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The three-electron quantum dot studied using hyperspherical coordinates

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Abstract. The hyperangular equation for three particles interacting via an inverse-square potential in a harmonic well was solved numerically by using the correlated hyperspherical harmonics as basis functions. The implications of permutational and rotational symmetries were analysed in detail. Some of the qualitative features of low-lying states were found to be determined completely by symmetries.

With molecular-beam epitaxy, experimentalists are now able to create quantum dots in semiconductors, each containing only a small number of electrons ($N = 1, 2, 3, \ldots$) and having discrete energy levels [1]. Such an artificially fabricated atomic system shows interesting many-body effects in a strong magnetic field. Series of *magic* numbers of angular momentum which minimize the interaction energy have been found. The ground-state energy has been measured in some recent experiments as a function of external magnetic field [1, 2]. This has stimulated extensive theoretical studies. Already, several methods have been proposed for obtaining the approximate ground-state energy of a quantum dot in a magnetic field by phenomenologically constructing the variational ground-state wave functions [3–5]. Exact numerical diagonalizations have also been carried out for systems containing a few electrons by using the Slater determinants composed of harmonic oscillator functions to obtain the ground-state energies [6, 7].

Recently [8, 9], Johnson and Quiroga suggested the use of an inverse-square potential, β/r^2 (β is the strength parameter), for the effective electron–electron interaction in the dots, and the introduction of hyperspherical coordinates to describe the system. With parabolic confinement $m^*\omega_0 r^2/2$ (m^* is the effective electron mass, ω_0 is a strength parameter) and a perpendicular magnetic field $\boldsymbol{B}$, the relative-motion Schrödinger equation for N electrons is then separated into a hyper-radial equation and a field-independent angular equation [8]:

$$\left\{-\frac{\hbar^2}{2m^*}\left[\frac{1}{\xi^{2N-3}}\frac{\mathrm{d}}{\mathrm{d}\xi}\xi^{2N-3}\frac{\mathrm{d}}{\mathrm{d}\xi}-\frac{\lambda(\lambda+2N-4)}{\xi^2}\right]+\frac{1}{2}m^*\omega^2\xi^2+\frac{\omega_c}{2}L\right\}R(\xi)=E_{rel}R(\xi) \tag{1}$$

$$\{\Gamma(\Omega)+U(\Omega)\}G_L(\Omega)=\lambda(\lambda+2N-4)G_L(\Omega) \tag{2}$$

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where: $\xi^2 = \sum_{i=1}^{N} \mu_i \eta_i^2 / m^*$, where ξ is the hyper-radius, $\{\eta_i\}$ is a set of Jacobi coordinates and μ_i is the corresponding reduced mass;

$$\omega = \sqrt{\omega_0^2 + \omega_c^2/4}$$

where $\omega_c = eB/m^*$ is the cyclotron frequency; L is the angular momentum for relative motion (which was denoted by J in reference [8]); $\Gamma(\Omega)$ is the grand orbital operator; and $U(\Omega) = m^*\beta \sum_{i>j} \xi^2 / r_{ij}^2$ is the interaction energy of the $\xi = 1$ hypersphere times the particle mass, where Ω denotes all of the angular variables for brevity. Physically, ξ measures the size, while Ω describes the shape and orientation of the system. The separability of the Schrödinger equation into equation (1) and (2) implies that changes of size and shape proceed independently. Only systems with quadratic and/or inverse-square pairwise interactions possess this property. Equation (1) is exactly solvable and its eigenvalue is $E_{rel} = \hbar\omega(2n + \lambda + N - 1) + \hbar\omega_c L/2$ $(n = 0, 1, 2, \ldots)$. For $N > 2$, equation (2) cannot be solved analytically without further simplification. In reference [8], Johnson and Quiroga found a set of approximate analytical solutions that are valid in the Wigner crystal regime (i.e. the large-β limit). However, since currently studied quantum dots are, like a fractional quantum Hall system, in the liquid regime, knowledge of particle correlations in the intermediate regime will be more demanding as regards the understanding of experimentally observed phenomena.

In the following, we will present a procedure for solving equation (2) numerically by using the eigenfunctions of $\Gamma(\Omega)$ as basis functions, and study the particle correlations. Since $N = 3$ is the simplest system with many-body effects, we will demonstrate the procedure explicitly for that case. Only the spin-polarized states are considered. Its extension to other N and other spins is straightforward.

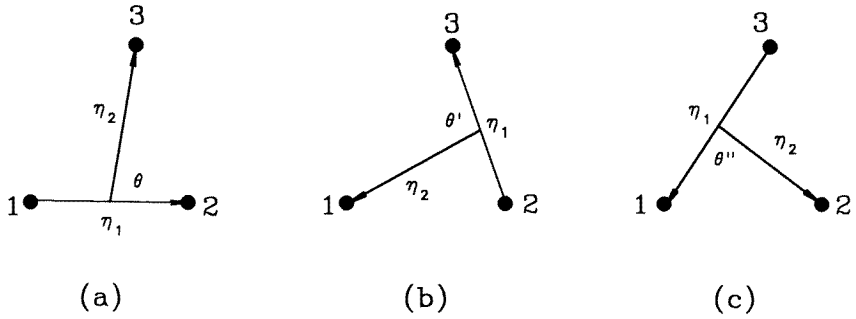

Figure 1. Jacobi coordinates for a three-body system.

With $N = 3$, the Jacobi coordinates that can be assigned to the system are depicted in figure 1. The hyper-radius and the hyperangle for the system are then defined through

$$\begin{aligned} \sqrt{\frac{1}{2}}\eta_1 &= \xi \sin\alpha \\ \sqrt{\frac{2}{3}}\eta_2 &= \xi \cos\alpha. \end{aligned} \tag{3}$$

The potential function $U(\Omega)$ is then given by

$$U(\Omega) = \beta m^* \left(\frac{1}{\cos^2\alpha} + \frac{1}{\cos^2\alpha'} + \frac{1}{\cos^2\alpha''} \right). \tag{4}$$

In this expression, we have used hyperangles defined in terms of different sets of Jacobi coordinates as variables to keep it simple. The grand orbital operator reads

$$\Gamma(\Omega) = \frac{\partial^2}{\partial\alpha^2} + \left(\frac{\cos\alpha}{\sin\alpha} - \frac{\sin\alpha}{\cos\alpha}\right)\frac{\partial}{\partial\alpha} - \frac{\hat{\ell}^2(\varphi_1)}{\cos^2\alpha} - \frac{\hat{\ell}^2(\varphi_2)}{\sin^2\alpha} \tag{5}$$

where $\hat{\ell}(\varphi_1) = -\mathrm{i}\,\partial/\partial\varphi_1$, φ_1 is the polar angle of η_1, etc. $\Gamma(\Omega)$ is translationally invariant, i.e. $\Gamma(\Omega) = \Gamma(\Omega') = \Gamma(\Omega'')$. The eigen-equation $\Gamma(\Omega)Y(\Omega) = \lambda_0(\lambda_0+2)Y(\Omega)$ can be solved analytically, with its eigenvalues and eigenfunctions given by

$$Y_{[\nu l_1 l_2]}(\Omega) = N_{\nu l_1 l_2} P_\nu^{l_1,l_2}(\alpha)\mathrm{e}^{\mathrm{i}l_1\varphi_1}\mathrm{e}^{\mathrm{i}l_2\varphi_2} \tag{6}$$

$$\lambda_0 = 2\nu + |l_1| + |l_2| \qquad L = \hbar(l_1 + l_2) \tag{7}$$

where

$$N_{\nu l_1 l_2} = \sqrt{(2\nu + |l_1| + |l_2| + 1)\nu!(\nu + |l_1| + |l_2|)!/[2\pi^2(\nu + |l_1|)!(\nu + |l_2|)!]}$$

is the normalization constant and $P_\nu^{l_1,l_2}$ is a Jacobi polynomial, defined by

$$P_\nu^{l_1,l_2}(\alpha) = \sum_{m=0}^{\nu}(-1)^{\nu-m}\binom{\nu+|l_2|}{m}\binom{\nu+|l_1|}{\nu-m}(\cos\alpha)^{2m+|l_1|}(\sin\alpha)^{2(\nu-m)+|l_2|}. \tag{8}$$

Since ξ is invariant under any particle permutations, the angular wavefunction $G_L(\Omega)$ defined in equation (2) should be antisymmetric for fermions. Let $\hat{A} = [1 - P_{(12)} - P_{(13)} - P_{(23)} + P_{(123)} + P_{(132)}]/6$ be the antisymmetrization operator, then an antisymmetrized harmonics with l_1 odd (there is no antisymmetric state for even l_1) can be expressed as

$$\hat{A}Y_{[\nu l_1 l_2]}(\Omega) = \frac{1}{3}[Y_{[\nu l_1 l_2]}(\Omega) + Y_{[\nu l_1 l_2]}(\Omega') + Y_{[\nu l_1 l_2]}(\Omega'')]. \tag{9}$$

The translational invariance of $\Gamma(\Omega)$ and the total angular momentum operator $\hat{L}$ implies that $Y_{[\nu l_1 l_2]}(\Omega')$ and $Y_{[\nu l_1 l_2]}(\Omega'')$ continue to be their common eigenfunctions with the same eigenvalues as those given by $Y_{[\nu l_1 l_2]}(\Omega)$. (Note that they are no longer eigenstates of $\hat{\ell}(\varphi_1)$ and $\hat{\ell}(\varphi_2)$.) Therefore they can be expanded in terms of $Y_{[\nu' l_1' l_2']}(\Omega)$, such that

$$\hat{A}Y_{[\nu l_1 l_2]}(\Omega) = \sum_{[\nu' l_1' l_2']} B^{[\nu l_1 l_2]}_{[\nu' l_1' l_2']} Y_{[\nu' l_1' l_2']}(\Omega) \tag{10}$$

where the ranges of sums are finite and subject to the constraints $l_1' + l_2' = l_1 + l_2 = L$ and $2\nu' + |l_1'| + |l_2'| = 2\nu + |l_1| + |l_2| = \lambda_0$; the expansion coefficient is given by

$$B^{[\nu l_1 l_2]}_{[\nu' l_1' l_2']} = \frac{1}{3}[\delta_{[\nu' l_1' l_2'],[\nu l_1 l_2]} + 2\langle Y_{[\nu' l_1' l_2']}(\Omega)|Y_{[\nu l_1 l_2]}(\Omega')\rangle]. \tag{11}$$

In obtaining equation (11), we have made use of the following identity:

$$\langle Y_{[\nu' l_1' l_2']}(\Omega)|Y_{[\nu l_1 l_2]}(\Omega'')\rangle = \begin{cases} \langle Y_{[\nu' l_1' l_2']}(\Omega)|Y_{[\nu l_1 l_2]}(\Omega')\rangle & \text{for } l_1' \text{ odd} \\ -\langle Y_{[\nu' l_1' l_2']}(\Omega)|Y_{[\nu l_1 l_2]}(\Omega')\rangle & \text{for } l_1' \text{ even.} \end{cases}$$

The bracket $\langle Y_{[\nu' l_1' l_2']}(\Omega)|Y_{[\nu l_1 l_2]}(\Omega')\rangle$ defines a transformation matrix for hyperspherical harmonics with two different sets of angular coordinates as variables. This was first discussed by Raynal and Revai for harmonics in three space dimensions [10] and later extended to harmonics in two space dimensions by Gan *et al* [11]. It is important to realize that a set of antisymmetric functions obtained from equation (10) are generally linearly dependent. In practice, we have used the Schmidt procedure to select out a set of orthonormalized antisymmetric basis states from harmonics with the same λ_0 and L. With antisymmetric basis states, each term in equation (4) gives the same contributions and the

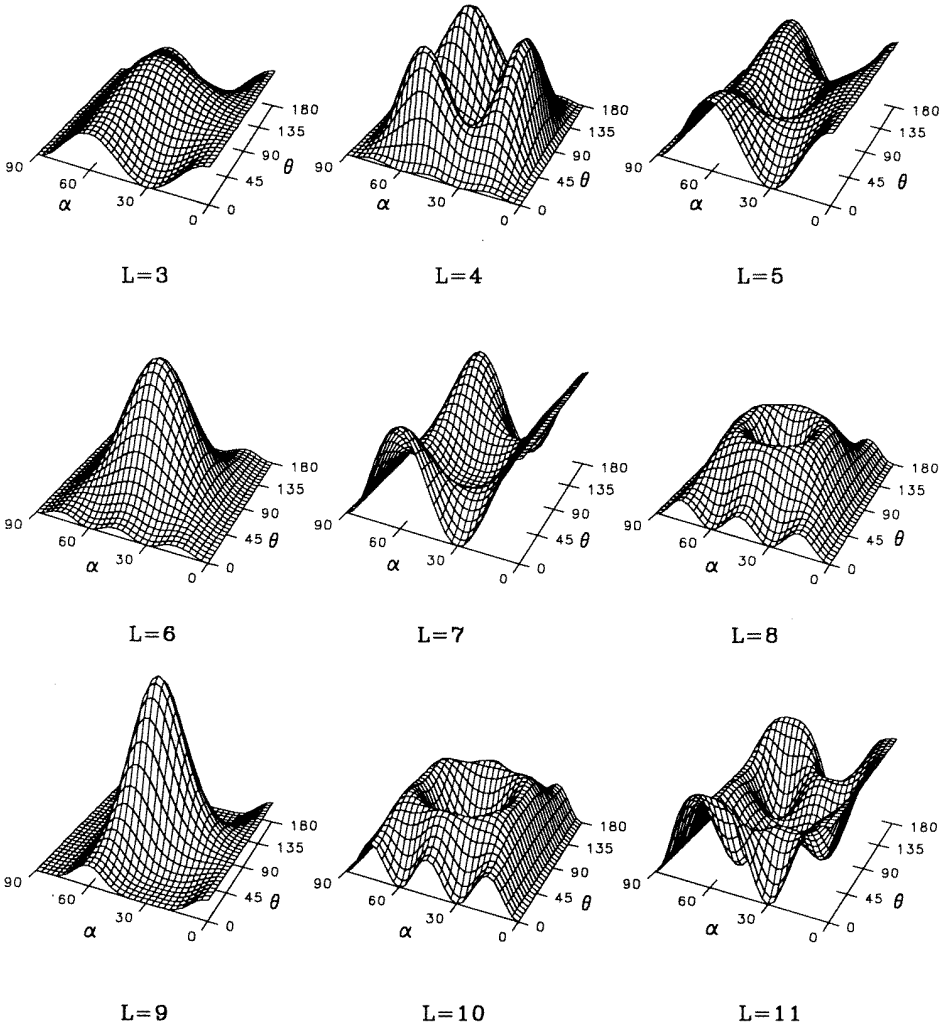

Figure 2. Density distributions of the lowest states with $\beta \to 0$ on the (α, θ) plane, where α ranges from 0 to 90° and θ from 0 to 180°.

matrix elements of $U(\Omega)$ can be calculated analytically. We diagonalized the Hamiltonian in a subspace restricted to $\lambda_0 < 24$ to obtain the eigenvalues and eigenfunctions.

As is well known, permutation symmetry has important effects on the quantum states of identical particles. For noninteracting systems, this can be described as a constraint on the ways in which one can fill the single-particle levels (i.e. the Pauli principle). For strongly correlated systems, the concept of single-particle levels is no longer valid. We need a new language to describe the constraint globally. For three interacting particles confined in a potential well, the equilibrium configuration is an equilateral triangle (ET) with an appropriate side length. In the ground state this configuration should be pursued to minimize the interaction energy. However, since in the ET configuration a rotation of 120° is equivalent to a cyclic permutation of the three particles (an odd permutation), we have $R(120^\circ)G_L(\mathrm{ET}) = -G_L(\mathrm{ET})$. The rotation operator $R(120^\circ)$ yields a phase factor of

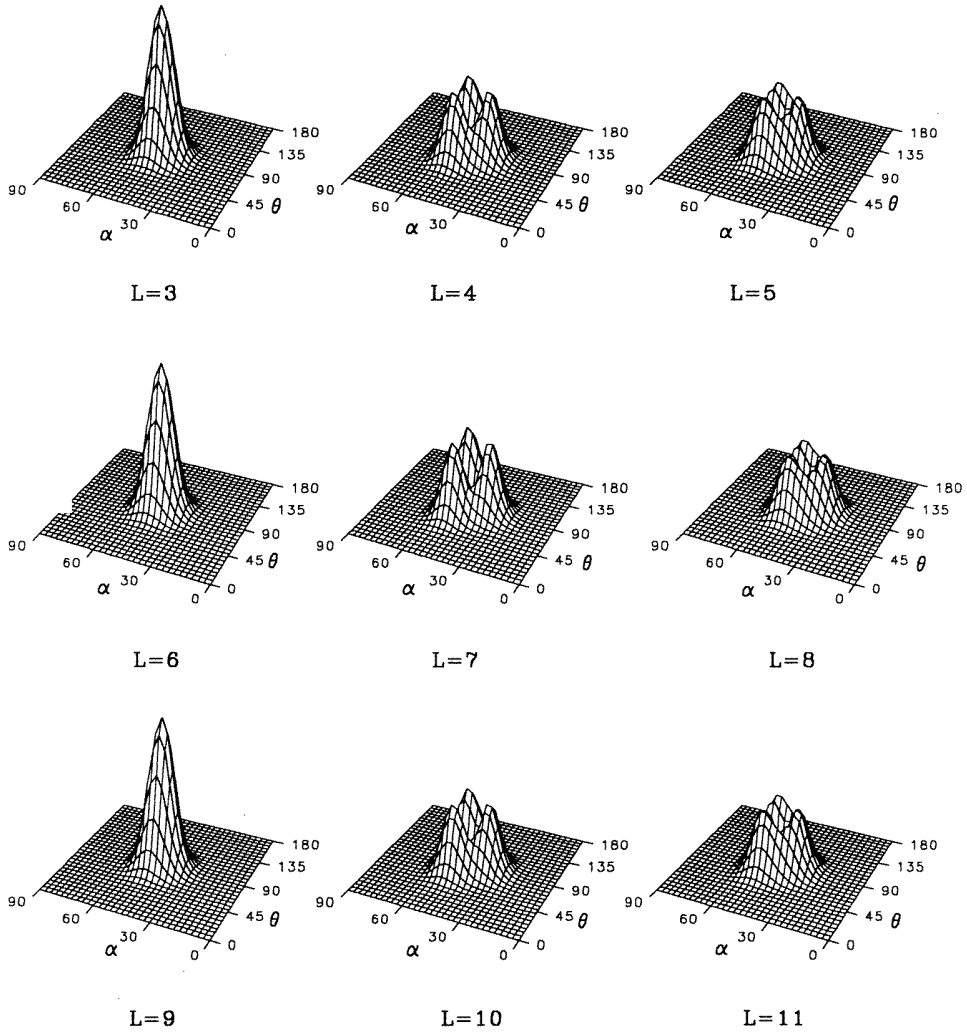

Figure 3. As figure 2, except that $\beta = 120m^*\hbar^2$.

$\exp(\mathrm{i}\,2\pi L/3)$. Thus we have $G_L(\mathrm{ET}) = 0$ unless $L = 3k$ (k being an integer). This implies that the ET configuration is only accessible in the $L = 3k$ states due to the symmetry constraint. Therefore it is reasonable to expect that both the average kinetic energy and interaction energy will be increased by the appearance of such a node in $L \neq 3k$ states. Another regular configuration of three particles is a dumb-bell with a third particle at the centre (denoted by CDB). It corresponds to a saddle point of the interaction energy in the multicoordinate space. The CDB configuration is inaccessible in $L =$ even states since in the CDB a rotation of 180° is equivalent to transposition of two particles at the ends. The CDB is structurally unstable. It cannot be so important as the ET when the latter is accessible by symmetries. Other nodes of an antisymmetric wavefunction occur at $r_{ij} = 0$, which prohibit the contact interaction of two fermions. All of the nodes that we have discussed here originate completely from symmetries; we call them inherent nodes hereafter. With all of the inherent nodes in mind, we present the numerical results as follows.

(i) To see the effect of antisymmetrization, in figure 2 we present the density function

$$\rho(\alpha, \theta) = |G_L(\Omega)|^2 \tag{12}$$

on the (α, θ) plane in the limit $\beta \to 0$, where $\theta = \varphi_2 - \varphi_1$ is the polar angle between η_1 and η_2. Only the lowest state of an L is considered. Within the (α, θ) plane, the line $\alpha = 90^\circ$ and the points $(30^\circ, 0)$ and $(30^\circ, 180^\circ)$ correspond to $r_{12} = 0$, $r_{23} = 0$ and $r_{31} = 0$ respectively; they are nodes of all of the antisymmetric wavefunctions. The central point $(45^\circ, 90^\circ)$ corresponds to the ET configuration which is a node of the wavefunction of the $L \neq 3k$ states. In $L = 3k$ states, the density function peaks at $(45^\circ, 90^\circ)$. Hence the ET is the dominant configuration of these states. The peak is sharper for larger L. The line $\alpha = 0$ and the points $(60^\circ, 0)$ and $(60^\circ, 180^\circ)$ correspond to the CDB configurations, which are nodes of the wavefunction of $L =$ even states. The CDB is the dominant configuration in $L = 5, 7, 11, \ldots$ states where the ET configuration is inaccessible. In all of the states shown in figure 2, there is no node except the inherent ones. As a result, states differing in L but having the same symmetry constraints look similar (compare, for example, $L = 4, 8, 10$ states). In the excited states, there are some other nodes originating from the dynamics and representing a more energetic internal motion.

(ii) To see the effects of particle–particle interaction, in figure 3 we present the results with strong interaction ($\beta = 120m^*\bar{h}^2$). In comparison with the situation discussed above, the main feature is retained; the only difference lies in the fact that the density distribution is now concentrated more at the central point $(45^\circ, 90^\circ)$ and in its vicinity, in order to minimize the interaction energy. Away from the neighbourhood of $(45^\circ, 90^\circ)$, $\rho(\alpha, \theta)$ tends to zero. In this case, whether or not $r_{ij} = 0$ and the CDB configuration are inherent nodes becomes unimportant. The dominant factor is the node representing an ET prohibition which occurs in the $L \neq 3k$ states. In reference [12], the geometrical structures of a four-electron quantum dot interacting via a Coulomb potential was studied in the Wigner crystal limit. It was found there that each state was characterized by several isolated peaks of the density function, and a mode of internal motion can be identified which transforms one regular configuration into another. In our present case, except for the $L = 3k$ states, the density distribution function does not have very sharp peaks but just looks like a volcano; hence the dominant structures and the mode of internal motion are not very well defined here. This may be relevant to the details of particle–particle potentials.

(iii) Figure 4 presents the λ-spectrum with $\beta = 120m^*\bar{h}^2$. A striking feature is that the lowest state of an $L = 3k$ sequence has particularly low energy compared to other

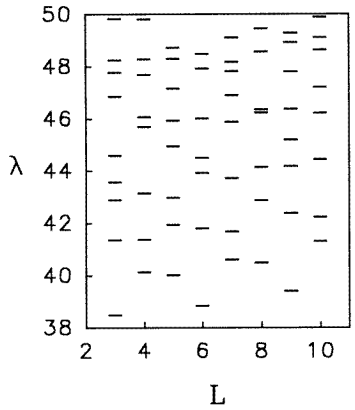

Figure 4. The quantum λ-spectrum with $\beta = 120m^*\bar{h}^2$.

sequences. This is entirely due to the favourable ET configuration being accessible in the state. There is a big energy gap between the lowest and the second states of an $L = 3k$ sequence. The width of the gap gives a measure to the stability of the lowest state. Since the lowest states of $L = 3k$ sequences have similar internal structures, they constitute the lowest rotational band of a three-electron Wigner molecule. We noticed that by assuming small zero-point oscillation energy for the relative motion, Johnson and Quiroga obtained an approximate analytical expression for the eigenvalues (see equation (12) in reference [8]). On taking $\beta = 120m^*\hbar^2$, our exact numerical diagonalization gives $\lambda = 38.5$ for the lowest state of $L = 3$, while the analytical result is $\lambda = 15.8$, indicating that the zero-point oscillation energy is still the dominant part here and there is a large cancellation in the analytical result. Further increasing the β-value may help to improve the analytical result but the numerical method then becomes computationally too intensive.

To summarize, we have demonstrated a procedure to numerically solve the three-body problem in hyperspherical coordinates. We have paid special attention to particle correlations in the lowest states. The separability of the radial part from the angular part has enabled us to fully and intuitively expose particle correlations in an interacting three-particle system, while the customary procedure for studying particle correlations by extracting the two-body density from the full wavefunction may lose some useful information. As we have found in several previous studies [12, 13], symmetries play a decisive role as regards the low-lying states of few-body systems, such that we can gain a deep insight into the qualitative features of low-lying spectrum and density distributions simply by analysing the symmetry constraints before diagonalizing the Hamiltonian.

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