

# Hyperspherical Expansion Approach for Study the Three Particle System

Kumari Priyanka<sup>1</sup>, B. B. Prasad<sup>1</sup> and Pramod Kumar<sup>2</sup>

<sup>1</sup>Department of Physics, VKSU, ARA

<sup>2</sup>Department of Botony, MU, Bodh Gaya

## Abstract

There are various methodologies of studies on scattering behavior of three-particle system. Among them, Hyperspherical harmonics methods are quite efficient to study three particle systems. An interesting approach which received good attention for treatment with local potentials is the method of hyperspherical harmonics (HH). The three-body wave function is expanded in a discrete orthonormal set of functions in five of six degrees of freedom. This expansion result in a set of coupled one dimensional differential equation and can be handled by standard procedures. This method appears to work well for soft core interactions

**Keywords:** *hyperspherical harmonics, three-particle, interaction, differential equation*

## 1. Introduction

The three-body system as the simplest many-body system which contain the different of transition from two-body to many-body treatments. These systems present a scene of theoretical laboratory for testing these approximations used in many-body studies.

The available two-body data (binding energy and scattering parameters) can be explained by analyzing the theoretical framework easily, but the data do not contain enough in formations for example,  $\Sigma$ -N scattering data is scarce and to derive such two-body potentials which fit the three-body experiment data is a major theoretical exercise. Moreover the two-body potentials can be constructed which has correct two-body “on shell”, properties but fail to reproduce “off shell” events; therefore, three-body studies are important in fixing up two-particle interactions.

There is various methodology of studies on three-particle like Variational, Faddeev and hyperspherical harmonics methods. An interesting approach which received good attention for treatment with local potentials is the method of hyperspherical harmonics (HH). The three-body wave function is expanded in a discrete orthonormal set of functions in five of six degrees of freedom. This expansion result in a set of coupled one dimensional differential equation and can be handled by standard procedures. This method appears to work well for soft core interactions. As one moves to hard cores the convergence becomes poorer.

## 2. Hyperspherical Expansion Approach

This method was pioneered by Delves [1,2] and by Simonov [3]. This method was improved by Favry [4]. It was reviewed by Simonov [3] in 1966 and Louck et al [5].

In the hyperspherical harmonics method the three particle system is described in a six-dimensional hyperspace having five angular coordinates and a radius vector called hyperradius. The Schrodinger equation expressed in this space involves hyperangular momentum operator, and the three particle wave function can be expanded in a set of hyperangular functions with the hyper radial part of the wave function as coefficient of the expansion. The system of three-particle wave equation can then be reduced to a set of coupled integral equation in a single variable *i.e.* the hyperradius, if the angular variables are integrated out. The eigen functions of hyperangular operators are called the hyperspherical harmonics.

The basic idea is to generalize the spherical harmonic used in two-body problem in a six dimensional hyperspace hence the name hyperspherical harmonics expansions of HHE method.

For the three particle system we use rationalized Jacobi co-ordinates

$$\vec{\xi} = \sqrt{\left(\frac{m_1 m_2}{m_1 + m_2}\right)} \times (\vec{r}_1 - \vec{r}_2) \quad (1)$$

$$\vec{\eta} = \sqrt{\frac{m_3 (m_1 + m_2)}{m_1 + m_2 + m_3}} \times \left(\frac{m_1 \vec{r}_1 + m_2 \vec{r}_2}{m_1 + m_2}\right) \quad (2)$$

Where  $r_1, r_2, r_3$ , are the position vector of the three particle 1, 2,3. The co-ordinate  $\xi$  is the distance between the particles 1 and 2 while  $\eta$  is the distance between the particle 3 and center of mass of particles 1 and 2.

Instead of two-body angular momenta

$$\vec{r}_{12} = \frac{\hbar}{i} \left[ \vec{r}_{12} \times \frac{\partial}{\partial r_{12}} \right] \quad (3)$$

Which does not commute with each other, we introduce “Jacobi” momenta:

$$\vec{l}_\xi = \frac{\hbar}{i} \left[ \vec{\xi} \times \frac{\partial}{\partial \xi} \right]; \vec{l}_\eta = \frac{\hbar}{i} \left[ \vec{\eta} \times \frac{\partial}{\partial \xi} \right] \quad (4)$$

and  $\vec{L} = \vec{l}_\xi + \vec{l}_\eta$

L is the total angular momentum of the system

The first step is to introduce the “hyperradius”  $\rho$  in the six- dimensional space.

$$\rho^2 = \xi^2 + \eta^2 \quad (5)$$

Our six-dimensional space comprise of one hyperradial length  $\rho$  and five angles ( $\theta_\eta, \phi_\eta, \phi_\xi, \theta_\xi, \beta$ ). Then all the angular variables separate in the kinetic energy operator, after the removal of the motion of center of mass of the system.

$$\hat{T} = \frac{1}{2\mu} \left\{ \frac{1}{\rho^5} \frac{\partial}{\partial \rho} \left( \rho^5 \frac{\partial}{\partial \rho} \right) + \frac{\Delta_\Omega}{\rho^2} \right\} \quad (6)$$

$\Delta_\Omega$  is the angular part of the six-dimensional Laplacian  $\Delta_6$  and the three-particle Schrodinger equation has the form

$$(\hat{T} + U_{123})\psi(\vec{\xi}, \vec{\eta}) = E\psi(\vec{\xi}, \vec{\eta}) \quad (7)$$

Next step in the hyperspherical harmonics approach is the choice of angular functions (harmonics); they are taken to be the eigenfunctions of  $\Delta_6$

$$\Delta_6 U_{K\alpha} = K^2 u_{K\alpha} = K(K+4) u_{K\alpha} \quad (8)$$

Here K is an integer and  $\alpha$  are all other quantum numbers.  $K^2$  is the hyperangular momentum operator with the eigen values  $-K(K+4)$  One can express  $u_{K\alpha}$  through harmonic polynomials

$$u_{K\alpha}(\Omega) = \rho^{-K} P_{K\alpha}(\vec{\xi}, \vec{\eta}) \quad (9)$$

Where,

$$\Delta_6 P_{K\alpha} = \left( \frac{\partial^2}{\partial \xi^2} + \frac{\partial^2}{\partial \eta^2} \right) P_{K\alpha} = 0 \quad (10)$$

K is the power of the polynomial  $P_{K\alpha}$ . The angular functions  $u_{K\alpha}$  hyperspherical harmonics with the properties (8 to 10) are called hyperspherical functions (H.F.)

The three-particle wave function in this representation is an expansion

$$\Psi = \sum_{K\alpha} \chi_{K\alpha}(\rho) u_{K\alpha}(\Omega) \tag{11}$$

The coefficients  $\chi_{K\alpha}$  are called partial waves. It is interesting to see what will happen if we use instead of space co-ordinates the momentum coordinates:  $\xi \rightarrow p_\xi$ ;  $\eta \rightarrow p_\eta$ ;  $R \rightarrow p$  The corresponding “hyperradius” is then simply the total kinetic energy (k.e) (the total energy of free particles before and after collision) with center of mass motion excluded.

$$p^2 = p_\xi^2 + p_\eta^2 = 2\eta E \tag{12}$$

Therefore, scattering or decay amplitudes depends on the angular variables  $\Omega_p$  with the hyperradius  $\rho_p$  fixed. The expansion (12) can now be used in two different ways. One is the kinematical natural [1,6]. Suppose  $\Psi$  is the scattering or decay amplitude, depending on the internal momenta.  $p_\xi$  and  $p_\eta$  with  $E$  fixed. Then equation (11) gives immediately a parametrization of the amplitude. In general H.H. satisfies orthonormality conditions.

$$\int u_{K\alpha}^*(\Omega) u_{K'\alpha'}(\Omega) d\Omega_\xi = \delta_{KK'} \delta_{\alpha\alpha'} \tag{13}$$

$$\text{where } d\Omega_\xi = \int_0^{\pi/2} \sin^2 \theta \cos \theta d\theta \int d\Omega_\xi d\Omega_\eta \tag{14}$$

$d\Omega_\xi$  and  $d\Omega_\eta$  are the respective elements of solid angle in the  $\xi$  and  $\eta$  directions. Taking in the momentum variables (14), one easily observes that (14) is no more than the phase space of 3-particles, which is present in the unitarity relation

$$\text{disc} \Psi_{n \rightarrow m}(\vec{p}_\xi) = \left( \Psi_{n \rightarrow A}(\vec{p}_\xi) \Psi_{m \rightarrow A}(\vec{p}_\xi) + \Psi_{n \rightarrow A}(\vec{p}_\eta) \Psi_{m \rightarrow A}(\vec{p}_\eta) d\Omega_\xi \right) \tag{15}$$

Where  $A=3$ . Now due to (13) the expansion (11) immediately diagonalizes the A-th part of the unitarity expression (15). This is one of the most important reasons why the expression (11) turned out to be useful in the analysis of an amplitude with A particles in the final state. One of the most important applications of this sort is the analysis of the Dalitz-Fabre plot [7] to parametrize the decay amplitude and to compare the experimental results of different groups.

Now we turn to the dynamics of  $A(=3)$  particles. Inserting (5) with into the Schrodinger equation, and multiplication by  $u_{K\alpha}(\rho)$  and utilization of the orthonormal property (13) we get an infinite coupled set of one-dimensional equation.

$$\chi_{K\alpha}(\rho) = \rho^{-S/2} P_{K\alpha}(\rho) \tag{16}$$

$$\left[ \frac{d^2}{d\rho^2} - \frac{\Lambda(\Lambda+1)}{\rho^2} + \frac{2\mu E}{\hbar^2} \right] P_{K\alpha}(\rho) = \frac{2\mu}{\hbar^2} \sum_{K'\alpha'} U_{K\alpha}^{K'\alpha'}(\rho) P_{K'\alpha'}(\rho) \tag{17}$$

Where the matrix elements of potentials are:

$$U_{K\alpha}^{K'\alpha'}(\rho) = \int U_{K\alpha}^*(\Omega) (U_{123}) U_{K'\alpha'}(\Omega) d\Omega_\xi, \tag{18}$$

and  $U_{123}$  is the potential operator. Equations (17) are the final product in the dynamical applications of the hyperspherical harmonic approach. They can be used both for (i) bound state problems when  $E < 0$  and (ii) scattering when  $E > 0$  in the later case one should write in addition to (17) the asymptotic conditions, describing the scattered waves and the possible presence of bound subsystem at infinite  $\rho$ . This causes much trouble because in this case the convergence is bad and the number of equations (17) to be solved is large. However, the convergence is bad due to the asymptotic terms, which can be written explicitly (in the case) of two outgoing subsystems [8]; therefore, the expansion of the remaining part of the wavefunction is convergent much better [9]. There are a number of studies giving the general formalism and calculations concerning this approach [8,10]. Most ambitious approach and a general one of this kind is the “Quasimolecular approach” or “Interpolation Method” suggested by Baz [11].

The case of three outgoing subsystems needs a more elaborate analysis, since the asymptotics are more complicated. In the case of bound states total wavefunction vanishes asymptotically. To understand the physical meaning of the global quantum no.  $K$ , we use the analogy to ordinary angular momentum. When a particle is

scattered from a potential  $V(r)$  the angular momentum decomposition of the scattering solution  $\Psi(r)$  is an expansion into components of different impact parameter  $p$ . classically, the impact parameter is the closest distant in which a particle of given angular momentum and given velocity  $v$  passes the scattering centre. In quantum mechanics the impact parameter has no sharp value. But we have still approximately

$$p = \frac{L\hbar}{v} \quad (19)$$

And thus, an expansion into angular momentum quantum numbers  $L$  is an expansion into impact parameters. When the potential  $V(r)$  is short-ranged and the velocity  $V$  is not too large, only the first few terms of the expansion will contribute to the scattering process.

The quantum number  $K$  has a quite similar meaning. We could call it a three-particle impact parameter. Thinking in terms of classical orbits, a large value of  $K$  means that the three particles cannot come close to each other at the same time. Either all three particles are far apart or, when two particles are close together, the third particle is far apart. When  $K = 0$ , on the other hand, all three particles meet in the scattering center. The minimum value of  $\rho$  is related to  $K$  just as the minimum value of  $r$  is related to  $L$ . for  $K=0$ , the particles seem to come right out of the scattering center. For higher values of  $K$ , they seem to have left the scattering center in a more and more “Crooked way”. Two advantages of the expansion into angular momentum eigenstates are not present in the hyperangular momentum expansion ( $K$ -harmonic expansion) of a scattering wavefunction. Firstly, a sum of two-particle interaction potentials is not spherically symmetric in the six-dimensional co-ordinate space except for the harmonic oscillator type potential. The operator  $K$ , therefore, does not commute with the Hamiltonian  $H$ , while  $L$  commutes with  $H$  for a spherical symmetrical potential  $V(r)$ . The various hyperspherical states are coupled by the interaction. Secondly and this may be even more important, higher-order terms of the expansion into hyperspherical functions become unimportant only in certain special cases. A sum of two-particle interaction potentials has an infinite range in  $\rho$ -space, that is  $V(\rho)$  does not tend to zero with  $\rho \rightarrow \infty$ .

Ballot and Fabre [12] made a significant improvement to this method, by introducing a linear combination of Simonov’s hyperspherical harmonic, which Fabre calls “Optimal subset” (also called “potential harmonics”). The subset is chosen so that a given type of potential will have all its non-zero matrix element between members of the subset. This choice adopted by Erens et al. [13] for central potential and by Fabre [12], and Efros [14] for tensor potentials, gives a substantial improvement in the speed of convergence e.g. in the central case, 27 members of Fabre’s subset take into account 75 members of Simonov’s original set.

Also, there is one most important aspect of the treatment is that energies of any excited states can be found out once the ground state energy has been obtained. In case of Simonov’s [15] treatment of triton, the first harmonics contributed to binding energy was of the order of 90%. Therefore, a fast convergence towards the total binding can be obtained with very few harmonics.

Hyperspherical harmonic method has used by other workers also calculating the binding energy of three-body nuclear systems. Notable work has been done by Ballot and Fabre [12,17]. Ballot [12] has prescribed method for use of optimal subset.

**Optimal Subset:** A potential independent of the angular variables in the H.H.E. is hypercentral. It is a function of the hyperradius  $\rho$  only. But except harmonic oscillator potential no two-body potential is hypercentral. In the 6-dimensional space all other potentials contain hyperspherical deformations described by the various components of the hyperspherical harmonics expansions of the potential. These components in turn generate hyperspherical deformation in the wavefunction. When the deformation of the potential is small with respect to the hypercentral term, it is justified to use a perturbation expansion of the wavefunction in terms of the deformed part of the potential. Assume that a state  $\Psi(\rho, \Omega)$  is described to a good approximation by a wavefunction  $\Psi_0(\rho, \Omega)$  in such a way that  $\langle \Psi | \Psi_0 \rangle \approx 1$

One defines an optimal subset with respect to this state by stating that any element  $\Psi_k(\rho, \Omega)$  orthogonal to  $\Psi_0(\rho, \Omega)$  must fulfil the condition

$$\langle \Psi_k | V(\rho) | \Psi_0 \rangle = \int d\Omega \Psi_k^*(\rho, \Omega) V(\rho) \Psi_0(\rho, \Omega) = 0 \quad (20)$$

In the case the exclusive use of the  $\Psi_k(\rho, \Omega)$  subset enables one to take completely into account a perturbative calculation up to the third order included. In the hyperspherical formulation  $\Psi_0(\rho, \Omega)$  is the product of  $\Psi_0(\rho)$  and a H.H.  $B_0(\Omega)$  fully antisymmetric. More detail is available in the reference [17].

The method of optimal subset has the advantage that instead of using infinite number of coupled differential equations only those equations come into play which contribute to the binding energy. This method has been widely used by Coelho, Das etc [16]. This method has the specific importance when efficient computers were not available to handle large determinants.

Also, a technique for the reduction of the system of coupled differential equations to three coupled equations for the hyperspherical harmonics formalism was proposed by Fabre [17]. But this technique was followed with a numerical application by Das et al.[16]. The same approximation has already been used for atoms by Macek [18] and C.D.Lin [19]. In their work Das et al. [16] have investigated the quality of approximation with nuclear potentials which exhibit rapid variations in short range. This method is also known as Uncoupled Adiabatic Approximation (UAA). They have worked with four different two-body potentials of Baker

Volkov, S3 and S4\40\ for the calculation of the triton binding energy. The result with UAA is found to be very close to those obtained with CDE (Coupled Differential Equations). The calculation of the eigen solution of a large number of coupled equations is extremely difficult. But with the use of UAA method this difficulty is simplified two ways first the computing time and second memory requirements.

Further, it is to be remarked that Macek [18] has shown that it should work well in the study of atomic systems.

Another important work on the adiabatic approximation in the three-body problem is due to Ballot, Fabre and Levinger [20]. In the framework of the hyperspherical formalism, they have studied the coupled adiabatic approximation (CAA) for the case of three-nucleons interacting via central spin-dependent two-body potentials. They have analyzed the convergence of the ground state eigen-values versus the grand orbital quantum number and compare the results to that coupled equations. They also compare with two simpler but less accurate approximations than the uncoupled adiabatic approximations called the extreme adiabatic approximation. The former provides an upper and the latter provides a lower bound to the ground state energy.

The idea of the adiabatic approximation was introduced by Born and Oppenheimer to solve the bound state of electrons and nuclei in a diatomic molecule. The authors [20] have discussed extreme adiabatic approximation (EAA), uncoupled adiabatic approximation (UAA) and coupled adiabatic approximation. They have demonstrated the basic inequalities

$$E(EAA) \leq E(CE) \leq E(CAA) \leq E(UAA) \quad (21)$$

Where E is the b.e. They have made the numerical calculations and compared the results. They authors finally comment that an extension of CAA method using a higher number of coupled equations is not interesting, because of the complicated nature of coupling amplitudes.

Powerful and exact approaches for three-body problem are the hyperspherical harmonic method, Faddeev equations and Yakubowski equations. For the bound state calculations, hyperspherical harmonic approach is more popular and adequate.

For the three-body problem for certain kinds of physical interactions, one cannot use the Faddeev equations in the t-matrix form because the Schmidt's norm of the kernel of these equations diverges. Hyperspherical harmonic method is an accurate method. A correlation between the Faddeev equation and hyperspherical harmonic expansion exists. Adhikari and Tomio [21] have proposed iterative method for solution of three-particle and four-particle one-dimensional homogenous integral equations of the method of hyperspherical functions in the momentum representation for solving the integral Faddeev equation in the case of separable potentials. The use of hyperspherical functions for solving Faddeev equations for the case of double hypernuclei and supernuclei has been made by Dzhibuti et al. [22, 23]. A new partial expansion for the Faddeev integral equations in the hyperspherical basis has been obtained by Dzhibuti et al. [22] as an application to the ground states of  $^3\text{H}$  and hypernucleus  $^9_{\Lambda}\text{Be}$  for various  $\Sigma$  local potentials has been studied. A good convergence in the number of the K-harmonics is demonstrated. A generalization to 4-body case is also possible.

### 3. Conclusions

There are many methodologies for the studies on three-particle and the more scientific are Variational, Faddeev and hyperspherical harmonics methods. The method of hyperspherical harmonics, provides an efficient approach to study three-particle system e.g.  $\Sigma^-$  - hypertriton in  $(\Sigma^- - n - n)$  model. The  $\Sigma^-$ -n potential have been derived which provide the limits to the hypertriton ground state energies corresponding to the binding energy of a bound sigma-minus deuteron ( $^d_{\Sigma^-}$ ) which is  $^+_{0} - ^{10}_{0}$  Mev.

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