An improved variational method*

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Abstract In order to improve the unitarity of the S-matrix, an improved variational formulism is derived by proposing new generating functionals and adopting proper asymptotic boundary conditions for trial relative wave functions. The formulas with the weighted line-column balance for the single-channel and multi-channel scatterings, where the non-central interaction is implicitly considered, are presented. A numerical check is performed with a soluble model in a four coupled channel scattering problem. The result shows that the high accuracy and the unitarity of the S-matrix are reached.

Key words variational method, Galerkin variational method, scattering matrix, unitary

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1 Introduction

Nowadays, many new hadronic states have been found in high energy experiments. Many of them might have a molecular-like structure. Understanding the structures and properties of these states is a challenging problem for physicists. Because of the non-Abelian character of the fundamental strong interaction theory, Quantum Chromodynamics (QCD), one of the most efficient methods to solve this problem is using a QCD model theory, for instance the chiral constituent quark model. However, due to the complicated interactions between quarks, one has to solve it numerically rather than analytically. In order to solve the bound state problem reliably, one needs to fix model parameters by explaining the available experimental data as much as possible, so that the model has predictive power. Up to now, the available data are mostly scattering data. The variational method is a powerful and commonly used approximation method to treat the scattering problem[4, 10]. The basic mathematical descriptions of the variational method are the Ritz and Galerkin variational methods. In fact, M. Kamimura has proposed a variational procedure[9] which is the generation of the Kohn-Hulthén-Kato variational method for the S-matrix in nuclear reactions. In this paper, we try to improve the Kamimura's method by proposing a generating functional where the non-central interaction is explicitly included, adopting a proper asymptotic boundary condition, so that the unitarity and the symmetry of the S-matrix can be ensured, and considering the weighted line-column balance to increase the numerical accuracy. In Sect. 2, we present the method for the case of a single scattering channel with a central potential, and the method in the case of a single scattering channel with an additional non-central potential and in the multi-channel case in Sects. 3 and 4, respectively. Finally, we present a numerical check in Sect. 5.

2 Single scattering channel with central potential

We consider the scattering of two hadrons. In the case of a spinless hadron moving in a finite-ranged central force field, the radial Schrödinger equation can be written as

$$\hat{\boldsymbol{K}}_l \; u_l(r) = 0 \; , \tag{1}$$

with

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$$\hat{\boldsymbol{K}}_l = -\frac{\hbar^2}{2\mu}\frac{\mathrm{d}^2}{\mathrm{d}r^2}+\frac{\hbar^2}{2\mu}\frac{l(l+1)}{r^2}+V(r)-E \ , \quad (2)$$

$$k = \frac{\sqrt{2\mu E}}{\hbar}, \quad (3)$$

and $u_l(r)$ being the reduced radial wave function of the relative motion between two hadrons. Because the potential between two hadrons is finite-ranged, the asymptotic boundary condition for the outgoing radial wave function should be

$$u_l(r)|_{r\to 0} \longrightarrow 0 \ , \quad (4)$$

$$u_l(r)|_{r\to\infty} \longrightarrow \frac{1}{2\mathrm{i}k}\left[s_l\ \hat{h}_l^+(kr)-\hat{h}_l^-(kr)\right]. \quad (5)$$

Let us define an auxiliary functional[1]

$$\boldsymbol{J}[u] = \frac{\hbar^2}{2\mu}\ s-2\mathrm{i}k\ \left(u,\ \hat{\boldsymbol{K}}_l\ u\right), \quad (6)$$

with the inner product defined as

$$\left(u,\hat{\boldsymbol{K}}v\right) = \int_{r=0}^{\infty}\mathrm{d}r u(r)\hat{\boldsymbol{K}}v(r). \quad (7)$$

Now, let us carry out a similar procedure as shown in Kamimura's paper[9]. Take a trial wave function $u_t(r)$ which satisfies the asymptotic boundary condition

$$u_t(r)|_{r\to 0} \longrightarrow 0 \ , \quad (8)$$

$$u_t(r)|_{r\to\infty} \longrightarrow \frac{1}{2\mathrm{i}k}\left[s_t\hat{h}_l^+(kr)-\hat{h}_l^-(kr)\right] \ , \quad (9)$$

and expand it as

$$u_t(r) = \sum_{i=0}^{n}c_i\ u_i(r) \ , \quad (10)$$

where the basis function

$$u_i(r) = \begin{cases}\alpha_i\ u_i^{(in)}(r), & r<r_\mathrm{C}\\ \dfrac{1}{2ik}\left[s_i\ \hat{h}_l^+(kr)-\hat{h}_l^-(kr)\right], & r>r_\mathrm{C}\end{cases} \quad (11)$$

is a class C^1 function and satisfies

$$u_i(r)|_{r\longrightarrow 0} = 0 \ , \quad (12)$$

$$\hat{\boldsymbol{K}}_l\ u_i(r)|_{r>r_\mathrm{C}} = 0 \ . \quad (13)$$

Comparing Eqs. (8, 9 and 11), we obtain the relation

$$\sum_{i=0}^{n}c_i = 1 \ , \quad (14)$$

$$\sum_{i=0}^{n}c_i s_i = s_t \ , \quad (15)$$

and consequently

$$u_t(r) = u_0(r)+\sum_{i=1}^{n}c_i\left[u_i(r)-u_0(r)\right] \ , \quad (16)$$

$$\delta u_t(r) = \sum_{i=1}^{n}\delta c_i\left[u_i(r)-u_0(r)\right] \ . \quad (17)$$

Moreover, using the connection conditions for $u_i(r)$ at $r=r_\mathrm{C}$, we get the expressions for α_i and s_i

$$\alpha_i = \frac{1}{\left|\begin{matrix}\hat{h}_l^+(kr) & u_i^{(in)}(r)\\ \dfrac{\mathrm{d}}{\mathrm{d}r}\hat{h}_l^+(kr) & \dfrac{\mathrm{d}}{\mathrm{d}r}u_i^{(in)}(r)\end{matrix}\right|_{r=r_\mathrm{C}}} \ , \quad (18)$$

$$s_i = \frac{\left|\begin{matrix}\hat{h}_l^-(kr) & u_i^{(in)}(r)\\ \dfrac{\mathrm{d}}{\mathrm{d}r}\hat{h}_l^-(kr) & \dfrac{\mathrm{d}}{\mathrm{d}r}u_i^{(in)}(r)\end{matrix}\right|_{r=r_\mathrm{C}}}{\left|\begin{matrix}\hat{h}_l^+(kr) & u_i^{(in)}(r)\\ \dfrac{\mathrm{d}}{\mathrm{d}r}\hat{h}_l^+(kr) & \dfrac{\mathrm{d}}{\mathrm{d}r}u_i^{(in)}(r)\end{matrix}\right|_{r=r_\mathrm{C}}} \ . \quad (19)$$

Carrying out the Galerkin variation, we have

$$\delta\boldsymbol{J}[u_t] = -4\mathrm{i}k\left(\delta u_t,\ \hat{\boldsymbol{K}}_l\ u_t\right) = 0 \ , \quad (20)$$

namely

$$\left(\delta u,\hat{\boldsymbol{K}}_l u\right) = 0 \ . \quad (21)$$

With the definition

$$(\boldsymbol{K}_l)_{ij} = \left(u_i,\hat{\boldsymbol{K}}_l u_j\right), \quad (22)$$

we rewrite the above equation into the form of linear equations

$$\sum_{j=1}^{n}(\mathcal{K}_l)_{ij}c_j = (\mathcal{M}_l)_i \quad i=1,2,3,\cdots,n, \quad (23)$$

where

$$(\mathcal{K}_l)_{ij} = (\boldsymbol{K}_l)_{ij}-(\boldsymbol{K}_l)_{i0}-(\boldsymbol{K}_l)_{0j}+(\boldsymbol{K}_l)_{00}, \quad (24)$$

$$(\mathcal{M}_l)_i = (\boldsymbol{K}_l)_{00}-(\boldsymbol{K}_l)_{i0}, \quad (25)$$

and the integral kernel $\mathcal{K}_l$ and $\boldsymbol{K}_l$ have the symmetry properties

$$(\mathcal{K}_l)_{ij} = (\mathcal{K}_l)_{ji} \quad (26)$$

and

$$(\boldsymbol{K}_l)_{ij}-(\boldsymbol{K}_l)_{ji} = -\frac{\hbar^2}{2\mu}\frac{1}{2\mathrm{i}k}(s_i-s_j), \quad (27)$$

respectively.

For deriving the integral kernel $(\boldsymbol{K}_l)_{ij}$ conveniently, we rewrite the basis function as

$$u_i(r) = \alpha_i\left(u_i^{(in)}(r)+u_i^{(ex)}(r)\right), \quad (28)$$

with

$$\alpha_i u_i^{(ex)}(r) = \begin{cases} 0, & r < r_{\rm C} \\ \dfrac{1}{2{\rm i}k}\left[s_i \hat{h}_l^+(kr) - \hat{h}_l^-(kr)\right] - \alpha_i u_i^{(in)}(r), & r > r_{\rm C} \end{cases} . \quad (29)$$

Apparently,

$$\hat{\boldsymbol{K}}_l u_i^{(in)}(r)\Big|_{r>r_{\rm C}} = -\hat{\boldsymbol{K}}_l u_i^{(ex)}(r)\Big|_{r>r_{\rm C}} . \quad (30)$$

Substituting this basis function into the definition (22), we get

$$(\boldsymbol{K}_l)_{ij} = \alpha_i\alpha_j\left[\left(\boldsymbol{K}_l^{(in)}\right)_{ij} - \left(\boldsymbol{K}_l^{(ex)}\right)_{ij}\right], \quad (31)$$

where

$$\left(\boldsymbol{K}_l^{(in)}\right)_{ij} = \int_{r=0}^{\infty} u_i^{(in)}(r)\hat{\boldsymbol{K}}_l u_j^{(in)}(r){\rm d}r , \quad (32)$$

$$\left(\boldsymbol{K}_l^{(ex)}\right)_{ij} = \int_{r=r_{\rm C}}^{\infty} u_i^{(in)}(r)\hat{\boldsymbol{K}}_l u_j^{(in)}(r){\rm d}r . \quad (33)$$

If we take

$$u_i^{(in)}(r) = 4\pi r\left(\frac{\mu\omega}{\pi}\right)^{\frac{3}{4}}\exp\left[-\frac{\mu\omega}{2}(r^2+S_i^2)\right]\times i_l(\mu\omega S_i r) , \quad (34)$$

where i_l is the l-th modified spherical Bessel function, $\left(\boldsymbol{K}_l^{(in)}\right)_{ij}$ can be calculated analytically and the correction part $\left(\boldsymbol{K}_l^{(ex)}\right)_{ij}$ should be evaluated numerically.

It should especially be mentioned that due to

$$u_i^{(in)}(r)\Big|_{r\to\infty} \propto \exp\left[\mu\omega S_i r - \frac{\mu\omega}{2}(r^2+S_i^2)\right]$$

and

$$\hat{h}_l^{\pm}(kr)|_{r\to\infty} \longrightarrow \exp\left[\pm{\rm i}\left(kr - l\frac{\pi}{2}\right)\right],$$

the value of α_i, and consequently the matrix element $(\boldsymbol{K}_l)_{ij}$, would severely increase with increasing $r_{\rm C}$, but not

$$\left(\tilde{\boldsymbol{K}}_l\right)_{ij} = \left(\boldsymbol{K}_l^{(in)}\right)_{ij} - \left(\boldsymbol{K}_l^{(ex)}\right)_{ij}. \quad (35)$$

Therefore, to make the calculation reliable, we further perform the operation of the weighted line-column balance. Define

$$\left(\tilde{\mathcal{K}}_l\right)_{ij} = \frac{1}{\alpha_i\alpha_j}(\mathcal{K}_l)_{ij}, \quad (36)$$

$$\left(\tilde{\mathcal{M}}_l\right)_i = \frac{1}{\alpha_i}(\mathcal{M}_l)_i, \quad (37)$$

$$\tilde{c}_j = \alpha_j c_j, \quad (38)$$

then

$$\begin{aligned}\left(\tilde{\mathcal{K}}_l\right)_{ij} = & \left[\left(\boldsymbol{K}_l^{(in)}\right)_{ij} - \left(\boldsymbol{K}_l^{(ex)}\right)_{ij}\right] - \\ & \frac{\alpha_0}{\alpha_j}\left[\left(\boldsymbol{K}_l^{(in)}\right)_{i0} - \left(\boldsymbol{K}_l^{(ex)}\right)_{i0}\right] - \\ & \frac{\alpha_0}{\alpha_i}\left[\left(\boldsymbol{K}_l^{(in)}\right)_{0j} - \left(\boldsymbol{K}_l^{(ex)}\right)_{0j}\right] + \\ & \frac{\alpha_0\alpha_0}{\alpha_i\alpha_j}\left[\left(\boldsymbol{K}_l^{(in)}\right)_{00} - \left(\boldsymbol{K}_l^{(ex)}\right)_{00}\right], \quad (39)\end{aligned}$$

$$\begin{aligned}\left(\tilde{\mathcal{M}}_l\right)_i = & \frac{\alpha_0\alpha_0}{\alpha_i}\left[\left(\boldsymbol{K}_l^{(in)}\right)_{00} - \left(\boldsymbol{K}_l^{(ex)}\right)_{00}\right] - \\ & \alpha_0\left[\left(\boldsymbol{K}_l^{(in)}\right)_{i0} - \left(\boldsymbol{K}_l^{(ex)}\right)_{i0}\right]. \quad (40)\end{aligned}$$

Finally, we obtain the linear equations

$$\sum_{j=1}^{n}\left(\tilde{\mathcal{K}}_l\right)_{ij}\tilde{c}_j = \left(\tilde{\mathcal{M}}_l\right)_i \quad i=1,2,3,\cdots,n . \quad (41)$$

Solving these coupled equations for $\tilde{c}_j$'s, we can evaluate

$$\boldsymbol{J}[c_1,c_2,\cdots,c_n] = \frac{\hbar^2}{2\mu}\sum_{i=0}^{n}c_i s_i - 2{\rm i}k\sum_{i=0}^{n}c_i(\boldsymbol{K}_l)_{0i} ,$$

and subsequently the stationary value of the S-matrix

$$\boldsymbol{S}_{\rm st} = \sum_{i=0}^{n}c_i s_i - \frac{2\mu}{\hbar^2}\cdot 2{\rm i}k\sum_{i=0}^{n}c_i(\boldsymbol{K}_l)_{0i} . \quad (42)$$

3 Single scattering channel with non-central potential

We first define an operator as

$$\hat{\boldsymbol{K}} = \begin{pmatrix} -\dfrac{\hbar^2}{2\mu}\dfrac{{\rm d}^2}{{\rm d}r^2} + \dfrac{\hbar^2}{2\mu}\dfrac{l_1(l_1+1)}{r^2} + V_{l_1l_1}(r) - E & V_{l_1l_2}(r) \\ V_{l_2l_1}(r) & -\dfrac{\hbar^2}{2\mu}\dfrac{{\rm d}^2}{{\rm d}r^2} + \dfrac{\hbar^2}{2\mu}\dfrac{l_2(l_2+1)}{r^2} + V_{l_2l_2}(r) - E \end{pmatrix}, \quad (43)$$

the wave function as

$$\boldsymbol{u}^{(l_1)} = \begin{pmatrix} u_{l_1} \\ u_{l_2} \end{pmatrix}^{(l_1)} = \begin{pmatrix} u_{l_1}^{(l_1)} \\ u_{l_2}^{(l_1)} \end{pmatrix}, \quad (44)$$

where the superscript (subscript) indicates the orbital angular momentum of the incoming (outgoing) partial-wave, and write the coupled channel Schrödinger equation as

$$\begin{cases} \left(\hat{\boldsymbol{K}}\right)_{l_1l_1} u_{l_1}^{(l_1)}(r) + \left(\hat{\boldsymbol{K}}\right)_{l_1l_2} u_{l_2}^{(l_1)}(r) = 0 \\ \left(\hat{\boldsymbol{K}}\right)_{l_2l_1} u_{l_1}^{(l_2)}(r) + \left(\hat{\boldsymbol{K}}\right)_{l_1l_2} u_{l_2}^{(l_2)}(r) = 0 \end{cases} . \quad (45)$$

Now we construct a generating functional for the S-matrix

$$\boldsymbol{J}\left[\boldsymbol{u}^{(l_1)}, \boldsymbol{u}^{(l_2)}\right] = \frac{\hbar^2}{2\mu}\boldsymbol{S}_{l_1l_2} - 2\mathrm{i}k\left(\boldsymbol{u}^{(l_1)}, \hat{\boldsymbol{K}}\boldsymbol{u}^{(l_2)}\right), \quad (46)$$

where $\boldsymbol{u}_{l_\delta}^{(l_\gamma)}$ satisfies the asymptotic boundary condition

$$\begin{cases} u_{l_\delta}^{(l_\gamma)}(r)\Big|_{r\to 0} \longrightarrow 0 \\ u_{l_\delta}^{(l_\gamma)}(r)\Big|_{r\to\infty} \longrightarrow \frac{1}{2\mathrm{i}k}\left[\boldsymbol{S}_{l_\delta l_\gamma}\hat{h}_{l_\delta}^{+}(kr) - \delta_{l_\delta l_\gamma}\hat{h}_{l_\delta}^{-}(kr)\right] \end{cases} , \quad (47)$$

and

$$\boldsymbol{J}\left[u^{(l_1)}, u^{(l_2)}\right] = \boldsymbol{J}\left[u^{(l_2)}, u^{(l_1)}\right]. \quad (48)$$

By a similar procedure as in the last section, we get the relations

$$\sum_{i=0}^{n_{l_\delta}} c_{l_\delta i}^{(l_\gamma)} = \delta_{l_\delta l_\gamma} , \quad (49)$$

$$\sum_{i=0}^{n_{l_\delta}} c_{l_\delta i}^{(l_\gamma)} s_{l_\delta i} = (\boldsymbol{S}_t)_{l_\delta l_\gamma} , \quad (50)$$

and

$$\alpha_{l_\delta i} = \frac{1}{\begin{vmatrix} \hat{h}_{l_\delta}^{+}(kr) & u_{l_\delta i}^{(in)}(r) \\ \frac{\mathrm{d}}{\mathrm{d}r}\hat{h}_{l_\delta}^{+}(kr) & \frac{\mathrm{d}}{\mathrm{d}r}u_{l_\delta i}^{(in)}(r) \end{vmatrix}_{r=r_\mathrm{C}}} , \quad (51)$$

$$s_{l_\delta i} = \frac{\begin{vmatrix} \hat{h}_{l_\delta}^{-}(kr) & u_{l_\delta i}^{(in)}(r) \\ \frac{\mathrm{d}}{\mathrm{d}r}\hat{h}_{l_\delta}^{-}(kr) & \frac{\mathrm{d}}{\mathrm{d}r}u_{l_\delta i}^{(in)}(r) \end{vmatrix}_{r=r_\mathrm{C}}}{\begin{vmatrix} \hat{h}_{l_\delta}^{+}(kr) & u_{l_\delta i}^{(in)}(r) \\ \frac{\mathrm{d}}{\mathrm{d}r}\hat{h}_{l_\delta}^{+}(kr) & \frac{\mathrm{d}}{\mathrm{d}r}u_{l_\delta i}^{(in)}(r) \end{vmatrix}_{r=r_\mathrm{C}}} . \quad (52)$$

Defining integral kernels

$$\boldsymbol{K}_{l_\gamma i, l_\delta j}^{(in)} = \int_{r=0}^{\infty} u_{l_\gamma i}^{(in)}(r)\hat{\boldsymbol{K}}u_{l_\delta j}^{(in)}(r)\mathrm{d}r \quad (53)$$

and the external correction

$$\boldsymbol{K}_{l_\gamma i, l_\delta j}^{(ex)} = \delta_{l_\gamma l_\delta}\int_{r=r_{l_\gamma C}}^{\infty} u_{l_\gamma i}^{(in)}(r)\hat{\boldsymbol{K}}u_{l_\gamma j}^{(in)}(r)\mathrm{d}r , \quad (54)$$

we get

$$\boldsymbol{K}_{l_\gamma i, l_\delta j} = \alpha_{l_\gamma i}\alpha_{l_\delta j}\left[\boldsymbol{K}_{l_\gamma i, l_\delta j}^{(in)} - \boldsymbol{K}_{l_\gamma i, l_\delta j}^{(ex)}\right]. \quad (55)$$

Carrying out the Galerkin variation, the coupled linear equations are obtained as

$$\begin{cases} \sum_{j=1}^{n_{l_\gamma}} \mathcal{K}_{l_\gamma i, l_\gamma j} c_{l_\gamma j}^{(l_\gamma)} + \sum_{j=1}^{n_{l_\delta}} \mathcal{K}_{l_\gamma i, l_\delta j} c_{l_\delta j}^{(l_\gamma)} = \mathcal{M}_{l_\gamma i}^{(l_\gamma)} \\ \sum_{j=1}^{n_{l_\gamma}} \mathcal{K}_{l_\delta i, l_\gamma j} c_{l_\delta j}^{(l_\gamma)} + \sum_{j=1}^{n_{l_\delta}} \mathcal{K}_{l_\delta i, l_\delta j} c_{l_\delta j}^{(l_\gamma)} = \mathcal{M}_{l_\delta i}^{(l_\gamma)} \end{cases} . \quad (56)$$

Solving these equations for $c_{l_\delta j}^{(l_\gamma)}$'s, one finally obtains the S-matrix elements

$$(\boldsymbol{S}_\mathrm{st})_{l_\gamma l_\gamma} = \sum_{i=0}^{n_{l_\gamma}} c_{l_\gamma i}^{(l_\gamma)} s_{l_\gamma i} - \frac{2\mu}{\hbar^2}\cdot 2\mathrm{i}k\sum_{i=0}^{n_{l_\gamma}} \boldsymbol{K}_{l_\gamma 0, l_\gamma i} c_{l_\gamma i}^{(l_\gamma)} - \frac{2\mu}{\hbar^2}\cdot 2\mathrm{i}k\sum_{i=0}^{n_{l_\delta}} \boldsymbol{K}_{l_\gamma 0, l_\delta i} c_{l_\delta i}^{(l_\gamma)} , \quad (57)$$

$$(\boldsymbol{S}_\mathrm{st})_{l_\delta l_\delta} = \sum_{i=0}^{n_{l_\delta}} c_{l_\delta i}^{(l_\delta)} s_{l_\delta i} - \frac{2\mu}{\hbar^2}\cdot 2\mathrm{i}k\sum_{i=0}^{n_{l_\gamma}} \boldsymbol{K}_{l_\delta 0, l_\gamma i} c_{l_\gamma i}^{(l_\delta)} - \frac{2\mu}{\hbar^2}\cdot 2\mathrm{i}k\sum_{i=0}^{n_{l_\delta}} \boldsymbol{K}_{l_\delta 0, l_\delta i} c_{l_\delta i}^{(l_\delta)} , \quad (58)$$

$$(\boldsymbol{S}_\mathrm{st})_{l_\gamma l_\delta} = \sum_{i=0}^{n_{l_\gamma}} c_{l_\gamma i}^{(l_\delta)} s_{l_\gamma i} - \frac{2\mu}{\hbar^2}\cdot 2\mathrm{i}k\sum_{i=0}^{n_{l_\gamma}} \boldsymbol{K}_{l_\gamma 0, l_\gamma i} c_{l_\gamma i}^{(l_\delta)} - \frac{2\mu}{\hbar^2}\cdot 2\mathrm{i}k\sum_{i=0}^{n_{l_\delta}} \boldsymbol{K}_{l_\gamma 0, l_\delta i} c_{l_\delta i}^{(l_\delta)} . \quad (59)$$

4 Multiple scattering channels

Similar to the derivation in the last section, we define operators

$$\begin{cases} \left(\hat{\boldsymbol{K}}_l\right)_{ii} = -\frac{\hbar^2}{2\mu_i}\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{\hbar^2}{2\mu_i}\frac{l(l+1)}{r^2} + V_{ii}(r) + M_i - E \\ \left(\hat{\boldsymbol{K}}_l\right)_{ij} = V_{ij}(r) \qquad i \neq j \end{cases} \quad (60)$$

and the wave function with orbital angular momentum l

$$\boldsymbol{u}_l^{(m)} = \begin{pmatrix} u_{1l}^{(m)} \\ u_{2l}^{(m)} \\ \cdots \\ u_{N_\mathrm{C}l}^{(m)} \end{pmatrix}, \quad (61)$$

with the superscript (subscript) indicating the incoming (outgoing) channel. To ensure the unitarity and symmetry of the S-matrix, we use the following boundary condition

$$\begin{cases} u_i^{(m)}(r)\Big|_{r\to 0} \longrightarrow 0 \\ u_i^{(m)}(r)\Big|_{r\to\infty} \longrightarrow \dfrac{1}{2\mathrm{i}k_i}\sqrt{\dfrac{\mu_i k_i}{\mu_m k_m}}\times \\ \qquad\qquad \left[s_{im}\hat{h}_l^{+}(k_i r)-\delta_{im}\hat{h}_l^{-}(k_i r)\right] \end{cases}. \quad (62)$$

Then the auxiliary functional for the S-matrix of the multichannel scattering can be written as

$$\boldsymbol{J}\left[\boldsymbol{u}^{(m)},\boldsymbol{u}^{(n)}\right] = \frac{\hbar^2}{2}\sqrt{\frac{1}{\mu_m\mu_n}}s_{mn} - 2\mathrm{i}\sqrt{k_m k_n}\left(\boldsymbol{u}^{(m)},\hat{\boldsymbol{K}}_l\boldsymbol{u}^{(n)}\right), \quad (63)$$

with

$$\left(\boldsymbol{u}_l^{(m)},\boldsymbol{K}_l\boldsymbol{u}_l^{(n)}\right) = \sum_{i=1}^{N_{\mathrm{C}}}\sum_{j=1}^{N_{\mathrm{C}}}\left(u_i^{(m)},\hat{\boldsymbol{K}}_l u_j^{(n)}\right)$$

and

$$\boldsymbol{J}\left[\boldsymbol{u}^{(m)},\boldsymbol{u}^{(n)}\right] = \boldsymbol{J}\left[\boldsymbol{u}^{(n)},\boldsymbol{u}^{(m)}\right]. \quad (64)$$

By expanding the trial wave function with the similar basis functions as shown in the former sections, we obtain the relations

$$\sum_{i=0}^{n_p} c_{pi}^{(m)} = \delta_{pm}, \quad (65)$$

$$\sum_{i=0}^{n_p} c_{pi}^{(m)} s_{pi} = \sqrt{\frac{\mu_p k_p}{\mu_m k_m}}\,(s_{\mathrm{t}})_{pm}. \quad (66)$$

Using the connection conditions, we get

$$\alpha_{pi} = \frac{1}{\begin{vmatrix} \hat{h}_l^{+}(k_p r) & u_{pi}^{(in)}(r) \\ \dfrac{\mathrm{d}}{\mathrm{d}r}\hat{h}_l^{+}(k_p r) & \dfrac{\mathrm{d}}{\mathrm{d}r}u_{pi}^{(in)}(r)\end{vmatrix}_{r=r_{\mathrm{C}}}}, \quad (67)$$

and

$$s_{pi} = \frac{\begin{vmatrix} \hat{h}_l^{-}(k_p r) & u_{pi}^{(in)}(r) \\ \dfrac{\mathrm{d}}{\mathrm{d}r}\hat{h}_l^{-}(k_p r) & \dfrac{\mathrm{d}}{\mathrm{d}r}u_{pi}^{(in)}(r)\end{vmatrix}_{r=r_{\mathrm{C}}}}{\begin{vmatrix} \hat{h}_l^{+}(k_p r) & u_{pi}^{(in)}(r) \\ \dfrac{\mathrm{d}}{\mathrm{d}r}\hat{h}_l^{+}(k_p r) & \dfrac{\mathrm{d}}{\mathrm{d}r}u_{pi}^{(in)}(r)\end{vmatrix}_{r=r_{\mathrm{C}}}}. \quad (68)$$

Apparently, this formulation ensures the unitarity of the S-matrix. Denoting the integral kernel as

$$(\boldsymbol{K}_l)_{pi,qj} = \int_{r=0}^{\infty} u_{pi}(r)\hat{\boldsymbol{K}}_l u_{qj}(r)\mathrm{d}r, \quad (69)$$

we can also prove the symmetry relation

$$(\boldsymbol{K}_l)_{pi,qj} - (\boldsymbol{K}_l)_{qj,pi} = -\frac{\hbar^2}{2\mu_p}\frac{1}{2\mathrm{i}k_p}(s_{pi}-s_{pj})\,\delta_{pq} \quad (70)$$

and provide a formula for the kernel as

$$(\boldsymbol{K}_l)_{pi,qj} = \alpha_{pi}\alpha_{qj}\left[\left(\boldsymbol{K}_l^{(in)}\right)_{pi,qj} - \left(\boldsymbol{K}_l^{(ex)}\right)_{pi,qj}\right], \quad (71)$$

with

$$\left(\boldsymbol{K}_l^{(in)}\right)_{pi,qj} = \int_{r=0}^{\infty} u_{pi}^{(in)}(r)\hat{\boldsymbol{K}}_l u_{qj}^{(in)}(r)\mathrm{d}r \quad (72)$$

and

$$\left(\boldsymbol{K}_l^{(ex)}\right)_{pi,qj} = \delta_{pq}\int_{r=r_{p\mathrm{C}}}^{\infty} u_{pi}^{(in)}(r)\boldsymbol{K}_l u_{pj}^{(in)}(r)\mathrm{d}r. \quad (73)$$

Carrying out the Galerkin variational procedure, we arrive at the final coupled linear equations

$$\sum_{q=1}^{N_{\mathrm{C}}}\sum_{j=1}^{n_q}\left(\tilde{\mathcal{K}}_l\right)_{pi,qj}\tilde{c}_{qj}^{(n)} = \left(\tilde{\mathcal{M}}_l^{(n)}\right)_{pi} \qquad i=1,2,3,\cdots,n, \quad (74)$$

with

$$\begin{aligned}\left(\tilde{\mathcal{K}}_l\right)_{pi,qj} = &\left[\left(\boldsymbol{K}_l^{(in)}\right)_{pi,qj} - \left(\boldsymbol{K}_l^{(ex)}\right)_{pi,qj}\right] - \\ &\frac{\alpha_{q0}}{\alpha_{qj}}\left[\left(\boldsymbol{K}_l^{(in)}\right)_{pi,q0} - \left(\boldsymbol{K}_l^{(ex)}\right)_{pi,q0}\right] - \\ &\frac{\alpha_{p0}}{\alpha_{pi}}\left[\left(\boldsymbol{K}_l^{(in)}\right)_{p0,qj} - \left(\boldsymbol{K}_l^{(ex)}\right)_{p0,qj}\right] + \\ &\frac{\alpha_{p0}\alpha_{q0}}{\alpha_{pi}\alpha_{qj}}\left[\left(\boldsymbol{K}_l^{(in)}\right)_{p0,q0} - \left(\boldsymbol{K}_l^{(ex)}\right)_{p0,q0}\right]\end{aligned} \quad (75)$$

and

$$\begin{aligned}\left(\tilde{\mathcal{M}}_l^{(n)}\right)_{pi} = &\frac{\alpha_{p0}\alpha_{q0}}{\alpha_{pi}}\left[\left(\boldsymbol{K}_l^{(in)}\right)_{p0,q0} - \left(\boldsymbol{K}_l^{(ex)}\right)_{p0,q0}\right] - \\ &\alpha_{q0}\left[\left(\boldsymbol{K}_l^{(in)}\right)_{pi,q0} - \left(\boldsymbol{K}_l^{(ex)}\right)_{pi,q0}\right],\end{aligned} \quad (76)$$

and the stationary value of the S-matrix

$$(\boldsymbol{S}_{st})_{mn} = \sqrt{\frac{\mu_n k_n}{\mu_m k_m}}\sum_{i=0}^{n_m} c_{mi}^{(n)} s_{mi} - \frac{4\mathrm{i}}{\hbar^2}\sqrt{\mu_m k_m \mu_n k_n}\sum_{q=1}^{N_{\mathrm{C}}}\sum_{j=0}^{n_q}\left(\hat{\boldsymbol{K}}_l\right)_{m0,qj} c_{qj}^{(n)}. \quad (77)$$

5 Numerical check with a soluble model

Here, we employ a square-well potential as the soluble model to examine the accuracy of the derived variational method. We calculate the scattering process with a four coupled channel and a potential

$$V(r)=\begin{cases} -\begin{pmatrix} -10 & -200 & -50 & 50 \\ -200 & -20 & -100 & 70 \\ -50 & -100 & -30 & 38 \\ 50 & 70 & 38 & -40 \end{pmatrix} & r<2\ \text{fm} \\ 0 & r>2\ \text{fm} \end{cases}. \tag{78}$$

The masses of the particles a and b in different channels are tabulated in Table 1. We first solved this scattering problem analytically[1]. The resultant values of the S-matrix are tabulated in Table 2. Then, we calculated the values of the S-matrix with the derived variational method by employing 10 trial basis functions with a local Gaussian shape[1]. The results are also tabulated in Table 2. From this table, one sees that the accuracy of the S-matrix elements from the derived variational method is quite high and can reach at least 7 significant digits. One also finds that the S-matrix is unitary by calculating

$$\sum_{i=1}^{4}|S_{i1}|^2 = 1 \tag{79}$$

and symmetric by equation (64).

Table 1. The masses of the particles a and b in different channels.

channel number	m_a/MeV	m_b/MeV
1	170	180
2	110	250
3	150	220
4	155	225

In summary, in order to improve the unitarity of the S-matrix, an improved variational formalism is derived by proposing new generating functionals and adopting proper asymptotic boundary conditions for the trial relative wave functions. Formulae with the weighted line-column balance for the single-channel and multi-channel scatterings, where the non-central interaction is implicitly considered, were presented. A numerical check has been performed with a soluble model in a four coupled channel scattering problem. The result shows that high accuracy and the unitarity of the S-matrix are reached.

Table 2. The values of S-matrix elements in a four coupled channel scattering problem with a square well potential. The incoming channel is number 1.

		30 MeV	90 MeV
S_{11}	analytical solution	(0.4473515, −0.68056643)	(6.895854×10^{-2}, −0.448038367)
	variational method	(0.4473519, −0.68056645)	(6.895851×10^{-2}, −0.448038363)
S_{21}	analytical solution	(−0.343851265, −0.13108581)	(−0.464547, 0.347278435)
	variational method	(−0.343851259, −0.13108579)	(−0.464547, 0.347278439)
S_{31}	analytical solution	(−0.262105725, −0.24491177)	(−0.51804951, -7.1553477×10^{-2})
	variational method	(−0.262105728, −0.24491176)	(−0.51804952, -7.1553476×10^{-2})
S_{41}	analytical solution	(0.1949905898, 0.185973840)	(0.423895405, 7.0125298×10^{-2})
	variational method	(0.1949905849, 0.185973836)	(0.423895404, 7.0125293×10^{-2})
		150 MeV	**500 MeV**
S_{11}	analytical solution	(1.4212612×10^{-2}, −0.272897362)	(0.364338585, -6.2302472×10^{-2})
	variational method	(1.4212618×10^{-2}, −0.272897344)	(0.364338581, -6.2302473×10^{-2})
S_{21}	analytical solution	(−0.31520531, 0.61034166)	(0.154766900, 0.817862838)
	variational method	(−0.31520530, 0.61034163)	(0.154766899, 0.817862832)
S_{31}	analytical solution	(−0.524048564, 6.7681866×10^{-2})	(−0.2757592835, 0.174463445)
	variational method	(−0.524048557, 6.7681872×10^{-2})	(−0.2757592853, 0.174463443)
S_{41}	analytical solution	(0.414182052, -5.1953794×10^{-2})	(0.18481194, −0.172879302)
	variational method	(0.414182048, -5.1953793×10^{-2})	(0.18481194, −0.172879304)

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