Description of Resonant States in the Shell Model[1]

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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 ^{5}He and ^{5}Li nuclei with JISP16 NN interaction.

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 Γ 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 Oscilla-

tor 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 ^{5}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 ℓ in a system of two particles with reduced mass $\mu = \dfrac{m_1 m_2}{m_1 + m_2}$ 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 $T_{N,N}$ and $T_{N,N\pm2}$ 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 $N' > \mathcal{N}$. In other words, we split the complete infinite oscillator basis space into two subspaces: the 'internal' subspace P spanned by oscillator functions with $N \leq \mathcal{N}$ where the complete Hamiltonian $H = T + V$ is used and 'external' subspace Q spanned by oscillator functions with $N > \mathcal{N}$ 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_ν and eigenvectors $\langle N|\nu\rangle$ of the Hamiltonian submatrix in the P space are known. E_ν and $\langle N|\nu\rangle$ fit the set of linear equations

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

$$N \leq \mathcal{N}, \quad \nu = 0,1,\ldots,d-1. \tag{1}$$

Here $d = (\mathcal{N}-\ell)/2+1$ 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]

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

where

$$G_{\mathcal{N},\mathcal{N}}(E) = -\sum_{\nu=0}^{d-1}\frac{|\langle\mathcal{N}|\nu\rangle|^2}{E_\nu - E}, \tag{3}$$

and $S_{N,\ell}(E)$ and $C_{N,\ell}(E)$ are the regular and irregular solutions of the free Hamiltonian in the oscillator representation which analytical expressions can be found in Ref. [11].

The HORSE formalism can be used in combination with any approach utilizing the oscillator basis expansion. In particular, it can be used to generalize the nuclear shell model for applications to the continuum spectrum. In this case, the P space should be associated with the many-body shell model basis space while the Q space is to be used to "open" a particular channel in the many-body system. The standard matrix equation defining the shell model eigenstates should be used as the P-space set of linear equations (1) where the relative motion wave function components in the oscillator basis $\langle N|\nu\rangle$ should be replaced by many-body oscillator shell-model components $\langle N[\alpha]J|\nu\rangle$ characterized by a given value of the total angular momentum J and an additional set of quantum numbers $[\alpha]$ which distinguish many-body oscillator states with the same N and J. The summation in Eq. (1) should run over all possible states with different $[\alpha]$ thus increasing drastically the P space dimensionality d. This increase of the P space dimensionality is however just a manifestation of the increase of basis space in a many-body system and is implemented in modern shell model codes. A more significant limitation for applications is the same increase of the number of summed terms in Eq. (3) where the last oscillator

components of the relative motion eigenfunctions $\langle\mathcal{N}|\nu\rangle$ should be replaced by the many-body oscillator components $\langle\mathcal{N}[\alpha]J\Gamma|\nu\rangle$ with the maximal total oscillator quanta in the P space $\mathcal{N}$ projected onto a desired channel Γ. Note, Eq. (3) requires summation over all shell model eigenstates E_ν with a given value of the total angular momentum J while the modern shell model codes usually are designed to calculate only a few lowest eigenstates. The high-lying eigenstates E_ν can contribute even to low-energy phase shifts since the increase of the denominator in Eq. (3) can be accompanied for some states by an increase of the numerator.

To overcome these difficulties, we propose a Single-State (SS) HORSE formalism. The conventional wisdom says that a shell model eigenstate E_ν 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:

$$\tan\delta_\ell(E_\nu) = -\frac{S_{\mathcal{N}+2,\ell}(E_\nu)}{C_{\mathcal{N}+2,\ell}(E_\nu)}. \tag{4}$$

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 $\langle\mathcal{N}[\alpha]J\Gamma|\nu\rangle$ defining the desired channel. Hence Eq. (4) can be used for scattering channels of any type. In the case of low-energy scattering when $E \ll \frac{1}{8}\hbar\Omega(\mathcal{N}+2-\ell)^2$, one can use asymptotic expressions for $S_{\mathcal{N}+2,\ell}(E_\nu)$ and $C_{\mathcal{N}+2,\ell}(E_\nu)$ at large $\mathcal{N}$ [13] to obtain

$$\tan\delta_\ell(E_\nu) = \frac{j_\ell(2\sqrt{E_\nu/s})}{n_\ell(2\sqrt{E_\nu/s})}, \quad s = \frac{\hbar\Omega}{\mathcal{N}+7/2}, \tag{5}$$

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 $\mathcal{N}$ individually but only on their combination s.

The shell model calculations are usually performed for sets of $\mathcal{N}$ and $\hbar\Omega$ values. Within the SS HORSE formalism, we can calculate the phase shift $\delta_\ell(E)$ at the respective set of eigenenergies $E = E_\nu(\mathcal{N},\hbar\Omega)$ 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:

$$S_\ell(k) = S_\ell^{-1}(-k). \tag{6}$$

Since $S_\ell = e^{2i\delta_\ell}$, the phase shift $\delta_\ell(E)$ is an odd function of k and its expansion in Taylor series of $\sqrt{E} \sim k$ includes only odd powers of $\sqrt{E}$:

$$\delta_\ell(E) = c\sqrt{E} + d(\sqrt{E})^3 + \dots \qquad (7)$$

More, since $\delta_\ell \sim k^{2\ell+1}$ 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 $k = ik_b$ or a pole associated with a low-energy resonance at the complex momentum $k = \kappa_r \equiv k_r - i\gamma_r$, it can be expressed as

$$S(k) = \Theta(k)S_p(k), \qquad (8)$$

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]

$$S_b(k) = -\frac{k + ik_b}{k - ik_b}, \quad S_r(k) = \frac{(k + \kappa_r)(k - \kappa_r^*)}{(k - \kappa_r)(k + \kappa_r^*)}. \qquad (9)$$

The respective phase shift

$$\delta_\ell(k) = \phi(k) + \delta_p(k), \qquad (10)$$

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

$$\delta_b(E) = \pi - \arctan\sqrt{\frac{E}{|E_b|}},$$
$$\delta_r(E) = -\arctan\frac{a\sqrt{E}}{E - b^2}. \qquad (11)$$

Here π in the expression for δ_b appears due to the Levinson theorem [14], $E_b = -\dfrac{\hbar^2 k_b^2}{2\mu} < 0$ is the bound state energy while the resonance energy E_r and its width Γ are

$$E_r \equiv \frac{\hbar^2}{2\mu}(k_r^2 - \gamma_r^2) = b^2 - a^2/2,$$
$$\frac{\Gamma}{2} \equiv \frac{\hbar^2}{\mu}k_r\gamma_r = a\sqrt{b^2 - a^2/4}. \qquad (12)$$

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:

$$\delta_0(E) = \pi - \arctan\sqrt{\frac{E}{|E_b|}} + c\sqrt{E} + d(\sqrt{E})^3. \qquad (13)$$

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

$$\delta_1(E) = -\arctan\frac{a\sqrt{E}}{E - b^2} - \frac{a}{b^2}\sqrt{E} + d(\sqrt{E})^3. \qquad (14)$$

This form guarantees that $\delta_1 \sim k^3$ 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 ^{5}He and ^{5}Li nuclei with the JISP16 NN interaction. However, we should note here that we first carefully verified the computational algorithm described below supposing α 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 N_{max}, 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, $\mathcal{N}$, which is entering the above SS HORSE formulas. In the case of ^{5}He and ^{5}Li nuclei, $\mathcal{N} = N_{max} + 1$. Note, even N_{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_{max} values. In particular, we perform here the NCSM calculations with $N_{max} = 2, 4, \dots, 16$ for $\frac{1}{2}^-$ and $\frac{3}{2}^-$ states and with $N_{max} = 1, 3, \dots, 15$ for $\frac{1}{2}^+$ state. We pick up for further scattering calculations the lowest NCSM eigenenergies E_0^{NCSM} in ^{5}He and ^{5}Li with $J^\pi = \frac{3}{2}^-, \frac{1}{2}^-$ 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^α is the ^{4}He ground state energy obtained in NCSM with the same $\hbar\Omega$ and the same N_{max} in the case of $\frac{1}{2}^-$

and $\frac{3}{2}^{-}$ states and with excitation quanta $N_{max} - 1$ in the case of unnatural parity $\frac{1}{2}^{+}$ states of ^{5}He and ^{5}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}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 $N_{max} \leq 16$ 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_{max} below some critical $\hbar\Omega$ value. This critical $\hbar\Omega$ value decreases with increasing N_{max}. More instructive are the phase shifts $\delta_1(E_0)$ 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_r and width Γ 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:

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

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_{max} and $\hbar\Omega$ values (note, $\hbar\Omega$ enters

definition of functions $S_{N,\ell}(E)$ and $C_{N,\ell}(E)$ 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_{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 $\delta_1(E)$ 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

$$-\frac{S_{N_{max}+3,0}(E_0)}{C_{N_{max}+3,0}(E_0)}$$
$$= \tan\left(\pi - \arctan\sqrt{\frac{E_0}{|E_b|}} + c\sqrt{E_0} + d(\sqrt{E_0})^3\right), \quad (16)$$

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_r and widths Γ obtained using Eq. (12) are presented in the table. We show in the table not only the results obtained from NCSM calculations with N_{max} ranging from 4 to 16 but also from calculations with $N_{max} \leq 6$ 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].
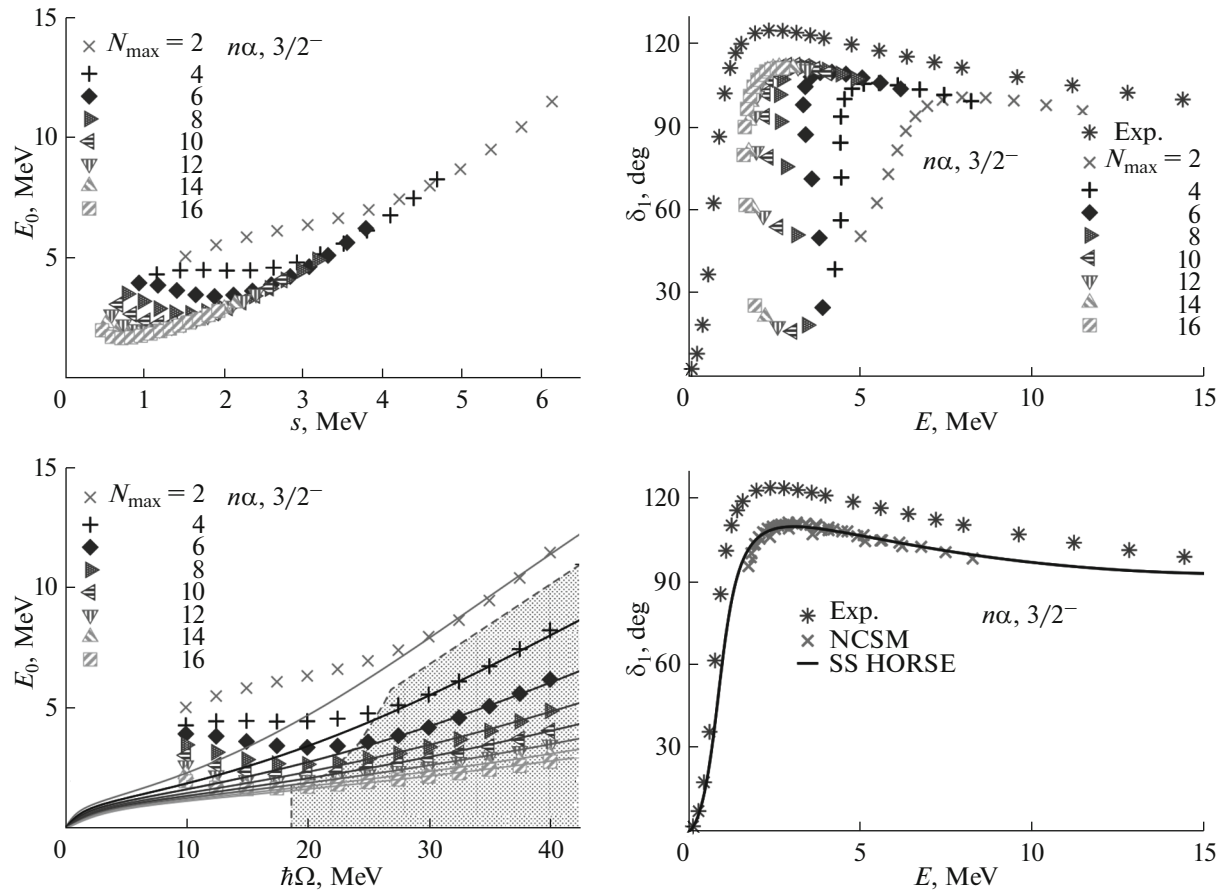
Fig. 1. $n\alpha$ scattering in the $\frac{3}{2}^-$ state. Left: eigenenergies E_0 obtained with various N_{max} vs scaling parameter s (upper panel) and vs $\hbar\Omega$ (lower panel). The shaded area shows the E_0 values selected for the SS HORSE analysis. The lines were obtained by Eq. (15) with fitted parameters. Right: the phase shift $\delta_1(E)$ obtained by Eq. (4) vs the $n\alpha$ 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].
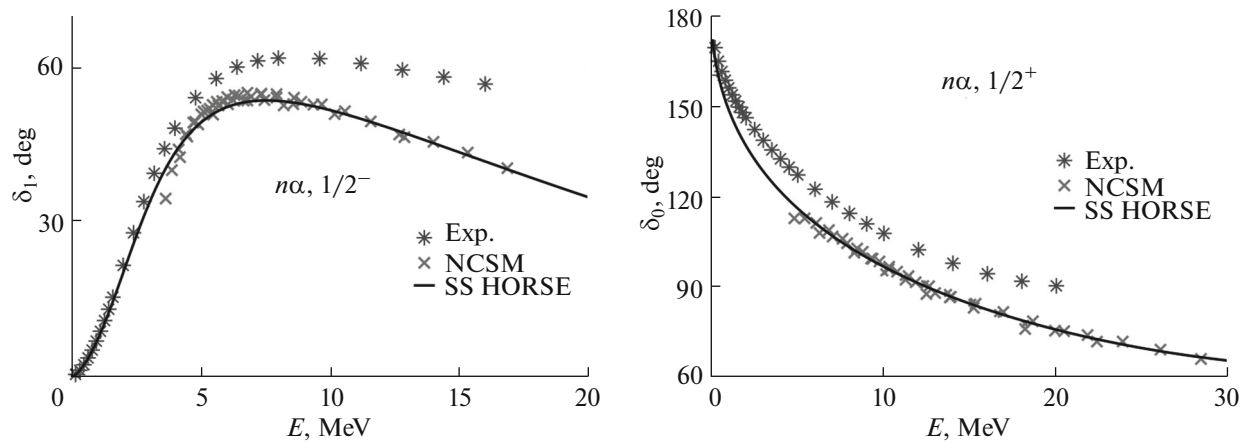

Fig. 2. $n\alpha$ scattering phase shifts in the $\frac{1}{2}^-$ (left) and $\frac{1}{2}^+$ (right) states. See Fig. 1 for details.

Energies E_r and widths Γ (in MeV) of ^{5}He and ^{5}Li resonant states

	^{5}He$\left(\frac{3}{2}^-\right)$		^{5}He$\left(\frac{1}{2}^-\right)$		^{5}Li$\left(\frac{3}{2}^-\right)$		^{5}Li$\left(\frac{1}{2}^-\right)$	
	E_r	Γ	E_r	Γ	E_r	Γ	E_r	Γ
N_{max} = 4–16	0.93	1.01	1.84	5.49	2.05	1.35	3.29	4.70
N_{max} = 4–6	0.97	1.07	1.82	5.61	2.72	1.27	3.83	4.57
R-matrix [19]	0.80	0.65	2.07	5.57	1.69	1.23	3.18	6.60

ACKNOWLEDGMENTS

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