Time-dependent optical potential for the Schrödinger solution in a truncated subspace

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A time-dependent imaginary optical potential is used to approximate the Schrödinger time evolution in a necessarily truncated subspace. The flux of probability into the neglected space, for which the ordinary unitary subspace Schrödinger solution does not account, can generally be well reproduced by an optical potential that is diagonal in energy and linear in time. This is demonstrated in a number of examples including the Lipkin model, Gaussian Hamiltonians, and a schematic heavy-ion collision model.

I. INTRODUCTION

The widespread use of the time-dependent Hartree-Fock description of heavy-ion collisions (see, e.g., Refs. 1–3) has motivated us to study alternative approximate solutions of the ordinary time-dependent Schrödinger equation for a complex system. Any such attempt is necessarily faced with the problem of truncating the total Hilbert space of the system to a subspace of sufficiently small dimension to make a numerical solution feasible. However, the straightforward solution of the truncated Schrödinger equation in the selected subspace is unphysical because the solution will be unitary with respect to the subspace, and does not allow for any flux of probability, mass, charge, or energy between the limited subspace and the rest of the Hilbert space.[4–6]

A similar deficiency occurs in stationary scattering theory with the customary restriction to a limited number of final channels. The flux into the neglected channels is usually accounted for by an appropriate additional imaginary potential (e.g., Ref. 7). It is therefore tempting to study if the undesirable effect of truncating a time-dependent calculation to a limited subspace can be remedied in a similar fashion by the use of a time-dependent imaginary potential.

The concept of a time-dependent optical potential has been discussed earlier in the literature (e.g., Ref. 8). In this paper we propose a simple parametrization of such a potential and apply it to a number of test cases. This functional form of the potential seems to be sufficiently general to account rather accurately for the flux into the neglected space in a variety of time-evolution cases, although a universal applicability (similar to the Woods-Saxon form of the stationary optical model) cannot be claimed on the basis of the cases studied.

We discuss in Sec. II the properties that are desirable for an optical potential in a time-dependent calculation, and derive an appropriate parametrization (Secs. III and IV). The accuracy of the optical-model solution is studied in a number of examples (Secs. V and VI) in comparison with the exact Schrödinger solution. Since the exact solution is not known in practical cases, an appropriate dissipative approximation to the exact solution must be used for the initial time behavior of the system (Sec. VII). The conclusions for the use of a time-dependent optical potential are summarized in Sec. VIII.

II. TIME-DEPENDENT OPTICAL MODEL

The time evolution of a system with given Hamiltonian H is, in principle, determined by the solution $|\Psi(t)\rangle$ of the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle = H|\Psi(t)\rangle \ , \tag{1}$$

for the initial state $|\Psi(0)\rangle$. In practice, however, the Schrödinger equation (1) will have to be solved in some restricted basis. If P denotes the projection onto the corresponding subspace, the truncation of the Schrödinger equation amounts to solving the time-evolution problem for PHP rather than for the original H,

$$i\hbar\frac{\partial}{\partial t}|\Phi_P(t)\rangle = PHP|\Phi_P(t)\rangle \ , \tag{2}$$

with solutions $|\Phi_P(t)\rangle$ that are contained in the subspace for all times. Therefore (even if the initial state $|\Psi(0)\rangle = |\Phi_P(0)\rangle$ is in the subspace), the solution $|\Phi_P(t)\rangle$ of Eq. (2) will generally differ from the projection $P|\Psi(t)\rangle$ of the exact Schrödinger solution $|\Psi(t)\rangle$ onto the subspace

$$|\Phi_P(t)\rangle \neq P|\Psi(t)\rangle \ , \tag{3}$$

simply because the subspace solution $|\Phi_P(t)\rangle$ does not allow for any flux of probability out of the selected subspace into the neglected part of the Hilbert space (and possibly back). It is the initial flux out of the subspace that the optical potential is expected to account for.

The problem then consists in finding within the subspace an appropriate imaginary matrix iW, the time-dependent optical potential, such that the solution $|\Phi_{\rm opt}(t)\rangle$ of the modified subspace equation

$$i\hbar\frac{\partial}{\partial t}\,|\,\Phi_{\rm opt}(t)\rangle=[PHP+iW(t)]\,|\,\Phi_{\rm opt}(t)\rangle \tag{4}$$

fits the projection of the exact solution $|\,\Psi(t)\rangle$ as closely as possible,

$$|\,\Phi_{\rm opt}(t)\rangle\approx P\,|\,\Psi(t)\rangle\ . \tag{5}$$

For this purpose the optical potential $iW(t)$ has to be parametrized by a sufficiently general (though practical) functional form, the parameters of which will then have to be determined in each individual case.

III. PARAMETRIZATION OF THE OPTICAL POTENTIAL

The subspace Schrödinger equation (2) can easily be solved, in principle, in the energy representation , i.e., the basis $|\,E_p\rangle$ that diagonalizes the subspace part PHP of the Hamiltonian matrix H (but not necessarily the full H)

$$PHP\,|\,E_p\rangle=E_p\,|\,E_p\rangle,\quad |\,E_p>\in P\text{ space}\ . \tag{6}$$

In this representation the most general functional form of the matrix $W(t)$ is given by

$$\langle E_p\,|\,iW(t)\,|\,E_{p'}\rangle=-i\hbar\sum_{\nu=0}^{N}|\,\alpha_\nu(E_p,E_{p'})\,|\,t^\nu/\nu! \tag{7}$$

with energy-dependent fit parameters $\alpha_\nu(E_p,E_{p'})$, and a sufficiently large order N of the power series. Since for vanishing $W(t)$ the amplitudes of the optical equation (4) are decoupled in the $|\,E_p\rangle$ representation, it is desirable to maintain this property in a suitable parametrization of $W(t)$, i.e., $W(t)$ should be diagonal in the energy representation of the subspace,

$$\alpha_\nu(E_p,E_{p'})=\alpha_\nu(E_p)\delta(E_p,E_{p'})\ . \tag{8}$$

Otherwise the required fits of the parameters α_ν could not be performed separately for each probability amplitude, and the fit procedure would not be practical for large spaces.

The optical solution that corresponds to the parametrization (8) of $W(t)$ is then given explicitly by

$$\langle E_p\,|\,\Phi_{\rm opt}(t)\rangle=\langle E_p\,|\,\Phi_{\rm opt}(t=0)\rangle\exp(-iE_pt/\hbar)\exp\left[-\sum_{\nu=1}^{N+1}|\,\alpha_{\nu-1}(E_p)\,|\,t^\nu/\nu!\right] \tag{9}$$

as can easily be verified by inserting the solution (9) into Eq. (4) with the optical potential given by (7) and (8). Equation (9) shows that this functional form of $W(t)$ leads to an exponential decay of each probability amplitude, whereas the complex phases $E_pt/\hbar$ remain unchanged.

IV. LINEAR APPROXIMATION

The simplest possible functional form of the time-dependent optical potential (9) is the linear case ($N=1$), i.e.,

$$\langle E_p\,|\,iW(t)\,|\,E_{p'}\rangle=-i\hbar\delta(E_p,E_{p'})[\alpha_0(E_p)+\alpha_1(E_p)t] \tag{10}$$

with two parameters α_0, $\alpha_1\geq 0$ for each energy eigenvalue E_p in the selected subspace. It turns out (cf. Sec. V) that this approximation is already sufficiently accurate, and higher-order terms do not improve the results obtained with the linear optical potential (10).

Moreover, a trivial fit of the optical solution (9) to only two points in time, t_1 and t_2, is generally rather accurate, as will be shown below. The parameter values α_0 and α_1 of Eq. (10) are then completely determined by the positive solutions (else $\alpha=0$) of the two linear equations

$$\alpha_0t_1+\tfrac{1}{2}\alpha_1t_1^2=-\ln A(t_1)\ , \tag{11a}$$

$$\alpha_0t_2+\tfrac{1}{2}\alpha_1t_2^2=-\ln A(t_2)\ , \tag{11b}$$

for each energy E_p where $A(t)$ denotes the relative amplitude

$$A(t)=\frac{|\,\langle E_p\,|\,\Psi(t)\rangle\,|}{|\,\langle E_p\,|\,\Psi(0)\rangle\,|}\ . \tag{11c}$$

In the examples discussed below, the solution (11) has been used as an initial guess for a least-squares fit. In all cases plotted in Secs. V and VI it turned out that the final result of the fit was almost identical to the approximation (11).

V. EXAMPLES

We have studied the optical-potential approximation for three different types of Hamiltonian matrices, the Lipkin model, Gaussian matrix parametrizations, and a schematic heavy-ion Hamiltonian that is discussed in Sec. VI. In each case we have computed the exact time-dependent Schrödinger solution $\Psi(t)$ in a finite-model Hilbert space, and compared the projection of $\Psi(t)$ onto a much smaller subspace with the result of solving the optical-model equation (4) within the subspace.

The Gaussian Hamiltonian matrix parametrization

$$H_{mn}=-V_0\exp\left[-\frac{\beta}{2}\frac{m+n}{2}-\frac{m-n}{2\sigma^2}\right] \tag{12}$$

has an exponential diagonal level density and a Gaussian falloff for the off-diagonal matrix elements. The parametrization comprises constant matrices ($\beta=0,\sigma\to\infty$), diagonal matrices ($\sigma\to 0$), C numbers ($\beta=0,\sigma\to 0$), and intermediate cases.

Figure 1 shows the rapid convergence of the power series (7) for the time dependence of the optical potential (9). Here the exact solution is for a 50×50 matrix H_{mn} projected onto the subspace associated with the first 5×5

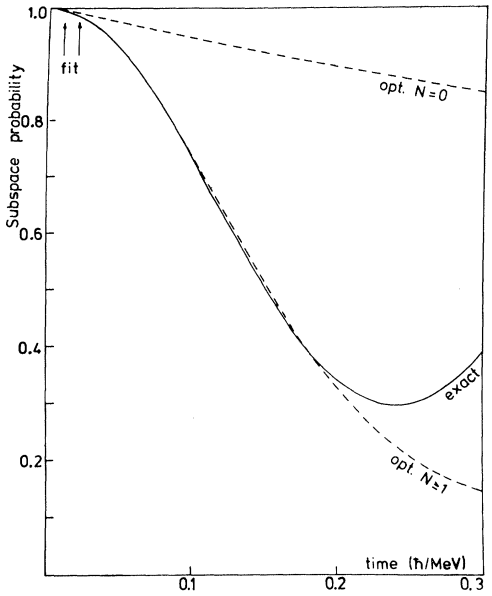

FIG. 1. Subspace probability as a function of time. The solid line is the exact solution for a 50×50 Gaussian Hamiltonian matrix projected onto a 5×5 subspace. The dashed lines show the rapid convergence of the optical-model approximations with imaginary potentials of order N in time. Here the parameter values are $\beta=0.1$, $\sigma=20$, and $V_0=1$ MeV. The time scale is in units of $\hbar/V_0$.

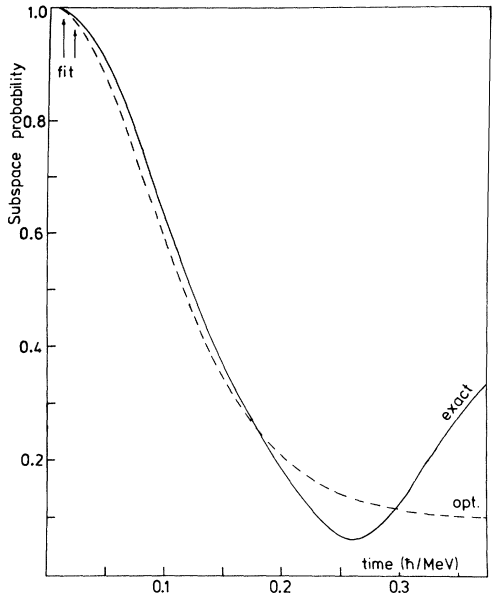

FIG. 2. Subspace probability for the ten-particle Lipkin model ($\epsilon=1$, $V=1$) projected onto a six-dimensional subspace in comparison to the linear optical-model result.

components of H_{mn}. The initial state $\Psi_P(t=0)$ has a binomial distribution with probability 0.5 (i.e., peaked at the third of five basis states). The optical potential, Eqs. (7) and (9), has been fitted to the exact solution in the time interval $t\leq0.02\hbar$/MeV which corresponds to a decrease in probability from 100% to 99% in the subspace. The figure shows that a constant optical potential [$N=0$ in Eq. (7)] does not fit at all, whereas the linear ($N=1$) and all higher powers in time coincide (within 10^{-4}). The $N\geq2$ approximations also coincide with the simplified linear two-point fit with parameter values determined from Eq. (11) for $t_1=0.01\hbar$/MeV and $t_2=0.02\hbar$/MeV corresponding to a loss of 0.3% and 1% of the initial probability in the subspace. Although the further decrease in probability is quite large, the optical approximation remains close to the exact solution until the flux of probability back into the selected subspace starts to dominate. The latter effect is, of course, outside the scope of an optical model. Thus in Fig. 1 the linear optical-potential model remains rather accurate over a period of time that extrapolates the initial fit interval by a factor of 10, and for a total loss in probability that is 70 times larger than what the optical approximation has been fitted to. We have studied many other cases of Gaussian matrices with various dimensions and widths as well as different initial distributions, and in every case the optical model works equally well.

As a further example we use the Lipkin model,[9–12] a popular test case for time-dependent approximations. The Hamiltonian is that of N fermions on two N-fold degenerate levels $\sigma=\pm1, p=1,\ldots,N$,

$$H=\tfrac{1}{2}\epsilon\sum_{p,\sigma}\sigma a^{\dagger}_{p\sigma}a_{p\sigma}+\tfrac{1}{2}V\sum_{p,p',\sigma}a^{\dagger}_{p\sigma}a^{\dagger}_{p'\sigma}a_{p-\sigma}a_{p'-\sigma}. \quad (13)$$

The exact solution can be obtained by writing the creation and annihilation operators of the corresponding single-particle states $|p,\sigma\rangle$ in terms of operators J_+,J_-, and J_z with the ordinary angular momentum commutation properties (for details see, e.g., Refs. 5, 11, and 13).

The example of Fig. 2 shows the ten-particle Lipkin model (i.e., dimension 11) truncated to the six-dimensional subspace spanned by the states $|J,-J\rangle$, $|J,-J+1\rangle,\ldots,|J,0\rangle$ of the standard basis, and a binomial initial distribution with probability 0.5 (i.e., peaked at the third and fourth of the six basis states). The plotted curve shows the subspace probability for the linear optical solution (10) with the parameter values (11) for $t=0.01\hbar$/MeV and $0.02\hbar$/MeV (i.e., 0.4% and 2% decrease in probability, respectively). The degree of approximation achieved in this case is almost as good as in the Gaussian matrix examples in spite of the peculiar sparse structure of the Lipkin Hamiltonian matrix. Again the optical model fails once a flux of probability from the neglected space back into the subspace sets in.

We note that in some cases the overall subspace probability is almost conserved over a certain interval of time while the probability distribution shifts towards initially unoccupied basis states within the subspace before a noticeable flux of probability out of the subspace occurs. It is then advantageous to choose the fit interval for the optical potential accordingly.

VI. SCHEMATIC HEAVY-ION MODEL

Heavy-ion collisions have been the main incentive for the use of time-dependent methods in nuclear physics.

This has motivated us to study the optical-potential approximation in the case of a (very schematic) heavy-ion model Hamiltonian. It consists of a single-particle Hamiltonian for each ion, $H_{sp}^{(1)}$ and $H_{sp}^{(2)}$, and an additional two-body interaction $V(1,2)$ acting between the ions

$$H=H_{sp}^{(1)}+H_{sp}^{(2)}+V(1,2)\ . \tag{14}$$

Rather than making a choice for the geometry and potential shape of the ions, and deriving the matrix elements of $H_{sp}^{(1)}$ and $H_{sp}^{(2)}$ from that, we assume, for simplicity, that the single-particle energies of each ion follow a pattern similar to level density formulas, i.e.,

$$H_{sp}^{(1)}\,|\,i\rangle=V_1\exp(-i/a_1)\,|\,i\rangle \tag{15a}$$

and

$$H_{sp}^{(2)}\,|\,j\rangle=V_2\exp(-j/a_2)\,|\,j\rangle\ , \tag{15b}$$

where $|\,i\rangle$ and $|\,j\rangle$ denote the appropriate basis for each ion, and V_1, V_2, a_1, and a_2 are parameters.

The two-body interaction matrix is defined in the product basis $|\,i\rangle\,|\,j\rangle$ as

$$\langle ij\,|\,V\,|\,kl\rangle=V_0\exp[-(\,|\,ij-kl\,|\,/a_0^2)] \tag{16}$$

with the parameters V_0 and a_0. This functional form is motivated by the requirement that the interaction should be large between two-ion states $|\,i\rangle\,|\,j\rangle$ and $|\,k\rangle\,|\,l\rangle$ that are either particularly simple (e.g., $|\,i\rangle$, $|\,j\rangle$, $|\,k\rangle$, and $|\,l\rangle$ low excited) or both very complicated (i.e., $|\,i\rangle$, $|\,j\rangle$, $|\,k\rangle$, and $|\,l\rangle$ highly excited), and small for matrix elements between states of different structure.

Figure 3 shows the time dependence of the subspace probability for the exact solution, and for the optical approximation for the case of six levels in each ion, i.e., a full space of dimension 36, truncated to a subspace of dimension 16 which contains the first four levels of each ion. The initial state is taken to be statistically distributed in the subspace with amplitudes

$$c_{mn}=\frac{\{\exp[-E_{12}(m,n)/kT]\}^{1/2}}{\left[\sum_{\mu,\nu\in P}\exp[-E_{12}(\mu,\nu)/kT]\right]^{1/2}}\ , \tag{17}$$

where $E_{12}(m,n)$ denotes the energy of the noninteracting two-ion system in the product state $|\,m\rangle\,|\,n\rangle$ of the P space. During the time interval plotted the probability in the subspace decreases from initially 100% to about 30% before a flux of probability back into the selected subspace occurs. The optical approximation is fitted for $t=0.05\hbar$/MeV and $0.1\hbar$/MeV when about 3% of the initial subspace probability is lost. Here again the optical-model extrapolation follows the exact solution until the flux of probability back into the selected subspace sets in. The extrapolation remains accurate over 6 times the period of time of the original fit, and for more than 20 times the loss of probability within the original fit interval. Similar results have been obtained for other temperatures kT in the initial distribution.

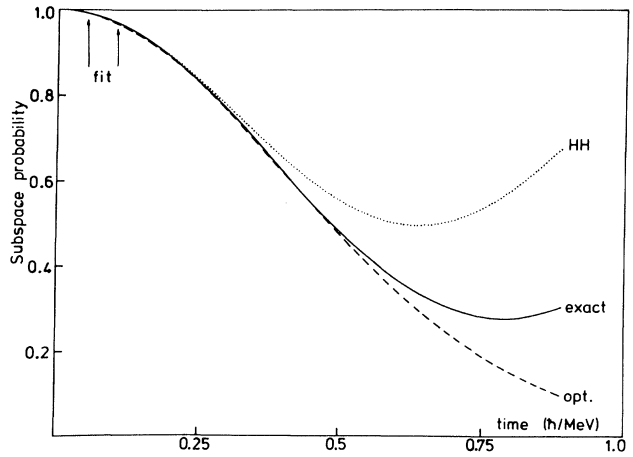

FIG. 3. Time dependence of the exact subspace probability of the schematic heavy-ion model, and the optical-potential approximation. The parameter values are $V_1=V_2=-2$ MeV, $V_0=-0.2$ MeV, $a_1=a_2=2$, $a_0=4$, and $kT=0.5$ MeV. The time interval for the optical-potential fit is indicated in the figure. The full space has dimension 36, the subspace is truncated to dimension 16. For comparison, the H^2 subspace time-evolution approximation of Sec. VII is also given (labeled *HH*).

We note that the schematic heavy-ion model result of Fig. 3 can also be fitted by assuming an explicit energy dependence of the parameters α_0 and α_1 of the form

$$\alpha_0(E)=\sum_{n=0}^{1}a_nE^n\ , \tag{18a}$$

$$\alpha_1(E)=\sum_{n=0}^{1}b_nE^n\ . \tag{18b}$$

In this way an almost identical fit can be achieved by using only the four parameters a_n and b_n for all sixteen amplitudes in the energy basis rather than two independent parameters α_0 and α_1 for each individual amplitude.

In a semiclassical treatment of time-dependent collisions the Hamiltonian is assumed to depend on the center-of-mass distance between the ions rather than on the individual particle coordinates only. In this case the Hamiltonian is explicitly time dependent, and the time-evolution calculation has to be performed in a finite number of short time steps (as in the time-dependent Hartree-Fock approximation). This requires, of course, for each consecutive time step a new set of parameters of the imaginary potential (7). The optical fits can easily be performed by using the trivial two-point formula (11), and should allow one to considerably increase the step size of the time-dependent calculation (cf. Sec. VII), and thus lead to a corresponding reduction in computer time.

VII. INITIAL TIME-EVOLUTION APPROXIMATION

In practical cases the exact solution will not be known. Therefore an initial approximation to the Schrödinger time-evolution in the subspace is required (e.g., a perturbation expansion[14]) from which the optical-potential solution can then be obtained. The fit serves then as an extrapolation over time intervals that are possibly much larger than the convergence interval of the original subspace approximation.

Such a short-term solution for the subspace time evolution has been discussed in Refs. 4–6. It has been demonstrated that for short time intervals a remarkably accurate approximation to the exact Schrödinger time evolution in the subspace can be obtained by solving the second-order time-differential equation in the subspace

$$-\hbar^2\frac{\partial^2}{\partial t^2}\,|\,\Psi_{\rm appr}(t)\rangle = PH^2P\,|\,\Psi_{\rm appr}(t)\rangle \tag{19}$$

with the initial condition

$$i\hbar\frac{\partial}{\partial t}\,|\,\Psi_{\rm appr}(t=0)\rangle = PHP\,|\,\Psi_{\rm appr}(t=0)\rangle \tag{20}$$

and a given initial state $|\,\Psi_{\rm appr}(t=0)\rangle$. The solution is equivalent to projecting each term of the power series for the exact time evolution $\exp(-iHt/\hbar)\,|\,\Psi(t)\rangle$ onto the subspace, and truncating the result to second order in time. Thus the exact time evolution can always be approximated to arbitrary precision by the solution of Eq. (19) in the subspace, if the time interval is chosen sufficiently small. This short-term subspace solution is also shown in Fig. 3. It is evident from the plot that this solution, when augmented by an optical-potential fit becomes applicable for a much larger interval of time than the second-order subspace approximation alone.

VIII. CONCLUSIONS

We conclude from the results of this study that the time evolution of a system in a necessarily truncated subspace can be described rather accurately by adding an imaginary time-dependent potential to the truncated Hamiltonian in the Schrödinger equation for the subspace. The imaginary optical potential can be chosen diagonal in the energy representation and linear in time with parameter values as given by Eq. (11). Such an optical potential can account very well for the flux of probability into the neglected space. In a perturbation approach for short time intervals, e.g., that of Eq. (19), the use of such an optical potential as an extrapolation can substantially improve the range of convergence. As one would expect, the optical model fails as soon as the flux of probability from the excluded space into the selected subspace starts to dominate.

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