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Application of multidimensional SSQM formalism to He atom

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Abstract : Usually the renormalized Numerov (RN) algorithm is used to solve the set of coupled differential equations of the few body system. The straight forward approach of this algorithm to the excited states faces some serious problems of convergence in binding energy. Here we present an alternative elegant approach using multidimensional super-symmetric quantum mechanics (SSQM) where the problem of convergence is avoided by searching for the ground states of the partner potentials. Application of this formalism to the first excited $^1S^e$ state of He atom gives excellent result, showing very fast convergence.

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1. Introduction

Hyperspherical harmonics expansion method (HHEM) is one of the most elegant approaches [1–5] for solving few body problems. Expanding the total wave function in the complete set of hyperspherical harmonics, one gets a set of coupled differential equations (CDEs). Usually the renormalized Numerov (RN) algorithm [6] is used to solve the set of CDEs. Convergence in the binding energy (BE) is achieved by increasing the number of harmonics kept in the calculation. For the ground state, convergence is usually not a serious problem. The main problem arises when one tries to solve the set of CDEs for excited states. Due to increase in excitation, the wave function extends in global dimensions, requiring higher order harmonics for a faithful representation. Hence proper convergence in BE requires a large number of harmonics, which in turn increases the dimension of the CDEs and creates a great computational difficulty. Here we propose an alternative elegant approach using supersymmetric quantum mechanics, where we look always for the ground state solutions of each member of the hierarchy of Hamiltonians [7,8], which correspond to the excited states of the original Hamiltonian. So the problem of convergence in BE can easily be circumvented by this new formalism.

The paper is organised as follows. In Section 2, we briefly review the HHEM method. In Section 3, we present the multidimensional supersymmetry (SUSY) algebra. In Section 4, we apply it to the Helium atom. In Section 5, we discuss the numarical results and draw our conclusions.

2. Hyperspherical harmonics expansion method (HHEM)

A general $(n+1)$ body Schrödinger equation has the form

$$\sum_{i=1}^{n+1}\left(-\frac{\hbar^2}{2m_i}\nabla_{r_i}^2\right)+\sum_{i<j=2}^{n+1}V_{\text{two}}(r_i-r_j)+V_{\text{many}}-E \times \psi(r_1,\ldots,r_{n+1})=0 \quad (1)$$

where $V_{\text{two}} \rightarrow$ two body interaction.

$V_{\text{many}} \rightarrow$ three and higher body interactions.

$r_i \rightarrow$ position vector of the i-th particle of mass m_i.

Next one introduces a set of Jacobi coordinates $\zeta_1, \zeta_2, \ldots, \zeta_n$ through

$$\zeta_1 = d_1(r_2 - r_1)$$

$$\zeta_2 = d_2\left[r_3 - \left(\frac{m_1 r_1 + m_2 r_2}{m_1 + m_2}\right)\right]$$

$$\zeta_j = d_j \; r_{j+1} - \frac{\left(\Sigma_{i=1}^{j} m_i r_i\right)}{\Sigma_{i=1}^{j} m_i} \qquad (j = 1, n) \tag{2}$$

Then the centre of mass motion will be automatically separated out and a relative motion is described by n Jacobi coordinates as

$$\left[-\frac{\hbar^2}{2m}\sum_{i=1}\nabla_{\zeta_i}^2 + V_{\text{tot}}(\zeta_1, \ldots, \zeta_n) - E\right] \times \psi(\zeta_1, \ldots, \zeta_n) = 0 \tag{3}$$

where V_{tot} represents the sum total of all interactions and m is an effective mass expressed in term of m_i's and d_i's. One next introduces the set of $3n$ hyperspherical variables. These are $2n$ polar angles $\{(\vartheta_i, \varphi_i),\ i = 1, n\}$ of the Jacobi vectors $\zeta_1, \ldots, \zeta_n$ and the "hyperradius" (r) defined through

$$r = \left[\sum_{i=1}^{n} \zeta_i^2\right]^{\frac{1}{2}}. \tag{4}$$

The remaining $(n-1)$ variables $\{\phi_2, \phi_3, \ldots, \phi_n\}$ are introduced through

$$\begin{aligned}
\zeta_n &= r\cos\phi_n \\
\zeta_{n-1} &= r\sin\phi_n \cos\phi_{n-1} \\
\zeta_{n-2} &= r\sin\phi_n \sin\phi_{n-1} \cos\phi_{n-2} \\
&\vdots \\
\zeta_2 &= r\sin\phi_n \sin\phi_{n-1} \ldots \sin\phi_3 \cos\phi_2 \\
\zeta_1 &= r\sin\phi_n \sin\phi_{n-1} \ldots \sin\phi_3 \sin\phi_2 \\
(\phi_1 &= 0)
\end{aligned} \tag{5}$$

which automatically satisfies eq. (4). The $(3n-1)$ angle variables are collectively called "hyperangles" and denoted by the abbreviated notation Ω_{3n}. The hyperradius (r) and the set of $(3n-1)$ hyperangles (Ω_{3n}) together form the $3n$ hyperspherical variables. In terms of the hyperspherical variables, the Schrödinger equation for the relative motion becomes

$$\left[-\frac{\hbar^2}{2m}\left\{\frac{1}{r^\nu}\frac{\partial}{\partial r}\left(r^\nu \frac{\partial}{\partial r}\right) - \frac{\hat{K}^2(\Omega_{3n})}{r^2}\right\} + V_{\text{tot}}(r, \Omega_{3n}) - E\right] \times \psi(r, \Omega_{3n}) = 0, \tag{6}$$

where $\nu = 3n - 1$ and $\hat{K}^2(\Omega_{3n})$ is the square of the hyperangular momentum operator [9]. The wave function $\psi(r, \Omega_{3n})$ is expanded in the complete basis of hyperspherical harmonicg (HH) $\{Y_{K\alpha}(\Omega_{3n})\}$:

$$\psi(r, \Omega_{3n}) = \sum_{K\alpha} \frac{u_{K\alpha}(r)}{r^{\frac{(3n-1)}{2}}} Y_{K\alpha}(\Omega_{3n}) \tag{7}$$

where $u_{K\alpha}(r)$ is called a hyper partial wave and $Y_{K\alpha}(\Omega_{3n})$ is the eigenfunction of $\hat{K}^2(\Omega_{3n})$ corresponding to the eigenvalue $K(K+3n-2)$, where α represents a set of $(3n-1)$ quantum numbers associated with $(3n-1)$ hyperangles. The factor $r^{-\frac{(3n-1)}{2}}$ is included in eq.(7) to remove the first derivative. Substitution of eq. (7) to eq. (6) and projection on a particular HH leads to the following set of CDEs in the single variable r :

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + \frac{\hbar^2}{2m}\frac{L_K(L_K+1)}{r^2} - E\right]u_{K\alpha}(r) + \sum_{K'\alpha'} < K\alpha \left| V_{\text{tot}}(r, \Omega_{3n}) \right| K'\alpha' > u_{K'\alpha'}(r) = 0, \tag{8}$$

where $L_K = K + \frac{(3n-3)}{2}$. The coupling matrix element is given by

$$\begin{aligned}
&\left\langle K\alpha \left| V_{\text{tot}}(r, \Omega_{3n}) \right| K'\alpha' \right\rangle \\
&= \int Y_{K\alpha}^*(\Omega_{3n}) V_{\text{tot}}(r, \Omega_{3n}) Y_{K'\alpha'}(\Omega_{3n}) d\Omega_{3n},
\end{aligned} \tag{9}$$

Actually the expansion basis in eq. (7) is an infinite set and the resulting CDE is also in finite set. For practical calculation one has to truncate the expansion basis which results in a finite set of CDEs. If the maximum number of basis functions chosen in the truncation be N then eq. (8) is replaced by

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} - E\right]u_k(r) + \sum_{k'=1}^{N} V_{kk'}(r) u_{k'}(r) = 0 \qquad (k = 1, N). \tag{10}$$

where the effective coupling potential matrix element, $V_{kk'}(r)$ is given by

$$V_{kk'}(r) = \left\langle k \left| V_{\text{tot}} \right| k' \right\rangle + \frac{\hbar^2}{2m}\frac{L_k(L_k+1)}{r^2}\delta_{kk'} \tag{11}$$

Here k is a single index combining the quantum numbers (K, α). One generally uses the renormalized Numerov algorithm [6] or hyperspherical adiabatic approximation [HAA] [10] to solve the set of CDE numerically.

3. Multidimensional supersymmetric quantum mechanics

For a one dimensional Schrödinger equation with a potential V_1 (in the shifted energy scale where the ground state energy of original potential V is zero), one can define a superpotential as

$$W(x) = -\frac{\psi_0'(x)}{\psi_0(x)}, \quad \frac{\hbar}{\sqrt{2m}} = 1 \tag{12}$$

where $\psi_0(x)$ is the ground state wave function. Then supersymmetric quantum mechanics (SSQM) [7] allows to construct a partner potential V_2 corresponding to a partner Hamiltonian H_2, where H_2 will have the same eigenspectrum as H_1 except the ground state of H_1 will be missing in H_2.

So solving H_2 for the ground state one can get the first excited state of H_1. Although the method is quite straightforward in one dimension, its generalization to a multidimensional bound state problem has only been proposed recently by us [8]. The problem arises in the definition of the superpotential. In multi-dimension the effective potential, eq (11), being a $N \times N$ matrix and the eigenfunction being a N component column vector the usual definition of W, given by eq.(12), is no longer valid. Here we circumvent the problem by a mathematical trick as mentioned in the next paragraph.

The set of CDEs, eq. (10), can be written in matrix form (with the choice of units according to eq. (12)) as :

$$-\frac{d^2}{dr^2} - E\Big)[I] + [V(r)]\Big\}\big|u(r)\big\rangle = 0, \tag{13}$$

where a symbol enclosed within a square bracket indicates a $N \times N$ square matrix and a symbol enclosed in a ket notation represents a N component column vector. In shifted energy scale as in one dimension [7] we have for the ground state

$$\frac{d^2}{dr^2}[I] + [V_1]\Big)\big|u^{(0)}\big\rangle_1 = 0. \tag{14}$$

The suffix 1 denotes the potential in the shifted energy scale. Next we define superpotential as a real symmetric matrix $[W(r)]$ which will satisfy the matrix equation

$$[W]\big|u^{(0)}\big\rangle_1 = -\big|u^{(0)\prime}\big\rangle_1, \tag{15}$$

where a prime denotes a differention with respect to the argument. Note that we could not construct $[W]$ from a generalization of eq. (12), since both $|u^{(0)}>_1$ and $|u^{(0)\prime}>_1$ are column vectors and their ratio is undefined. Then it is easy to verify that

$$[V_1] = [W^2] - [W']. \tag{16}$$

Define the matrix operators as :

$$[A] = \frac{d}{dr}[I] + [W]$$

$$[A'] = -\frac{d}{dr}[I] + [W]. \tag{17}$$

Then the many body Hamiltonian matrix $[H_1]$ can be factorized as

$$[H_1] = [A'][A]. \tag{18}$$

The partner many body Hamiltonian

$$[H_2] = [A][A']$$

$$= -\frac{d^2}{dr^2}[I] + [V_2], \tag{19}$$

corresponds to a partner potential matrix

$$[V_2] = [W^2] + [W']. \tag{20}$$

Then following the treatment of the one dimensional case, one can show that the eigenspectrum of $[H_1]$ and $[H_2]$ are related as

$$E_{n+1}^{(1)} = E_n^{(2)}$$

$$E_0^{(1)} = 0$$

$$u^{n+1}\big\rangle_1 = \frac{1}{\sqrt{E^{(2)}}}[A']\big|u^{(n)}\big\rangle_2$$

$$u^{(n)}\big\rangle_2 = \frac{1}{\sqrt{E_{n+}^{(1)}}}[A]\big|u^{(n+1)}\big\rangle_1 \tag{21}$$

$$n = 0, 1, 2, \ldots$$

The derivations are quite straightforward and left for interested readers.

So the main outcome of SUSY is that the partner potential matrix $[V_2]$ has the same eigenspectrum as that of $[V_1]$, only the ground state of $[V_1]$ is missing in $[V_2]$. The ground state of $[V_2]$ corresponds to first excited state of $[V_1]$. Next starting from $[V_2]$ as a new potential and repeating the SUSY algebra, one can construct a new partner $[V_3]$ having same eigenspectrum as of $[V_2]$ and the ground state of $[V_3]$ will correspond to second excited state of $[V_1]$. In this way one can construct a hierarchy of Hamiltonians (Figure 1) until all the bound states of $[H_1]$ be exhausted. Now solving each member of the hierarchy for ground state only, one can get the full eigenspectrum of $[H_1]$.

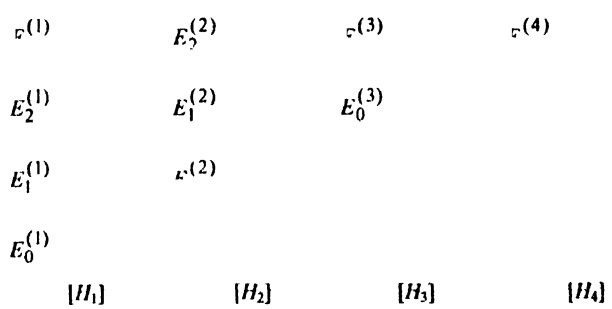

Figure 1. Energy level diagram of the hierarchy of Hamiltonains and their energy spectra.

The main advantage of this new formalism is to overcome the problem of convergence in BE when one tries to solve the CDEs by RN method. In the traditional methods [6], one has to solve the CDEs for ground and excited states. The accuracy in BE depends on the number of harmonics kept in the calculation. In ground state the wavefunction has no node and the wave function is fairly compact in the hyperradius, so a small number of harmonics is sufficient to