent all these expressions are quasiperiodic functions in $T$, and all the other periodic minima are irrelevant). A more detailed discussion of this can be found in Ref. 3.

Now let us discuss the computation $U(N,t)$, based on Eq. (1.6), for any real time $t$. The first question is: What

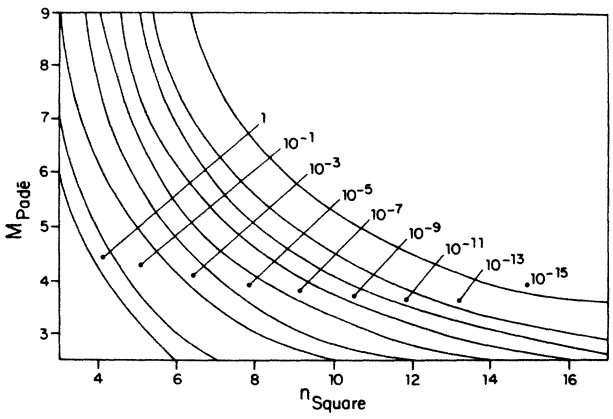


FIG. 2. Comparison of the two alternative methods for the time evolution. Discrepancy $\delta_U(N,T,M,n)$ [Eq. (3.1)] as a function of $M$, the order of the diagonal Padé approximant, and of $n$, the number of squaring operations. The curves connect points of the same discrepancy. The region between the curves is characterized by $\delta_U<\epsilon$, where $\epsilon$ is given in the figure. The cutoff is $\Lambda=10.0\ \text{fm}^{-1}$, the dimension of the basis is $N=10$, the scattering time is $T=0.0152034\ \text{MeV}^{-1}$, chosen as the minimum of $\Delta\langle\ \rangle(N,T)$.

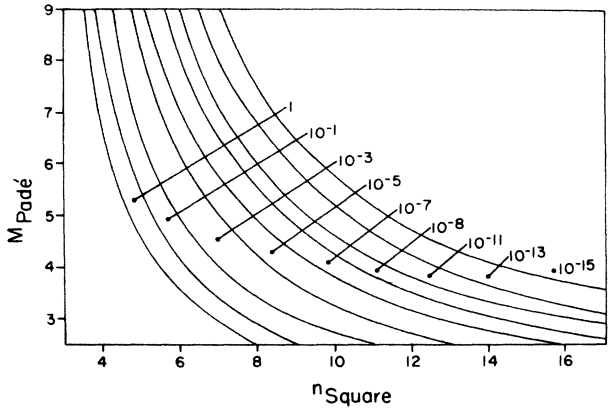


FIG. 3. Same as Fig. 2, but $N=20$, $T=0.0304069\ \text{MeV}^{-1}$.

is a suitable value of $m$, i.e., what $\tau=t/m$ do we choose? A condition for selecting $\tau$ is

$$\|H(N)\tau\| \ll 1 \ . \tag{2.6}$$

Because it is inconvenient to compute the norm of $H(N)$, it is useful to have an estimate of it from the norm of $H^0$. If the interaction is negative definite, which holds in our case, one has

$$\|H(N)\| < \|H^0(N)\| \ . \tag{2.7}$$

If the interaction does not have this property, then the norm of $H^0(N)$ is only a rough estimate of the norm of $H(N)$: however, one has

$$\|H(N)\| - \|H^0(N)\| \sim 0, \quad \Lambda \to \infty \ . \tag{2.8}$$

For any value of $\tau$, obeying Eq. (2.6), we compute $\exp[iH(N)\tau]$ using Padé approximants. In Ref. 2 the use of operator Padé approximants has been discussed. Because we want to avoid matrix inversions, we compute the Padé approximant for each matrix element

$$f(\tau)=\langle j \mid \exp(iH(N)\tau) \mid k \rangle \ . \tag{2.9}$$

The Padé approximants are based on the Taylor expan-

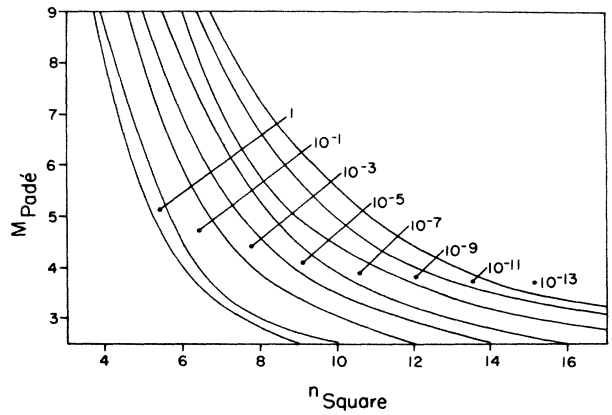


FIG. 4. Same as Fig. 2, but $N=30$, $T=0.0405426\ \text{MeV}^{-1}$.

sion of $f(\tau)$ at $\tau=0$. We use the diagonal Padé approximants $f[M,M](\tau)$ which are defined as a rational functions in $\tau$ of degree $M$ over $M$, such that the Taylor expansion coefficients at $\tau=0$ of $f(\tau)$ and $f[M,M](\tau)$ agree up to the order $2M$. The Padé approximants have been calculated from recursive relations which are discussed in Ref. 10. Then according to Eq. (1.6), the resulting matrix is squared $n=\log_2(m)$ times, to give $U(N,t)$. It is clear that errors in this procedure arise from two sources. The first kind is the error due to the Padé approximation, and the second one is the numerical error due to the repeated squaring of matrices. The relation between these errors will be studied in Sec. III.

## III. NUMERICAL RESULTS

For the wave packet, given by Eqs. (2.2), we have computed the exact $S$ matrix element in a standard way from the Lippmann-Schwinger equation, giving the reference value $S=0.976\,930+0.198\,743i$. Then we have computed the matrix element of the approximate $S$ matrix $S(N,T)$ by the strong approximation of Moller wave operators (SAM) using diagonalization of the approximate Hamiltonian $H(N)$. In these calculations the cutoff parameter has been set to $\Lambda=10.0\ \mathrm{fm}^{-1}$. The results are displayed in Fig. 1 which shows the action $\langle E\rangle T$ and the relative error of the $S$ matrix $\Delta_S(N,T)$, given by Eq. (2.3), as a function of the number $N$ of the expansion functions. For each $N$ the scattering time $T$ corresponds to the value which gives a minimum of $\Delta\langle\ \rangle(N,T)$. One observes that $\langle E\rangle T\gg 1$, i.e., the time evolution is long. The approximate $S$ matrix converges fairly rapidly towards its reference value. In particular, one observes a kind of exponential falloff behavior of the error $\Delta_S(N,T)$ as a function of $N$ over a fairly wide range of $N$ values. Now we want to compare the time evolution and the $S$ matrix using the two alternative methods, i.e., by the SAM method once via diagonalization and secondly via the Padé method and squaring. The results for the time evolution are shown in Figs. 2–4 and the results for the $S$ matrix are shown in Figs. 5–7. We have computed, for $N=10$, 20, and 30, and for the corresponding scattering time $T$, determined as the minimum of $\Delta_{\langle\ \rangle}(N,T)$, the time evolution via diagonalization [Eq. (1.4)], denoted by $U^{\mathrm{diag}}(N,T)$, and the time evolution via the Padé approximant and squaring [Eq. (1.6)], denoted by $U^{\mathrm{pasq}}(N,T,M,n)$. The latter depends on the following approximation parameters: $M$ the order of the diagonal Padé approximants and $n$ the number of squaring operations. We display the discrepancy

$$\delta_U(N,T,N,n)=\left[\sum_{i,j=1}^{N}\left|U^{\mathrm{diag}}(N,T)_{ij}-U^{\mathrm{pasq}}(N,T,M,n)_{ij}\right|^2\right]^{1/2} \tag{3.1}$$

as a function of $M$ and $n$. The curves connect points of the same error. They all have approximately a hyperbola shape. These curves have been produced using quadrupole precision on an IBM 4381 machine which has an

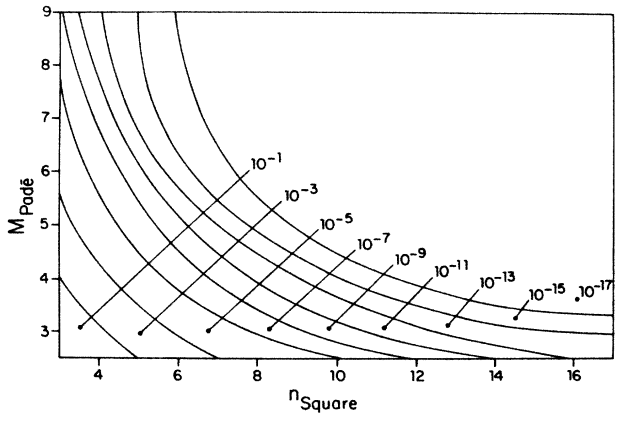


FIG. 5. Comparison of the two alternative methods for the $S$ matrix. Discrepancy $\delta_S(N,T,M,n)$ [Eq. (3.2)] as a function of $M$, the order of the diagonal Padé approximant, and of $n$ the number of squaring operations. The wave-packet parameters are $q_{\mathrm{low}}=1.0\ \mathrm{fm}^{-1}$. $q_{\mathrm{up}}=4.0\ \mathrm{fm}^{-1}$. The cutoff is $N=10.0\ \mathrm{fm}^{-1}$; the dimension of the basis is $N=10$; the scattering time is $T=0.015\,203\,4\ \mathrm{MeV}^{-1}$, chosen as the minimum of $\Delta\langle\ \rangle(N,T)$.

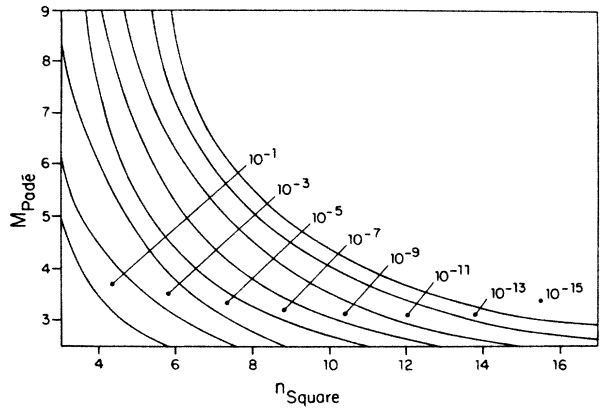


FIG. 6. Same as Fig. 5, but $N=20$, $T=0.030\,406\,9\ \mathrm{MeV}^{-1}$.

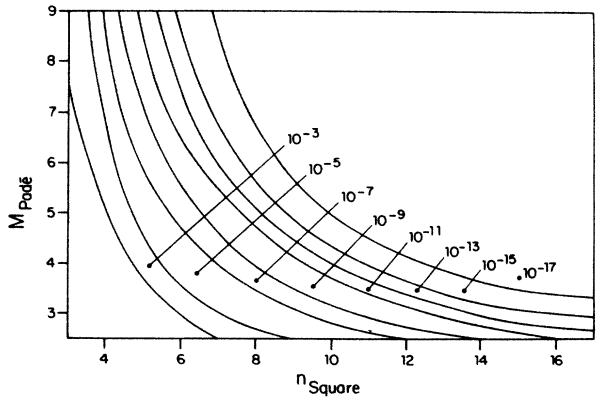


FIG. 7. Same as Fig. 5, but $N=30$, $T=0.040\,542\,6\ \mathrm{MeV}^{-1}$.

internal precision of about 30 digits. One observes that the discrepancy can be made very small, i.e., we obtain numerical agreement up to half the number of digits of internal machine precision. Comparing Figs. 2–4 one observes that $\delta_U(N,T,M,n)$ increases as a function of $N$, due to the increased number of matrix elements summed over. In order to estimate the average discrepancy per matrix element one should consider $\delta_U(N,T,M,n)/N$. For the same set of parameters $N$ and $T$ we have computed the $S$ matrix via Eq. (1.2). We denote by $S^{\text{diag}}$ the expression obtained by inserting $U^{\text{diag}}$ for the time evolution in Eq. (1.2), and we denote by $S^{\text{pasq}}$ the expression corresponding to $U^{\text{pasq}}$. We display in Figs. 5–7 the discrepancy

$$\delta_S(N,T,M,n) = | \langle \phi^{\text{as}} | S^{\text{diag}}(N,T) - S^{\text{pasq}}(N,T,M,n) | \phi^{\text{as}} \rangle | \ . \quad (3.2)$$

As expected, the discrepancy of the $S$ matrix elements lies in the same range of order of magnitude as the average discrepancy per matrix element of the time evolution. In particular, comparison of Fig. 1 and Figs. 5–7 shows that the discrepancy $\delta_S(N,T,M,n)$ is several orders of magnitude smaller than the error $\Delta_S(N,T)$, i.e., the error introduced into the time evolution by using a perturbed generator is much larger than the discrepancy coming from the two different methods to compute the perturbed time evolution. In this sense the two methods yield equivalent results.

## IV. CONCLUSIONS

In this paper we have compared computational methods for the time evolution and the $S$ matrix of a Schrödinger system. In particular, we have considered a two-nucleon system interacting via a short-range Yamaguchi potential. We have shown that the generator of the time evolution, the Hamiltonian, can be perturbed to a finite-dimensional Hamiltonian, and to each perturbed Hamiltonian corresponds a finite scattering time $T$, for which the error in the perturbed $S$ matrix becomes minimal. We have given methods to determine a finite scattering time, based on the principle of minimizing the violation of energy conservation in a scattering process. In all cases considered, we find a long scattering time $T$, i.e., $\langle E \rangle T \gg \hbar$, where $\langle E \rangle$ is the energy. We have compared two ways to compute for a long scattering time $T$ the perturbed time evolution corresponding to the perturbed generator. One way to do it is to diagonalize the finite-dimensional Hamiltonian and compute the perturbed time evolution in the eigenrepresentation. As an alternative, we have suggested in this paper computing the perturbed time evolution for a short time using Padé approximants and obtaining the long-time evolution by iterative squaring. The numerical results show that both ways are equivalent. In our opinion the new alternative offers advantages in the following respect: When applied to systems with a large number of degrees of freedom ($N$-body with $N > 3$) which correspond to large matrices, it seems to be easier to apply out-of-core routines and vector computing. Also, because matrix multiplication is related to multiple integrals, which have been treated successfully with Monte Carlo methods, it seems more likely for the new alternative that statistical methods can be merged successfully. This aspect would also be relevant for cases with a large number of degrees of freedom.

## ACKNOWLEDGMENT

Two of the authors (R. G. and H. K.) are grateful for support from the Natural Science and Engineering Research Council of Canada.

---

*Present address: Max-Planck-Institut für Kernphysik, D-6900 Heidelberg 1, West Germany.

†Present address: Department of Biochemistry and Molecular Biology, Mayo Foundation, Rochester, MN 55905.

[1]H. Kröger, J. Math. Phys. **25**, 1875 (1984).

[2]C. Moler and C. Van Loan, SIAM (Soc. Ind. Appl. Math.) Rev. **20**, 801 (1978).

[3]M. Batinić, Ž, Bajzer, and H. Kröger, Phys. Rev. C **33**, 1187 (1986).

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

[5]W. O. Amrein, J. M. Jauch, and K. B. Sinha, *Scattering Theory in Quantum Mechanics,* Vol. 16 of *Lecture Notes and Supplements in Physics* (Benjamin, New York, 1977).

[6]A. J. Dragt, in *Lectures on Nonlinear Orbit Dynamics (Fermilab, 1982),* Proceedings of the Conference on Physics of High Energy Particle Accelerators, AIP Conf. Proc. No. 87, edited by R. A. Carrigan and F. R. Huson (AIP, New York, 1982), p. 147.

[7]E. Forest, Superconducting Super Collider Central Design Group Publication No. SSC-111 (1987).

[8]H. Kröger, Phys. Rev. A **35**, 4525 (1987).

[9]R. Girard and H. Kröger, Phys. Rev. D **34**, 1824 (1986).

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