NUCLEI Theory

SS-HORSE Method for Studying Resonances

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Abstract—A new method for analyzing resonance states based on the Harmonic-Oscillator Representation of Scattering Equations (HORSE) formalism and analytic properties of partial-wave scattering amplitudes is proposed. The method is tested by applying it to the model problem of neutral-particle scattering and can be used to study resonance states on the basis of microscopic calculations performed within various versions of the shell model.

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1. INTRODUCTION

In recent years, considerable advances have been made in developing microscopic methods for describing continuum states of nuclei, the widths of their resonance states, and nuclear reactions. Some of these methods are worthy of special note. These include the method that is based on the integral Lorentz transformation [1, 2] which was implemented in the hyperspherical-harmonic approximation and was extended [3] in such a way as to employ it together with the No-Core Shell Model (NCSM); the continuum shell model [4]; first attempts at studying nucleon scattering by nuclei within the quantum Monte Carlo method [5]; and the Gamow shell model-in particular, the no-core Gamow shell model [6]. The most significant results in the modern ab initio theory of nuclear reactions were obtained by employing the NCSM approach in combination with the resonating-group method (for reviews, see [2, 7, 8]).

In the present study, we develop a simple method for estimating the resonance energies E_r and widths Γ and for approximating phase shifts at low energies on the basis of the dependence of the energy of the lowest state $E_0(\hbar\Omega)$ on the oscillator parameter $\hbar\Omega$ and on the dimension of the model space. Our group proposed this method earlier [9–11] and used it to analyze resonance states in the ⁵He nucleus [9–11] and in the four-neutron system (tetraneutron) [12, 13]. The method relies on that version of the *J*-matrix formalism of scattering theory [14] which employs the harmonic-oscillator basis—this is the so-called HORSE (Harmonic-Oscillator Representation of

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Scattering Equations) method [15]. Here, we propose developing the method introduced in [9-11] in such a way as to ensure a correct behavior of phase shifts in the region of low energies on the basis of analytic properties of partial-wave scattering amplitudes.

The method is tested by applying it to a model two-body problem with a potential is fitted to neutron scattering by alpha particle in the $3/2^-$ and $1/2^-$ partial waves [16].

2. SS-HORSE METHOD

Let us consider the HORSE equations describing the scattering of neutral particles having the reduced mass $\mu = m_1 m_2/(m_1 + m_2)$ and interacting via the potential V in the partial wave characterized by the orbital angular momentum l. Within the HORSE method [15], the wave function for relative particle motion is expanded in an infinite series in harmonicoscillator functions. The basis functions are characterized by the oscillator parameter $\hbar\Omega$, the radial quantum number n, and the orbital angular momentum l.

In the harmonic-oscillator basis, the kineticenergy matrix is tridiagonal, its nonzero elements $T_{n,n}$ and $T_{n,n\pm 1}$ becoming larger in magnitude as the radial quantum number n grows. At the same time, the matrix elements $V_{n,n'}$ of the short-range potential decrease with increasing n and n'. Starting from some n or n' > N, it is therefore possible to disregard the matrix elements $V_{n,n'}$. As a result, the space of basis states splits into the internal region $n \le N$, where the interaction is fully taken into account, and the external region n > N, where only the matrix elements of the kinetic energy are retained in the Hamiltonian.

The eigenvectors of the infinite matrix of this Hamiltonian can be found if the eigenenergies E_{ν}

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and the eigenvectors $\langle n|\nu\rangle$ of the Hamiltonian matrix $H_{n,n'}^N$ in the internal region $n, n' \leq N$ are known. The quantities E_{ν} and $\langle n|\nu\rangle$ satisfy the set of linear equations

$$\sum_{n'=0}^{N} H_{n,n'}^{N} \langle n' | \nu \rangle = E_{\nu} \langle n | \nu \rangle, \qquad (1)$$
$$n < N, \quad \nu = 0, 1, ..., N.$$

The eigenvectors $\langle n | \nu \rangle$ are orthonormalized; that is,

$$\sum_{n'=0}^{N} \langle \nu' | n' \rangle \langle n' | \nu \rangle = \delta_{\nu\nu'}, \qquad (2)$$
$$\sum_{\nu'=0}^{N} \langle n' | \nu' \rangle \langle \nu' | n \rangle = \delta_{nn'}.$$

The phase shifts can be calculated by the formula [15]

$$\tan \delta_l(E)$$
(3)
= $-\frac{S_{N,l}(E) - G_{N,N}(E)T_{N,N+1}S_{N+1,l}(E)}{C_{N,l}(E) - G_{N,N}(E)T_{N,N+1}C_{N+1,l}(E)},$

where

$$G_{N,N}(E) = -\sum_{\nu=0}^{N} \frac{|\langle N|\nu\rangle|^2}{E_{\nu} - E}$$
(4)

and $S_{n,l}(E)$ and $C_{n,l}(E)$ are, respectively, the regular and the irregular harmonic-oscillator solution for the free Hamiltonian. The explicit form of these solutions is known from [15].

The calculation of scattering observables becomes substantially simpler if the energy coincides with one of the eigenvalues. In particular, it follows from Eqs. (3) and (4) that, under the condition $E_{\nu} > 0$, the phase shift reduces to a very simple expression,

$$\tan \delta_l(E_{\nu}) = -\frac{S_{N+1,l}(E_{\nu})}{C_{N+1,l}(E_{\nu})}.$$
 (5)

It is important that not only does the summation over the entire set of eigenstates disappear, but also the dependence on the wave-function components $\langle N | \nu \rangle$ becomes nonexistent. The phase shift $\delta_l(E_\nu)$ is fully determined by the eigenenergy E_ν alone. The eigenenergies depend on the boundary N at which the internal region Hamiltonian is truncated and on the parameter $\hbar\Omega$ of the harmonic-oscillator basis. It follows that, by varying $\hbar\Omega$ and N within reasonable limits, one can calculate, with the aid of Eq. (5), phase shifts in the respective range of energies $E_\nu(\hbar\Omega)$. Expressions similar to that in (5) can also be obtained for other scattering attributes—in particular, for the S matrix and for the partial-wave scattering amplitude. In the following, we will refer to this method for calculating the features of scattering as the Single-State (SS) HORSE method [9–11], since, from the standard HORSE formalism, we use the energy of only one eigenstate, E_{ν} , and the explicit expressions for the harmonic-oscillator solutions $S_{n,l}(E)$ and $C_{n,l}(E)$.

It should be noted that, if the dependence of phase shifts on the energy $\delta_l(E)$ is known—for example, from an analysis of experimental data—Eq. (5) at fixed values of the parameters N and $\hbar\Omega$ can be considered as a transcendental equation for determining the eigenvalues E_{ν} . Thus, one can find, on the basis of Eq. (5), values that the eigenenergies of a finite Hamiltonian matrix should have within a theory that employs an expansion of wave functions in terms of a harmonic-oscillator basis—for example, within standard versions of the nuclear shell modelin order to be consistent with experimental data on scattering. The use of Eq. (5) simplifies substantially the approach that our group proposed earlier [17] in studying resonance nucleon scattering by alpha particle within the inverse scattering approach.

By and large, the developed SS-HORSE method can be applied together with other approaches that employ a harmonic-oscillator basis. In particular, it can be used to extend the applicability range of the nuclear shell model to problems dealing with the continuous spectrum. In that case, the internal subspace is associated with the model space of the multiparticle shell-model basis, while the external subspace is used to describe open channels. Within the shell model, the basis space is usually specified by the maximum number of excitation quanta, N_{max} . For each specific problem, one can readily establish the correspondence between N_{max} and the parameter Nof the SS HORSE method.

Within the SS-HORSE formalism, we can calculate the phase shifts $\delta_l(E)$ at the energies $E^{(i)} =$ $E_{\nu}(N^{(i)}, \hbar \Omega^{(i)})$ that cover some interval. Parametrizing the values obtained for the phase shifts $\delta_l(E)$, we can extrapolate $\delta_l(E)$ to a broader energy range and, if the system being studied has a resonance state, calculate the resonance energy and width. For this, the result of a complete diagonalization of the Hamiltonian matrix is not needed, which is especially important for applications in many-body problemsfor example, in the shell model—where the number of basis states grows exponentially with N_{max} ; we are interested only in the energy of only one or few lowest eigenstates of the system. It is also of importance that Eq. (5) does not feature a dependence on wavefunction components—that is, this equation is valid for any channel. It should also be noted that, in principle, the phase shift can be continued analytically to the region of negative energies in order to obtain information about the properties of bound states such a continuation is briefly discussed in the following [see expressions (13)-(15) below].

The convergence of the results of HORSE calculations depends on the choice of values for the parameters N and $\hbar\Omega$ and has specific features inherent in each specific problem. The following fact permits simplifying the problem of choosing modelparameter values for employing them within the SS-HORSE method. In the low-energy region, the use of large-N asymptotic expressions for $S_{N+1,l}(E_{\nu})$ and $C_{N+1,l}(E_{\nu})$ [18] under the condition

$$E_{\nu} \ll \frac{1}{8}\hbar\Omega(N+1)^2 \tag{6}$$

makes it possible to obtain

$$\tan \delta_l(E_\nu) = \frac{j_l(2\zeta_\nu)}{n_l(2\zeta_\nu)},\tag{7}$$

$$\zeta_{\nu} = \sqrt{E_{\nu}/s}, \quad s = \frac{\hbar\Omega}{2N + l + 7/2},$$

where $j_l(x)$ and $n_l(x)$ are spherical Bessel and Neumann functions. Expression (7) reflects the following scaling property: the phase shift does not depend on *N* and $\hbar\Omega$ individually, but it depends on their ratio, which is a scaling variable *s*.

In calculations with the harmonic-oscillator basis, the scaling was first proposed in [19] in studying bound states. In contrast to *s*, the scaling variable

$$L = \sqrt{2(2N + l + 7/2)/(\hbar\Omega)}$$
(8)
 $\times \sqrt{\hbar^2/\mu} \sim 1/\sqrt{s},$

which was introduced in [19] with the correction proposed in [20], has the dimensions of length. Expression (7), which we obtained from the HORSE equations, generalizes the scaling property to scattering states.

It should be noted that, under the additional condition

$$\frac{4E_{\nu}}{s} \gg 1,\tag{9}$$

which is equivalent to

$$E_{\nu} \gg \frac{\hbar\Omega}{4(2N+l+7/2)},$$
 (10)

the asymptotic expressions can be used for the spherical Bessel and Neumann functions in question. As a result, expression (7) reduces to a simpler form; that is,

$$\delta_l = -2\sqrt{E/s} + \pi l/2. \tag{11}$$

Figure 1 shows that the values of the function

$$f_{N,l} = -\arctan\left(S_{N,l}(E_{\nu})/C_{N,l}(E_{\nu})\right)$$
(12)

are in excellent agreement with the asymptotic expression $\arctan(j_l(2\sqrt{E/s})/n_l(2\sqrt{E/s}))$ in the region of low energies even in the case of N = 1; as N increases, the energy range over which the approximation being considered is valid becomes broader. At the same time, the asymptotic expression (11) is valid in the region of large values of the argument $\sqrt{E/s}$, and higher are the values of l, larger are the $\sqrt{E/s}$ values at which this asymptotic expression becomes valid. The case of l = 0, in which the asymptotic expressions for the spherical Bessel and Neumann functions under study at large values of the argument in terms of sines and cosines coincide with the functions $j_0(x)$ and $n_0(x)$ themselves, is an exception. Thus, the energy range in which it is legitimate to use expression (11) becomes broader with increasing Nand decreasing *l*. But while the simplified scaling relation (11) cannot be applied at low values of the energy E_{ν} , in which case the inequality in (10) is invalid, the more general scaling relation (7) can be used down to zero energy.

Here, it is of interest to consider in more detail the connection with the expressions from [19, 20] for bound-state energies. It is well known that, in the vicinity of a ground-state pole, the S matrix can be approximated as [21]

$$S_l \equiv \exp(2i\delta_l) = \frac{D_l}{k - ik_b},\tag{13}$$

where $E = -\hbar^2 \varkappa^2 / 2\mu$, $E_b = -\hbar^2 k_b^2 / 2\mu$ is the boundstate energy, $\varkappa = k/i$ and k_b are the respective imaginary parts of the momenta, and D_l is expressible in terms of the asymptotic normalization constant A_l as [21]

$$D_l = (-1)^{l+1} i |A_l|^2, (14)$$

and is purely imaginary. Expression (7) remains valid at negative energies. From Eqs. (7), (13), and (14), we can then obtain

$$\varkappa_{\nu} = k_b - |A_l|^2 \exp\left(-\frac{4\varkappa_{\nu}\hbar}{\sqrt{2\mu s}}\right), \qquad (15)$$

where $E_{\nu} = -\hbar^2 \varkappa_{\nu}^2 / 2\mu$. Instead of this, the authors of [19, 20] proposed the expression, which, in our notation, takes the form

$$E_{\nu} = E_b + C_l \exp\left(-\frac{4k_b\hbar}{\sqrt{2\mu s}}\right). \tag{16}$$

Expressions (15) and (16) are similar, but there are also substantial distinctions between them: Eq. (16) for the bound-state eigenenergies E_{ν} in a finite harmonic-oscillator basis involves these energies themselves and the energy E_b that one could expect in the limit the infinite basis, while Eq. (15), which we derived, contains, instead of the energies, the

respective momenta $\varkappa_{\nu} \sim \sqrt{|E_{\nu}|}$ and $k_b \sim \sqrt{|E_b|}$; moreover, the constant k_b appears in the exponential function in (16), but the momentum \varkappa_{ν} , which changes as a function of the energy E_{ν} , takes its place in the exponent in our equation (15). A detailed comparison of Eqs. (15) and (16) and especially of the energy estimates obtained with the aid of them in an infinite harmonic-oscillator basis, E_b , in particular nuclear-physics problems, is of a great interest for applications. We plan to perform such an investigation in our future studies.

In general, the phase shift should be a smooth function of the scaling parameter s. In accordance with Eq. (7), the eigenenergies E_{ν} calculated for different sets of model parameters N and $\hbar\Omega$ should therefore lie on the same smooth curve representing the dependence $E_{\nu}(s)$. A deviation of any result from this curve would indicate that we have not reached the convergence and that it is necessary to exclude the respective value from the data set for the further analysis within the SS-HORSE framework. By considering a model problem, we will demonstrate below the selection of the eigenenergies E_{ν} .

3. PARAMETRIZATION OF PHASE SHIFTS IN THE LOW-ENERGY REGION ON THE BASIS OF ANALYTIC PROPERTIES OF SCATTERING AMPLITUDES

Let us consider a quantum system that has one resonance state in a partial wave characterized by the orbital angular momentum l. Resonance states are associated with the *S*-matrix poles (or the poles of the partial-wave scattering amplitude f_l) situated on the second (unphysical) sheet of complex energy at the point $E_p = E_r - i\Gamma/2$ (or at the point $k_p = k_r - i\gamma$ of the lower half-plane of the complex momentum) [21–23]. The resonance energy (E_r) and width (Γ) are related to the respective momentum pole by the following obvious equations:

$$E_r = \frac{\hbar^2}{2\mu} (k_r^2 - \gamma^2), \quad \frac{\Gamma}{2} = \frac{\hbar^2}{\mu} k_r \gamma.$$

The partial-wave scattering amplitude for neutral particles, $f_l(E)$, is expressed in terms of the partial-wave S matrix $S_l(E)$ and the partial-wave phase shift $\delta_l(E)$ as

$$f_{l}(E) = \frac{S_{l}(E) - 1}{2ik} = \frac{e^{i\delta_{l}(E)} \sin \delta_{l}(E)}{k}$$
(17)
$$= \frac{k^{2l}}{k^{2l+1} \cot \delta_{l}(E) - ik^{2l+1}},$$

where $E = \hbar^2 k^2 / 2\mu$ is the c.m. energy of relative particle motion. The additional factor k^{2l} in the numerator and denominator on the right-hand side of

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the last equality in (17) was introduced for the sake of convenience, since, in the region of $E \rightarrow 0$, the effective-range expansion yields [23]

$$k^{2l+1} \cot \delta_l(E) = -\frac{1}{a_l} + \frac{r_l}{2}k^2 - \frac{P_l}{4}k^4 + \dots$$

Below, we restrict ourselves to the approximation where one retains only the first three terms of the exact expansion; that is,

$$k^{2l+1}\cot\delta_l(E) \simeq -\frac{1}{a_l} + \frac{r_l}{2}k^2 - \frac{P_l}{4}k^4.$$
 (18)

It should be noted that the function $k^{2l+1} \cot \delta_l(E)$ can be expanded in a series in even powers of the momentum k (or in integer powers of the relativemotion energy E) not only in the low-energy region but also at any energies.

In order to parametrize scattering amplitudes and phase shifts, we will generalize the method proposed in [24] to the case of resonance scattering. For this purpose, we introduce an auxiliary complex-valued function F_l defined as

=

$$F_{l}(E) \equiv R_{l}(E) + iI_{l}(E)$$
(19)
= $\frac{k^{2l+1}\cot\delta_{l}(E) - i(k_{r} - i\gamma)^{2l+1}}{E - (E_{r} - i\Gamma/2)}.$

The numerator of the function F_l coincides with the denominator of the scattering amplitude upon the substitution of a fixed value $k_p = (k_r - i\gamma)$ for the variable k in the second term. The function F_l does not have singularities at $E = E_r - i\Gamma/2$, so that we can approximate it by a polynomial in energy, but, by construction, the function F_l then leads automatically to the appearance of a pole in the scattering amplitude $f_l(E)$ at the resonance energy $E = E_r - i\Gamma/2$.

We now introduce the following notation:

$$Q_r = \operatorname{Re}\left[i(k_r - i\gamma)^{2l+1}\right], \qquad (20)$$
$$Q_i = \operatorname{Im}\left[i(k_r - i\gamma)^{2l+1}\right].$$

As a result, the following expressions can readily be obtained for the real and imaginary parts of the function F_l :

$$R_{l}(E)$$
(21)
= $\frac{(k^{2l+1}\cot\delta_{l} - Q_{r})(E - E_{r}) - \frac{1}{2}Q_{i}\Gamma}{(E - E_{r})^{2} + (\Gamma/2)^{2}},$
 $I_{l}(E)$ (22)
 $\frac{1}{2}(k^{2l+1}\cot\delta_{r} - Q_{r})\Gamma + Q_{r}(E - E_{r})$

$$= -\frac{\frac{1}{2}(k^{2l+1}\cot\delta_l - Q_r)\Gamma + Q_i(E - E_r)}{(E - E_r)^2 + (\Gamma/2)^2}.$$

By construction of the auxiliary function $F_l(E)$ and due to the effective-range expansion (18), both the

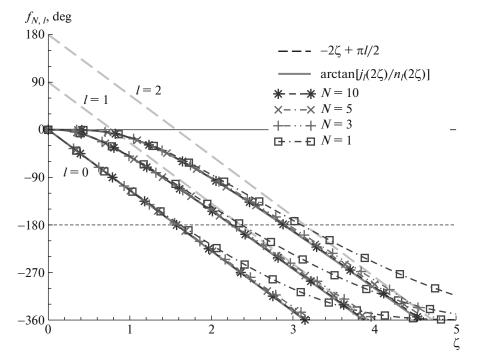


Fig. 1. Illustration of the scaling property. The curves endowed with symbols represent the functions $f_{N,l}$ [see Eq. (12)] versus $\zeta = \sqrt{E/s}$ for various values of N. The solid curves correspond to Eq. (7); the regions where they agree with the respective functions $f_{N,l}$ are regions of the scaling behavior. The dashed straight lines correspond to the asymptotic expression (11).

real $[R_l(E)]$ and the imaginary $[I_l(E)]$ parts of this function can be expanded in a series in even powers of k on the real momentum axis.

The function $I_l(E)$ is unambiguously determined by the function $R_l(E)$. Indeed, we can obtain the following relation from Eqs. (21) and (22):

$$I_{l}(E)(E - E_{r}) = -\frac{1}{2}R_{l}(E)\Gamma - Q_{i}.$$
 (23)

Obviously, the function $I_l(E)$ then does not have a singularity at the point $E = E_r$ only if the free term in the expansion of the function $R_l(E)$ in the Taylor series in powers of $(E - E_r)$ coincides with $-2Q_i/\Gamma$. In particular, the approximation of the function $R_l(E)$ by a second-order polynomial $\mathcal{R}_l^{(2)}(E - E_r)$ in $(E - E_r)$ should have the form

$$\mathcal{R}_{l}^{(2)}(E - E_{r})$$
(24)
= $\frac{2}{\Gamma} \left[-Q_{i} + w_{1}(E - E_{r}) + w_{2}(E - E_{r})^{2} \right].$

One can readily see that, in this case, the approximation (18) is valid in the low-energy region; finding $k^{2l+1} \cot \delta_l$ from Eq. (21) and taking into account Eq. (24), we can then obtain the following expressions for the scattering length a_l and the effective range r_l :

$$a_l = -\frac{\Gamma}{2} \bigg[Q_r \frac{\Gamma}{2} + Q_i E_r \tag{25}$$

+
$$(w_1 - w_2 E_r) \left(E_r^2 + (\Gamma/2)^2 \right) \Big]^{-1}$$
,

$$r_{l} = \frac{\hbar^{2}}{\mu} \frac{2}{\Gamma}$$
(26)
 $\times \left[-Q_{i} - 2w_{1}E_{r} - w_{2} \left(3E_{r}^{2} - (\Gamma/2)^{2} \right) \right].$

Thus, a parametrization of phase shifts that guarantees their correct behavior both in the vicinity of the threshold and in the resonance region can be constructed on the basis of Eq. (21) alone. The procedure used to fit the parameter values is as follows. Let $E_0^{(i)}$ (i = 1, 2, ..., d) be the set of lowest positive eigenvalues E_0 calculated at various values of the model parameters $N^{(i)}$ and $\hbar\Omega^{(i)}$ (*d* is the number of energies in this set). At some fixed values of w_1, w_2 , E_r , and Γ , we find those energies $\mathcal{E}^{(i)}$ for each of the values of $N^{(i)}$ and $\hbar\Omega^{(i)}$ that satisfy the equation

$$\frac{\left(\frac{C_{N+1,l}(E)}{S_{N+1,l}(E)}k^{2l+1} + Q_r\right)(E - E_r) + \frac{1}{2}Q_i\Gamma}{(E - E_r)^2 + (\Gamma/2)^2} \quad (27)$$
$$= \frac{2}{\Gamma} \left[Q_i - w_1(E - E_r) - w_2(E - E_r)^2\right],$$

which combines Eqs. (5), (21), and (24). The ultimate values of the adjustable parameters are determined by

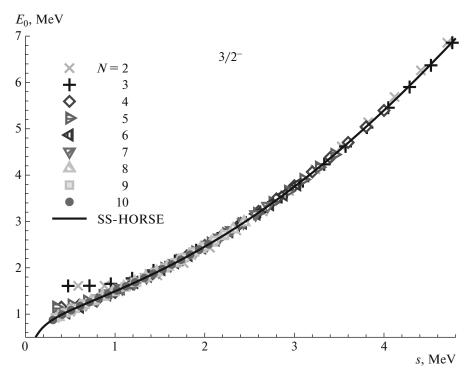


Fig. 2. Energies E_0 of the lowest state as a function of the scaling variable *s* in the $p_{3/2}$ partial wave. The solid line represents the solution of Eq. (29).

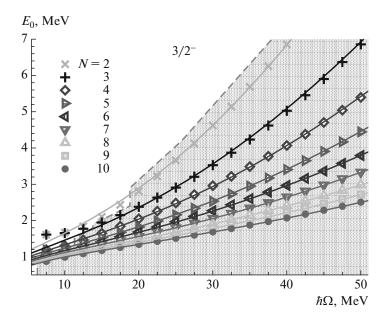


Fig. 3. Energies E_0 of the lowest state as a function of $\hbar\Omega$ in the $p_{3/2}$ partial wave. The results lying outside the shaded region are not used in the SS-HORSE calculations. The solid curves represent the solution of Eq. (29) after rescaling for each model space.

minimizing the functional

$$\Xi = \sqrt{\frac{1}{d} \sum_{i=1}^{d} \left(E_0^{(i)} - \mathcal{E}^{(i)} \right)^2}.$$
 (28)

From Eqs. (7), (21), and (24), one can readily obtain the transcendental equation

$$\frac{2}{\Gamma} \left[-Q_i + w_1 (E - E_r) + w_2 (E - E_r)^2 \right]$$
(29)

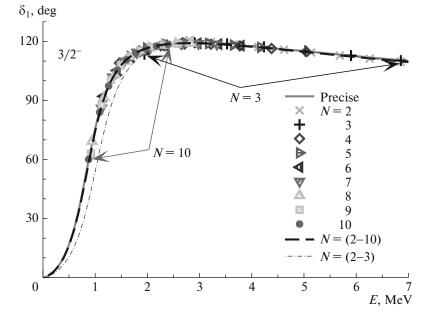


Fig. 4. Phase shifts in the $3/2^-$ partial wave. The solid curve stands for precisely calculated phase shifts, while the dashed and dash-dotted curves represent the phase shifts approximated on the basis of the SS-HORSE method [calculations according to Eq. (31)] for, respectively, the N = (2-10) and the N = (2-3) versions; the results obtained in the rest versions are indistinguishable from the N = (2-10) curve in the scale of the figure. Symbols display the calculations according to Eq. (5) in various model spaces specified by the value of N. The arrows indicate the boundaries of the values of $\delta_l(E_0^{(i)})$ in the calculations for N = 3 and N = 10.

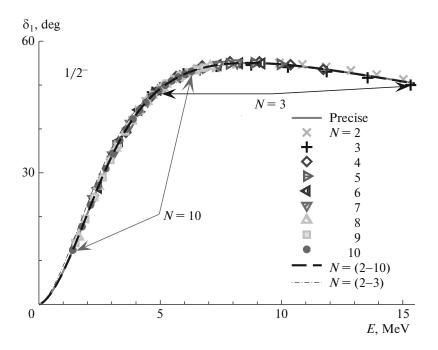


Fig. 5. Same as Fig. 4, but for the $1/2^{-}$ partial wave.

$$=\frac{\left(k^{2l+1}\frac{n_l\left(2\sqrt{E/s}\right)}{j_l\left(2\sqrt{E/s}\right)}-Q_r\right)(E-E_r)-\frac{1}{2}Q_i\Gamma}{(E-E_r)^2+(\Gamma/2)^2}.$$

tain a smooth dependence of the energy on the scaling variable, E(s), for fixed values of the adjustable parameters w_1 and w_2 and the resonance parameters E_r and Γ .

Solving this equation with respect to *E*, we can ob-

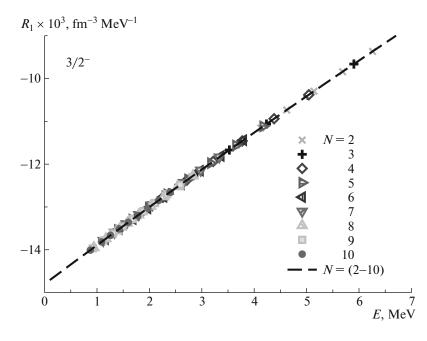


Fig. 6. Comparison of the functions $\mathcal{R}_l^{(2)}(E - E_r)$ (dashed line) obtained by the fit using the selected set of eigenvalues $E_0^{(i)}$ from the N = (2–10) model spaces with the set of values that was calculated for the function $\mathcal{R}_l(E_0^{(i)})$ according to expression (21) with the phase shifts $\delta_l(E_0^{(i)})$ obtained using the results $E_0^{(i)}$ of the diagonalization of the Hamiltonian, expression (5) and the fitted values of the $3/2^-$ -resonance from the N = (2-10) version.

4. ILLUSTRATION OF HOW THE METHOD WORKS

We will now demonstrate how the method works by applying it to a model problem of neutral-particle scattering on a Woods–Saxon potential with a surface spin–orbit term,

$$V_{n\alpha} = \frac{V_0}{1 + \exp\left[(r - R_0)/\alpha_0\right]}$$
(30)

+
$$(\mathbf{l} \cdot \mathbf{s}) \frac{1}{r} \frac{a}{dr} \frac{v_{ls}}{1 + \exp\left[(r - R_1)/\alpha_1\right]}$$
.

With the parameter [16] $V_0 = -43.0$ MeV, $V_{ls} = -40.0$ MeV fm², $R_0 = 2.0$ fm, $\alpha_0 = 0.70$ fm, $R_1 = 1.5$ fm, and $\alpha_1 = 0.35$ fm, this potential simulates well phase shifts and resonance features for neutron scattering by alpha particle—in particular, a comparatively narrow resonance in the $p_{3/2}$ partial wave and a broader resonance in the $p_{1/2}$ partial wave. The precise values obtained for resonance-state energies and widths in the case of scattering on the potential (30) from calculations with the reduced mass $\mu = \frac{4}{5}m_{nucl}$ (where m_{nucl} is the nucleon mass) are given in the table.

We have calculated the energy of the lowest state, E_0 , by diagonalizing the Hamiltonian matrix with this potential in a harmonic-oscillator basis for $N = 2, 3, \ldots, 10$ at $\hbar\Omega$ values varied between 7.5 and 50 MeV with a step of 2.5 MeV. The calculated eigenvalues E_0 for the $p_{3/2}$ partial wave are given in Fig. 2 versus the scaling variable *s*. One can see that these results mostly lie on a smooth curve. This is not so only for the results obtained in the case of model spaces where *N* and $\hbar\Omega$ are small, in which case the values of *s* are also modest. These results were discarded and were not taken into account in the subsequent analysis. The selection of the results of diagonalization are visualized in Fig. 3, which gives the dependence $E_0(\hbar\Omega)$.

The results for our analysis of scattering in the $p_{1/2}$ partial wave were selected in a similar way.

The phase shifts $\delta_l(E_i^0)$ calculated within the SS-HORSE approach according to Eq. (5) for the eigenenergies E_i^0 selected in the way outlined above are in excellent agreement with the precise phase shifts in the $p_{3/2}$ and $p_{1/2}$ partial waves (see Fig. 4 and 5, respectively). We note that the SS-HORSE calculations at small values of N lead to phase shifts lying higher in energy and outside the resonance region. As N increases, the $\delta_l(E_i^0)$ values are shifted to the region of resonance energies.

Our numerical calculations reveal that, in order to parametrize the function $R_l(E)$, it is sufficient to use a second-order polynomial $\mathcal{R}_l^{(2)}(E - E_r)$ in $(E - E_r)$ [see expression (24)]. This parametrization is

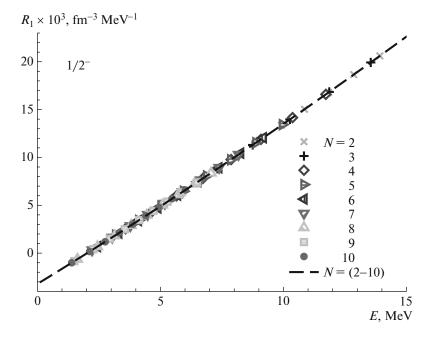


Fig. 7. Same as Fig. 6, but for the $1/2^{-}$ partial wave.

illustrated in Figs. 6 and 7. These figures show that the approximations $\mathcal{R}_l^{(2)}(E - E_r)$ (dashed curves) are in excellent agreement with the values calculated for the functions $R_l(E_0^{(i)})$ (points) by using Eq. (21) with the phase shifts $\delta_l(E_0^{(i)})$ obtained by means of expression (5) and the results $E_0^{(i)}$ of diagonalization of the Hamiltonian together with the fitted values of the resonance energies and widths.

The parameters w_1 and w_2 of the function $\mathcal{R}_l^{(2)}(E - C)$ E_r) and the resonance parameters E_r and Γ were determined by minimizing the functional Ξ . The fitted results and the root-mean-square deviations of Ξ are given in the table for various versions of the calculation. Versions of SS-HORSE calculations differ by sets of the results of diagonalization of the Hamiltonian matrix that are used in these calculations. By way of example, we indicate that we use in the N = (2-3) version the eigenenergies E_0 from the shaded region in Fig. 3 that correspond to the calculations for N = 2 and 3; the eigenenergies from the shaded region in the N = (2-4) version correspond to the calculations for N = 2, 3, and 4; and so on. In the N = (2-10) version, we use all eigenenergies E_0 from the shaded region in Fig. 3.

The table demonstrates that the resonance energies and widths converge rather fast to precise values as the set of energies E_0 is extended. It is important to note, however, that, even in the minimal version of those considered in our present study [N = (2-3)], where the input data are beyond the resonance region, we obtain reasonable estimates for resonance parameters, and this is of particular importance for multiparticle applications within the shell model, where the computational burden increases rapidly with the basis size.

A smooth energy dependence of phase shifts at the fitted values of the parameters w_1 , w_2 , E_r , and Γ can be calculated by the formula

$$k^{2l+1}\cot\delta_l = Q_r \tag{31}$$

+
$$\frac{\mathcal{R}_l^{(2)}(E-E_r)\left[(E-E_r)^2 + (\Gamma/2)^2\right] + \frac{1}{2}Q_i\Gamma}{E-E_r}$$
,

which, upon taking into account Eq. (24), follows from Eq. (21). The result given by this formula differs from the precise dependence $\delta_l(E)$ only in the case of employing the parameters of the minimal version [N = (2-3)], this being due primarily to an overestimated (underestimated) energy of the $3/2^-$ ($1/2^-$) resonance as compared to the respective precise values. On the scales of Figs. 4 and 5, the results obtained within other versions are virtually undistinguishable from precise phase-shift values. That the phase shifts are accurately reproduced within the SS-HORSE approach is demonstrated also by good agreement of the scattering lengths and effective ranges calculated on the basis of Eqs. (25) and (26) with their precise counterparts (see table).

| | 1 | I | r | 1 | | | |
|-------------------|-------------|----------------|-------------------------|--------------------------|--|--|--------|
| | E_r , MeV | Γ , MeV | a_l , fm ³ | r_l , fm ⁻¹ | w_1 , fm ⁻³ MeV ⁻¹ | w_2 , fm ⁻³ MeV ⁻² | Ξ, keV |
| $3/2^-$ resonance | | | | | | | |
| N = (2 - 3) | 1.016 | 0.861 | -41.6 | -1.031 | 6.815×10^{-4} | -2.128×10^{-5} | 121 |
| N = (2 - 4) | 0.888 | 0.787 | -53.6 | -0.881 | 4.628×10^{-4} | -1.067×10^{-5} | 268 |
| N = (2 - 5) | 0.882 | 0.785 | -54.4 | -0.871 | 4.485×10^{-4} | -9.783×10^{-6} | 232 |
| $N = (2{-}10)$ | 0.848 | 0.777 | -59.6 | -0.806 | 3.501×10^{-4} | -2.782×10^{-6} | 181 |
| Precise value | 0.837 | 0.780 | -61.7 | -0.777 | | | |
| $1/2^-$ resonance | | | | | | | |
| N = (2 - 3) | 1.371 | 5.384 | -20.0 | -0.126 | 3.562×10^{-3} | 4.878×10^{-5} | 174 |
| N = (2 - 4) | 1.752 | 5.533 | -15.5 | -0.362 | 4.711×10^{-3} | 1.821×10^{-5} | 155 |
| N = (2 - 5) | 1.718 | 5.559 | -15.8 | -0.330 | 4.566×10^{-3} | 2.446×10^{-5} | 157 |
| N = (2 - 10) | 1.688 | 5.556 | -16.1 | -0.309 | 4.459×10^{-3} | 2.810×10^{-5} | 90 |
| Precise value | 1.66 | 5.58 | -16.3 | -0.273 | | | |

Energies E_r and widths Γ of the $3/2^-$ and $1/2^-$ resonances, along with the scattering lengths a_l in the model problem of neutron scattering by alpha particle (given for various versions of the SS HORSE calculation are the parameters of the $\mathcal{R}_l^{(2)}$ parametrization and the root-mean-square deviations Ξ obtained by the fit)

5. CONCLUSIONS

In the present study, we have proposed a new approach to analyzing resonance states. This approach relies on the SS-HORSE method, which permits calculating phase shift by using the eigenenergy value alone. The parametrization constructed above for the phase shifts in the low-energy region based on analytic properties of partial-wave scattering amplitudes, makes it possible to describe correctly the behavior of these phase shifts not only in the resonance region but also for $E \rightarrow 0$.

Testing this method by applying it to the model problem of neutral-particle scattering, we have shown that, as the size of the truncated-Hamiltonian matrix corresponding to the internal region of the HORSE model space grows, the method provides a rapid convergence to precise results. The resonance energies and widths calculated for the above model problem agree with their precise counterparts.

The fact that the phase shifts in the low-energy region and the resonance parameters can be obtained by exclusively employing the results deduced from an analysis of the dependence of the energy of a continuum state on the harmonic-oscillator-basis parameters $\hbar\Omega$ and N, is obviously an advantage of the proposed method. The method can widely be used to study resonances and nuclear reactions in the region of low energies on the basis of microscopic calculations within the no-core shell model and within other models and approaches that involve harmonic-oscillator basis functions.

The method can be extended to the case of charged-particle scattering. An extension of the SS-HORSE method to the case of Coulomb scattering will be the subject of our next publication.

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