

Scattering theory on the lattice and with a Monte Carlo method

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We present an alternative time-dependent method of calculating the S matrix in quantum systems governed by a Hamiltonian. In the first step one constructs a new Hamiltonian that describes the physics of scattering at energy E with a reduced number of degrees of freedom. Its matrix elements are computed with a Monte Carlo projector method. In the second step the scattering matrix is computed algebraically via diagonalization and exponentiation of the new Hamiltonian. Although we have in mind applications in many-body systems and quantum field theory, the method should be applicable and useful in such diverse areas as atomic and molecular physics, nuclear physics, high-energy physics and solid-state physics. As an illustration of the method, we compute s -wave scattering of two nucleons in a nonrelativistic potential model (Yamaguchi potential), for which the S matrix is known exactly.

I. INTRODUCTION

The determination of dynamical observables like scattering amplitudes, decay amplitudes, cross sections, etc., from quantum theory is a theme of central importance in many areas of physics, e.g., atomic physics, molecular physics, nuclear physics, high-energy particle physics, and also in condensed-matter physics. In this paper we are particularly interested in the scattering problem in many-body systems. In quantum field theory (QFT), there are two rigorous approaches to the scattering problem. First, there is the Lehmann-Symanzik-Zimmermann (LSZ)¹ reduction formula, which relates S -matrix elements to Green's functions. Second, there is the Haag-Ruelle^{2,3} formulation, which constructs the S matrix from asymptotic states, which are localized, having a definite particle number, mass, and other quantum numbers, via suitable operators applied to the vacuum.

A breakthrough to obtain nonperturbative quantitative solutions in quantum field theory has come with the formulation of field theory on the lattice (LFT). The formulation of field theory on a space-time lattice and its simulation on supercomputers has proven to be very useful in the systematic and nonperturbative study of many static properties in quantum chromodynamics (QCD). These include the hadronic mass spectrum,⁴ the heavy quark potential at zero temperature,⁵ as well as the equation of state of the quark-gluon plasma at high temperature.⁶ However, if one tries to compute scattering observables on a space-time lattice, one is confronted with several difficulties.

(i) Because of limitations in computing power [storage space and CPU speed], most lattices have spatial extensions between 1 and 2 fm. This seems to be too small if one wants to describe scattering of baryons (the size of a nucleon is roughly 1 fm).

(ii) If one computes Euclidean Green's functions, then the Minkowski Green's function, which is relevant for scattering amplitudes, can in principle be obtained from analytic continuation of the Euclidean Green's function. In practice, however, difficulties have been encountered.⁷

(iii) If one tries to compute the time evolution $\exp(iHt)$ for real time t from an Euclidean lattice, one also has observed difficulties,⁸ which corresponds to taking into account a complex action. Thus there is a general belief that scattering data cannot be obtained in a reliable way using an Euclidean space-time lattice formulation.

Hence, attempts have been made to tackle the scattering problem in alternative ways.

(i) Information related to deep inelastic scattering in QCD has been obtained from QCD lattice calculations by Martinelli and Sachrajda.⁹ They have computed the lowest two moments of the quark distribution function of the pion and the proton.

(ii) Lüscher¹⁰ has suggested computation of the scattering amplitude by extraction from finite-size effects on large lattices. Wiese¹¹ has extended this to extract resonance parameters from finite-size effects. In order to obtain reasonable accuracy, this requires very large lattices.

(iii) A time-dependent method to compute the time evolution and the S matrix has been suggested by Kröger

and collaborators, based on a discretization of the Hamiltonian and an algebraic evaluation of the S matrix. This scheme has been applied to the ϕ_{1+1}^4 model,¹² the massive Thirring model,¹³ and quantum electrodynamics (QED)₁₊₁.¹⁴

(iv) There have been other approaches, such as that by Garczynski,¹⁵ which derives scattering perturbation theory from a lattice.

On the other hand, many fruitful ideas and techniques have been developed in order to solve for the ground state. The techniques are mostly based on Monte Carlo methods. In particular, there are the Monte Carlo Green's-function method,¹⁶ the Monte Carlo projector method,¹⁷ the guided-random-walk technique,¹⁸ the coupled-cluster method,¹⁹ and similar techniques. They have been applied to compute, e.g., the binding energy of the α particle,²⁰ the properties of liquid helium ^3He ,²¹ and the glueball mass from QCD.²²

In this paper we want to discuss how to compute scattering observables in a many-body system. We propose to join the time-dependent Hamiltonian method for the S matrix¹²⁻¹⁴ with a stochastic method, in particular the Monte Carlo projector method,¹⁷ in order to reduce the number of degrees of freedom. Let us briefly describe it. We use a Hamiltonian formulation, use renormalization-group ideas and the Monte Carlo projector method to compute the Minkowski S matrix

$$\langle \phi_{\text{out}} | S | \phi_{\text{in}} \rangle = \lim_{t \rightarrow \infty} \langle \phi_{\text{out}} | \exp(iH^{\text{as}}t) \exp(-i2Ht) \times \exp(iH^{\text{as}}t) | \phi_{\text{in}} \rangle, \quad (1.1)$$

where H^{as} denotes an asymptotic Hamiltonian, and the asymptotic states are assumed to have a wave-packet distribution in energy in the interval $[E_{\text{low}}, E_{\text{up}}]$. In field theory, the Hamiltonian has infinitely many degrees of freedom. In the scattering process described by the above matrix element, only the degrees of freedom corresponding to energies in $[E_{\text{low}}, E_{\text{up}}]$ play a role. Thus we have the freedom to replace the Hamiltonian H by a new Hamiltonian H^{block} such that it has fewer degrees of freedom, but with the constraint to give the same physics for energies in the relevant energy interval. The transition $H \rightarrow H^{\text{block}}$ can be considered as a renormalization-group transformation. We suggest the construction of H^{block} as follows: One constructs a finite-dimensional basis of so-called broad states $|\phi_v^{\text{broad}}\rangle$. Then one constructs so-called focused states

$$|\psi_v^{\text{focus}}(\tau_{\text{focus}})\rangle = \int_{E_{\text{low}}}^{E_{\text{up}}} dE \exp[-(H-E)^2 \tau_{\text{focus}}] |\phi_v^{\text{broad}}\rangle. \quad (1.2)$$

In the limit $\tau_{\text{focus}} \rightarrow \infty$, the contributions of the broad states corresponding to energies E exterior to $[E_{\text{low}}, E_{\text{up}}]$ are filtered out. The block Hamiltonian is constructed by taking matrix elements of the original Hamiltonian between the focused states. The projection operator is positive (τ_{focus} is a real parameter) with a rapid exponential

falloff behavior for contributions corresponding to an energy outside of $[E_{\text{low}}, E_{\text{up}}]$. It is suitable for application of the Monte Carlo projector method.¹⁷ The S matrix is replaced by a block S matrix by substituting $H \rightarrow H^{\text{block}}$ in Eq. (1.1) and replacing the time limit by a finite scattering time. The numerical computation of the block S matrix is straightforward after algebraic diagonalization of the block Hamiltonian.

We suggest working in momentum space, i.e., using a momentum lattice. Momentum variables seem to be the natural coordinates because they describe the asymptotics in a simple way. Momentum lattices have been used in Refs. 12 and 13, and a light-cone momentum lattice has been used by Eller, Pauli, and Brodsky²³ to study QED. Stochastic quantization and the conservation of $\text{SU}(n)$ gauge invariance on a momentum lattice has been discussed in Ref. 24.

In this paper we want to demonstrate the feasibility of our approach by an application in few-body physics. We compute nucleon-nucleon (N - N) scattering in a nonrelativistic potential model (Yamaguchi potential). Although it is not the ideal application, we have chosen it because it has an analytical solution. The application is not ideal in the sense that solving a one-dimensional integral by Monte Carlo integration is much inferior to a fixed-node integration. However, for many-dimensional integrals, Monte Carlo integration is by far superior to fixed-node integration. Thus the ideal application is a system with many degrees of freedom. Here the S matrix of the Yamaguchi model provides a benchmark to test the accuracy of the method under variation of the coupling constant, the lattice size and other parameters.

In Sec. II, we introduce the idea of blocking of a Hamiltonian in order to reduce the number of degrees of freedom and we discuss the computation of a real-time S matrix on a lattice. In Sec. III, we explain the working of the Monte Carlo projector method. In Sec. IV, numerical results for N - N scattering are presented. In Sec. IV, we give a conclusion.

II. TIME-DEPENDENT FORMULATION OF SCATTERING

Let us consider a system, the dynamics of which is governed by a Hamiltonian H . Let us suppose we want to compute a scattering matrix element, determined by the boundary conditions that at $t = +\infty$ ($-\infty$) the scattering states asymptotically approach the Hilbert states ϕ_{out} (ϕ_{in}). Moreover, we suppose that there is an asymptotic Hamiltonian H^{as} [not necessarily the same for $t = +\infty$ ($-\infty$)]. Then the S matrix in time-dependent language is given by Eq. (1.1). We assume that the asymptotic states ϕ_{out} (ϕ_{in}) have a wave-packet distribution in energy, say in the energy interval $[E_{\text{low}}, E_{\text{up}}]$, and the scattering energy $E_{\text{scat}} = \langle H^{\text{as}} \rangle$ lies in this interval. The computation of the S -matrix element proceeds in two steps: (i) the reduction of the number of degrees of freedom by introducing a block Hamiltonian and its computation using the Monte Carlo projector method; (ii) the algebraic computation of the block S matrix.

A. Blocking approximations (reduction of the number of degrees of freedom)

In most physical systems, the Hamiltonian has a large number of degrees of freedom (this is already the case in few-body systems, if one considers, e.g., three-nucleon scattering with realistic N - N potentials). How can the number of degrees of freedom involved in a scattering reaction be reduced? Let us assume for the moment that $\phi_{\text{out}}/\phi_{\text{in}}$ are sharp eigenstates of H^{as} to the energy E . Then the S -matrix element given by Eq. (1.1) would not change if we replaced $H \rightarrow H' = P(E)HP(E)$, with $P(E)$ being the spectral projector corresponding to energy E . Now H' describes the same physics at energy E as H does, but has a much smaller number of degrees of freedom. Now $P(E)$ is an object which is numerically inconvenient to compute. In our case, however, $\phi_{\text{out}}(\phi_{\text{in}})$ are wave packets covering at energy interval $[E_{\text{low}}, E_{\text{up}}]$. Hence a suitable new Hamiltonian would be

$$H \rightarrow H' = P[E_{\text{low}}, E_{\text{up}}]HP[E_{\text{low}}, E_{\text{up}}], \quad (2.1)$$

and analogously for the asymptotic Hamiltonian

$$H^{\text{as}} \rightarrow H'^{\text{as}} = P^{\text{as}}[E_{\text{low}}, E_{\text{up}}]H^{\text{as}}P^{\text{as}}[E_{\text{low}}, E_{\text{up}}]. \quad (2.2)$$

Thus

$$\langle \phi_{\text{out}} | S' | \phi_{\text{in}} \rangle = \lim_{t \rightarrow \infty} \langle \phi_{\text{out}} | \exp(iH'^{\text{as}}t) \exp(-i2H't) \times \exp(iH'^{\text{as}}t) | \phi_{\text{in}} \rangle \quad (2.3)$$

gives the same matrix element as Eq. (1.1), i.e.,

$$\langle \phi_{\text{out}} | S | \phi_{\text{in}} \rangle = \langle \phi_{\text{out}} | S' | \phi_{\text{in}} \rangle. \quad (2.4)$$

However, $S \neq S'$. The expression, given by Eq. (2.3), is suitable for a numerical computation. This can be done as follows. We construct a ‘‘broad’’ basis of states

$|\phi_{\nu}^{\text{broad}}\rangle$, $\nu=1, \dots, N$, which are elements of Hilbert space. The broad states can be chosen quite arbitrarily, but are usually wave packets. They are supposed to have nonzero overlap with eigenstates of the original Hamiltonian H , corresponding to eigenvalues from the interval $[E_{\text{low}}, E_{\text{up}}]$. Moreover, they have to be linearly independent. Then we construct a basis of ‘‘focused’’ states $|\psi_{\nu}^{\text{focus}}\rangle$, $\nu=1, \dots, N$, via Eq. (1.2). Because of

$$P[E_{\text{low}}, E_{\text{up}}] = \lim_{\tau \rightarrow \infty} \left[\frac{\tau}{\pi} \right]^{1/2} \int_{E_{\text{low}}}^{E_{\text{up}}} dE \exp[-(H-E)^2\tau], \quad (2.5)$$

the states $|\psi_{\nu}^{\text{focus}}(\tau_{\text{focus}})\rangle$ have the property of ‘‘focusing’’ onto the eigenstates of H in the interval $[E_{\text{low}}, E_{\text{up}}]$ when $\tau_{\text{focus}} \rightarrow \infty$, and to exponentially suppress all degrees of freedom which correspond to eigenstates of H exterior to $[E_{\text{low}}, E_{\text{up}}]$. The focused states are neither orthogonal nor normalized. One can construct a projector onto the focused states

$$P^{\text{block}} = \sum_{\nu, \mu=1}^N |\psi_{\nu}^{\text{focus}}\rangle \langle \psi_{\mu}^{\text{focus}}|, \quad (2.6)$$

$$\sigma_{\nu\mu} = \langle \psi_{\nu}^{\text{focus}} | \psi_{\mu}^{\text{focus}} \rangle, \quad (2.7)$$

where we have suppressed the dependence on the approximation parameter τ_{focus} . With the help of P^{block} , we construct a block Hamiltonian

$$H^{\text{block}} = P^{\text{block}}HP^{\text{block}}. \quad (2.8)$$

Analogously to $|\phi_{\nu}^{\text{broad}}\rangle$, $|\psi_{\nu}^{\text{focus}}\rangle$, P^{block} , and H^{block} corresponding to the Hamiltonian H , one can construct the analogous expressions $|\phi_{\nu}^{\text{as, broad}}\rangle$, $|\psi_{\nu}^{\text{as, focus}}\rangle$, $P^{\text{as, block}}$, and $H^{\text{as, block}}$ corresponding to the asymptotic Hamiltonian H^{as} . Then the block S matrix is given by

$$\langle \phi_{\text{out}} | S^{\text{block}}(t) | \phi_{\text{in}} \rangle = \langle \phi_{\text{out}} | \exp(iH^{\text{as, block}}t) \exp(-i2H^{\text{block}}t) \exp(iH^{\text{as, block}}t) | \phi_{\text{in}} \rangle. \quad (2.9)$$

If, e.g., one chooses $|\phi_{\nu}^{\text{broad}}\rangle$ such that H^{as} is diagonal in that basis, then in order to compute the block S matrix one has to evaluate only the following matrix elements:

$$\sigma_{\nu\mu} = \langle \psi_{\nu}^{\text{focus}} | \psi_{\mu}^{\text{focus}} \rangle = \int_{E_{\text{low}}}^{E_{\text{up}}} dE \int_{E_{\text{low}}}^{E_{\text{up}}} dE' \langle \phi_{\nu}^{\text{broad}} | \exp[-(H-E)^2\tau_{\text{focus}}] \exp[-(H-E')^2\tau_{\text{focus}}] | \phi_{\mu}^{\text{broad}} \rangle, \quad (2.10)$$

$$H_{\nu\mu}^{\text{block}} = \langle \psi_{\nu}^{\text{focus}} | H | \psi_{\mu}^{\text{focus}} \rangle = \int_{E_{\text{low}}}^{E_{\text{up}}} dE \int_{E_{\text{low}}}^{E_{\text{up}}} dE' \langle \phi_{\nu}^{\text{broad}} | \exp[-(H-E)^2\tau_{\text{focus}}] H \exp[-(H-E')^2\tau_{\text{focus}}] | \phi_{\mu}^{\text{broad}} \rangle, \quad (2.11)$$

$$\phi_{\text{out}, \nu} = \langle \phi_{\text{out}} | \psi_{\nu}^{\text{focus}} \rangle = \int_{E_{\text{low}}}^{E_{\text{up}}} dE \langle \phi_{\text{out}} | \exp[-(H-E)^2\tau_{\text{focus}}] | \phi_{\nu}^{\text{broad}} \rangle, \quad (2.12)$$

$$\phi_{\text{in}, \nu} = \langle \phi_{\text{in}} | \psi_{\nu}^{\text{focus}} \rangle = \int_{E_{\text{low}}}^{E_{\text{up}}} dE \langle \phi_{\text{in}} | \exp[-(H-E)^2\tau_{\text{focus}}] | \phi_{\nu}^{\text{broad}} \rangle. \quad (2.13)$$

Let us give two comments on the blocking procedure. In principle, τ_{focus} should go to infinity. In practical applications, it has to be finite. Convergence with respect to τ_{focus} has to be verified numerically. Another remark concerns the projection operator $\exp[-(H-E)^2\tau_{\text{focus}}]$ introduced in Eq. (1.2). The latter contrasts to the projection operator $\exp(-H\tau_{\text{focus}})$ used in ground

state computations. If, instead we would take for scattering $\exp[-(H-E)\tau_{\text{focus}}]$, this would fail, because contributions coming from eigenstates corresponding to energies $E' < E$ would blow up exponentially.

Let us discuss possible choices for the broad states. One possible choice for a basis of broad states is such that H^{as} becomes diagonal in that basis. This brings about a

simplification for the evaluation of $\exp(iH^{\text{as,block}}t)$. Another choice would be such that the noninteracting Hamiltonian H^0 becomes diagonal in the basis of broad states. In order to define such a basis, we introduce a momentum lattice of broad resolution. Let the lattice be defined by the sites p_ν , $\nu=1, \dots, N$, which form a regular D -dimensional lattice. The volume of the elementary cube is $(\Delta p)^D$. The lattice may be viewed as a decomposition of the total lattice volume into disjoint elementary cubes c_ν , $\nu=1, \dots, N$, such that p_ν is located at the center of C_ν . Then one can define a basis of step functions $|p_\nu\rangle$, $\nu=1, \dots, N$ via $\langle p|p_\nu\rangle=1$ if $p \in C_\nu$ and vanishes elsewhere.

In a one-body Hamiltonian, one can choose $|\phi_\nu^{\text{broad}}\rangle = |p_\nu\rangle$, $\nu=1, \dots, N$. In a many-body Hamiltonian, step functions can occur in all sectors of Fock space, e.g., in the m -body sector $|p_{\nu_1}, \dots, p_{\nu_m}\rangle$. This would still lead to a very large set of basis functions. However, the broad basis can be chosen actually to be much smaller. First, one can restrict the broad basis by the requirement

$$E_\nu^{\text{as}} = \langle \phi_\nu^{\text{broad}} | H^{\text{as}} | \phi_\nu^{\text{broad}} \rangle \in [E_{\text{low}}, E_{\text{up}}]. \quad (2.14)$$

For the case $H^{\text{as}} = H^0$, and considering a one-body Hamiltonian on a one-dimensional lattice, this is illustrated in Fig. 1. Secondly, let us assume that the asymptotic states ϕ_{out} (ϕ_{in}) belong to an m -particle sector, e.g., $m=2$. Then one can restrict the broad basis to be chosen from only the $m=2$ particle sector (the focused states, via the interaction included in the full Hamiltonian, have contributions from other particle-number sectors). Then H^{block} , given by Eq. (2.11), can be viewed as a Hamiltonian in the $m=2$ particle sector, while the original Hamiltonian H acts in the whole Fock space. This is another way of looking at the above statement that $H \rightarrow H^{\text{block}}$ can be regarded as a renormalization-group transformation. H and H^{block} are quite different Hamiltonians, but they should describe the same physics in the energy interval $[E_{\text{low}}, E_{\text{up}}]$. However, there are many other possible choices for the basis of broad states, and in general it is not necessary that they are eigenstates of the noninteracting Hamiltonian. There is no general rule, except (i) basis states should be constructively simple, and (ii) they should not yield too-small matrix elements, i.e., elements which are zero compared to the statistical noise.

We have noted the fact that H^{block} corresponds to a

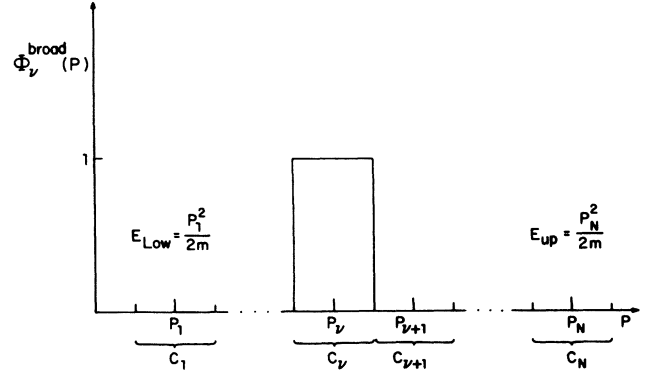


FIG. 1. The definition of a “broad” state in momentum space.

finite-dimensional Hamiltonian matrix and thus its eigenvalues E_ν [Eq. (2.14)] are expected to lie in the interval $[E_{\text{low}}, E_{\text{up}}]$. This is strictly valid in the limit $\tau_{\text{focus}} \rightarrow \infty$, but for some large but finite τ_{focus} the eigenvalues are expected to be located in the neighborhood of this interval. Numerically, this is desirable, because it corresponds to a well-conditioned matrix, in contrast to the original Hamiltonian H , which has an unbounded spectrum, with eigenvalues extending from 0 to ∞ , and hence H can be considered an ill-conditioned matrix.

B. Computation of the block S matrix

In Sec. II A, we have described how to reduce the number of degrees of freedom of a Hamiltonian H by construction of a block Hamiltonian H^{block} . H^{block} corresponds to a finite-dimensional Hamiltonian matrix. Hence we can compute the block time evolution $U^{\text{block}}(t) = \exp(iH^{\text{block}}t)$ and the block S matrix by algebraic diagonalization:

$$H^{\text{block}}|\eta_\nu\rangle = E_\nu|\eta_\nu\rangle, \quad \nu=1, \dots, N, \quad (2.15)$$

$$H^{\text{as,block}}|\eta_\nu^{\text{as}}\rangle = E_\nu^{\text{as}}|\eta_\nu^{\text{as}}\rangle, \quad \nu=1, \dots, N. \quad (2.16)$$

As mentioned above, it is convenient to choose

$$|\phi_\nu^{\text{broad}}\rangle \equiv |\eta_\nu^{\text{as}}\rangle, \quad \nu=1, \dots, N. \quad (2.17)$$

Then the block S matrix given by Eq. (2.9) reads, using Eqs. (2.15) and (2.16),

$$\langle \phi_{\text{out}} | S^{\text{block}}(t) | \phi_{\text{in}} \rangle = \sum_{\nu, \mu, \sigma=1}^N \langle \phi_{\text{out}} | \eta_\nu^{\text{as}} \rangle \exp(iE_\nu^{\text{as}}t) \langle \eta_\nu^{\text{as}} | \eta_\mu \rangle \exp(-i2E_\mu t) \langle \eta_\mu | \eta_\sigma^{\text{as}} \rangle \exp(iE_\sigma^{\text{as}}t) \langle \eta_\sigma^{\text{as}} | \phi_{\text{in}} \rangle. \quad (2.18)$$

The questions to ask now are the following: (i) Under which conditions does this yield a systematic and reliable approximation of the original S matrix? (ii) What does the parameter t mean? How is it chosen? One can give several answers to question (i). The mathematical answer is that H^{block} has to approximate H in the sense of strong resolvent convergence.²⁵ The physical answer is that H^{block} has to be a good approximation of H in the spec-

tral neighborhood of the scattering energy E_{scat} . The answer from the practical point of view is that one constructs H^{block} from H by the blocking procedure, based on a lattice discretization. One has to vary the approximation parameter, e.g., the block dimension, lattice size and spacing, until the block S matrix yields converging results. The answer to question (ii) is that the parameter t , which has nothing to do with the parameter τ_{focus} , is a

real-time parameter which has to be chosen large but finite. [Neither $\lim_{t \rightarrow \infty} U^{\text{block}}(t)$ nor $\lim_{t \rightarrow \infty} S^{\text{block}}(t)$ does exist, because the generator of the time evolution is a finite-dimensional operator.] The ideal choice for the parameter t would be such that $\Delta S = |S - S^{\text{block}}(t)|$ would be minimal. In practice, where the exact solution for S is unknown, one can fix the parameter t by the physical requirement that the violation of energy in the scattering process becomes minimal. The energy violation can be measured by

$$\Delta_{\langle E \rangle}(t) = |\langle \psi^{\text{scat}}(t) | H^{\text{block}} | \psi^{\text{scat}}(t) \rangle - \langle \phi_{\text{in}} | H^{\text{as,block}} | \phi_{\text{in}} \rangle|, \quad (2.19)$$

where

$$|\psi^{\text{scat}}(t)\rangle = U^{\text{block}}(t) U^{\text{as,block}}(-t) |\phi_{\text{in}}\rangle \quad (2.20)$$

corresponds to a scattering state. This definition for the parameter t , called scattering time t_{scat} , has been tested for several nonrelativistic²⁶ and relativistic models^{12–14}, and it has been observed that the ideal definition and the working definition, Eq. (2.19), give very close answers, i.e., the parameter determined from the working definition yields a stable S matrix, close to its reference value.

Let us close this section with a remark on the behavior of $U^{\text{block}}(t)$ and $S^{\text{block}}(t)$. First, matrix elements of both $U(t)$ and $U^{\text{block}}(t)$ have an oscillatory behavior with increasing $t \rightarrow \infty$. However, matrix elements of $U(t)U^{\text{as}}(-t)$ converge with $t \rightarrow \infty$, thus matrix elements of $S^{\text{block}}(t)$ are expected to be smooth and stable functions in t , at least in some reasonably wide time interval, which includes the scattering time. Secondly, S is unitary and $S^{\text{block}}(t)$, by construction, is also unitary for any real value of t . This implies bounds on the numerical solution, and is very useful from the practical point of view.

III. MONTE CARLO PROJECTOR METHOD

In this section, we want to describe how to compute the matrix elements $\sigma_{\nu\mu}$, $H_{\nu\mu}^{\text{block}}$, $\phi_{\text{out},\nu}$, $\phi_{\text{in},\nu}$ given by Eqs. (2.10)–(2.13) necessary to compute the block S matrix. We introduce another momentum lattice, which is of fine resolution δk with $\delta k < \Delta p$ (i.e., it has a finer resolution than the p lattice of the broad states). We denote the lat-

tice by sites k_i , $i = 1, \dots, M$, which form a regular D -dimensional lattice. The volume of the elementary cube is $(\delta k)^D$. Correspondingly, we introduce a basis which should span the whole Hilbert space via the step functions, as introduced in Sec. II. We consider elementary cubes C_i of volume $(\delta k)^D$ centered at k_i , and define a one-body step function $|k_i\rangle$, defined by $\langle k | k_i \rangle = \text{const}$, if $k \in C_i$, and vanishes elsewhere. The constant is chosen to normalize $|k_i\rangle$: $\langle k_i | k_i \rangle = 1$. In a many-body system, e.g., for one species of bosons, one has to build the basis from all particle-number sectors, e.g., in the m -particle sector $|k_{i_1}, \dots, k_{i_m}\rangle$. For convenience of notation, we denote the basis by $|k_i\rangle$, also including the many-body case. Then we write

$$1 = \sum_{k_i} |k_i\rangle \langle k_i|, \quad (3.1)$$

which means that the states $|k_i\rangle$ span a complete basis, which is strictly valid only if the lattice momentum cutoff goes to infinity and the lattice momentum resolution δk goes to zero. Having defined the broad lattice (Sec. II A) and the fine-resolution lattice, then the conversion of a function given in terms of the broad lattice onto the fine lattice (or vice versa) is given by the scalar products $\langle p_i | k_j \rangle$, $i = 1, \dots, N$, $j = 1, \dots, M$ ($M > N$). The noninteracting Hamiltonian is diagonal in the basis:

$$\langle k_i | H^0 | k_j \rangle = \epsilon^0(k_i) \delta_{ij}. \quad (3.2)$$

Then in order to compute the matrix element $H_{\nu\mu}^{\text{block}}$, we apply the Monte Carlo projector method. We split the Hamiltonian into two parts:

$$H = H^0 + V. \quad (3.3)$$

Then we write

$$H_{\nu\mu}^{\text{block}} = \int_{E_{\text{low}}}^{E_{\text{up}}} dE \int_{E_{\text{low}}}^{E_{\text{up}}} dE' h_{\nu\mu}(E, E'), \quad (3.4)$$

$$h_{\nu\mu}(E, E') = \langle \phi_{\nu}^{\text{broad}} | \exp[-(H - E)^2 \tau_{\text{focus}}] \times H \exp[-(H - E')^2 \tau_{\text{focus}}] | \phi_{\mu}^{\text{broad}} \rangle. \quad (3.5)$$

The operator $\exp[-(H - E)^2 \tau_{\text{focus}}]$ is broken into L time slices, between which the momentum basis of fine resolution $|k_i\rangle$ is inserted:

$$\begin{aligned} h_{\nu\mu}(E, E') = & \sum_{i_1, \dots, i_{2L+2}} \langle \phi_{\nu}^{\text{broad}} | k_{i_1} \rangle \langle k_{i_1} | \exp[-(H - E)^2 \Delta\tau] | k_{i_2} \rangle \times \dots \\ & \times \langle k_{i_L} | \exp[-(H - E)^2 \Delta\tau] | k_{i_{L+1}} \rangle \langle k_{i_{L+1}} | H | k_{i_{L+2}} \rangle \times \dots \\ & \times \langle k_{i_{2L+1}} | \exp[-(H - E')^2 \Delta\tau] | k_{i_{2L+2}} \rangle \langle k_{i_{2L+2}} | \phi_{\mu}^{\text{broad}} \rangle, \end{aligned} \quad (3.6)$$

where $\Delta\tau = \tau_{\text{focus}}/L$. Thus one has to evaluate the matrix element

$$g_{ij}(E) = \langle k_i | \exp[-(H - E)^2 \Delta\tau] | k_j \rangle. \quad (3.7)$$

One has

$$\begin{aligned} \exp[-(H - E)^2 \Delta\tau] = & \exp[-(H^0 - E)^2 \Delta\tau] \\ & \times \exp[-(V^2 + V H^0 + H^0 V \\ & \quad - 2VE) \Delta\tau] \\ & + O(\Delta\tau^2). \end{aligned} \quad (3.8)$$

Hence, due to $\Delta\tau \ll 1$,

$$g_{ij}(E) \cong \langle k_i | \exp[-(H^0 - E)^2 \Delta\tau] | k_i \rangle \\ \times \langle k_i | 1 - \Delta\tau(V^2 + VH^0 + H^0V - 2VE) | k_j \rangle . \quad (3.9)$$

This can be evaluated explicitly. Then in order to evaluate the matrix element $h_{\nu\mu}(E, E')$ by Monte Carlo methods, we introduce “scores” S_{ij} and “weights” P_{ij} via

$$g_{ij} = S_{ij} P_{ij} , \quad (3.10)$$

$$\sum_i P_{ij} = 1 , \quad (3.11)$$

$$P_{ij} = P_{ji} . \quad (3.12)$$

Apart from the constraints given by Eqs. (3.10)–(3.12), the splitting of g_{ij} into S_{ij} and P_{ij} is arbitrary. For the case of N - N scattering, considered in Sec. IV, we have considered two choices:

$$P_{ij}^{(a)} = \text{const} \times \exp[-(k_i^2 - 2mE)^2 / \sigma^2] , \quad (3.13)$$

$$P_{ij}^{(b)} = \text{const} \times \exp(-|H_{ii} - H_{jj}| / \sigma^2) . \quad (3.14)$$

Putting Eqs. (3.6)–(3.12) into Eq. (3.6) defines a Monte Carlo procedure, where the amplitude for momentum k_i at some intermediate time slice is generated with probability P_{ij} . In the process, the scores S_{ij} are accumulated. The generation of configurations of momenta $\{k_{i_1}, \dots, k_{i_{2L+2}}\}$ for all time slices and hence the product $S_{i_1 i_2} \dots S_{i_L i_{L+1}} H_{i_{L+1} i_{L+2}} S_{i_{L+2} i_{L+3}} \dots S_{i_{2L+1} i_{2L+2}}$ is repeated many times in order to carry out the sum in Eq. (3.6). Finally the evaluation of $h_{\nu\mu}(E, E')$ is repeated for many values of E, E' (corresponding to the moments on the k lattice) in order to obtain $H_{\nu\mu}^{\text{block}}$ by integration as defined in Eq. (3.4). The same technique is applied to compute the other matrix elements $\sigma_{\nu\mu}, \phi_{\text{out}, \nu}, \phi_{\text{in}, \nu}$.

In principle, the resulting answers should be independent of the choice of the probability matrix P_{ij} . In practice, where the number of sweeps is finite, some choices are better than others. Form (ii) is certainly better than form (i) for the Yamaguchi Hamiltonian, considered in Sec. IV. There exist many other ways of improving the Monte Carlo algorithm described above, such as the EPMC (Ref. 27) and the wave-function guided walk.¹⁸ We do not wish to use those schemes here, as we are more interested in studying the behavior of the S matrix from an imperfect knowledge of the matrix element $h_{\nu\mu}$.

IV. NONRELATIVISTIC N - N SCATTERING

As outlined above in Secs. II and III, we want to avoid computing $\langle \exp(iHt) \rangle$ numerically, but rather compute $\langle H^{\text{block}} \rangle$, for which Monte Carlo algorithms have been used widely.^{16–18, 22, 27} The success of our approach therefore rests on the accurate determination of matrix elements of the block Hamiltonian and also on the propagation of the errors from the block Hamiltonian to the block S matrix. In this section we discuss this issue for a model describing nonrelativistic N - N scattering with the

separable Yamaguchi potential. We have chosen this model because it has an analytical solution for the S matrix.

A. The model

In order to describe two-body scattering, one separates the c.m. motion from the relative motion by using Jacobi coordinates, and correspondingly writing the Hamiltonian $H_{\text{total}} = H_{\text{c.m.}} + H_{\text{rel}}$. Then we split the relative motion Hamiltonian into a free and an interacting part, as in Eq. (3.3). The free Hamiltonian H^0 is given by

$$H^0 | \mathbf{q} \rangle = \frac{q^2}{2m} | \mathbf{q} \rangle , \quad (4.1)$$

where \mathbf{q} denotes the Jacobi relative momentum and $m = \frac{1}{2} m_{\text{nucl}}$ is the reduced mass. We have taken the nucleon mass to be $m_{\text{nucl}} = 938.259$ MeV. In order to describe N - N scattering at low energies, the separable Yamaguchi potential²⁸ can be used. It describes the phase shifts fairly well up to 100 MeV. The potential is separable of rank one, with an s -wave form factor

$$V = | \chi \rangle \lambda \langle \chi | , \quad (4.2)$$

$$\langle \mathbf{q} | \chi \rangle = 1 / (q^2 + \beta^2) . \quad (4.3)$$

The parameters λ and β are fitted to reproduce the effective range parameters, singlet scattering length, and singlet effective range. We have taken $\lambda = -0.0278811$ fm⁻² and $\beta = 1.12747$ fm⁻¹. The S matrix is related to the T matrix via

$$\langle \mathbf{q}' | S | \mathbf{q} \rangle = \delta(\mathbf{q}' - \mathbf{q}) - 2\pi i \delta(E'_q - E_q) \\ \times \lim_{\epsilon \rightarrow 0^+} \langle \mathbf{q}' | T(E_q + i\epsilon) | \mathbf{q} \rangle . \quad (4.4)$$

Because V is separable, one obtains an analytic solution for the T -matrix

$$T(z) = | \chi \rangle \frac{\lambda}{1 - \lambda \Delta(z)} \langle \chi | , \quad (4.5)$$

$$\lim_{\epsilon \rightarrow 0^+} \Delta(E_q + i\epsilon) = \frac{2\pi^2 m}{\beta^2 (q/\beta + i)^2} . \quad (4.6)$$

We have computed the S matrix in a partial-wave representation, in particular in the s wave.

In partial-wave representation, the momentum q runs from 0 to ∞ . We have used a momentum cutoff $\Lambda = 10.0$ fm⁻¹. We have chosen the energy interval $[E_{\text{low}}, E_{\text{up}}]$ set by $q_{\text{low}} = 1.0$ fm⁻¹ and $q_{\text{up}} = 4.0$ fm⁻¹. We have taken as asymptotic state $\phi_{\text{out}} = \phi_{\text{in}}$, given by a wave-packet state, defined in the interval $[q_{\text{low}}, q_{\text{up}}]$ by

$$\phi_{00}(q) = \kappa \left[1 - \cos \left[2\pi \frac{q - q_{\text{low}}}{q_{\text{up}} - q_{\text{low}}} \right] \right] , \quad q_{\text{low}} \leq q \leq q_{\text{up}} , \quad (4.7)$$

and vanishing elsewhere. The constant κ is chosen to normalize the state to unity. This wave packet is bell shaped, having a peak at $(q_{\text{up}} + q_{\text{low}})/2$ and a width of $(q_{\text{up}} - q_{\text{low}})/2$.

We have introduced the broad resolution lattice by discretizing the interval $[q_{\text{low}}, q_{\text{up}}]$ into $N=3$ and 6 subintervals, i.e., $\Delta q=1.0$ and 0.5 fm^{-1} , respectively. We have chosen as broad basis functions the step functions (see Fig. 1) corresponding to those subintervals. We have introduced a fine-resolution lattice by discretizing the interval $[0, \Lambda]$ into $M=20$ and 40, subintervals, respectively, i.e., $\delta q=0.5$ and 0.25 fm^{-1} , and used as basis functions the step functions corresponding to those subintervals. It has turned out that the exact analytical solution for the S matrix and the numerical solution from the lattice with fine resolution agree to less than 10^{-3} .

The other approximation parameters correspond to the Monte Carlo simulation. We have used focus time steps $\Delta\tau$ of 0.014, 0.020, 0.033, and 0.071 fm, and a total number of focus time slices $L=3, 5, 7,$ and 11. For the Yamaguchi model, we found that τ_{focus} of about 0.2–0.5 was already good enough to obtain convergence, as is shown below in the results. For the given magnitude of the coupling constant λ , it turns out that the probability given by Eq. (3.12) is a good choice to perform the random walk in phase space.

The computation of the on-diagonal matrix elements of H^{block} required only a few thousand sweeps (up to 10^4) in order to get an accuracy of less than 10%. The off-diagonal matrix elements, on the other hand, involve more work, namely up to 10^5 sweeps.

B. Numerical results

We have computed the S matrix in three ways. (i) First, we have taken the analytical expression from time-independent stationary scattering theory for the on-shell T matrix, Eqs. (4.5) and (4.6), and integrated numerically over the energies which contribute to the asymptotic wave packet, Eq. (4.7). This is considered as exact solution, referred to as reference solution. (ii) Secondly, we have computed the time-dependent block S matrix, Eq. (2.9), by computing the block Hamiltonian, Eq. (2.11), from the fine-resolution lattice (k lattice). We have replaced in Eq. (2.11) the original Hamiltonian H by the Hamiltonian defined on the fine-resolution lattice. We have diagonalized it and hence computed the exponentials in Eq. (2.11) in its eigenrepresentation. This is considered as the reference solution for the block Hamiltonian and the block S matrix. (iii) Finally, we have computed the block S matrix from the block Hamiltonian via the Monte Carlo projector method. This is the solution we want to study. In this way, information on the error from the blocking method is obtained by comparing the exact solution with the blocking reference solution, and information on the error from Monte Carlo methods is obtained by comparing the blocking reference solution with the blocking Monte Carlo solution.

The point of our numerical example is not to attempt to get the most accurate value for the S matrix as possible using the best available Hamiltonian projector Monte Carlo method. We have used a conventional Monte Carlo method and limited statistics because the goal is instead to attempt to see whether acceptable values for the scattering matrix can be obtained with imperfectly

known Hamiltonian matrix elements. The fact is that an accurate calculation of the S matrix in the context of the Yamaguchi model could not imply the success of our general approach for more complicated and more realistic theories. What is more likely, however, is that in the latter case the numerical calculation of the block Hamil-

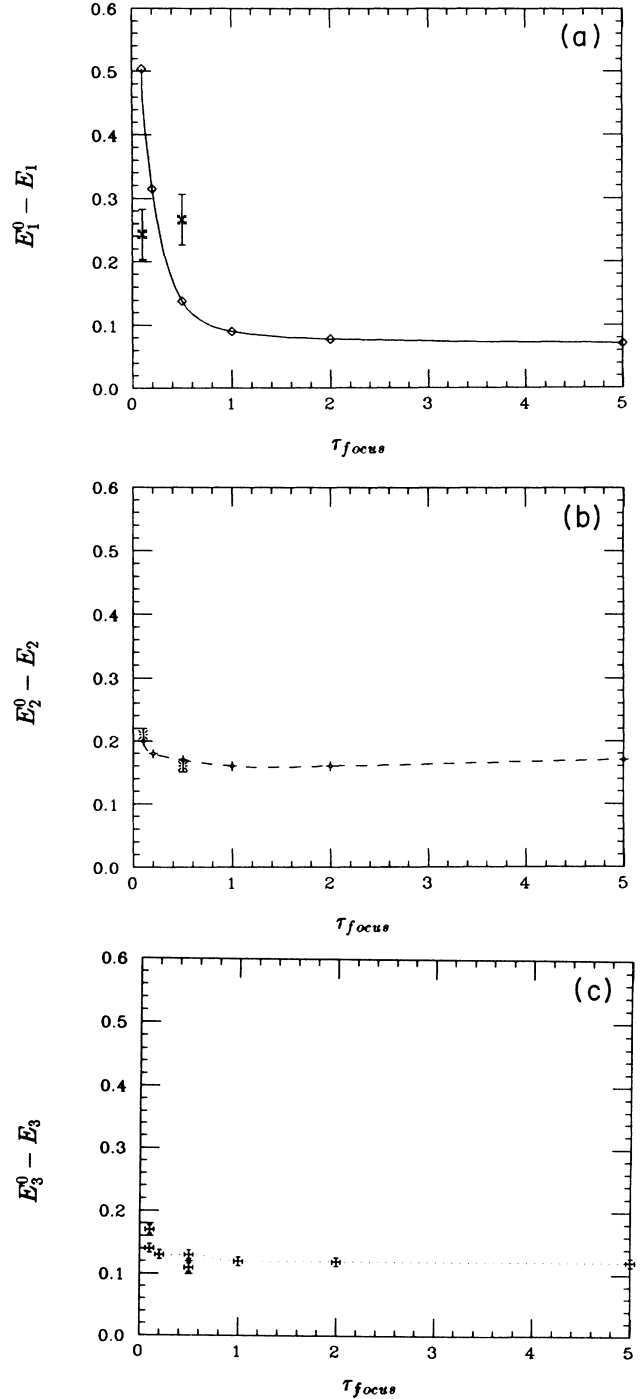


FIG. 2. The difference between the eigenvalues of the asymptotic and the full block Hamiltonians vs τ_{focus} . $\lambda=0.278811 \text{ fm}^{-2}$, $N=3$, and $M=40$. The diamonds, crosses, and pluses correspond to the reference values. The solid squares represent the Monte Carlo data. The lines are a guide for the eye.

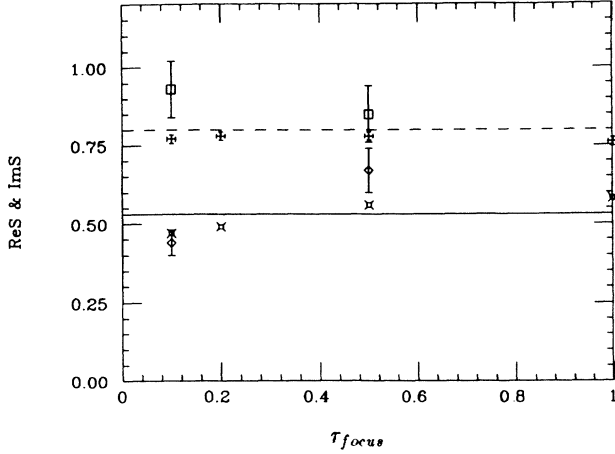


FIG. 3. Block S matrix vs τ_{focus} . $\lambda=0.278\,811\text{ fm}^{-2}$. The continuous line ($\text{Re } S$) and the dashed line ($\text{Im } S$) correspond to the exact solution. The symbols (\times) and ($+$) correspond to $\text{Re } S$ and $\text{Im } S$, respectively, of the reference block S matrix. The open diamonds and open squares correspond to $\text{Re } S$ and $\text{Im } S$, respectively, of the Monte Carlo block S matrix.

tonian matrix elements will be known with mediocre accuracy (10–20%), given the size of the problem and the complexity of the interactions.

In general, the Monte Carlo method described in Sec. III yields the matrix elements of the full and asymptotic block Hamiltonian. In our application, we have chosen to use for the matrix elements of the asymptotic block Hamiltonian the exact values, in order to reduce the errors. In most applications in many-body theory, the calculation of the matrix elements of the asymptotic block Hamiltonian is likely to be simple enough to permit an exact solution.

In Fig. 2 we show the difference of the eigenvalues

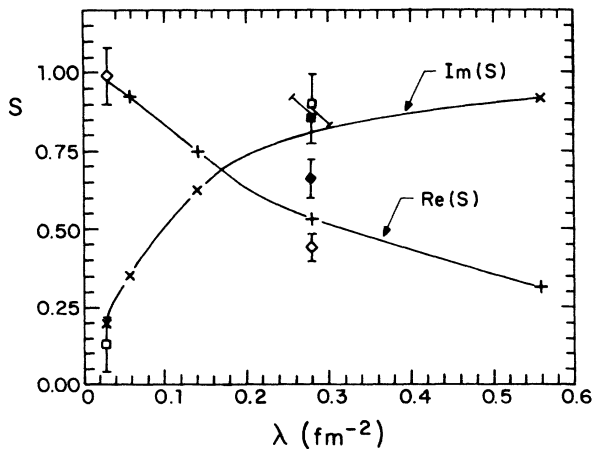


FIG. 4. Block S matrix vs coupling parameter λ . $N=3$, $M=40$. The symbols ($+$) and (\times) correspond to $\text{Re } S$ and $\text{Im } S$, respectively, of the reference block S matrix. The continuous lines are a guide for the eye. The Monte Carlo data are given by diamonds ($\text{Re } S$) and squares ($\text{Im } S$). The open symbols correspond to $\tau_{\text{focus}}=0.1\text{ fm}$ and the solid symbols correspond to $\tau_{\text{focus}}=0.5\text{ fm}$.

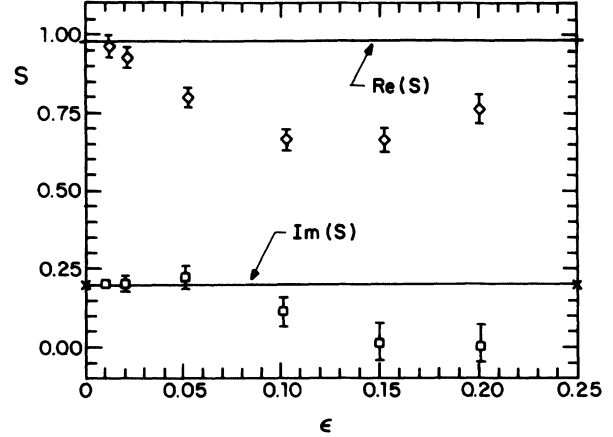


FIG. 5. Block S matrix as a function of the error ϵ , Eq. (4.8), in the block Hamiltonian. $\lambda=0.0278\,811\text{ fm}^{-2}$, $\tau_{\text{focus}}=0.1\text{ fm}$, $N=3$, $M=40$. 150 random numbers were used to generate the Gaussian distribution.

$E_v^0 - E_v$, $v=1,2,3$ corresponding to the asymptotic and full block Hamiltonian as a function of τ_{focus} . This corresponds to taking $\lambda=-0.278\,811\text{ fm}^{-2}$ (ten times the value of the Yamaguchi model), $N=3$ broad states, and $M=40$ on the fine-resolution lattice. We display the reference results and the Monte Carlo results from the block Hamiltonian. One observes convergence of the reference block Hamiltonian as a function τ_{focus} starting at about $\tau_{\text{focus}}=0.5\text{ fm}$. Except for the lowest eigenvalue ($v=1$), the eigenvalues obtained from Monte Carlo methods show good agreement. Because the asymptotic state has only a small contribution from the $v=1$ broad states, the deviation in the lowest eigenvalue from Monte Carlo methods does not strongly influence the block S matrix. This is shown in Fig. 3, which gives the exact S matrix, the reference block S matrix, and the Monte Carlo block S matrix. Again one observes rapid convergence of the reference block S matrix as a function of τ_{focus} . For $\tau_{\text{focus}}=0.5\text{ fm}$, the relative error between the exact S matrix and the block S matrix is less than 3%. This is remarkable, in view of the small dimension N of the block Hamiltonian and strong coupling parameter λ . From this we conclude in this model that the idea of the block S matrix works. The Monte Carlo data have larger errors, but follow the trend of the reference block S matrix. This can be seen clearly from Fig. 4, where we have plotted the same results as a function of the coupling parameter λ .

Because the eventual application of the method in a many-body system requires the evaluation of the block Hamiltonian by Monte Carlo methods, the question of how statistical errors from the block Hamiltonian propagate to the block S matrix is crucial. We have studied this by a simulation, introducing a “noisy” block Hamiltonian

$$H^{\text{block}} \rightarrow H^{\text{block}}(1 + \epsilon x), \quad (4.8)$$

where ϵ is a real-error parameter and x is a Gaussian stochastic variable ($\langle x \rangle = 0$, $\langle x^2 \rangle = 1$). The results are

shown in Fig. 5. This corresponds to the coupling constant λ from the Yamaguchi model. Concerning the error propagation from the block Hamiltonian to the block S matrix, two observations can be made. (i) In the region of small ϵ (<0.05), there is a linear relation between the error of the block Hamiltonian and the block S matrix. (ii) In the region of large ϵ (<0.2), the error of the block S matrix shows some saturation. This is due to the built-in unitarity of the block time evolution and the block S matrix, which puts an upper bound on the block S -matrix elements.

However, looking at Figs. 3–5, with respect to unitarity, one observes $\text{Re}^2(S) + \text{Im}^2(S) < 1$. This is due to the fact that we do not scatter an asymptotic state of sharp energy, but rather a wave packet covering a finite range of energies.

V. CONCLUSIONS

We have proposed and tested a new formalism for the calculation of the scattering matrix which should be applicable for a wide variety of scattering problems. The method consists of reducing the number of degrees of freedom of the Hamiltonian, in order to describe scattering in a finite-energy interval. The matrix elements of the new block Hamiltonian are computed using a momentum lattice and the Monte Carlo projection method. This Hamiltonian is diagonalized algebraically, which yields the corresponding block S matrix. We have investigated the role of errors associated with the matrix elements of

the full and the asymptotic Hamiltonians on the scattering matrix, and have found that acceptable results can be obtained with error levels of 10% or less (the typical errors in the Monte Carlo method). We are now in the process of applying this method to compact quantum electrodynamics on the lattice in order to test its performance in gauge theories.²⁹

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