Description of Resonant States in the Shell Model

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Abstract—A technique for describing scattering states within the nuclear shell model is proposed. This technique is applied to scattering of nucleons by α particles based on ab initio No-Core Shell Model calculations of $^3$He and $^5$Li nuclei with JISP16 $NN$ interaction.

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1. INTRODUCTION

There is noticeable progress in the microscopic description of nuclear reactions, continuum spectra and widths of nuclear resonant states. In particular, we mention the Lorentz Integral Transform method [1, 2] which was mainly utilized within the Hyperspherical Harmonics approach and was generalized [3] for the use in combination with the No-Core Shell Model (NCSM), the Continuum Shell Model [4], the first attempts to study scattering of nucleons by nuclei within the Quantum Monte Carlo approach [5], the Gamow Shell Model including the ab initio No-Core Gamow Shell Model (NCGSM) [6]. The main achievement in modern ab initio theory of nuclear reactions is a description of various reactions with light nuclei within a combination of NCSM with Resonating Group Method (RGM, see reviews [2, 7, 8]).

In this contribution, we formulate a simple method for calculating low-energy phase shifts and for extracting resonant energies $E_r$ and widths $\Gamma$ directly from the shell model eigenstates without additional complexities like introducing additional Berggren basis states as in NCGSM or additional RGM calculations as in the combined NCSM/RGM approach. The method is based on the $J$-matrix formalism in scattering theory [9]. The $J$-matrix approach utilizes a diagonalization of the Hamiltonian in one of two bases: the so-called Laguerre basis that is of a particular interest for atomic physics applications and the oscillator basis that is appropriate for nuclear physics. The version of the $J$-matrix formalism with the oscillator basis is also sometimes referred to as an Algebraic Version of RGM [10] or as a HORSE (Harmonic Oscillator Representation of Scattering Equations) method [11]. We use the latter nomenclature in what follows.

The proposed method is applied to the analysis of resonant states in scattering of nucleons by α particle based on ab initio calculations of $^3$He and $^5$Li nuclei within NCSM [8] with the JISP16 $NN$ interaction [12].

2. HORSE AND SS HORSE FORMALISMS

We start with a short description of the HORSE formalism in the case of scattering in a partial wave with the orbital momentum $\ell$ in a system of two particles with reduced mass $\mu = \frac{m_1m_2}{m_1 + m_2}$ interacting via potential $V$. The relative motion wave function is expanded in infinite series of oscillator functions with the oscillator frequency $\hbar\Omega$ labeled by the principal quantum number $n = 0, 1, 2, \ldots, \infty$ or by the oscillator quanta $N = 2n + \ell$.

The kinetic energy matrix in the oscillator basis is tridiagonal, its non-zero matrix elements $T_{N,N'}$ are increasing linearly with $N$. On the other hand, the potential energy matrix elements $V_{N,N'}$ are decreasing with $N$ and/or $N'$. Therefore a reasonable approximation is to neglect the potential energy matrix elements $V_{N,N'}$ with respect to $T_{N,N}$ if $N$ or $N' > N$. In other words, we split the complete infinite oscillator basis space into two subspaces: the ‘internal’ subspace $P$ spanned by oscillator functions with $N \leq N'$ where the complete Hamiltonian $H = T + V$ is used and ‘external’ subspace $Q$ spanned by oscillator functions with $N > N'$ corresponding to the free

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motion where the Hamiltonian includes only the kinetic energy.

The eigenvectors of the infinite Hamiltonian matrix including only kinetic energy matrix elements in the \(Q\) space and both potential and kinetic energy matrix elements in the \(P\) space can be found if the eigenenergies \(E_\nu\) and eigenvectors \(\langle N|\nu \rangle\) of the Hamiltonian submatrix in the \(P\) space are known. \(E_\nu\) and \(\langle N|\nu \rangle\) fit the set of linear equations

\[
\sum_{n'=0}^{d-1} H_{N,2n'+\nu} \langle 2n' + \nu |\rangle = E_\nu \langle N|\nu \rangle,
\]

where \(d \equiv (N - \ell)/2 + 1\) is the dimensionality of the \(P\) space. All scattering observables at any energy \(E\) can be extracted from the eigenvectors of this infinite Hamiltonian matrix. For example, the scattering phase shifts \(\delta_\ell(E)\) can be calculated as [11]

\[
\tan \delta_\ell(E) = \frac{S_{N,\ell}(E) - G_{N,N}(E)T_{N,N+2}S_{N+2,\ell}(E)}{C_{N,\ell}(E) - G_{N,N}(E)T_{N,N+2}C_{N+2,\ell}(E)},
\]

where

\[
G_{N,N}(E) = \sum_{\nu} \frac{|\langle N|\nu \rangle|^2}{E_\nu - E}.
\]

To overcome these difficulties, we propose a Single-State (SS) HORSE formalism. The conventional wisdom says that a shell model eigenstate \(E_\nu\) defines all the properties of a nearby resonant state. So, let us calculate the phase shift \(\delta_\ell(E_\nu)\) at this energy. From Eqs. (2), (3) we obtain a very simple expression:

\[
\tan \delta_\ell(E_\nu) = -\frac{S_{N+2,\ell}(E_\nu)}{C_{N+2,\ell}(E_\nu)}.
\]

Note, we get rid not only of the need to sum over a huge number of eigenstates as in Eq. (3) but also from the shell model wave function component \(\langle N|\alpha J|\nu \rangle\) defining the desired channel. Hence Eq. (4) can be used for scattering channels of any type. In the case of low-energy scattering when \(E < \frac{1}{8} \hbar \Omega(N + 2 - \ell)^2\), one can use asymptotic expressions for \(S_{N+2,\ell}(E_\nu)\) and \(C_{N+2,\ell}(E_\nu)\) at large \(N\) [13] to obtain

\[
\tan \delta_\ell(E_\nu) = \frac{j_\ell(2\sqrt{E_\nu/s})}{n_\ell(2\sqrt{E_\nu/s})}, \quad s = \frac{\hbar \Omega}{N + 7/2},
\]

where \(j_\ell(x)\) and \(n_\ell(x)\) are spherical Bessel and Neumann functions. Equation (5) exhibits a scaling property of low-energy scattering: the phase shift \(\delta_\ell(E)\) at shell model eigenenergies \(E = E_\nu\) does not depend on the shell model parameters \(\hbar \Omega\) and \(N\) individually but only on their combination \(s\).

The shell model calculations are usually performed for sets of \(N\) and \(\hbar \Omega\) values. Within the SS HORSE formalism, we can calculate the phase shift \(\delta_\ell(E)\) at the respective set of eigenenergies \(E = E_\nu(N, \hbar \Omega)\) covering some energy interval. Next we can extrapolate the phase shift on a larger energy interval using accurate parametrizations of \(\delta_\ell(E)\) at low energies.

3. LOW-ENERGY PHASE SHIFT PARAMETRIZATION

The scattering \(S\)-matrix as a function of momentum \(k\) is known [14] to have the following symmetry property:

\[
S_\nu(k) = S_\nu^{-1}(-k).
\]
Since \( S_r = e^{2i\delta_r} \), the phase shift \( \delta_r(E) \) is an odd function of \( k \) and its expansion in Taylor series of \( \sqrt{E - k^2} \) includes only odd powers of \( \sqrt{E} \):

\[
\delta_r(E) = c\sqrt{E} + d(\sqrt{E})^3 + \ldots \quad (7)
\]

More, since \( \delta_r - k^{2+1} \) in the limit \( k \to 0 \), \( c = 0 \) in the case of \( p \)-wave scattering, \( c = d = 0 \) in the case of \( d \)-wave scattering, etc.

If the \( S \)-matrix has a pole associated with a bound state at the imaginary momentum \( k = i\kappa \) or a pole associated with a low-energy resonance at the complex momentum \( k = \kappa_r + i\gamma_r \), it can be expressed as

\[
S(k) = \Theta(k)S_p(k),
\]

where \( \Theta(k) \) is a smooth function of \( k \) and the pole term \( S_p(k) \) in the case of a bound state \( (p = b) \) or a resonant state \( (p = r) \) is [14]

\[
S_p(k) = \frac{k + ik_b}{k - ik_b}, \quad S_p(k) = (k + \kappa_r)(k - \kappa_r^*) \quad (9)
\]

The respective phase shift

\[
\delta_r(k) = \phi(k) + \delta_p(k),
\]

where the pole contribution \( \delta_p(k) \) takes the form

\[
\delta_p(E) = \pi - \arctan \frac{E}{\sqrt{|E_b|}}
\]

\[
\delta_r(E) = -\arctan \frac{a\sqrt{E}}{E - b^2}.
\]

(11)

Here \( \pi \) in the expression for \( \delta_p \) appears due to the Levinson theorem [14], \( E_b = -\frac{\hbar^2 k_b^2}{2\mu} < 0 \) is the bound state energy while the resonance energy \( E_r \), and its width \( \Gamma \) are

\[
E_r = \frac{\hbar^2}{2\mu} (k_r^2 - \gamma_r^2) = b^2 - a^2/2,
\]

\[
\Gamma = \frac{\hbar^2}{2\mu} k_r \gamma_r = a\sqrt{b^2 - a^2}/4.
\]

(12)

In applications to the non-resonant \( n\alpha \) scattering in the \( \frac{1}{2}^+ \) state, we therefore are using the following parametrization of the phase shift:

\[
\delta_0(E) = \pi - \arctan \frac{E}{\sqrt{|E_b|}} + c\sqrt{E} + d(\sqrt{E})^3.
\]

The bound state pole contribution here is associated with the so-called Pauli-forbidden state. There are resonances in the \( n\alpha \) scattering in the \( \frac{1}{2}^- \) and \( \frac{3}{2}^- \) states; hence we parametrize the phase shifts as

\[
\delta_r(E) = -\arctan \frac{a\sqrt{E}}{E - b^2} - \frac{a}{b^2} \sqrt{E} + d(\sqrt{E})^3.
\]

(14)

This form guarantees that \( \delta_r - k^3 \) in the limit of \( E \to 0 \) [see Eq. (7) and discussion below it].

## 4. APPLICATION TO \( n\alpha \) SCATTERING

We calculate the \( n\alpha \) scattering phase shifts and resonant parameters using the results of the NCSM calculations of \( ^3\)He and \( ^3\)Li nuclei with the JISP16 \( NN \) interaction. However, we should note here that we first carefully verified the computational algorithm described below supposing \( \alpha \) as a structureless particle and using phenomenological \( N\alpha \) potentials. In this case, the scattering phase shifts and resonant pole locations can be calculated numerically. Our SS HORSE approach was found to be very accurate.

The NCSM model space is conventionally truncated using the maximal excitation oscillator quanta. This NCSM model space should be associated with the \( P \) space of the SS HORSE method which is defined using total oscillator quanta in the many-body system, \( N \), which is entering the above SS HORSE formulas. In the case of \( ^3\)He and \( ^3\)Li nuclei, \( N = N_{\text{max}} + 1 \). Note, even \( N_{\text{max}} \) values should be used to calculate the natural parity states \( \frac{1}{2}^- \) and \( \frac{3}{2}^- \) in these nuclei while the unnatural parity state \( \frac{1}{2}^+ \) is obtained in the NCSM calculations with odd \( N_{\text{max}} \) values. In particular, we perform here the NCSM calculations with \( N_{\text{max}} = 2, 4, \ldots, 16 \) for \( \frac{1}{2}^- \) and \( \frac{3}{2}^- \) states and with \( N_{\text{max}} = 1, 3, \ldots, 15 \) for \( \frac{1}{2}^+ \) state. We pick up for further scattering calculations the lowest NCSM eigenenergies \( E_0^{NCSM} \) in \( ^3\)He and \( ^3\)Li with \( J^\pi = \frac{3}{2}^- \) and \( \frac{1}{2}^+ \); note, all these \( E_0^{NCSM} < 0 \) since they are defined regarding to the 5-nucleon decay threshold. The SS HORSE method requires however positive eigenenergies \( E_0 \) defined in respect to the \( N + \alpha \) threshold. We obtain these eigenenergies as \( E_0 = E_0^{NCSM} - E_0^\alpha \) where \( E_0^\alpha \) is the \( ^4\)He ground state energy obtained in NCSM with the same \( \hbar \Omega \) and the same \( N_{\text{max}} \) in the case of \( \frac{1}{2}^- \)
and $\frac{3^-}{2}$ states and with excitation quanta $N_{\text{max}} - 1$ in the case of unnatural parity $\frac{1^+}{2}$ states of $^5\text{He}$ and $^5\text{Li}$.

After defining eigenenergies $E_0$, we note that not all of them can be used for phase shift calculations due to convergence patterns of eigenstates in the harmonic oscillator basis. Our SS HORSE formalism results in relations for phase shifts similar to those obtained in Ref. [15]. Using the nomenclature of Ref. [15], we should use only eigenenergies $E_0$ which are not influenced by infra-red corrections. As an example, we discuss the selection of eigenenergies $E_0$ in the case of $n\alpha$ scattering in the $\frac{3^-}{2}$ state. The $^5\text{He}$ calculations were performed with $\hbar\Omega$ ranging from 10 to 40 MeV in steps of 2.5 MeV and, as was mentioned above, with $N_{\text{max}} \leq 16$ using the code MFDn [16]. The obtained $E_0$ values are depicted in the left panels of Fig. 1. Due to the scaling property (5), we expect all eigenenergies $E_0$ as function of the scaling parameter $s$ to lie on a single curve. We see however deviations from such a curve on the left upper panel of Fig. 1 that occur for each set of $E_0$ obtained with a given $N_{\text{max}}$ below some critical $\hbar\Omega$ value. This critical $\hbar\Omega$ value decreases with increasing $N_{\text{max}}$. More instructive are the phase shifts $\delta(E_0)$ obtained by Eq. (4) which are also expected to form a single curve. The deviations from this curve are seen in the upper right panel of Fig. 1 to be more pronounced. For the calculation of the phase shifts and resonant parameters, we select the $E_0$ values which form approximately single curves on upper panels of Fig. 1. This selection is illustrated by lower panels of Fig. 1.

The resonant $n\alpha$ scattering phase shifts in the $\frac{3^-}{2}$ and $\frac{1^-}{2}$ states are described by Eq. (14). We need to fit the parameters $a$, $b$ and $d$ of this equation. The resonance energy $E_c$ and width $\Gamma$ can then be obtained by Eq. (12). From Eqs. (4) and (14) we derive the following relation for resonant $n\alpha$ scattering in the $\frac{3^-}{2}$ and $\frac{1^-}{2}$ states:

$$\frac{S_{N_{\text{max}}+3,1}(E_0)}{C_{N_{\text{max}}+3,1}(E_0)} = \tan \left[ -\frac{a\sqrt{E_0}}{E_0 - b^2} - \frac{a^2}{b^2}\sqrt{E_0} + d(\sqrt{E_0})^3 \right].$$ \hspace{1cm} (15)

We assign some values to the parameters $a$, $b$ and $d$ and solve this equation to find $E_0$ for each desired combination of $N_{\text{max}}$ and $\hbar\Omega$ values (note, $\hbar\Omega$ enters the definition of functions $S_{N_{\text{max}}}(E)$ and $C_{N_{\text{max}}}(E)$ see, e.g., Ref. [11]). The resulting set of $E_0$ is compared with the set of selected eigenvalues obtained from NCSM and we minimize the rms deviation between these two sets to find the optimal values of the parameters $a$, $b$ and $d$. The behavior of $E_0$ as functions of $\hbar\Omega$ dictated by Eq. (15) with the fitted optimal parameters $a$, $b$ and $d$ for various $N_{\text{max}}$ values is depicted by curves on the lower left panel of Fig. 1. It is seen that these curves accurately describe the selected eigenvalues from the shaded area. The phase shifts $\delta(E_0)$ obtained by Eq. (14) with fitted parameters are shown in the lower right panel of Fig. 1. It is seen that our theoretical predictions are in a reasonable correspondence with the results of phase shift analysis of experimental scattering data of Ref. [17].

A wider $\frac{1^-}{2}$ resonance and non-resonant $n\alpha$ scattering phase shifts in the $\frac{1^-}{2}$ state are described in the same manner (see Fig. 2). The only difference in the case of the $\frac{1^-}{2}$ scattering is that instead of Eq. (15), we are using

$$\frac{S_{N_{\text{max}}+3,0}(E_0)}{C_{N_{\text{max}}+3,0}(E_0)} = \tan \left[ \pi - \arctan \left( \sqrt{\frac{E_0}{E_b}} + c\sqrt{E_0} + d(\sqrt{E_0})^3 \right) \right].$$ \hspace{1cm} (16)

which can be easily obtained from Eqs. (4) and (13). The phase shift analysis of experimental data is also reasonably described in these cases.

The formalism presented in Refs. [11, 18] can be used to generalize the SS HORSE approach to charged particle scattering. This generalization yields a more complicated formula for the SS HORSE phase shifts than Eq. (4) and to other relations derived from it like Eqs. (15) and (16). However, a modified scaling property (5) can also be obtained in this case and we can use generally the same fitting algorithm for the parameters describing the phase shifts.

Resonance energies $E_c$ and widths $\Gamma$ obtained using Eq. (12) are presented in the table. We show in the table not only the results obtained from NCSM calculations with $N_{\text{max}}$ ranging from 4 to 16 but also from calculations with $N_{\text{max}} \leq 6$ which demonstrate that the resonant parameters only slightly change when the fit is performed using the NCSM results restricted to an essentially smaller model space. This is very encouraging for future applications to heavier nuclear systems. Our results are in a good agreement with $R$-matrix analysis of experimental data of Ref. [19].
Fig. 1. \( na \) scattering in the \( \frac{3}{2}^- \) state. Left: eigenenergies \( E_0 \) obtained with various \( N_{\text{max}} \) vs scaling parameter \( s \) (upper panel) and vs \( h\Omega \) (lower panel). The shaded area shows the \( E_0 \) values selected for the SS HORSE analysis. The lines were obtained by Eq. (15) with fitted parameters. Right: the phase shift \( \delta_1(E) \) obtained by Eq. (4) vs the \( na \) c. m. energy. The symbols on the upper panels shows the phase shifts obtained from all \( E_0 \) values while the lower panel depicts the phase shifts generated by the selected \( E_0 \) values. The line was obtained by Eq. (14) with fitted parameters. The experimental phase shifts are taken from Ref. [17].

Fig. 2. \( na \) scattering phase shifts in the \( \frac{1}{2}^- \) (left) and \( \frac{1}{2}^+ \) (right) states. See Fig. 1 for details.
Energies $E_r$ and widths $\Gamma$ (in MeV) of $^5\text{He}$ and $^5\text{Li}$ resonant states

| $N_{\text{max}} = 4$–$16$ | $^5\text{He}(3^-_2)$ | $^5\text{He}(1^-_2)$ | $^5\text{Li}(3^-_2)$ | $^5\text{Li}(1^-_2)$ |
|-----------------------------|-----------------|-----------------|-----------------|-----------------|
| $E_r$ | $\Gamma$ | $E_r$ | $\Gamma$ | $E_r$ | $\Gamma$ | $E_r$ | $\Gamma$ |
| 0.93 | 1.01 | 1.84 | 5.49 | 2.05 | 1.35 | 3.29 | 4.70 |
| 0.97 | 1.07 | 1.82 | 5.61 | 2.72 | 1.27 | 3.83 | 4.57 |
| 0.80 | 0.65 | 2.07 | 5.57 | 1.69 | 1.23 | 3.18 | 6.60 |

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