NON-SPURIOUS HARMONIC OSCILLATOR STATES WITH ARBITRARY PERMUTATIONAL SYMMETRY

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Abstract

An algorithm for the construction of non-spurious harmonic oscillator (h.o.) wave functions with arbitrary permutational symmetry is presented. The h.o. wave functions, expressed in Jacobi coordinates, are calculated recursively using a new type of h.o. coefficients of fractional parentage. These coefficients are the eigenvectors of the two-cycle class operator of the permutation group in the appropriate basis. The matrix elements of the class operators are evaluated by using a specific version of the h.o. brackets. A procedure is developed to transform the resultant h.o. states from Jacobi into single particle coordinates. The procedures proposed are expected to enhance the effectiveness of computations involving h.o. basis sets.

I. Construction of non-spurious harmonoic oscillator states with arbitrary permutational symmetry

Harmonic oscillator wave functions have been widely used in computational molecular, atomic and nuclear physics, and recently also in non-relativistic quark calculations[1]. In all these applications the eigenvectors of a translationally invariant hamiltonian are evaluated in terms of h.o. eigenstates. The h.o. states used in these calculations should be constructed in such a way that the trivial center-of-mass (c.m.) motion is explicitly separated: Spurious states, in which the c.m. is excited, must be eliminated.

In order to construct non-spurious states for n identical isotropic three-dimensional h.o.s we must use a set of coordinates where the c.m. is separated from the $n-1$ internal coordinates. Among the various sets of coordinates satisfying this requirement the normalized Jacobi coordinates

$$\vec{\rho}^{(n)} = \vec{R} = \frac{1}{\sqrt{n}}\sum_{j=1}^{n}\vec{r}_j \quad ; \quad \vec{\rho}_i = \sqrt{\frac{i-1}{i}}\left(\vec{r}_i - \frac{1}{i-1}\sum_{j=1}^{i-1}\vec{r}_j\right) \quad i = 2,3,\ldots,n \qquad (1)$$

were found to be preferable because each internal coordinate $\vec{\rho}_i$ $i = 2,\ldots,n$ depends on the first i single particle coordinates only. This property enables the formulation of a recursive procedure for constructing the set of h.o. non-spurious states[2].

The h.o. wave functions expressed in Jacobi coordinates are naturally separated into an internal and a c.m. wave function. The c.m. wave function is totally symmetric with respect to permutations of the particle coordinates. On the other hand, the internal coordinates do not have simple symmetry properties with respect to permutation of particle indices. Our aim is to construct internal wave functions, consisting of $n-1$ h.o.s, which belong to an irrep of the permutation group, S_n.

The permutational symmetry of an internal wave function of n-particles can be specified by a sequence of Young frames $\Gamma_2\Gamma_3\ldots\Gamma_n$, where Γ_i is the i-particle Young frame. This sequence is equivalent to the Yamanouchi symbol Y_n[3]. Additional good quantum numbers are the *resultant* internal angular momentum Λ_n and internal energy ($\hbar\omega\left(\epsilon_n + \frac{3}{2}(n-1)\right)$ where ϵ_n is an internal energy parameter). However, the angular momenta and energies of less than n particles are not good quantum numbers. One can construct a complete set of states labeled by $|Y_n\Lambda_n\epsilon_n\alpha_n>$ where α_n is an additional label that takes care of the remaining degeneracies. For simplicity we denote the combination of quantum numbers $\Lambda_n\epsilon_n\alpha_n$ by Φ_n. $\eta^{(i)}$ stands for the individual h.o. radial and angular quantum numbers N_i and L_i corresponding to the i'th Jacobi coordinate.

The two particle internal wavefunction can be written as

$$|\Gamma_2\,\Lambda_2\,\epsilon_2\,;\vec{\rho}_2>=|\Gamma_2\,\Phi_2\,;\vec{\rho}_2>=\Psi_{N_2L_2}(\vec{\rho}_2)=|\eta^{(2)};\vec{\rho}_2> \tag{2}$$

where $\epsilon_2 = 2N_2 + L_2$, Λ_2 is the internal angular momentum and $L_2 = \Lambda_2$. Γ_2 is determined by L_2: $\Gamma_2 = [2]$ for even L_2 and $\Gamma_2 = [1^2]$ for odd L_2. The value of the z component of the angular momentum is suppressed.

Let us assume that the $(n-1)$-particle wave functions, symmetry adapted to S_{n-1}, have already been constructed. The general expression for the n-particle internal wave function, symmetry adapted to S_n, can than be written in the form

$$|Y_n\Phi_n;\vec{\rho}_2\vec{\rho}_3\ldots\vec{\rho}_n>=\sum_{\substack{\Phi_{n-1}\eta^{(n)}\\(\epsilon_n=\epsilon_{n-1}+2N_n+L_n)}}\left[Y_{n-1}\Phi_{n-1}\eta^{(n)}\Lambda_n|\}Y_n\Phi_n\right]|Y_{n-1}\Phi_{n-1}\eta^{(n)}\Lambda_n;\vec{\rho}_2\vec{\rho}_3\ldots\vec{\rho}_n> \tag{3}$$

where $Y_n = Y_{n-1}\Gamma_n$ and the coefficients [|}] are the h.o. coefficients of fractional parentage (hocfps).

The hocfps defined in Eq. (3) satisfy orthogonality and completeness relations[2] similar to those satisfied by the single shell cfps for arbitrary permutational symmetry, defined in ref. [4]. On the other hand, here, the n'th particle state $|\eta^{(n)};\vec{\rho}_n>=|N_nL_n;\vec{\rho}_n>$ is not unique. We have to sum over all the different single particle states consistent with the angular momentum coupling $\vec{\Lambda}_{n-1}+\vec{L}_n=\vec{\Lambda}_n$ and the energy relation $\epsilon_n=\epsilon_{n-1}+2N_n+L_n$, since the elements of S_n couple all those states. This is the price paid for using the Jacobi rather than single particle coordinates.

The hocfps are evaluated recursively by diagonalizing the transposition class operator (the sum of all the different transpositions)

$$\mathrm{C}^2\,[S_n]=\sum_{i<i'}^{n}(i,i') \tag{4}$$

within sets of states having common ϵ_n, Λ_n and Y_{n-1}. The eigenvalues of this operator *uniquely* determine the various irreps of S_n obtained from a given irrep of S_{n-1} by adding one box[4]. The eigenvectors are the desired hocfps.

The evaluation of the matrix elements of the transposition class operator is presented in ref. [2]. It involves a passage to a new set of coordinates $\vec{\tilde{\rho}}_{n-1}$ and $\vec{\tilde{\rho}}_n$, which are either symmetric or antisymmetric in the coordinates $\vec{r}_{n-1}$ and $\vec{r}_n$. This passage is achieved under a rotation by an angle β satisfying $cos\beta = \sqrt{\frac{n-2}{2(n-1)}}$ and $sin\beta .= \sqrt{\frac{n}{2(n-1)}}$

$$\begin{aligned}
\bar{\vec{\rho}}_{n-1} &= \vec{\rho}_{n-1}cos\beta - \vec{\rho}_n sin\beta = \frac{1}{\sqrt{2}}(\vec{r}_{n-1} - \vec{r}_n) \\
\bar{\vec{\rho}}_n &= \vec{\rho}_{n-1}sin\beta + \vec{\rho}_n cos\beta = \sqrt{\frac{n-2}{2n}}\left[(\vec{r}_{n-1} + \vec{r}_n) - \frac{2}{n-2}\sum_{i=1}^{n-2}\vec{r}_i\right]
\end{aligned} \tag{5}$$

The phase problem associated with degenerate irreps is discussed in ref. [2]

II. Transformation of the harmonic oscillator states from Jacobi into single particle coordinates

The internal h.o. states with arbitrary symmetry, derived in the previous section, are expressed in terms of the normalized Jacobi coordinates (Eq. (1)). However, in many calculations in atomic and nuclear physics it is desirable to have expressions for the wave functions in terms of the single particle coordinates. This is particularly important when the h.o. states are used as a basis set in a calculation involving non-harmonic potentials, which are not easily expressible in Jacobi coordinates.

The total n-particle h.o. wave function is obtained by coupling the c.m. wave function to the internal wave function, obtaining

$$|Y_n\Phi_n c^{(n)}\mathcal{L}_n; \vec{\rho}_2\vec{\rho}_3\ldots\vec{\rho}_n\vec{\rho}^{(n)} > \tag{6}$$

where $\mathcal{L}_n$ is the total angular momentum and $c^{(n)}$ stands for the n-particle c.m. quantum numbers $N^{(n)}$ and $L^{(n)}$. The permutational symmetry of this coupled state is determined by that of the internal state, as was shown in the previous section. For n-particle non-spurious states the c.m. wave function is always in the ground state and therefore $L^{(n)} = 0$ and $\mathcal{L}_n = \Lambda_n$.

The coordinates $\vec{\rho}_n$ and $\vec{\rho}^{(n)}$ can be rewritten in terms of the first $(n-1)$-particle c.m. coordinate, $\rho^{(n-1)} = \frac{1}{\sqrt{n-1}}(\vec{r}_1 + \ldots + \vec{r}_{n-1})$, and the n'th particle coordinate $\vec{r}_n$. Inserting this relation we obtain[5]

$$\begin{aligned}
\vec{\rho}^{(n-1)} &= \vec{\rho}^{(n)}cos\beta - \vec{\rho}_n sin\beta \\
\vec{r}_n &= \vec{\rho}^{(n)}sin\beta + \vec{\rho}_n cos\beta
\end{aligned} \tag{7}$$

where $cos\beta = \sqrt{\frac{n-1}{n}}$.

The h.o. wavefunctions expressed in terms of the coordinates $\vec{\rho}_n$ and $\vec{\rho}^{(n)}$ can be transformed into h.o. wave functions expressed in terms of the coordintes $\vec{\rho}^{(n-1)}$ and $\vec{r}_n$ by using the h.o. brackets for different masses[6].

After separating the wavefunction of the last coordinate ($\vec{r}_n$) by using a change of coupling transformation[7], we obtain

$$\begin{aligned}
|Y_n\Phi_n c^{(n)}\mathcal{L}_n; \vec{\rho}_2\vec{\rho}_3\ldots\vec{\rho}_n\vec{\rho}^{(n)} > = \sum_{\Phi_{n-1}c^{(n-1)}\mathcal{L}_{n-1}h^{(n)}} C^{Y_n\Phi_n c^{(n)}\mathcal{L}_n}_{\Phi_{n-1}c^{(n-1)}\mathcal{L}_{n-1}h^{(n)}} \\
|Y_{n-1}\Phi_{n-1}c^{(n-1)}\mathcal{L}_{n-1}h^{(n)}\mathcal{L}_n; \vec{\rho}_2\vec{\rho}_3\ldots\vec{\rho}_{n-1}\vec{\rho}^{(n-1)}\vec{r}_n >
\end{aligned} \tag{8}$$

where the coefficients are

$$
\begin{aligned}
C^{Y_n \Phi_n c^{(n)} \mathcal{L}_n}_{\Phi_{n-1} c^{(n-1)} \mathcal{L}_{n-1} h^{(n)}} &= \sqrt{(2\Lambda_n + 1)(2\mathcal{L}_n + 1)} \\
&\sum_{\eta^{(n)}} \left[Y_{n-1} \Phi_{n-1} \eta^{(n)} \Lambda_n | \} Y_n \Phi_n \right] \sum_{\lambda} (2\lambda + 1) \\
&\left\{ \begin{array}{ccc} \Lambda_{n-1} & \mathcal{L}_n & \lambda \\ L^{(n)} & L_n & \Lambda_n \end{array} \right\} \left\{ \begin{array}{ccc} \Lambda_{n-1} & \mathcal{L}_n & \lambda \\ \tilde{L}_n & L^{(n-1)} & \mathcal{L}_{n-1} \end{array} \right\} < (c^{(n-1)} h^{(n)}) \lambda | (\eta^{(n)} c^{(n)}) \lambda >
\end{aligned}
\tag{9}
$$

and where the $h^{(n)}$ stands for quantum numbers $\tilde{N}_n$, $\tilde{L}_n$ of the h.o. wave function in the single particle coordinate $\vec{r}_n$. The summation over the quantum numbers N_n and L_n (denoted by $\eta^{(n)}$) is restricted by the condition $\epsilon_n = \epsilon_{n-1} + 2N_n + L_n$, where ϵ_n and ϵ_{n-1} are specified by Φ_n and Φ_{n-1}. Note that the Yamanouchi symbol Y_n determines the Yamanouchi symbol Y_{n-1}. In order to transform completely to the single particle coordinates we have to apply Eq. (8) recursively $(n-1)$ times.

In conclusion we point out that the straightforward construction of an n-particle basis in terms of h.o. wave functions generates a large number of spurious states, involving c.m. motion. A common device employed to eliminate these states is the addition of an appropriate operator with a relatively large coefficient to the hamiltonian, in order to push them up in energy. An obvious drawback is that a huge basis set is employed, a substantial part of which is totally ineffective.

The explicit elimination of the spurious states presently proposed results in a very significant reduction in the size of the basis employed. Moreover, the states constructed in our method have a definite permutational symmetry. This property is essential for calculations involving multiple angular momentum quantum numbers, such as non-relativistic quark calculations.

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