A model study of scattering of a composite object

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Abstract. A sound simultaneous description of the structure and reaction features in a many-body nuclear system is at the very heart of understanding the short-lived nucleonic matter in the laboratory and in the universe. In this brief presentation we discuss some aspects and techniques related to reactions involving composite objects that explicitly make a connection between the structure and reaction properties of nuclei. Here we concentrate on a specific pedagogical example that highlights difficulties and clarifies the path towards solutions.

1. Introduction

The so-called configuration interaction approach, together with its specific application to the nuclear structure known as the Nuclear Shell Model, forms a well-established technique for treating stationary many-body problems. This approach can become challenging when applied to modestly sized systems, due to the large dimension of the corresponding Hilbert space. Nevertheless, numerous successful techniques, for example Lanczos diagonalization, Monte Carlo methods, coupled-cluster methods, and importance truncation, to name a few, exist both for dealing with such Hilbert spaces numerically and for truncating the space efficiently [1, 2]. Another useful approach is to renormalize interactions so as to facilitate convergence and reduce the Hilbert space dimension.

The success of configuration interaction techniques for stationary many-body problems has encouraged extension of its applications to problems of reactions, which are inherently non-stationary. For example, the Gamow formulation [3] and alternative Continuum Shell Model approaches [4, 5, 6] have been widely applied. It is, however, unclear whether the stationary state methods mentioned above would be applicable to or be as effective for the non-stationary problems. The goal of this presentation is to address this question using a particular simple example.

2. The Model

In order to illustrate the issue, we present here a model shown in Fig. 1. Let us consider a one-dimensional problem where the projectile is a composite object with unit mass made up of two particles which have masses $\mu_1$ and $\mu_2$, so that $\mu_1 + \mu_2 = 1$. In addition to that we select units so that $\hbar^2/2 = 1$. The particles are bound by a potential $v(x_1 - x_2)$ where the particles’ coordinates are $x_1$ and $x_2$. This composite system interacts with an external potential $V(x_1, x_2)$. Let us assume that only the second particle interacts with the potential, that is, $V(x_1, x_2) \rightarrow V(x_2)$, and that the potential is represented by an infinite wall: $V(x_2) = \infty$ for $0 < x_2$, and $V(x_2) = 0$ otherwise. Having defined the center-of-mass and relative coordinates,
Figure 1. Schematic picture of scattering

\[ X = \mu_1 x_1 + \mu_2 x_2 \] and \[ x = x_1 - x_2 \], respectively, we can write the Hamiltonian for the system as

\[ H = -\frac{\partial^2}{\partial X^2} + V(x_1, x_2) + h, \quad \text{where} \quad h = -\frac{1}{\mu} \frac{\partial^2}{\partial x^2} + v(x). \] (1)

Here \( h \) is the intrinsic Hamiltonian of the composite system, and \( \mu = \mu_1 \mu_2 \) is the reduced mass thereof. We view the intrinsic Hamiltonian \( h \) as being analogous to the Shell Model Hamiltonian with some eigenstates \( \psi_n(x) = \langle x|n \rangle \) that correspond to intrinsic energies \( \epsilon_n \):

\[ h\psi_n(x) = \epsilon_n \psi_n(x), \quad n = 0, 1, 2, \ldots \]

We assume (see Fig. 1) that the incident beam is traveling from the left and contains the projectiles in an intrinsic state (channel) \( n \). This boundary condition, together with the Schrödinger equation with the Hamiltonian (1), determines the wave function

\[ \Phi(X, x) = \frac{e^{iK_nX}}{\sqrt{|K_n|}} \psi_n(x) + \sum_{m=0}^{\infty} \frac{R_{mn}}{\sqrt{|K_m|}} e^{-iK_mX} \psi_m(x), \] (2)

where

\[ K_n(E) = \sqrt{(E - \epsilon_n)} \] (3)

is the center-of-mass momentum of the nucleus with energy \( E \), while in the \( n^{th} \) intrinsic state. The second boundary condition

\[ \Phi(X, x) = 0 \text{ at } x_2 = 0, \] (4)

due to the impenetrable wall, is to be used for determining the set of coefficients \( R_{mn} \).

If the energy \( E \geq \epsilon_n \) for a certain channel \( n \), then the channel is open and the corresponding momentum \( K_n \) is real. For \( E < \epsilon_n \) the channel \( n \) is closed and \( K_n \) is purely imaginary. For both cases the principal value of the square root in Eq. (3) is to be used for finding \( K_n \).

The reflection amplitudes \( R_{mn} \) are normalized in such a way that \( |R_{mn}|^2 \) for an open channel \( m \) represents the probability for the incoming beam in channel \( n \) to reflect in channel \( m \). The conservation of particle-number in all the open channels implies \( \sum_{m \in \text{open}} |R_{mn}|^2 = 1 \). Thus, the reflection amplitudes for the open channels form the scattering matrix for the problem. In addition, \( R_{nm} = R_{mn} \) follows from time-reversal invariance.

3. The Projection Method

The location \( x_2 = 0 \) sets the center-of-mass coordinate to \( X = \mu_1 x \) where we denote \( x \equiv x_1 \), and thus the boundary condition (4) effectively contains the intrinsic coordinate \( x \) only:
\( \Phi(\mu_1 x, x) = 0. \) In our Projection Method, this equation is then projected onto an intrinsic basis state, which leads to the following linear equation

\[
\sum_m D_{n'm} \left[ -i\mu_1 (K_n + K_m) \right] \sqrt{|K_m|} = -\delta_{n'm} \sqrt{|K_n|}, \tag{5}
\]

where the matrix \( D \) is defined as

\[
D_{mn}(\kappa) = \langle m\mid \exp(\kappa x)\mid n \rangle. \tag{6}
\]

Equation (5) represents a Shell Model like approach to the problem; it is a linear problem for the \( S \)-matrix. Inversion of the \( D \)-matrix defined above, which is a complex function of energy, is equivalent to finding the propagator for the intrinsic Hilbert space spanned by the intrinsic basis states \( |n\rangle \). Formally, the approach is exact and should lead to an exact solution. We would like to draw a parallel between this method and the Continuum Shell Model approach [4, 5, 6]. The latter involves projections in a similar manner that allows the reaction variables to be removed, leading to a problem of matrix inversion - where the propagator contains some complex and energy-dependent effective Hamiltonian.

In order to highlight the challenges and the hidden problems that could emerge within this approach, we consider some specific examples that are simple yet illustrative. If the two particles forming a composite nucleus are bound by, for example, a harmonic oscillator confinement or an infinite well confinement, the \( D \)-matrix is then found to be analytic. One can truncate the channel space at some large number \( N \) and then solve Eq. (5) numerically.

Numerical instability is the first immediate problem that emerges in this treatment. The matrix element \( D_{mn}(\kappa) \) for a real \( \kappa \) (due to an imaginary momentum, associated with a virtual channel) is real and exponentially large. Thus, the matrix inversion in Eq. (5) is numerically difficult. This problem was dealt with in Ref. [7] through a linear transformation from the intrinsic basis set to a set of configuration localized states. In our approach we implement a singular value decomposition technique. Technical difficulties arise also from the fact that \( R_{mn} \) diverges for increasingly remote virtual channels. For the square well, where \( R_n \sim \exp \left[ \frac{\pi n}{2} \sqrt{\mu_1 \mu_2} \right] \) approximately (for an incident beam with particles in the ground state), the dependence of these coefficients on the outgoing channel number \( n \) is illustrated in the left panel of Fig. 2.

Thus, the matrix equation (5) formulated in a truncated channel space can in principle be solved, but only using high-precision numerical techniques due to this divergence. This can be understood also from the boundary condition (4) which is to be satisfied at any value of \( x \). If \( x \) is small enough for the intrinsic wave functions \( \psi_n(x) \) to have non-zero values for large \( n \)'s, then the terms in the sum (2) diverge with \( n \). One must be capable of treating large and small terms simultaneously, while dealing with a finite sum of this sort that is set equal to zero.

While the numerical problem just mentioned can be resolved, the approach is still ill-formulated in a strict mathematical sense. Seemingly convergent results can be found [7, 10] for a certain subset of ‘good’ parameters. However, in general, as \( N \) increases, the results start oscillating. We demonstrate this in the right panel of Fig. 2 where a harmonic oscillator confinement has been used as the example for \( v(x) \). It was observed in [11] that there is no numerical convergence with increasing \( N \). As can be seen from this figure, satisfactory answers can be easily found for the cases where the mass of the non-interacting particle is small, while this approach fails in more critical situations where the non-interacting particle is heavy and therefore penetrates the wall to a large extent.

4. Solution with the Variable Phase Method (VPM) and Convergence

Despite the complications within the approach discussed above, the same scattering problem can be solved either with time-dependent methods or with techniques that solve the problem in
Figure 2. **Left panel:** This refers to a system bound by an infinite square well confinement, with $\mu_1 = \mu_2$ and energy $E = 1.1\epsilon_0$, where $\epsilon_{n-1} = n^2$. Absolute values of its amplitudes of reflection in the virtual channels $n$, as calculated with the Projection Method with different truncations $N$, are plotted as different functions of $n$. These curves closely follow the straight line $\exp(\pi n/2)$ initially, and then deviate due to truncation. **Right panel:** This figure refers to a system of two particles bound by a harmonic oscillator confinement which collides with an infinite wall. The energy is exactly half-way between those of the ground state and of the first excited state, so that only the ground state channel is open. The single phase shift in this case is defined through $e^{2i\delta} = -R_{00}$, and is plotted as a function of $N$. The curves are oscillatory, and the phase-shift values become extremely unstable for large $\mu_1$'s. The curves represent phase-shifts for different mass ratios $\mu_1/\mu_2 = 1, 2, 3, 5, 10$, as labeled. The convergent values, as obtained with a different method (VPM [8, 9]), are shown by the horizontal grid lines with tic-marks on the right. Even for small $\mu_1$'s, where the value seems to be convergent initially, the curves behave erratically at considerably larger values of $N$ (see inset for $\mu_1/\mu_2 = 3$, extended up to $N = 160$).

In most problems that do not allow for an analytic solution, the exact solution to any level of precision can be reached with some convergence technique. It is crucial to understand the convergence and be able to manipulate modern computational techniques to achieve it. It was found in Ref. [14] and in several other studies that followed works in Refs. [15, 16] that the eigenvalues of the most general Shell Model Hamiltonians converge exponentially with truncation. This exponential convergence can be proved analytically by reducing the corresponding matrix to a tridiagonal matrix. An exception to the exponential convergence occurs when, at high energies, the asymptotic value of the diagonal element is exactly twice that of the adjacent off-diagonal elements [14]. A power-law convergence is expected in this particular case. Figure 4 demonstrates convergence of the phase shift, obtained through the VPM, to its

the coordinate space. Figure 3 shows the results for the infinite square well obtained with such a method, namely, the Variational Phase Method (VPM) [8, 9]. It displays features that are expected for a multi-channel reaction [10]; for example, it displays cusps at thresholds, which is a consequence of unitarity [12, 13]. In addition to that, there are weak oscillations which become more pronounced (not shown) for more massive non-interacting particles.
asymptotic value \( \delta \) with increasing \( N \). Plotted on a log-log scale, \( \delta - \delta(N) \) is a linear curve, Fig. 4(b), implying a power-law. The convergence is of \( 1/N \)-type for the square well confinement and of \( 1/\sqrt{N} \)-type for an oscillator confinement. This means that the difference \( \delta - \delta(N) \) is inversely proportional to the absolute value of the corresponding virtual momentum \( |K_N| \).

In reactions, especially at high energies, a pivotal role is played by the kinetic energy operator which, when discretized in the coordinate space, leads to an exact 2:1 ratio of diagonal to non-diagonal components, showing a slow power-law convergence instead of an exponential convergence.

5. Summary
For this short conference contribution we concentrated on a particular example of the reaction problem involving a composite object. Our primary goal was to follow the steps in projecting the reaction problem onto an intrinsic Shell Model space. The procedure and the resulting matrix inversion problem in the Shell Model Hilbert space are similar to those in different versions of the Shell Model approach modified to treat the continuum. This example helps the understanding of the nature of the effective intrinsic dynamics of a system undergoing a reaction process. However, most importantly, it allows one to see some of the essential differences between the two Shell Model matrix formulations (the usual Shell Model formulation and the one modified to treat continuum). This example also identifies some possible pitfalls which we can summarize as follows: Reaction physics involves quantities of exponential scales and therefore could yield erroneous solutions if not obtained through numerical tools that are capable of handling those scales. The Projection Method, while formally correct, may not be able to provide a path converging to a solution, requiring explicit coordinate- or time-dependent methods to be used. While the Shell Model Hamiltonians generally have exponential convergence as a function of truncation, convergence in reaction problems is somewhat slower, which is related to the dominance of the kinetic energy operator in the Hamiltonian.

This presentation describes, in details, some aspects of a much broader subject of scattering of composite objects, described in a large body of work [17] which aims at unification of structure and reaction in many-body physics. The Variable Phase Method (VPM) has known convergence properties, and is therefore a powerful tool for studying scattering, breakup, and tunneling.
Figure 4. Panel (a): Phase shifts (in degrees) calculated through the VPM as functions of truncation $N$. The solid curve refers to a system bound by an infinite well confinement, and the dotted curve, to an oscillator confinement. The energy in both cases lies exactly half way between the ground state energy and that of the first excited state of the confining potential, so that only the ground state channel is open. The single phase shift $\delta$ in this case is defined through $e^{2i\delta} = -R_{00}$. The phase shifts $\delta(N)$, as calculated with $N$ channels included, in the two cases converge to their asymptotic values, $\delta = -23.04^\circ$ and $\delta = -22.98^\circ$, respectively. Note that the asymptotic value for the oscillator matches with the one shown in Fig. 2(b), as obtained through the Projection Method. Panel (b): For both confinements, $\delta - \delta(N)$ as functions of $N$ are straight lines on a log-log scale, implying power-law convergence.

with realistic systems, and obtaining satisfactory/convergent solutions. Lessons learnt from this example have been utilized in other tools like Time-dependent Continuum Shell Model [18].

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