Spurious states in the Faddeev formalism for few-body systems

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We discuss the appearance of spurious solutions of few-body equations for Faddeev amplitudes. The identification of spurious states, i.e., states that lack the symmetry required for solutions of the Schrödinger equation, as well as the symmetrization of the Faddeev equations is investigated. As an example, systems of three and four electrons, bound in a harmonic-oscillator potential and interacting by the Coulomb potential, are presented. [S0556-2813(99)05002-5]

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I. INTRODUCTION

One of the most viable approaches for solving the few-body problem is the Faddeev method [1]. It has been successfully applied to solve the three-nucleon bound-state problem for various nucleon-nucleon potentials [2–5]. The most complex calculations of this kind include up to 50 channels, when all the $j \leqslant 6$ waves are taken into account [6].

The Hamiltonian in the Schrödinger equation is Hermitian and the solutions for a system of fermions, for example, are antisymmmetrized. On the other hand, the Faddeev equations are non-Hermitian and the trial wave functions used for a system of fermions, e.g., are not fully antisymmetrized. Also, there are three Faddeev equations for the three-body system acting on the same variables as in the Schrödinger equation. One, therefore, could expect that there should be three times as many solutions as for the Schrödinger equation. Then, it is not surprising that spurious solutions of the Faddeev equations exist. A spurious solution is an eigenstate, which does not have the symmetry required by the Schrödinger equation, e.g., antisymmetry for a system of identical fermions. A spurious component in a solution of the Faddeev equations was found analytically for the first time for the ground state of three identical particles bound in the harmonic-oscillator (HO) potential by Friar *et al.* [7]. Spurious components of the Faddeev amplitudes were then observed also for the excited states in extensions of this work for three identical particles [8], three nonidentical particles [9], as well as for four identical spinless particles [10]. Spurious solutions of Faddeev-like equations were investigated by Evans and Hoffman [11], and the existence of spurious solutions of Faddeev equations for three identical particles was recently demonstrated by Rudnev and Yakovlev [12]. In Ref. [12] such solutions were constructed for states of zero total angular momentum. In addition, spurious solutions of the Faddeev equations for three nonidentical particles interacting by central potentials were investigated by Pupyshev [13]. In Ref. [14], we noted the appearance of spurious solutions, whose number exceeded the number of physical solutions, of the Faddeev equations for a three-nucleon system solved in an HO basis in a shell-model approach. Also, a spurious solution was reported recently in a three-body model calculation of ${}^{9}_{\Lambda}$Be [15].

In the present paper we investigate the appearance of spurious states in the Faddeev formalism and their identification in a systematic manner. We use three- and four-electron systems bound in an HO potential as an example for illustration and quantification of the problem.

In Sec. II we discuss the three fermion system. A generalization for the four-body system is presented in Sec. III. Conclusions are given in Sec. IV.

II. THREE-BODY SYSTEM

Our discussion is quite general. However, we prefer to illustrate our points by using a particular simple example, namely, a system of electrons bound by an HO potential and interacting by the Coulomb potential. We consider, therefore, the following Hamiltonian:

$$H=\sum_{i=1}^{A}\left[\frac{\vec{p}_i^{\,2}}{2m}+\frac{1}{2}m\Omega^2\vec{r}_i^{\,2}\right]+\sum_{i<j}^{A}V_{\mathrm{C}}(\vec{r}_i-\vec{r}_j). \tag{1}$$

Eigenstates of the Hamiltonian (1) are antisymmetric with respect to the exchange of any electron pair.

In the Faddeev formalism for a system of three identical particles, i.e., $A=3$, the following transformation of the coordinates

$$\vec{r}=\sqrt{\frac{1}{2}}(\vec{r}_1-\vec{r}_2), \tag{2a}$$

$$\vec{y}=\sqrt{\frac{2}{3}}\left[\frac{1}{2}(\vec{r}_1+\vec{r}_2)-\vec{r}_3\right], \tag{2b}$$

and, similarly, of the momenta, is introduced. It brings the one-body HO Hamiltonian from Eq. (1) into the form

$$H_0=\frac{\vec{p}^{\,2}}{2m}+\frac{1}{2}m\Omega^2\vec{r}^{\,2}+\frac{\vec{q}^{\,2}}{2m}+\frac{1}{2}m\Omega^2\vec{y}^{\,2}, \tag{3}$$

with the trivial center-of-mass term omitted. Eigenstates of H_0,

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$$|nlsj,\mathcal{N}\mathcal{L}\mathcal{J},J\rangle, \tag{4}$$

can be used as the basis for the Faddeev calculation. Here n,l and $\mathcal{N},\mathcal{L}$ are the HO quantum numbers corresponding to the harmonic oscillators associated with the coordinates and momenta $\vec{r},\vec{p}$ and $\vec{y},\vec{q}$, respectively. The quantum numbers s,j describe the spin and angular momentum of the relative-coordinate partial channel of particles 1 and 2, $\mathcal{J}$ is the angular momentum of the third particle relative to the center of mass of particles 1 and 2 and J is the total angular momentum. It is obvious that the basis (4) (similarly for trial states used in traditional Faddeev calculations), while antisymmetrized with respect to the exchange of particles $1\leftrightarrow 2$, is not antisymmetrized with respect to the exchanges of particles $1\leftrightarrow 3$ and $2\leftrightarrow 3$. On the other hand, the physical solutions corresponding to the solutions of the Schrödinger equation must be totally antisymmetrized. For our example system, the states (4) form a complete orthonormal basis. The physical solutions are such linear combinations of the basis states that have the proper antisymmetry for all the particle exchanges. On the other hand, one must expect that there are more basis states (4) than the total possible number of linearly independent antisymmetrized linear combinations of the states (4). Consequently, it is natural that spurious states will appear, when the calculation is performed using a basis of the type (4).

The first Faddeev equation can be written in the differential form as

$$(H_0+V_3-E)\phi_3=-V_3(\phi_1+\phi_2), \tag{5}$$

where V_3 is the two-body interaction between particles 1 and 2 and ϕ_1, ϕ_2, and ϕ_3 are the three Faddeev components. The other two Faddeev equations are cyclical versions of Eq. (5). Equation (5) can be rewritten in the form

$$\tilde{H}|\psi\rangle_{\mathrm{K}}=E|\psi\rangle_{\mathrm{K}}, \tag{6}$$

with

$$\tilde{H}=H_0+V(\vec{r})\mathcal{T}. \tag{7}$$

Here, $V(\vec{r})$ is the interaction between particles 1 and 2, e.g., V_3 of Eq. (5) or $V_{\mathrm{C}}(\sqrt{2}\vec{r})$ of Eq. (1); $|\psi\rangle_{\mathrm{K}}$ corresponds to the Faddeev amplitude ϕ_3 in Eq. (5); and $\mathcal{T}$, which has the properties of a metric operator [3,16], is given by

$$\mathcal{T}=1+\mathcal{T}^{(-)}+\mathcal{T}^{(+)}, \tag{8}$$

with $\mathcal{T}^{(+)}$ and $\mathcal{T}^{(-)}$ the cyclic and the anticyclic permutation operators, respectively.

For the basis (4), which we use as an example in the present paper, we obtain a formula for the matrix elements of $\mathcal{T}^{(-)}+\mathcal{T}^{(+)}$ by simplification of the expression (10) in Ref. [14], namely

$$\begin{aligned}
&\langle n_1 l_1 s_1 j_1,\mathcal{N}_1\mathcal{L}_1\mathcal{J}_1,J|\mathcal{T}^{(-)}+\mathcal{T}^{(+)}|n_2 l_2 s_2 j_2,\mathcal{N}_2\mathcal{L}_2\mathcal{J}_2,J\rangle \\
&\quad=\delta_{N_1,N_2}\sum_{LS}\hat{L}^2\hat{S}^2\hat{j}_1\hat{j}_2\hat{\mathcal{J}}_1\hat{\mathcal{J}}_2\hat{s}_1\hat{s}_2(-1)^L
\begin{Bmatrix} l_1 & s_1 & j_1 \\ \mathcal{L}_1 & \frac{1}{2} & \mathcal{J}_1 \\ L & S & J \end{Bmatrix}
\begin{Bmatrix} l_2 & s_2 & j_2 \\ \mathcal{L}_2 & \frac{1}{2} & \mathcal{J}_2 \\ L & S & J \end{Bmatrix}
\begin{Bmatrix} \frac{1}{2} & \frac{1}{2} & s_1 \\ \frac{1}{2} & S & s_2 \end{Bmatrix} \\
&\quad\times[(-1)^{s_1+s_2-\mathcal{L}_1-l_1}\langle\mathcal{N}_1\mathcal{L}_1 n_1 l_1 L|n_2 l_2\mathcal{N}_2\mathcal{L}_2 L\rangle_3+\langle n_1 l_1\mathcal{N}_1\mathcal{L}_1 L|\mathcal{N}_2\mathcal{L}_2 n_2 l_2 L\rangle_3],
\end{aligned} \tag{9}$$

where $N_i=2n_i+l_i+2\mathcal{N}_i+\mathcal{L}_i$, $i\equiv 1,2$, $\hat{j}=\sqrt{2j+1}$ and $\langle\mathcal{N}_1\mathcal{L}_1 n_1 l_1 L|n_2 l_2\mathcal{N}_2\mathcal{L}_2 L\rangle_3$ is the general HO bracket for two particles with mass ratio 3 as defined, e.g., in Ref. [17]. Similar expressions for different bases are described, e.g., in Refs. [18,19]. It follows from the symmetry properties of the states (4) and of the HO brackets that the contributions of $\mathcal{T}^{(-)}$ and $\mathcal{T}^{(+)}$ in Eq. (9) are identical.

We note that the eigensystem of the operator $\mathcal{T}$ (8) consists of two subspaces. The first subspace has eigenstates with the eigenvalue 3, which form totally antisymmetric physical states, while the second subspace has eigenstates with the eigenvalue 0, which form a not completely antisymmetric, unphysical subspace of states. Although we found these properties of $\mathcal{T}$ by direct calculation using the relation (9), it is, in fact, a general result. The same structure of eigenstates was also reported in Ref. [12] using a different basis. The eigenvalue structure follows from the fact that $\frac{1}{3}\mathcal{T}$ has the properties of a projection operator.

The Hamiltonian $\tilde{H}$ (7) is non-Hermitian. By solving Eq. (6) one obtains the right (ket) eigenstates, while by acting with $\tilde{H}$ to the left, one gets the bi-orthogonal left (bra) eigenstates. In the basis with physical and spurious states separated, e.g., those obtained from the diagonalization of $\mathcal{T}$, the Hamiltonian matrix takes the form

$$\begin{pmatrix} \langle\mathrm{Ph}|\tilde{H}|\mathrm{Ph}\rangle & 0 \\ \langle\mathrm{Sp}|\tilde{H}|\mathrm{Ph}\rangle & \langle\mathrm{Sp}|\tilde{H}|\mathrm{Sp}\rangle \end{pmatrix}. \tag{10}$$

Formally we obtain the Hamiltonian matrix (10) from the Hamiltonian matrix in the basis of the type (4) by an orthogonal transformation that transforms the basis (4) into the eigenstates of the operator $\mathcal{T}$ (8). In fact, this situation is very much analogous to the well-known properties of the Dyson boson-mapped systems [20]. It follows from the structure of the Hamiltonian matrix (10) that its right spurious eigen-

TABLE I. Results for three-electron system bound in a HO potential are presented. The first line shows the total of HO quanta corresponding to the relative motion in the basis states. The dimensions corresponding to the state $J^\pi = 1/2^-$ are shown in lines 2–4. Line 2 displays the full dimension (D), while lines 3 and 4 present the number of spurious (Sp) and physical (Ph) states, respectively. Lines 5 and 6 show calculated ground-state and first-excited-state energies, respectively. The calculations were done for $\hbar\Omega = 0.5$ a.u. The ground-state center-of-mass energy (0.75 a.u.) is not included in the energies shown. Energies corresponding to a particular N were obtained in calculations, where all physical basis states up to N were included.

N	1	3	5	7	9	11	13	15	17	19	21
D	3	10	21	36	55	78	105	136	171	210	253
Sp	2	7	14	24	37	52	70	91	114	140	169
Ph	1	3	7	12	18	26	35	45	57	70	84
E_1	3.4105	3.2787	3.2699	3.2669	3.2656	3.2649	3.2645	3.2643	3.2641	3.2639	3.2638
E_2		4.1002	4.0497	4.0472	4.0459	4.0453	4.0450	4.0449	4.0448	4.0447	4.0447

states $|\psi;\mathrm{Sp}\rangle_\mathrm{K}$ are not contaminated by the physical states. Similarly, the left physical eigenstates ${}_\mathrm{B}\langle\psi;\mathrm{Ph}|$ are not contaminated by the spurious ones. On the other hand, its right physical eigenstates $|\psi;\mathrm{Ph}\rangle_\mathrm{K}$ may have spurious admixtures; similarly the left spurious eigenstates ${}_\mathrm{B}\langle\psi;\mathrm{Sp}|$ may have physical admixtures. As a right spurious eigenstate has no physical admixtures, it must be annihilated by the action of the operator $\mathcal{T}$ (8), e.g.,

$$\mathcal{T}|\psi;\mathrm{Sp}\rangle_\mathrm{K} = 0. \tag{11}$$

The action of the opeartor $\mathcal{T}$ on the right eigenstates, thus, serves as a test for identification of spurious states among the calculated eigenstates, in analogy to identification of spurious states in the Dyson boson mapping by the means of the (so-called) $\mathcal{R}$ operator [21]. The relation (11) can be expressed in terms of the Faddeev amplitudes appearing in Eq. (5) as $\phi_1 + \phi_2 + \phi_3 = 0$. We note that the sum of the three Faddeev components has to be identified with the solution of the Schrödinger equation. If one finds solutions of the Faddeev equations, which are unphysical, e.g., that do not have the proper symmetry with respect to the particle exchanges, the corresponding three Faddeev components have to add up to zero. This is the only possibilty to avoid a contradiction.

It is possible to avoid the spurious state problem completely by Hermitizing the Hamiltonian (7) on the physical subspace, where it is quasi-Hermitian (see the discussion of quasi-Hermitian operators, e.g., in Ref. [16]). The Hermitized Hamiltonian takes the form

$$\overline{H} = H_0 + \overline{\mathcal{T}}^{1/2} V(\vec{r}) \overline{\mathcal{T}}^{1/2}, \tag{12}$$

where $\overline{\mathcal{T}}$ operates on the physical subspace only, e.g., it has only the eigenvalues 3.

Let us mention several relations between the eigenstates of the Faddeev Hamiltonian $\tilde{H}$ (7) and the symmetrized Hamiltonian $\overline{H}$ (12). First, we have for the left and right eigenstates of $\tilde{H}$

$${}_\mathrm{B}\langle\psi;\mathrm{Ph}| = {}_\mathrm{K}\langle\psi;\mathrm{Ph}|\mathcal{T}. \tag{13}$$

The eigenvectors $|\Psi\rangle$ of the Hamiltonian $\overline{H}$ (12) are related to the eigenvectors of the Hamiltonian $\tilde{H}$ (7) by

$$|\Psi\rangle = \mathcal{T}^{1/2}|\psi;\mathrm{Ph}\rangle_\mathrm{K}, \tag{14a}$$

$$\langle\Psi| = {}_\mathrm{B}\langle\psi;\mathrm{Ph}|\overline{\mathcal{T}}^{-1/2}. \tag{14b}$$

Note that we write explicitly $\overline{\mathcal{T}}$ instead of $\mathcal{T}$ only when an inversion is needed. For matrix elements of a general operator O we then have

$$\langle\Psi_f|O|\Psi_i\rangle = {}_\mathrm{B}\langle\psi_f;\mathrm{Ph}|\overline{\mathcal{T}}^{-1/2} O \mathcal{T}^{1/2}|\psi_i;\mathrm{Sp}\rangle_\mathrm{K}. \tag{15}$$

In addition to the relation (11), there is another possibility of identification of spurious states. It follows from the properties of the matrix elements of a general operator O between the physical and spurious eigenstates of $\tilde{H}$ (7), namely

$${}_\mathrm{B}\langle\psi_f;\mathrm{Ph}|\overline{\mathcal{T}}^{-1/2} O \mathcal{T}^{1/2}|\psi_i;\mathrm{Sp}\rangle_\mathrm{K} = 0, \tag{16a}$$

$${}_\mathrm{B}\langle\psi_f;\mathrm{Sp}|\overline{\mathcal{T}}^{-1/2} O \mathcal{T}^{1/2}|\psi_i;\mathrm{Ph}\rangle_\mathrm{K} \neq 0. \tag{16b}$$

These relations follow from the properties of the left and right eigenstates as discussed in the paragraph after Eq. (10). For an operator that commutes with $\mathcal{T}$ the square roots of $\mathcal{T}$ may be omitted in Eqs. (15) and (16). Also, in the above relations the substitution $\Sigma_{i<j} O_{ij} = \mathcal{T}^{1/2} O(\vec{r}) \mathcal{T}^{1/2}$ can be used for a two-body operator O_{ij} depending on $(\vec{r}_i - \vec{r}_j)$.

Let us return to our specific system example. The metric $\mathcal{T}$ (8) is diagonal in $N = 2n + l + 2\mathcal{N} + \mathcal{L}$. It follows from the expression (9) that any basis truncation other than one of the type $N \leq N_{\max}$ would lead, in general, to mixing of physical and unphysical states. Here, $N_{\max}$ characterizes the maximum of total allowed harmonic-oscillator quanta in the basis. At the same time, the truncation into total allowed oscillator quanta $N \leq N_{\max}$ preserves the equivalence of the Hamiltonians (7) and (12) on the physical subspace. A general consequence of this observation is that an improper truncation in the treatment of $\mathcal{T}$ leads to physical and spurious state mixing.

In Table I we present the dimensions (D) of the basis (4)

corresponding to a particular $N=2n+l+2\mathcal{N}+\mathcal{L}$ together with the number of physical states (Ph) and spurious states (Sp) for the three-electron system with $J^\pi=1/2^-$. Apparently, the number of physical states is about a third of all basis states. We also present the ground state and the first excited state energies obtained with the basis restricted by $N\leqslant N_{\max}$, where $N_{\max}$ corresponds to the number in the first row. We used the HO energy $\hbar\Omega=0.5$ atomic units (a.u.). The physical eigenenergies are shown without the trivial center-of-mass contribution. It is immediately seen from Eqs. (7) and (11) that the spurious states have the energies corresponding to the unperturbed Hamiltonian H_0 (3). Typically in the search for a bound state in the Faddeev calculations the lowest state would be physical and the spurious state existence would be unnoticed. The present electron system with a repulsive Coulomb interaction is interesting because of the fact that the physical ground state is the tenth state as can be deduced from the Table I. There are 2 spurious states with the unperturbed HO energy 2 a.u. and 7 spurious states with the energy 3 a.u. We note that for the discussed system the ground-state energy obtained by the stochastic variational method (SVM) [22] is 3.26324 a.u. [23] (after subtracting 0.75 a.u. for the center-of-mass energy). In our HO basis calculation two-decimal place precision is obtained rather rapidly. A further improvement of the precision is, however, slow. We performed calculations up to $N_{\max}=39$, where we obtained the ground state energy of 3.2634 a.u. and 4.0446 a.u. for the first-excited state. A substantial acceleration of convergency can be achieved by employing the effective interaction approach in a manner similar to that discussed in Ref. [14]. By replacing the interaction $V(\vec{r})$ in Eqs. (7) and (12) by $V_{\rm eff}(\vec{r})$ we reach the SVM ground-state result for $N_{\max}=27$ and for the first excited state we then obtain 4.04458 a.u.

III. FOUR-BODY SYSTEM

To demonstrate that the problems discussed prevail also for the Faddeev-type approach to systems with more than three particles, we present briefly the extension of the studied system to four electrons. We use the Hamiltonian (1) with $A=4$. By introducing the coordinate (and momenta) transformation

$$\vec{r}=\sqrt{\frac{1}{2}}(\vec{r}_1-\vec{r}_2), \tag{17a}$$

$$\vec{y}=\sqrt{\frac{2}{3}}\left[\frac{1}{2}(\vec{r}_1+\vec{r}_2)-\vec{r}_3\right], \tag{17b}$$

$$\vec{z}=\frac{\sqrt{3}}{2}\left[\frac{1}{3}(\vec{r}_1+\vec{r}_2+\vec{r}_3)-\vec{r}_4\right], \tag{17c}$$

the one-body part of the Hamiltonian (1) is obtained as

$$H_0=\frac{\vec{p}^2}{2m}+\frac{1}{2}m\Omega^2\vec{r}^2+\frac{\vec{q}^2}{2m}+\frac{1}{2}m\Omega^2\vec{y}^2+\frac{\vec{o}^2}{2m}+\frac{1}{2}m\Omega^2\vec{z}^2, \tag{18}$$

with the trivial center-of-mass term omitted.

A possible generalization of the Faddeev equation (6) for four identical particles can be written in the form

$$\widetilde{H}|\psi_{(123)4}\rangle=E|\psi_{(123)4}\rangle, \tag{19}$$

with

$$\widetilde{H}|\psi_{(123)4}\rangle\equiv H_0|\psi_{(123)4}\rangle+\frac{1}{2}(V_{12}+V_{13}+V_{23})(|\psi_{(123)4}\rangle+|\psi_{(432)1}\rangle+|\psi_{(134)2}\rangle+|\psi_{(142)3}\rangle), \tag{20}$$

and

$$(|\psi_{(123)4}\rangle+|\psi_{(432)1}\rangle+|\psi_{(134)2}\rangle+|\psi_{(142)3}\rangle)=(1-\mathcal{T}_{14}-\mathcal{T}_{24}-\mathcal{T}_{34})|\psi_{(123)4}\rangle\equiv\mathcal{T}_4|\psi_{(123)4}\rangle. \tag{21}$$

Here, $|\psi_{(123)4}\rangle$ is a four-fermion Faddeev amplitude completely antisymmetrized for particles 1, 2, and 3. There are three other equations that can be obtained from Eq. (19) by permuting particle 4 with particles 1, 2, and 3. Their sum then leads to the Schrödinger equation. We note that the present equations are different from the traditional Faddeev-Yakubovsky equations [24], which combine Faddeev amplitudes depending on two sets of Jacobi coordinates. As we are working with a complete orthonormal basis, it is sufficient and convenient to use a single set of Jacobi coordinates defined by the relations (17). Unlike the Faddeev amplitudes used typically in the Faddeev-Yakubovsky equations, the amplitudes appearing in Eq. (19) are antisymmetrized with respect to the first three particles. The present equations allow to employ easily three-body interactions or three-body effective interactions. The latter property makes them particularly useful for an extension of shell-model calculations for four nucleons [25].

The starting point for the present four-electron calculation is the basis

$$|N_1iJ_1,n_zl_z\mathcal{J}_4,J\rangle, \tag{22}$$

with the three-fermion part given by the antisymmetrized eigenstates of $\mathcal{T}$ (8) corresponding to eigenvalue 3, e.g.,

$$|N_1iJ_1\rangle=\sum c^{N_1iJ_1}_{nlsj\mathcal{N}\mathcal{L}\mathcal{J}_3}|nlsj,\mathcal{N}\mathcal{L}\mathcal{J}_3,J_1\rangle, \tag{23}$$

where $N_1=2n+l+2\mathcal{N}+\mathcal{L}$ and i counts the eigenstates of $\mathcal{T}$ with the eigenvalue 3 for given N_1 and J_1.

As for the three-particle transposition operators (9), a compact formula can be derived for the matrix elements of the four-particle transposition operators in the basis (22), e.g.,

$$\langle N_{1L} i_L J_{1L}, n_{zL} l_{zL} \mathcal{J}_{4L}, J | \mathcal{T}_{14} + \mathcal{T}_{24} + \mathcal{T}_{34} | N_{1R} i_R J_{1R}, n_{zR} l_{zR} \mathcal{J}_{4R}, J \rangle$$

$$= -\delta_{N_L,N_R} \sum c^{N_{1L} i_L J_{1L}}_{n_L l_L s_L j_L \mathcal{N}_L \mathcal{L}_L \mathcal{J}_{3L}} c^{N_{1R} i_R J_{1R}}_{n_R l_R s_R j_R \mathcal{N}_R \mathcal{L}_R \mathcal{J}_{3R}} \hat{L}^2_{1L} \hat{L}^2_{1R} \hat{S}^2_{1L} \hat{S}^2_{1R} \hat{L}^2_2 \hat{S}^2_2 \hat{j}_L \hat{j}_R \hat{\mathcal{J}}_{3L} \hat{\mathcal{J}}_{3R} \hat{\mathcal{J}}_{4L} \hat{\mathcal{J}}_{4R} \hat{J}_{1L} \hat{J}_{1R} (-1)^{S_{1L}+S_{1R}}$$

$$\times \begin{Bmatrix} \frac{1}{2} & s_R & S_{1R} \\ \frac{1}{2} & S_2 & S_{1L} \end{Bmatrix} \begin{Bmatrix} l_L & s_L & j_L \\ \mathcal{L}_L & \frac{1}{2} & \mathcal{J}_{3L} \\ L_{1L} & S_{1L} & J_{1L} \end{Bmatrix} \begin{Bmatrix} l_R & s_R & j_R \\ \mathcal{L}_R & \frac{1}{2} & \mathcal{J}_{3R} \\ L_{1R} & S_{1R} & J_{1R} \end{Bmatrix} \begin{Bmatrix} L_{1L} & S_{1L} & J_{1L} \\ l_{zL} & \frac{1}{2} & \mathcal{J}_{4L} \\ L_2 & S_2 & J \end{Bmatrix} \begin{Bmatrix} L_{1R} & S_{1R} & J_{1R} \\ l_{zR} & \frac{1}{2} & \mathcal{J}_{4R} \\ L_2 & S_2 & J \end{Bmatrix}$$

$$\times \hat{L}'^2 (-1)^{L'} \begin{Bmatrix} l_R & L_2 & L' \\ l_{zR} & \mathcal{L}_R & L_{1R} \end{Bmatrix} \begin{Bmatrix} l_R & L_2 & L' \\ l_{zL} & l' & L_{1L} \end{Bmatrix} \Bigg[\hat{s}_L \hat{s}_R \begin{Bmatrix} \frac{1}{2} & \frac{1}{2} & s_R \\ \frac{1}{2} & S_{1L} & s_L \end{Bmatrix}$$

$$\times (-1)^{l_{zR}+L_{1L}} ((-1)^{l_{zL}} \langle n' l' n_{zL} l_{zL} L' | n_{zR} l_{zR} \mathcal{N}_R \mathcal{L}_R L' \rangle_8 \langle n_L l_L \mathcal{N}_L \mathcal{L}_L L_{1L} | n' l' n_R l_R L_{1L} \rangle_3$$

$$+ (-1)^{s_R - s_L + \mathcal{L}_R - l_L - \mathcal{L}_L} \langle n_{zL} l_{zL} n' l' L' | \mathcal{N}_R \mathcal{L}_R n_{zR} l_{zR} L' \rangle_8 \langle \mathcal{N}_L \mathcal{L}_L n_L l_L L_{1L} | n_R l_R n' l' L_{1L} \rangle_3)$$

$$+ \delta_{l_L,l_R} \delta_{s_L,s_R} \delta_{\mathcal{N}_L,n'} \delta_{\mathcal{L}_L,l'} (-1)^{\mathcal{L}_R + l_{zR}} \langle n_{zL} l_{zL} \mathcal{N}_L \mathcal{L}_L L' | \mathcal{N}_R \mathcal{L}_R n_{zR} l_{zR} L' \rangle_8 \Bigg], \tag{24}$$

where $N_X = 2n_X + l_X + 2\mathcal{N}_X + \mathcal{L}_X + 2n_{zX} + l_{zX} = N_{1X} + 2n_{zX} + l_{zX}$, X≡L,R. We will give more details on the derivation, symmetry properties, as well as a generalization that includes the isospin quantum numbers, elsewhere [25].

As the structure of Eq. (19) is the same as the Faddeev equation (6), the discussion of the spurious state problem for the three-fermion system can be extended to the four-fermion system as well. In particular, eigenstates of the operator $\mathcal{T}_4$ defined by the relation (21) can be subdivided into two subspaces. A physical subspace corresponding to the eigenvalue 4 spanned by totally antisymmetric states and a spurious subspace spanned by eigenvectors corresponding to the eigenvalue 0. In the basis of the $\mathcal{T}_4$ eigenstates, the Hamiltonian $\tilde{H}$ appearing in Eq. (19) has the same structure as shown in Eq. (10). Its spurious eigenstates can be identified by the action of $\mathcal{T}_4$ on the right eigenstates, like in Eq. (11), e.g., $\mathcal{T}_4 |\psi_{(123)4}; \mathrm{Sp}\rangle_K = 0$.

It is possible to symmetrize the Hamiltonian $\tilde{H}$ on the physical subspace and eliminate the spurious state problem at the same time. The symmetrized Hamiltonian then takes the form

$$\overline{H} = H_0 + \overline{\mathcal{T}_4}^{1/2} \tfrac{1}{2} (V_{12} + V_{13} + V_{23}) \overline{\mathcal{T}_4}^{1/2}, \tag{25}$$

where $\overline{\mathcal{T}_4}$ operates only on the physical subspace.

In Table II we show the dimensions (D) of the basis (22) corresponding to particular $N = N_1 + 2n_z + l_z$ together with the number of physical states (Ph) and spurious states (Sp) for the four-electron system with $J^\pi = 0^+$. The relative number of physical states decreases with N and approaches about a fourth of all basis states for larger N. In the last two rows of Table II we present the ground state and the first excited state energies obtained in the calculations with the basis restricted by $N \leqslant N_{\max}$, where $N_{\max}$ corresponds to the number in the first row. As in the three-electron calculations the physical eigenenergies, which were obtained with the HO energy $\hbar\Omega = 0.5$ a.u., are shown without the trivial center-of-mass contribution. We note that the studied system, when described by Eq. (19), has a spurious ground state with the energy 3.25 a.u., corresponding to the unperturbed HO Hamiltonian H_0 (18). We note that the preliminary result of the ground-state energy of the studied system obtained by the SVM is 5.6002 [23] (after subtracting 0.75 a.u. for the center-of-mass energy). As for the three-electron calculations, we get a fast convergence to two-decimal place preci-

TABLE II. Results for four-electron system bound in a HO potential are presented. The first line shows the total of HO quanta corresponding to the relative motion in the basis states. The dimensions corresponding to the state $J^\pi = 0^+$ are shown in lines 2–4. Line 2 displays the full dimension (D), while lines 3 and 4 present the number of spurious (Sp) and physical (Ph) states, respectively. Lines 5 and 6 shows calculated ground-state and first-excited-state energies, respectively. The calculations were done for $\hbar\Omega = 0.5$ atomic units. The ground-state center-of-mass energy (0.75 a.u.) is not included in the energies shown. Energies corresponding to a particular N were obtained in calculations where all physical basis states up to N were included.

N	0	2	4	6	8	10	12	14
D	0	4	21	68	178	391	767	1390
Sp	0	2	14	48	128	284	564	1024
Ph	0	2	7	20	50	107	203	366
E_1		5.8829	5.6346	5.6094	5.6043	5.6022	5.6012	5.6006
E_2		6.0239	5.7396	5.7116	5.7034	5.7003	5.6988	5.6979

sion in our HO basis calculation. A further improvement of the precision is slow and requires larger model spaces. As in the three-electron calculation, a substantial acceleration of convergence can be achieved by employing the effective interaction approach [14]. By replacing the interaction V by a two-body effective interaction, we obtained a ground-state energy of 5.5991 a.u. and a first-excited-state energy of 5.6958 a.u. for $N_{\max}=14$. An additional speeding up of the rate of convergence can be achieved by using the three-body effective interaction [25].

IV. CONCLUSIONS

To summarize, we have investigated the appearance of spurious states in the Faddeev formalism for few-body systems. Depending on the studied system, such states may appear even among the lowest eigenstates. We have also discussed how the spurious states can be identified and how they can be eliminated by symmetrization of the Faddeev equations. We also noted that any improper truncation in the treatment of the particle exchange operators (e.g., $\mathcal{T},\mathcal{T}_4$) may lead, in general, to the mixing of physical and spurious states.

We used three- and four-electron systems bound in an HO potential as an example. Due to the repulsive character of the Coulomb interaction, such systems have spurious ground states, when solved in the Faddeev formalism. By examining the basis dimensions, we have illustrated that the number of physical states for the three-electron system is about a third of the total number of basis states. (It is exactly one-third, when the total number of basis states is divisible by three.) For the four-electron system we formulated equations for the Faddeev amplitudes antisymmetrized for the first three particles. Using this approach we observed that almost 3/4 of all the states were spurious.

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