EJTP **7, No. 23** (2010) 137–144 *Electronic Journal of Theoretical Physics*

A generalization of the Three-Dimensional Harmonic Oscillator Basis for Wave Functions with Non-Gaussian Asymptotic Behavior

Maurizio De Sanctis *

Departamento de Física, Universidad Nacional de Colombia, Bogotá D. C., Colombia

Received 10 January 2010, Accepted 8 March 2010, Published 20 March 2010

Abstract: Starting from the standard harmonic oscillator basis, we construct new sets of orthonormal wave functions with non-Gaussian asymptotic spatial dependence. These new wave functions can be used to study at numerical level two-body bound systems like mesons and baryons within quark-diquark models. Generalized hyperradial functions for three-quark models are also studied.

Keywords: Solutions Of Wave Equations: Bound States; Nonrelativistic Quark Models; Relativistic Quark Models
PACS (2008): 03.65.Ge; 12.39.Jh;12.39.Ki

1. Introduction

In order to study hadronic systems by means of constituent quark models, numerical variational methods (with the diagonalization of the Hamiltonian matrix) are generally used to find approximate eigenvalues and eigenfunctions for the Hamiltonian operator of the chosen model. We point out that, for those Hamiltonians, especially in relativized models, no analytic study is practically possible. On the other hand, the variational-diagonalization methods require to introduce a *basis*, that is a *complete* set of orthonormal (normalizable) *trial* wave functions. The most widely used (for its good analytic properties) is that given by the eigenfunctions of the nonrelativistic harmonic oscillator (HO) Hamiltonian. Coulombic bound state wave functions are also used but, due to the presence of the *continuum* states, they do not really represent a (complete) basis. Furthermore, we recall that they depend on the *energy* of each state.

* mdesanctis@unal.edu.co

As for the HO wave functions, their Gaussian asymptotic behavior is not compatible with other potentials, different from the HO one. As a consequence of this inconsistency a poor determination of the energy eigenvalues may be obtained. Moreover, the spatial behavior of the wave functions, that is used to study the electroweak hadronic form factors, is not correctly reproduced unless a very large number of HO wave functions is considered in the diagonalization procedure.

Aim of this note is to generalize the HO basis for the case of a different asymptotic behavior of the wave functions. We shall construct a *complete set* of orthonormal spatial wave functions for two-body bound systems such as mesons in quark-antiquark models [1], [2] and baryons in quark-diquark models [3], [4]. Furthermore, with the same technique, we shall generalize the hyperradial wave functions for studying three-body baryonic systems [5], [6]. The generalization is essentially obtained by replacing the standard argument of the HO (Gaussian) wave functions, proportional to r^2, with other spatial dependences and using, with a change of variable, the orthogonality of the Laguerre polynomials. For clarity, we derive our results in coordinate space but we also show how to construct, exactly in the same manner, the momentum space wave functions. These latter wave functions are strictly necessary for the numerical study of relativistic problems with strongly nonlocal interactions.

The remainder of this note is organized as follows. In sect. 2 we shall concisely revise the standard HO case. In sect. 3 we shall describe the generalization procedure for two-body problems and, in sect. 4 we shall study the generalization of the hyperradial functions for three-body systems. Finally, in sect. 5, some concluding remarks will be drawn.

2. The Standard HO Case

As starting point we take the usual nonrelativistic Schrödinger equation for a 3-dimensional HO

$$\left[\frac{\vec{p}^2}{2m} + \frac{1}{2}m\omega^2\vec{r}^2\right]\psi_{nlm_l}(\vec{r}) = E_{nl}\psi_{nlm_l}(\vec{r}) \tag{1}$$

where, for a two-body system, $\vec{r}$ represents the interparticle distance, $\vec{p}$ the conjugate momentum operator, m the reduced mass and ω the oscillator frequency. A standard procedure [7] allows to separate, for every central potential, the angular momentum eigenfunctions $Y_{lm_l}(\theta,\phi)$, so that the total wave functions are written as

$$\psi_{nlm_l}(\vec{r}) = \widehat{R}_{nl}(r)Y_{lm_l}(\theta,\phi) \ . \tag{2}$$

We need to analyze and generalize only the *radial part* of the wave functions, *i.e.* $\widehat{R}_{nl}(r)$. We recall that the HO is one of the few cases of physical interest in which their form can be determined analytically. In particular, they can be written as

$$\widehat{R}_{nl}(r) = \frac{1}{\bar{r}^{3/2}}s^l\widehat{Q}_{nl}(s)\exp\left[-\frac{1}{2}\widehat{F}(s)\right] \ . \tag{3}$$

In the present section the *hat* denotes all the spatial functions for the specific HO case. In the previous equation the following quantities have been introduced:
a) the paramenter $\bar{r}$, with dimensions of a *length*; when solving eq. (1) it takes the form $\bar{r} = (m\omega/\hbar)^{-1/2}$; on the other hand, it represents the variational parameter for the numerical solution in the nonanalytic cases;
b) the adimensional spatial variable $s = r/\bar{r}$;
c) the argument of the asymptotic exponential function $\widehat{F}(s) = s^2$, determined by the presence of the HO potential in eq. (1);
d) the polynomial factor

$$\widehat{Q}_{nl}(s) = c_{nl} L_n^{\alpha}(s^2) \ , \tag{4}$$

where the Laguerre polynomials $L_n^{\alpha}(u)$ are defined as in [8], with

$$\alpha = l + 1/2 \tag{5}$$

and, finally, the normalization constants

$$c_{nl} = \left[\frac{2(n!)}{\Gamma(n+\frac{3}{2})} \right]^{1/2} \quad . \tag{6}$$

Note that in eq. (3) the factor s^l gives the standard short range behavior of the wave functions. We also recall that the HO energy eigenvalues appearing in eq. (1) are

$$E_{nl} = \hbar\omega(2n + l + \frac{3}{2}) \tag{7}$$

where $N = 2n + l$ is often introduced.

For the following developments we also recall explicitly the integration rule of the Laguerre polynomials [8]

$$\int_0^{\infty} du \ u^{\alpha} L_{n'}^{\alpha}(u) L_n^{\alpha}(u) \exp(-u) = \frac{n!}{\Gamma(\alpha + n + 1)} \cdot \delta_{n'n} \tag{8}$$

from which, by means of a standard change of variable, the orthonormality equation for the radial HO wave functions is easily obtained

$$\int_0^{\infty} dr \ r^2 \widehat{R}_{n'l}(r) \widehat{R}_{nl}(r) = \delta_{n'n} \ . \tag{9}$$

3. The Generalized Basis for Two-Body Systems

For the radial wave functions of the generalized orthonormal basis we take the same structure as that of eq. (3)

$$R_{nl}(r) = \frac{1}{\bar{r}^{3/2}} s^l Q_{nl}(s) \exp\left[-\frac{1}{2} F(s) \right] \tag{10}$$

where s is the adimensional spatial variable, defined as is sect. 2. The function $F(s)$ is a positive, growing function of s. In particular, we require that:

(1) $Q_{nl}(0) = q_{nl}$, where the q_{nl} are constants;
(2) for $s \to \infty$, $Q_{nl}(s) \approx s^p$, where p is a positive real (finite) number;
(3) for $s \to 0$, $F(s) \approx s^f$, where f is a positive real number.

In more detail,

- requirement 1 will be used to ensure that the $R_{nl}(r)$ have the standard s^l behavior near the origin;
- requirement 2 and the form of the exponential function of $-\frac{1}{2}F(s)$ ensure that the wave functions are normalizable; finally,
- requirement 3 will be used to construct $Q_{nl}(s)$ that satisfy requirement 1. An upper limit for f will be also fixed.

To explain more clearly the following developments, we introduce the functions

$$G_{nl}(s) = s^{l+1} Q_{nl}(s) \ . \tag{11}$$

In terms of these functions the condition of orthonormality for the $R_{nl}(r)$ takes the form

$$\int_0^\infty dr\ r^2 R_{n'l}(r) R_{nl}(r) = \int_0^\infty ds\ G_{n'l}(s) G_{nl}(s) \exp[-F(s)] = \delta_{n'n} \ . \tag{12}$$

On the other hand, the orthonormality condition of the Laguerre polynomials given in eq. (8), by means of the following change of variable

$$u = F(s) \ , \quad F'(s) ds = du \ , \tag{13}$$

can be easily put in the form

$$\int_0^\infty ds\ F'(s)[F(s)]^\alpha \left(\frac{n'!}{\Gamma(\alpha+n'+1)}\right)^{1/2} L_{n'}^\alpha(F(s)) \times \left(\frac{n!}{\Gamma(\alpha+n+1)}\right)^{1/2} L_n^\alpha[F(s)] \exp(-F(s)) = \delta_{n'n} \ . \tag{14}$$

In consequence, comparing the previous equation with the orthonormality condition of eq. (12), we can write the $G_{nl}(s)$ as

$$G_{nl}(s) = \left(\frac{n!}{\Gamma(\alpha+n+1)}\right)^{1/2} [F'(s)(F(s))^\alpha]^{1/2} L_n^\alpha(F(s)) \ . \tag{15}$$

Then, by means of eq. (11), the $Q_{nl}(s)$ obviously take the form

$$Q_{nl}(s) = s^{-(l+1)} G_{nl}(s) \ . \tag{16}$$

By taking into account requirement 3, we can now fix the value of the index α in order to satisfy requirement 1. Considering the behavior of the $Q_{nl}(s)$ of eq. (15), with the help of (16), for $s \to 0$, one easily finds

$$\alpha = \frac{2l+3}{f} - 1 \ . \tag{17}$$

Furthermore, in the Laguerre polynomials one necessarily has $\alpha \geq 0$. In consequence, one determines, by means of the previous equation, the upper limit for f. Recalling that the wave functions with $l = 0$ must be always included, one has

$$f \leq 3 \ . \tag{18}$$

The previous equations complete the definition of the generalized basis. Note that, for the case $F(s) = s^2$, that implies $f = 2$, the standard H.O. case is easily recovered. For $F(s) = s$, that means $f = 1$, the Coulomb-Sturmian wave functions are obtained. These wave functions have been recently used to study the bound-state problem by means of an integral equation, incorporating the kinetic energy and the confining term into the Green's operator [9].

We point out that, in general, the argument of the Laguerre polynomials appearing in eq. (15) is not an integer power of s, so that our generalized functions do not have the standard structure *polynomial*$\times$*Gaussian function* as the HO ones.

One can repeat *exactly* the same procedure to construct radial momentum space functions. Analogously to eq. (10), they have the form

$$R_{nl}(p) = \frac{1}{\bar{p}^{3/2}} q^l Q_{nl}(q) \exp\left[-\frac{1}{2}F(q)\right] \tag{19}$$

where p is the relative momentum variable, $\bar{p}$ is the *dimensional* parameter and $q = p/\bar{p}$. The functions $Q_{nl}(q)$ and $F(q)$ are determined in the same way as in coordinate space. Obviously, the Fourier transform of $R_{nl}(r)$ maintains, in the momentum space, the *same* functional form (apart from a phase factor), *only* in the HO case.

4. The Generalized Hyperradial Wave Functions

Three-body systems are conveniently described in terms of the Jacobi coordinates $\vec{\rho}$ and $\vec{\lambda}$

$$\vec{\rho} = \frac{1}{\sqrt{2}}(\vec{r}_1 - \vec{r}_2), \qquad \vec{\lambda} = \frac{1}{\sqrt{6}}(\vec{r}_1 + \vec{r}_2 - 2\vec{r}_3) \tag{20}$$

after removing the center of mass coordinate $\vec{R}$. Then, instead of the Jacobi coordinates, one can introduce the hyperspherical ones [6], which are given by the angles $\Omega_\rho = (\theta_\rho, \phi_\rho)$ and $\Omega_\lambda = (\theta_\lambda, \phi_\lambda)$ together with the hyperradius, x, and the hyperangle, ξ, respectively defined as

$$x = \sqrt{\vec{\rho}^2 + \vec{\lambda}^2}, \qquad \xi = arctg(\frac{\rho}{\lambda}) \ . \tag{21}$$

Considering a *nonrelativistic* three-body Hamiltonian, if an hypercentral potential $V(x)$ is taken, the total wave function can be factorized into a product of a hyperspherical harmonic function $Y_{[\gamma]l_\rho l_\lambda}(\Omega_\rho, \Omega_\lambda, \xi)$ and a hyperradial function $\psi_{n\gamma}(x)$. The grand-angular quantum number is $\gamma = 2\nu + l_\rho + l_\lambda$, with $\nu = 0, 1, ...$, and l_ρ, l_λ representing the angular momenta associated to $\vec{\rho}$ and $\vec{\lambda}$, respectively.

In the hyperradial function $\psi_{n\gamma}(x)$, the quantum number n identifies the *different*, orthonormal, wave functions with the same γ. All these wave functions are completely symmetric with respect to particle interchange, given that the hyperradius x is symmetric. Suitable linear combinations of the hyperspherical harmonics are constructed to obtain wave functions with definite permutational symmetry [6]. The hyperradial functions $\psi_{n\gamma}(x)$ can be determined analitically in two cases of physical interest. First, when the interaction is represented by a HO two-body potential, that can be easily written as a hypercentral harmonic potential. In this case the hyperradial wave fuctions have a standard Gaussian behavior in x. Second, when the interaction is a hyperCoulomb (also called six-dimensional Coulomb) potential. The basis derived from the former approach has been widely used for the study of baryonic spectroscopy [10]; the wave functions derived from the latter [6] have improved the reproduction of several physical observables of the nucleon and have been recently used also for the study of triple heavy flavour baryons [11]. However, analogously to the case of two-body sistems, the (bound state) eigenfunctions of the hyperCoulomb nonrelativistic Hamiltonian do not represent a complete basis and depend on the energy of the state.

The orthonormality condition takes, in general, the form

$$\int_0^\infty dx x^5 \psi^*_{n'\gamma}(x)\psi_{n\gamma}(x) = \delta_{n'n} \tag{22}$$

where the factor x^5 is introduced when changing the variables $\vec{\rho}$ and $\vec{\lambda}$ with the hypercentral ones of eq. (21). For our generalization, analogously to eq. (10), we introduce

$$\psi_{n\gamma}(x) = \frac{1}{\bar{r}^3} y^\gamma \tilde{Q}_{n\gamma}(y) \exp\left[-\frac{1}{2}\tilde{F}(y)\right] \tag{23}$$

where $\bar{r}$, as in sect. 3, is the dimensional parameter of the model and $y = x/\bar{r}$ represents the adimensional hyperradius variable. For the functions $\tilde{Q}_{n\gamma}(y)$ and $\tilde{F}(y)$ we make the same requirements as those made in sect. 3 for the corresponding (untilded) functions. In this way, the standard x^γ behavior (when $x \to 0$) for the hyperradial functions, is obtained. We also introduce, for clarity

$$\tilde{G}_{n\gamma}(y) = y^{\gamma+5/2}\tilde{Q}_{n\gamma}(y) \ . \tag{24}$$

Following exactly the same procedure of eqs. (12)-(15), but using here the orthonormality condition of eq. (22) instead of eq. (12), one can finally write the $\tilde{G}_{n\gamma}(y)$ in terms of Laguerre polynomials of $\tilde{F}(y)$, obtaining the *same expression* as that given in eq. (15), with l replaced here by γ:

$$\tilde{G}_{n\gamma}(y) = \left(\frac{n!}{\Gamma(\tilde{\alpha}+n+1)}\right)^{1/2} [\tilde{F}'(y)(\tilde{F}(y))^{\tilde{\alpha}}]^{1/2} L_n^{\tilde{\alpha}}(\tilde{F}(y)) \ . \tag{25}$$

In this case, the value of $\tilde{\alpha}$ for the hyperradial functions is

$$\tilde{\alpha} = \frac{2\gamma+6}{f} - 1 \ . \tag{26}$$

Recalling that, as in sect. 3, $\tilde{\alpha} \geq 0$ and that the value $\gamma = 0$ must be included, one finds the upper limit for f:

$$f \leq 6 \quad . \tag{27}$$

Obviously, from eq. (24), one has

$$\tilde{Q}_{n\gamma}(y) = y^{-(\gamma+5/2)} \tilde{G}_{n\gamma}(y) \ . \tag{28}$$

In order to construct the new basis in momentum space, we previously introduce the *hypermomentum* k and the corresponding hyperangular variable χ in the following form

$$k = \sqrt{\vec{p}_\rho^2 + \vec{p}_\lambda^2}, \qquad \chi = arctg(\frac{p_\rho}{p_\lambda}) \tag{29}$$

where $\vec{p}_\rho$ and $\vec{p}_\lambda$ respectively represent the conjugate momenta of the spatial variables $\vec{\rho}$ and $\vec{\lambda}$ defined in eq. (20). All the permutational symmetry properties are exactly the same as in coordinate space. One can factorize in the same way the hyperangular momentum functions $Y_{[\gamma]l_\rho l_\lambda}(\Omega_{p_\rho}, \Omega_{p_\lambda}, \chi)$ and introduce the hypermomentum functions

$$\psi_{n\gamma}(k) = \frac{1}{\bar{p}^3} \kappa^\gamma \tilde{Q}_{n\gamma}(\kappa) \exp\left[-\frac{1}{2}\tilde{F}(\kappa)\right] \tag{30}$$

with the adimensional hypermomentum $\kappa = k/\bar{p}$. Analogously to the two-body case, the hypermomentum functions have the same form (apart from a phase factor) as the hyperradial one, only in the HO case, that is with $\tilde{F}(\kappa) = \kappa^2$.

Conclusions

In this note we have presented a method to construct a basis of wave functions with non-Gaussian asymptotic behavior. This mathematical tool has been developed for the study of both two-body and three-body problems. In the latter case the hyperspheric formalism has been used. The new basis can be constructed both in coordinate and momentum space.

References

[1] D. Ebert, R.N. Faustov and V.O. Galkin, *Eur. Phys. J.* **C47**, 745 (2006), arXiv:hep-ph/051109

[2] J. Eiglsperger, *Quarkonium Spectroscopy: Beyond One-Gluon Exchange*, Diploma Thesis, Technische Universität München, Physik-Department, January 2007, arXiv:0707.1269v1

[3] E. Santopinto, *Phys. Rev.* **C72**, 022201(R) (2005)

[4] C.L. Gutierrez, M De Sanctis, *Pramana - J. Phys.* **72**, 451 (2009)

[5] T. Melde, W. Plessas and B. Sengl, *Phys. Rev.* **D77**, 114002 (2008), arXiv:0806.1454

[6] E. Santopinto, F. Iachello and M.M. Giannini, *Eur. Phys. J.* **A1**, 307 (1998)

[7] L.D. Landau and E M Lifshitz, *Quantum Mechanics (Non-relativistic Theory)* (Elsevier, Butterworth Heinemann, Oxford 1981)

[8] I.S. Gradstein and I.M. Ryzhik, *Table of integrals, series and products* (Academic Press, New York, 1980)

[9] J. Day, J. McEwen and Z. Papp, arXiv:0905.3482v1

[10] N. Isgur and G. Karl, *Phys. Rev.* **D18** 4187 (1978); **D19**, 2653 (1979); **D20** 1191 (1979)

[11] Bhavin Patel, Ajay Majethiya and P.C. Vinodkumar, *Pramana - J. Phys.* **72**, 679 (2009)