Simple connection between Faddeev's and the K-harmonic approaches

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By employing a system for three bound identical bosons, a simple connection is made between Faddeev's and the K-harmonic approaches.

[NUCLEAR STRUCTURE Quantum few-body problem.]

Some progress has been made in the last decade concerning the quantum three-body problem. Faddeev's equations[1] and the K-harmonic method[2,3] provide, in principle, the possibility of solving that problem exactly. However, cases where those approaches present convergence difficulties are sometimes encountered. Although both approaches have a common origin in the Schrödinger equation and are exact in their context they can lead to different results. This is mainly because they are structurally represented by different equations and hence their numerical solutions can follow different paths of convergence. As a simple way to analyze their convergences, one can start from Faddeev's equations and expand the wave functions in terms of K-harmonics. The numerical solution of the set of equations obtained can be compared with the corresponding K harmonics. This procedure[4] can be done for different classes of pairwise interactions. For each method certain classes of potentials will give solutions which are not convergent. For pairwise functions, examples of this type are Coulomb potentials, r^n potentials,[5] etc., in Faddeev equations, and $r^{-n}(n>2)$ potentials, for K harmonics.[6] On the other hand, it is possible to select a common set of potentials where solutions can be obtained from either of the approaches. This is the case, for instance, for Gaussian, exponential, etc. forces. We are interested in this common situation.

For definiteness and facility to conceptualize, a description for three identical bosons is considered here. Certainly, a generalization of this case can be made.

An appropriate choice of Jacobi coordinates useful in the three-body problem is the following:

$$\vec{\eta}_i = (\tfrac{1}{2})^{1/2}(\vec{r}_j - \vec{r}_k)\,,$$

$$\vec{\xi}_i = (\tfrac{2}{3})^{1/2}\left(\frac{\vec{r}_j+\vec{r}_k}{2} - \vec{r}_i\right),$$

where i,j,k are the three numbers of the set $(1,2,3)$. The sign of $\vec{\eta}_i$ is fixed by the condition that (ijk) should form a cyclic permutation of (1 2 3). The above equation defines three equivalent sets of coordinates $i=1,2,3$ for the description of the three-body problem. A relation[7] among them can easily be found. Faddeev's equations for three-body bound states are given by[1]

$$(H_0+V_\mu-E)\psi_\mu = -V_\mu(\psi_\nu+\psi_\lambda)\,, \tag{1}$$

where $(\mu,\nu,\lambda)=(1,2,3)$ signifies a cyclic permutation, $V_\mu = V_{\lambda\nu}(|\vec{r}_\lambda - \vec{r}_\nu|)$, H_0 is the kinetic energy operator, and E is the binding energy.

For identical particles, the functional dependence ψ_μ is obviously the same for $\mu=1,2,3$. In this case, the total wave function Ψ can be written in terms of the permutation operator P as

$$\begin{aligned}\Psi &= (1+P_{12}P_{31}+P_{12}P_{32})\psi_3 \\ &= (1+P_{31}+P_{32})\psi_3 = (1+P)\psi_3\,,\end{aligned} \tag{2}$$

since $P_{12}\psi_3=\psi_3$, and the coupling in Eq. (1) is removed. We obtain the differential equation

$$(H_0-E)\psi_3(\vec{\xi}_3,\vec{\eta}_3) = -V_3(\vec{\xi}_3,\vec{\eta}_3)(1+P)\psi_3(\vec{\xi}_3,\vec{\eta}_3)\,. \tag{3}$$

By applying the symmetrizer $(1+P)$ on Eq. (3) we obviously get back the Schrödinger equation. This simple connection will be used later.

The K-harmonic or hyperspherical approach[2] consists in expressing the 3-body coordinates in generalized spherical coordinates (a hyperradius $\rho^2=\xi_1^2+\eta_1^2=\xi_2^2+\eta_2^2=\xi_3^2+\eta_3^2$ plus 5 angles $\{\hat{\xi}_i,\hat{\eta}_i,\theta_i\}$, θ_i defined by $\xi_i=\rho\sin\theta_i$, $\eta_i=\rho\cos\theta_i$, $0\leq\theta_i\leq\pi/2$). The total wave function is then expanded in a complete set of angular functions, the K harmonics or hyperspherical harmonics:

$$\psi = \sum_{K\alpha_3}[\phi_{K\alpha_3}(\rho)/\rho^{5/2}]|K\alpha_3\rangle\,, \tag{4}$$

where $\{K,\alpha_3\}$ stands for the appropriate quantum numbers necessary to specify the systems and $\{|K\alpha_3\rangle\}$ the complete set of angular functions. The kinetic energy operator is diagonal in this representation and contains only derivatives with respect to the hyperradius vector and a generalized centrifugal term which acts to suppress the

high partial waves. The two-body potentials are not in general diagonal,[2] but if they are local they will remain so in the hyperradius vector. Hence the K-harmonic method converts the original three-body Schrödinger equation to an infinite set of coupled ordinary differential equations[2,8]

$$(H_0-E)\phi_{K\alpha_3}(\rho)=-3\sum_{K'\alpha_3'}\langle K\alpha_3|V_3(\rho\cos\theta_3)|K'\alpha_3'\rangle \times\phi_{K'\alpha_3'}(\rho),\quad K=0,\ldots,\infty \tag{5}$$

where

$$H_0=\frac{\hbar^2}{2m}\left[\frac{d^2}{d\rho^2}-\frac{\Lambda(\Lambda+1)}{\rho^2}\right],\quad \Lambda=K+\tfrac{3}{2} \tag{6}$$

and the factor 3 in Eq. (5) appears since we are treating a system of three identical particles with angular functions of definite symmetry. The hope is that the centrifugal term in Eq. (6) and the form of the potentials will allow early truncation of the set given by Eq. (4) (at least for bound states). Although it is not difficult to establish the mathematical criteria for this truncation,[3] little serious work has been done along these lines.[9]

One may represent the Faddeev equation (3) and the Schrödinger equation (6) in subspaces spanned by a finite number of K harmonics. One cannot choose the same sets of K harmonics since the Faddeev component ψ_3 and the total wave function Ψ have to fulfill different symmetry requirements. Thus ψ_3 is a symmetric only with respect to the exchange of the pair (1,2) whereas Ψ is fully symmetric. For ψ_3 the following set is convenient[3]:

$$|K,LM,l_{\xi_i}l_{\eta_i}\rangle\equiv|K,\mathfrak{L},\lambda_i\rangle=N_i\sum_{m_{\xi_i}m_{\eta_i}}\langle\lambda_i m_{\xi_i}m_{\eta_i}|\mathfrak{L}\rangle\,Y_{l_{\xi_i}m_{\xi_i}}(\hat{\xi}_i)Y_{l_{\eta_i}m_{\eta_i}}(\hat{\eta}_i)(\sin\theta_i)^{l_{\xi_i}}(\cos\theta_i)^{l_{\eta_i}} \times P^{l_{\xi_i}+1/2,\,l_{\eta_i}+1/2}_{(K-l_{\xi_i}-l_{\eta_i})/2}(\cos2\theta_i) \tag{7}$$

where we are supposing a system of 3 identical bosons (0^+) with a definite total angular momentum L. We should notice that N_i is the normalization constant, $P_\alpha^{\beta,\gamma}(x)$ the Jacobi polynomials, and $\{\theta,\hat{\xi},\hat{\eta}\}$ the 5 angles in the 6-dimensional hyperspace of the 3 particles from which the c.m. motion was removed. Choosing l_{ξ_3} even, the symmetry in the pair (1,2) is guaranteed. Moreover, that set is specially suited if one can restrict the pair interaction V_3 to act only on a certain number of partial wave states.

For Ψ we need totally symmetric basis functions. We may choose as basis states the set $|K\alpha_3\rangle\equiv|K,LM,\nu\Omega\rangle$, as constructed in Ref. 2.

We now pose the question of how many basis states are necessary in the expansions of ψ_3 and Ψ, respectively, to achieve the same accuracy for the energy eigenvalue and eigenfunction. This question can be answered unambiguously, as we shall show below. For definiteness we will restrict ourselves to $L=0\Rightarrow l_{\xi_i}=l_{\eta_i}\equiv l$. Hence[2,3] the two types of states will be represented by $|Kl\rangle$ and $|K\nu\rangle$, respectively.

The Faddeev Eq. (3) in the space spanned by a finite number of states $|Kl\rangle$ reads

$$(H_0-E)\sum_{Kl}|Kl\rangle\langle Kl|\psi_3\rangle =-\sum_{Kl,K'l'}|Kl\rangle\langle Kl|V_3(1+P)|K'l'\rangle\langle K'l'|\psi_3\rangle. \tag{8}$$

Projecting onto $|Kl\rangle$ we obtain the coupled set of ordinary differential equations

$$(H_0-E)\Phi_{Kl}(\rho)=-\sum_{K'l'}\langle Kl|V_3(1+P)|K'l'\rangle\Phi_{K'l'}(\rho), \tag{9}$$

where $\Phi_{Kl}(\rho)\equiv\langle Kl|\psi_3\rangle$.

How can we compare the above set with the one used in Eq. (5)? Let us apply the symmetrization operator $(1+P)$ on Eq. (8). Clearly $(1+P)|Kl\rangle$ is a totally symmetric K harmonics and allows, therefore, the representation

$$(1+P)|Kl\rangle=\sum_\nu A_{K\nu}^{(l)}|K\nu\rangle. \tag{10}$$

Thus Eq. (8) becomes

$$(H_0-E)\sum_{Kl\nu}A_{K\nu}^{(l)}\Phi_{Kl}(\rho) =-\sum_{K\nu,K'\nu'\,l,l'}A_{K\nu}^{(l)}|K\nu\rangle\langle Kl|V_3|K'\nu'\rangle A_{K'\nu'}^{(l')}\Phi_{K'l'}(\rho). \tag{11}$$

If we define

$$\phi_{K\nu}(\rho)=\sum_l A_{K\nu}^{(l)}\Phi_{Kl}(\rho), \tag{12}$$

Eq. (11) takes the form

$$(H_0-E)\sum_{K\nu}|K\nu\rangle\phi_{K\nu}(\rho) =-\sum_{l,K\nu,K'\nu'}|K\nu\rangle A_{K\nu}^{(l)}\langle Kl|V_3|K'\nu'\rangle\phi_{K'\nu'}(\rho), \tag{13}$$

which is already close to Eq. (5) (resulting from the Schrödinger equation).

The decisive step now is to show that

$$\sum_l A^{(l)}_{K\nu}\langle Kl| = 3\langle K\nu| \,. \tag{14}$$

To do this we should note that the fully symmetric state $|K\nu\rangle$ can be represented[3] as a superposition of the states $|Kl\rangle$:

$$|K\nu\rangle = \sum_l C^{(\nu)}_{Kl}|Kl\rangle \,. \tag{15}$$

Furthermore, according to Eq. (10), we have

$$A^{(l)}_{K\nu} = \langle K\nu|(1+P)|Kl\rangle \,. \tag{16}$$

Since $(1+P)$ is Hermitian, we may apply it to the left, picking up a resulting factor of 3, and using Eq. (15), we immediately obtain

$$A^{(l)}_{K\nu} = 3C^{(\nu)*}_{Kl} \,, \tag{17}$$

which proves Eq. (14).

Hence Eq. (13) writes

$$(H_0 - E)\sum_{K\nu}|K\nu\rangle\phi_{K\nu}(\rho) = -3\sum_{K\nu,K'\nu'}|K\nu\rangle\langle K\nu|V_3|K'\nu'\rangle\phi_{K'\nu'}(\rho) \,, \tag{18}$$

or finally

$$(H_0 - E)\phi_{K\nu}(\rho) = -3\sum_{K'\nu'}\langle K\nu|V_3|K'\nu'\rangle\phi_{K'\nu'}(\rho) \,. \tag{19}$$

We find that there is a unique relation between the Faddeev and Schrödinger equations represented in the respective K-harmonics sets $\{|Kl\rangle\}$ and $\{|K\nu\rangle\}$. Using the same $K = K_{\max}$, the energy eigenvalue will be exactly the same calculated by either Eq. (5) or (19). Also the resulting eigenfunctions coincide:

$$\Psi = (1+P)\sum_{Kl}|Kl\rangle\Phi_{Kl}(\rho) = \sum_{Kl\nu}A^{(l)}_{K\nu}|K\nu\rangle\Phi_{Kl}(\rho) = \sum_{K\nu}|K\nu\rangle\phi_{K\nu}(\rho) \,. \tag{20}$$

However, the number of coupled equations may be different in general. Thus up to $K = 10$ only one totally symmetric state exists (ν takes only one value; see Ref. 2, Table II), whereas several l values come into play. Therefore, there are several states $|Kl\rangle$, for each $|K\nu\rangle$. If the situation is such that a relatively small $K_{\max}$ value is enough to achieve convergence, the Schrödinger equation for Ψ leads to a smaller number of coupled equations. The situation may be different if one considers short-range interactions which are effective only for s waves (or for few low l states). Then a corresponding reduced number of $|Kl\rangle$ states occur furnishing a reduced number of coupled equations in the Faddeev approach. In contrast, the above assumption for V_3 does not lead to a reduction of $|K\nu\rangle$ states.[2] Since the dependence on ν in the states $|K\nu\rangle$ increases with K, it is conceivable that the Faddeev set (9) is more advantageous in a situation where large K values are needed.

Finally, we should mention that for one-dimensional systems of three identical bosons the two approaches are absolutely equivalent.[9,10]

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