Interdimensional degeneracies for a quantum three-body system in $D$ dimensions

Xiao-Yan Gu * and Zhong-Qi Ma †

CCAST (World Laboratory), P.O.Box 8730, Beijing 100080, China

and Institute of High Energy Physics, Beijing 100039, China

Bin Duan ‡

Max Planck Institute for the Physics of Complex Systems,

Noethnitzer Str. 38, 01187, Dresden, Germany

A new approach is developed to derive the complete spectrum of exact interdimensional degeneracies for a quantum three-body system in $D$-dimensions. The new method gives a generalization of previous methods.

I. INTRODUCTION

The property of quantum systems in high dimensions and its relationship with that in three dimensions has aroused great interest in statistic mechanics, particle physics, and nuclear physics [1–5]. A characteristic feature for a quantum few body system in $D$ dimensions is existence of exact interdimensional degeneracies. For any central force problem in D dimensions an isomorphism exists between angular momentum $L$ and dimension $D$ such that each unit increment in $L$ is equivalent to two-unit increment in D, as perhaps first noticed by Van Vleck [6]. For one-electron system states related by the dimensional link $D, l \leftrightarrow (D-2), (l+1)$ are exactly degenerate [7]. For

*Electronic address: guxy@mail.ihep.ac.cn
†Electronic address: mazq@sun.ihep.ac.cn
‡Electronic address: duanb@mpipks-dresden.mpg.de
two-electron system Herrick and Stillinger found exact interdimensional degeneracies between the states $^{1,3}P^e$ and $^{1,3}D^o$ in $D = 3$ and the states $^{3,1}S^e$ and $^{3,1}P^o$ in $D = 5$, respectively [8]. These interdimensional degeneracies [5,7–14] were supposed [12,9] to permit that the accurate energies for the states $^{1,3}P^e$ and $^{1,3}D^o$ in $D = 3$ may be calculated with reduced effort by implementing the same procedures which calculate the states $^{3,1}S^e$ and $^{3,1}P^o$ in $D = 5$, respectively. The pattern of approximate interdimensional degeneracies among doubly excited states of two-electron atoms has also been nicely elucidated [13] by means of the molecular orbital description. This link, between dimension and orbital angular momentum as a pervasive feature, can be used to classify groups of quasidegenerate doubly excited atomic energies and to explain striking similarities among certain pairs of hyperspherical or molecular-orbital two-electron potential curves [13]. Interdimensional degeneracies can also be used to construct part of the D-dimensional spiked harmonic oscillator and anharmonic oscillator bound-state spectra [15,16].

As is well known, dimensional scaling methods provide a powerful approach for studying atomic and molecular systems in D dimensions [5,17–22], but much work has been confined to S-wave states and some $P^e$ states [7–9] which were obtained by exploiting a known interdimensional degeneracies between $S^e$ states in 5 dimensions and $P^e$ states in 3 dimensions. Applications of dimensional scaling methods to higher angular momentum states of multi-electron systems are sparse [5,7–14]. Recently, by the method of group theory, Dunn and Watson developed a formalism for the N-electron D-dimensional Schwartz expansion [23,24], and applied the principle method to the Schrödinger equation for two-electron system in an arbitrary $D$-dimensional space [25,26]. The resulting set of coupled differential equations in the internal variables, enabling the methods of dimensional scaling to be applied to higher-angular-momentum states. In addition, the coupled differential equations can show the complete spectrum of exact interdimensional degeneracies of two-electron system [25,26].

Despite the achievements outlined above, the method by Dunn and Watson [23–26]
seems quite complicated. To apply the methods of dimensional scaling to higher-angular-momentum states, a formalism needs to be developed which factors the D-dimensional rotational degrees of freedom from the internal degrees of freedom. They have to make several steps to decompose an n-rank tensor to irreducible tensors by making use of the method of group theory [27,28]. They first decomposed an n-rank tensor space into (a + 1)-fold traceless tensor subspaces. Then, they applied the Young operators on the one-fold traceless tensor space to project it into the irreducible invariant tensor subspace. At last, they analyze the equivalence of those representations and pick up the independent basis of the angular momentum belonging to the given irreducible representation by the generalized Schwartz identities. Each step in the decomposition is very complicated.

It is worth pointing out that the set of variables $r^{(1)}, \ldots, r^{(N)}, r^{(1,2)}, r^{(1,3)}, \ldots, r^{(N-1,N)}$ is not a complete set of internal variables even in three dimensions [29] because they cannot describe the configuration uniquely. One can convince himself by the following counter example. For three-electron system in three-dimensions the six variables $r^{(1)}, r^{(2)}, r^{(3)}, r^{(1,2)}, r^{(1,3)},$ and $r^{(2,3)}$ cannot distinguish two states related by spatial inversion in the body-fixed frame.

Another complicated problem occurs in the formalism for N-electron system in D-dimensions. Since a right-hand rectangular coordinate frame in D-dimensions is determined by $(D - 1)$ vectors which are linearly independent, the situations for N-electron system with $N > D - 1$ and $N \leq D - 1$ are very different [29]. On the other hand, the possible irreducible representations of SO($D$) are different for $D > 2N$, $D = 2N$, and $D < 2N$. Unfortunately, the complicated situations were not discussed in the formalism [23,24] in detail.

In our recent paper [30], we presented a new method of separating the rotational degrees of freedom from the internal degrees of freedom for three-body system in D-dimensions. After removing the motion of the center of mass there are two Jacobi coordinate vectors for a three-body system, just like two position vectors in two-electron...
system where the mass of nucleus is assumed to be infinite. An angular momentum state for a three-body system in \( D \) dimensions is described by the irreducible representation of \( \text{SO}(D) \) denoted by a two-row Young diagram \([\mu, \nu]\). Two states in three dimensions with the same angular momentum \( l \) and the different parities belong to the same irreducible representation of \( \text{SO}(3) \), but in \( D \)-dimensions where \( D > 3 \) they belong to different irreducible representations denoted by the Young diagrams \([l, 0]\) and \([l, 1]\) of \( \text{SO}(D) \). We explicitly find the independent base-function for the highest weight state of each irreducible representation \([\mu, \nu]\), which is a homogeneous polynomial of the components of two Jacobi coordinate vectors and satisfies the Laplace equation. Its partners can be calculated from it by the lowering operator. Any wave function of this system with a given angular momentum \([\mu, \nu]\) can be expressed as a combination of the base-functions where the coefficients are called the generalized radial functions. The generalized radial equations satisfied by the generalized radial functions are easily derived explicitly [30]. The general interdimensional degeneracies for any angular momentum \([\mu, \nu]\) can be found from the generalized radial equations, which is the main purpose of this Letter.

The plan of this Letter is as follows. In Sec. II, we outline the method given in our recent paper [29] we separated completely the global rotational degrees of freedom in the Schrödinger equation for an \( N \)-body system in the three-dimensional space from the internal ones. We have determined a complete set of \((2l + 1)\) inde-
dependent base-functions for a given total orbital angular momentum \( l \), which are the homogenous polynomials in the components of the Jacobi coordinate vectors and do not contain the Euler angles explicitly. The generalized radial equations which depend solely on internal variables are established. For the typical three-body system in three dimensional space, such as a helium atom \([31–33]\) and a positronium negative ion \([34]\), the generalized radial equations have been solved numerically with high precision. This method was generalized to the arbitrary dimensional space for a three-body system.

After removing the motion of center of mass, the Schrödinger equation with a spherically symmetric potential \( V \) in \( D \)-dimensions can be expressed in terms of the Jacobi coordinate vectors \( x \) and \( y \), where the atomic units \( (e = \hbar = 1) \) are used for simplicity, \([30]\):

\[
\left\{ \nabla_x^2 + \nabla_y^2 \right\} \Psi(x, y) = -2 \left\{ E - V(\xi_1, \xi_2, \xi_3) \right\} \Psi(x, y),
\]

\[
x = \left[ \frac{m_1 m_2}{m_1 + m_2} \right]^{1/2} \{ r_2 - r_1 \},
\]

\[
y = \left[ \frac{(m_1 + m_2)m_3}{m_1 + m_2 + m_3} \right]^{1/2} \{ r_3 - \frac{m_1 r_1 + m_2 r_2}{m_1 + m_2} \},
\]

\[
\xi_1 = x \cdot x, \quad \xi_2 = y \cdot y, \quad \xi_3 = x \cdot y,
\]

where \( r_j \) and \( m_j \) are the position vector and the mass of the \( j \)-th particle, respectively.

The orbital angular momentum in \( D \)-dimensions is described by the irreducible representation of \( \text{SO}(D) \), denoted by a two-row Young diagram \([\mu, \nu]\). We only need to find the base-function of angular momentum corresponding to the highest weight \( M \) of the representation \([\mu, \nu]\). Its partners can be calculated from it by the angular momentum operator \( L_{ab} \) \([30]\). It was proved that the following harmonic polynomial \( Q_{q}^{\mu \nu}(x, y) \) construct the independent and complete set of the highest weight states of \([\mu, \nu]\):

\[
Q_{q}^{\mu \nu}(x, y) = \frac{X_{12}^{q-\nu} Y_{12}^{\mu-q}}{(q - \nu)! (\mu - q)!} (X_{12} Y_{34} - Y_{12} X_{34})^\nu, \quad 0 \leq \nu \leq q \leq \mu.
\]

\[
X_{12} = x_1 + i x_2, \quad X_{34} = x_3 + i x_4, \quad Y_{12} = y_1 + i y_2, \quad Y_{34} = y_3 + i y_4.
\]

The formula for \( Q_{q}^{\mu \nu}(x, y) \) holds for \( D = 3 \) \( (x_4 = y_4 = 0, \nu = 0 \text{ or } 1) \) \([30]\) and \( D > 4 \).
When \( D = 4 \) we denote the highest weight states by \( Q^{(S)\mu\nu}_q(x, y) \) and \( Q^{(A)\mu\nu}_q(x, y) \) for the selfdual representations and the antiselfdual representations, respectively:

\[
Q^{(S)\mu\nu}_q(x, y) = \frac{X_{12}^{\mu-q}Y_{12}^{\nu-q}}{(q-\nu)(\mu-q)}(X_{12}Y_{34} - Y_{12}X_{34})^\nu \\
Q^{(A)\mu\nu}_q(x, y) = \frac{X_{12}^{\mu-q}Y_{12}^{\nu-q}}{(q-\nu)(\mu-q)}(X_{12}Y_{34}' - Y_{12}X_{34}')^\nu
\]

(3)

\( X_{34}' = x_3 - iy_4, \quad Y_{34}' = y_3 - ix_4. \)

Obviously, the base-function \( Q^{\mu\nu}_q(x, y) \) is a homogeneous polynomial of degree \( q \) and \( (\mu + \nu - q) \) in the components of the Jacobi coordinate vectors \( x \) and \( y \), respectively, and does not contain any angle variables explicitly. It is easy to check that \( Q^{\mu\nu}_q(x, y) \) satisfies following formulas:

\[
\nabla^2_x Q^{\mu\nu}_q(x, y) = \nabla^2_y Q^{\mu\nu}_q(x, y) = \nabla_x \cdot \nabla_y Q^{\mu\nu}_q(x, y) = 0, \\
x \cdot \nabla_x Q^{\mu\nu}_q(x, y) = qQ^{\mu\nu}_q(x, y), \\
y \cdot \nabla_y Q^{\mu\nu}_q(x, y) = (\mu + \nu - q)Q^{\mu\nu}_q(x, y), \\
y \cdot \nabla_x Q^{\mu\nu}_q(x, y) = (\mu - q + 1)Q^{\mu\nu}_{q-1}(x, y), \\
x \cdot \nabla_y Q^{\mu\nu}_q(x, y) = (q - \nu + 1)Q^{\mu\nu}_{q+1}(x, y).
\]

(4)

Any wave function of this system corresponding to the highest weight \( M \) of the representation \([\mu, \nu]\) can be expressed as a combination of the base-functions \( Q^{\mu\nu}_q(x, y) \),

\[
\Psi_M^{[\mu,\nu]}(x, y) = \sum_{q=\nu}^{\mu} \psi^{\mu\nu}_q(\xi_1\xi_2\xi_3)Q^{\mu\nu}_q(x, y),
\]

(5)

where the coefficients \( \psi^{\mu\nu}_q(\xi_1\xi_2\xi_3) \) are called the generalized radial functions. When applying the Laplace operator \( \nabla^2_x + \nabla^2_y \) to the wave function \( \Psi_M^{[\mu,\nu]}(x, y) \), the calculation consists of three parts. The first is to apply the Laplace operator to the generalized radial functions \( \psi^{\mu\nu}_q(\xi_1\xi_2\xi_3) \), which can be calculated by replacement of variables. The second is to apply it to \( Q^{\mu\nu}_q(x, y) \), which is vanishing due to Eq. (4). The last part is the mixed application

\[
2 \left\{ (\partial_{\xi_1}\psi^{\mu\nu}_q)2x + (\partial_{\xi_3}\psi^{\mu\nu}_q)y \right\} \cdot \nabla_x Q^{\mu\nu}_q + 2 \left\{ (\partial_{\xi_2}\psi^{\mu\nu}_q)2y + (\partial_{\xi_3}\psi^{\mu\nu}_q)x \right\} \cdot \nabla_y Q^{\mu\nu}_q,
\]

(6)
which can be calculated by Eq. (4) easily. Hence, we obtain the generalized radial equations, satisfied by the \((\mu - \nu + 1)\) functions \(\psi_{q}^{\mu \nu}(\xi_{1} \xi_{2} \xi_{3})\)

\[
\begin{align*}
\{4\xi_{1}\partial_{\xi_{1}}^{2} + 4\xi_{2}\partial_{\xi_{2}}^{2} + 2(D + 2q)\partial_{\xi_{1}} + 2(D + 2\mu + 2\nu - 2q)\partial_{\xi_{2}} + (\xi_{1} + \xi_{2})\partial_{\xi_{3}}^{2} \\
+ 4\xi_{3}(\partial_{\xi_{1}} + \partial_{\xi_{2}})\partial_{\xi_{3}}\} \psi_{q}^{\mu \nu} + 2(\mu - q)\partial_{\xi_{3}}\psi_{q+1}^{\mu \nu} + 2(q - \nu)\partial_{\xi_{3}}\psi_{q-1}^{\mu \nu} = -2(E - V)\psi_{q}^{\mu \nu}.
\end{align*}
\]

(7)

III. THE GENERAL INTERDIMENSIONAL DEGENERACIES

The radial equations (7) were derived without any approximation. This equations for \(\psi_{q}^{\mu \nu}\) in \(D + 2\) dimensions is

\[
\begin{align*}
\{4\xi_{1}\partial_{\xi_{1}}^{2} + 4\xi_{2}\partial_{\xi_{2}}^{2} + 2(D + 2q + 2)\partial_{\xi_{1}} + 2(D + 2\mu + 2\nu - 2q + 2)\partial_{\xi_{2}} + (\xi_{1} + \xi_{2})\partial_{\xi_{3}}^{2} \\
+ 4\xi_{3}(\partial_{\xi_{1}} + \partial_{\xi_{2}})\partial_{\xi_{3}}\} \psi_{q}^{\mu \nu} + 2(\mu - q)\partial_{\xi_{3}}\psi_{q+1}^{\mu \nu} + 2(q - \nu)\partial_{\xi_{3}}\psi_{q-1}^{\mu \nu} = -2(E - V)\psi_{q}^{\mu \nu}.
\end{align*}
\]

The radial equations for \(\psi_{q'}^{\mu' \nu'}\) in \(D\) dimensions where \(\mu' = \mu + 1, \nu' = \nu + 1\) and \(q' = q + 1\) is

\[
\begin{align*}
\{4\xi_{1}\partial_{\xi_{1}}^{2} + 4\xi_{2}\partial_{\xi_{2}}^{2} + 2(D + 2q + 2)\partial_{\xi_{1}} + 2(D + 2\mu + 2\nu - 2q + 2)\partial_{\xi_{2}} + (\xi_{1} + \xi_{2})\partial_{\xi_{3}}^{2} \\
+ 4\xi_{3}(\partial_{\xi_{1}} + \partial_{\xi_{2}})\partial_{\xi_{3}}\} \psi_{q'}^{\mu' \nu'} + 2(\mu - q)\partial_{\xi_{3}}\psi_{q'+1}^{\mu' \nu'} + 2(q - \nu)\partial_{\xi_{3}}\psi_{q'-1}^{\mu' \nu'} = -2(E - V)\psi_{q'}^{\mu' \nu'}.
\end{align*}
\]

It is evident that the radial equations (7) are invariant under the replacement

\[
\mu, \nu, q, (D + 2) \leftrightarrow (\mu + 1), (\nu + 1), (q + 1), D,
\]

yielding the complete spectrum of the exact interdimensional degeneracies between the \([\mu, \nu]\) state in \((D + 2)\)-dimensions and the \([\mu + 1, \nu + 1]\) state in \(D\)-dimensions. The parities of both states on two sides of correspondence (8) have the same value \((-1)^{\mu - \nu}\).

In comparison with the interdimensional degeneracies discussed in literatures [5,7–14], \(\mu = l, \nu = 0\), and the parity is \((-1)^{l}\).

Consider a system where two electrons move around a nucleus, such as a \(D\)-dimensional helium atom. It is a typical three-body system where the first and second particles are chosen to be two electrons and the third one is the nucleus. In the
non-relativistic quantum mechanics, the concept of spin comes from the experimental results, not from the equation. As usual [5,3], we also assume that the spin of an electron in the $D$-dimensional space is $1/2$, just as that in the real three dimensional space, and the total wave function of two electrons is antisymmetric in the permutation of them. Since the Jacobi coordinate vector $\mathbf{x}$ changes its sign in the permutation $R$ of two electrons and $y$ keeps invariant, we obtain from Eq. (2) that the permutation parity of the base-function $Q_{q}^{\mu\nu}(\mathbf{x}, y)$ is $(-1)^{q}$:

$$R\ Q_{q}^{\mu\nu}(\mathbf{x}, y) = (-1)^{q}\ Q_{q}^{\mu\nu}(\mathbf{x}, y).$$  \hspace{1cm} (9)

In the permutation of two electrons $Q_{q}^{\mu\nu}(\mathbf{x}, y)$ and $Q_{q+1}^{(\mu+1)(\nu+1)}(\mathbf{x}, y)$ have the opposite permutation parities. Therefore, two states in the interdimensional degeneracy (8) must have the different spin $S = 1$ and $S = 0$, respectively. In summary, we obtain the complete spectrum of the exact interdimensional degeneracies as follows. For a given parameter $a = 0$ or $1$, all the states with the orbital angular momentum $[\mu + n, \nu + n]$, the spin $S = [1 + (-1)^{a+n}]/2$, and the parity $(-1)^{\mu-\nu}$ in the dimension $D - n$ are interdimensional degenerate where $n$ is an arbitrary integer satisfying $D \geq n \geq -\nu$. These general interdimensional degeneracies include all those degeneracies discovered in literatures [5,7–14].

**IV. CONCLUSIONS**

In this Letter we have provided a systematic procedure for analysis of observed degeneracies among different states in different dimensions and yielded considerable insight into the energy spectra of three body system. Since the generalized radial equations (7) for a quantum three-body system with a spherically symmetric potential $V$ in $D$-dimensions are derived without any approximation [30], the interdimensional degeneracies given at the end of the preceding section are exact and general. This general interdimensional degeneracies for a three-body systems should be generalized to $N$-body system, which is our future task.
Before ending this Letter we would like to make a remark. The energy $E$ is completely determined by the solution of the coupled differential equations (7) with a suitable boundary conditions, although we could not solve Eq. (7) analytically but only numerically. Since the equations for two states in the general interdimensional degeneracies are exactly the same, their energies must be the same. However, in the practical numerical calculations [31–34] we expanded the solutions as a Taylor series in the orthogonal bases, which depend on the integral in the configuration space. As pointed out in Eq. (44) of our recent paper [30] the volume element of the configuration space contains a factor $(\xi_1 \xi_2 - \xi_3^2)^{(D-3)/2}$, which depends on the dimension $D$. On the other hand, a straightforward calculation shows that the integrals over the angular variables for the base-function $Q^{(\mu+1)(\nu+1)}_{q+1}(x, y)$ in $D$-dimensions contains one more factor $(\xi_1 \xi_2 - \xi_3^2)$ than that for the base-function $Q_{q}^{\mu \nu}(x, y)$ in $(D + 2)$-dimensions so that two wave functions of the states in the general interdimensional degeneracies have the same integral in the configuration space.

ACKNOWLEDGMENTS. This work was supported by the National Natural Science Foundation of China.


