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Exact bound-state solutions of the cut-off Coulomb potential in N-dimensional space

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Abstract. Exact solutions of the potential $V(r) = -Ze^2/(r+\beta)$, $\beta > 0$ are obtained in the N-dimensional space for certain values of β by means of factorization of infinite Hill determinant. We discuss some features of the radial wave Schrödinger equation in the N-dimensional space.

Keywords. N-dimensional Schrödinger equation; cut-off Coulomb potential; factorization of Hill determinant.

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1. Introduction

Recently De Meyer and Vanden Berghe (1990) and Sinha and Roychoudhury (1990) constructed a few exact bound-state solutions of the cut-off Coulomb potential

$$V(r) = -Ze^2/(r+\beta), \quad \beta > 0 \tag{1}$$

for certain β values. De Meyer and Vanden Berghe also obtained the bound-state energies of the potential to a good accuracy by means of dynamical group method for any positive β value. Sinha and Roychoudhury showed by using the formalism of supersymmetric quantum mechanics that the potential admits exact solutions when β and ℓ satisfy some constraints. This potential, studied by Mehta and Patil (1978) within the framework of dispersion theory, may be considered as an approximation to the potential due to smeared charge distribution. An approximation formula for the energy eigenvalues of various states for any angular momentum state has been established by Ray and Mahata (1989) in the framework of shifted $1/N$ expansion method. Exton (1991) has recently reduced the problem of cut-off Coulomb potential to solutions of the confluent Heun equation. The eigenvalue problem of attractive truncated Coulomb potential (1) has also been studied numerically (Singh *et al* 1985).

We apply the infinite Hill determinant method to cut-off Coulomb potential (1) and find that for some values of energy the determinant of infinite order factors into two determinants of which one is of finite size. The zeros of the determinant of finite size give the values of β for which the eigensolutions are exact. By this general approach all the exact analytical solutions in N-dimensional space including those given by De Meyer and Vanden Berghe (1990) and Sinha and Roychoudhury (1990) can be obtained easily for any angular momentum state.

2. Schrödinger equation in N-dimensional space

The radial wave Schrödinger equation for a spherically symmetric potential $V(r)$ in the N-dimensional space

$$-\frac{\hbar^2}{2m}\left[\frac{d^2R}{dr^2}+\frac{N-1}{r}\frac{dR}{dr}\right]+\left[\frac{\ell(\ell+N-2)\hbar^2}{2mr^2}\right]R=[E-V(r)]R \tag{2}$$

is transformed to another Schrödinger-type equation in $(2N-4)$-dimensional space

$$-\frac{\hbar^2}{2m}\left[\frac{d^2F}{d\rho^2}+\frac{(2N-5)}{\rho}\frac{dF}{d\rho}\right]+\frac{[2N+4\ell(\ell+N-2)-5]\hbar^2}{2m\rho^2}F=[\hat{E}-\hat{V}(\rho)]F \tag{3}$$

by substituting $r=1/2\alpha\rho^2$ and $R=F(\rho)/\rho$, where $\hat{E}-\hat{V}(\rho)=E\alpha^2\rho^2-\alpha^2\rho^2V(\frac{1}{2}\alpha\rho^2)$ and the parameter α is adjusted suitably. Comparing (3) with (2) we put $N'=2N-4$, $L(L+N'-2)=2N+4\ell(\ell+N-2)-5$ and we find that $L=(2\ell+1)$. Thus by this transformation in general the N-dimensional radial wave Schrödinger equation with angular momentum ℓ can be transformed to $(2N-4)$-dimensional problem with angular momentum $2\ell+1$. If we choose $\alpha^2=1/|E|$, the perturbed Coulomb problem $V(r)=-a/r+br+cr^2$ can be transformed to a sextic anharmonic oscillator problem

$$\hat{V}(\rho)=\rho^2+\frac{b}{2|E|^{3/2}}\rho^4+\frac{c}{4|E|^2}\rho^6$$

with eigenvalue $\hat{E}=2a/|E|^{1/2}$ and the Coulomb problem is reduced to a harmonic oscillator problem in $(2N-4)$-dimensional space.

If we define the reduced radial wave function by

$$y(r)=r^{(N-1)/2}R(r), \tag{4}$$

the N-dimensional Schrödinger equation (2) is transformed to

$$-\frac{\hbar^2}{2m}\frac{d^2y}{dr^2}+\left[\frac{(N+2\ell-1)(N+2\ell-3)\hbar^2}{8mr^2}+V(r)\right]y=Ey. \tag{5}$$

For the bound states of the potential (1) the reduced radial wave equation (5) in the N-dimensional space is converted to the confluent Heun equation (Exton 1991) in the variable $z=-r/\beta$

$$\begin{aligned}z^2(1-z)^2\frac{d^2y}{dz^2}=[&-2\beta^2Ez^4+2\beta(2\beta E+1)z^3\\&+\{(N+2\ell-1)(N+2\ell-3)/4-2\beta(\beta E+1)\}z^2\\&-(N+2\ell-1)(N+2\ell-3)z/2\\&+(N+2\ell-1)(N+2\ell-3)/4]y\end{aligned} \tag{6}$$

where we use $m=\hbar=Ze^2=1$ (atomic units).

3. Hill determinant approach

The radial wave Schrödinger equation (2) in the N-dimensional space is reduced to

$$g''(r)+\left[-2v+\frac{N-1}{r}\right]g'(r)$$
$$+\left[v^2-\frac{(N-1)v}{r}-\frac{\ell(\ell+N-2)}{r^2}+\frac{2m}{\hbar^2}(E-V(r))\right]g(r)=0 \quad (7)$$

by substituting

$$R(r)=\exp(-vr)g(r). \quad (8)$$

Next we try a series solution for $g(r)$

$$g(r)=\sum_{k=0}^{\infty} a_k r^{k+\lambda} \quad (9)$$

and substitute (9) into (7). We obtain the following relations

$$\lambda=\ell \quad (10)$$

$$R_k a_{k-3}+S_k a_{k-2}+T_k a_{k-1}+U_k a_k=0, \quad k\geqslant 1$$

and

$$a_{-1}=a_{-2}=a_{-3}=\ldots=0 \quad (11)$$

with

$$R_k=v^2+2E, \quad (12a)$$

$$S_k=\beta(v^2+2E)-v(2k+2\ell+N-5)+2, \quad (12b)$$

$$T_k=(k+\ell-1)(k+\ell+N-2\beta v-3)$$
$$-\beta v(N-1)-\ell(\ell+N-2), \quad (12c)$$

$$U_k=\beta k(k+2\ell+N-2). \quad (12d)$$

The eigenvalue condition of the Hill determinant for large n is

$$\mathrm{Det}\, D_n=0 \quad (13)$$

with

$$D_n=\begin{pmatrix} T_1 & U_1 & 0 & 0 & \cdots \\ S_2 & T_2 & U_2 & 0 & \cdots \\ R_3 & S_3 & T_3 & U_3 & \cdots \\ 0 & R_4 & S_4 & T_4 & \cdots \\ . & . & . & . & . \\ . & . & . & . & . \\ . & . & . & . & . \end{pmatrix} \quad (14)$$

The zeros of D_n as a function E give the energy eigenvalues of the problem.

For exact solutions of the problem we equate $R_k=0$ by putting $v^2=-2E$ where

$E<0$ for the bound states. Now if we put $S_k=0$ the Hill determinant factors in the form

$$\mathrm{Det}\, D_n = \mathrm{Det}\begin{pmatrix} \mathrm{A} & \mathrm{C} \\ \mathrm{O} & \mathrm{B} \end{pmatrix} = \mathrm{Det\,A.\ Det\,B}.$$

The zeros of Det A will give us the exact solutions by reducing the function $g(r)$ to a polynomial in r, whereas Det B is a determinant of infinite order.

4. Results and discussion

Let us consider some special cases for the exact bound-state solutions of the cut-off Coulomb potential with $\beta>0$ in N-dimensional space:

1. The conditions $S_3=0$ and

$$\begin{vmatrix} T_1 & U_1 \\ S_2 & T_2 \end{vmatrix} = 0$$

produce

$$E=-2/(2\ell+N+1)^2, \quad \beta=\ell+\tfrac{1}{2}(N+1)$$

and

$$R(r)=r^{\ell}(1+a_1 r)\exp(-vr)$$

with

$$a_1=-T_1/U_1=v=2/(2\ell+N+1).$$

Since the wavefunctions $R(r)$ do not have any zero in the interval $0<r<\infty$, the states are identified with $1s$, $2p$, $3d\ldots$ states for $\ell=0,1,2,\ldots$ respectively.

2. For $S_4=0$ and $D_3=0$, we have

$$E=-2/(2\ell+N+3)^2$$

and

$$v(1-v)\beta^2-3(1-v)\beta+2\ell+N=0.$$

The wavefunction $R(r)=r^l(1+a_1 r+a_2 r^2)\exp(-vr)$ is given by

$$a_1=v=2/(2\ell+N+3),$$
$$a_2=[v^2\beta(2\ell+N+1)-2]/2\beta(2\ell+N)$$

The exact solutions of this type for $\ell=0,1,2,3$ in 3-dimensional space are presented in table 1.

3. The conditions $S_5=0$ and $D_4=0$ yield

$$E=-2/(2\ell+N+5)^2,$$
$$v^4(A^3+9A^2+23A+15)\beta^3-12v^2(A^2+4A+3)\beta^2$$
$$+4(4A^2v+8Av+3A+3)-12A(A+1)=0$$

where $A=2\ell+N$.

Table 1. The exact solutions of the cut-off Coulomb potential in 3-dimensional space with the wavefunction $R(r) = r^l(1 + a_1 r + a_2 r^2)\exp(-a_1 r)$.

ℓ	E	β	a_1	a_2	State of the level
0	−1/18	1·901 924	1/3	−0·101 187	2*s*
		7·098 076	1/3	0·027 113	1*s*
1	−1/32	2·944 950	1/4	−0·030 413	3*p*
		9·055 050	1/4	0·015 413	2*p*
2	−1/50	3·964 466	1/5	−0·013 177	4*d*
		11·035 534	1/5	0·009 912	3*d*
3	−1/72	4·975 078	1/6	−0·006 901	5*f*
		13·024 922	1/6	0·006 901	4*f*

Table 2. The exact solutions of the cut-off Coulomb potential in 3-dimensional space with the wavefunction $R(r) = r^l(1 + a_1 r + a_2 r^2 + a_3 r^3)\exp(-a_1 r)$.

ℓ	E	β	a_1	$(a_2 \times 10^{-2})$	$(a_3 \times 10^{-3})$	State of the level
0	−1/32	1.871 645	1/4	−13·6430	8·262	3*s*
		6·610 815	1/4	−0·8756	−3·584	2*s*
		15·517 541	1/4	2·0186	0·530	1*s*
1	−1/50	2·920 685	1/5	−4·4477	1·463	4*p*
		8·761 673	1/5	0·1173	−0·985	3*p*
		18·317 642	1/5	1·3082	0·281	2*p*
2	−1/72	3·945 628	1/6	−2·0333	0·421	5*d*
		10·836 298	1/6	0·2690	−0·385	4*d*
		21·218 074	1/6	0·9140	0·165	3*d*
3	−1/98	4·960 258	1/7	−1·1062	0·157	6*f*
		12·879 632	1/7	0·2711	−0·183	5*f*
		24·160 110	1/7	0·6739	0·105	4*f*

The wavefunction $R(r) = r^l(1 + a_1 r + a_2 r^2 + a_3 r^3)\exp(-\nu r)$ is then given by

$$a_1 = \nu = 2/(A + 5),$$

$$a_2 = [\beta\nu^2(1 + A) - 2]/2A\beta,$$

$$a_3 = -\{\nu[2 - \nu(A + 1)] + a_2[2A - \beta\nu(A + 3)]\}/3\beta(A + 1).$$

The exact solutions for this case in 3-dimensional space with $\ell = 0, 1, 2, 3$ are presented in table 2.

4. Next we consider $S_6 = 0$ and $D_5 = 0$ which produce

$$E = -\nu^2/2 = -2/(2\ell + N + 7)^2$$

Table 3. The exact solutions of the cut-off Coulomb potential in 3-dimensional space with the wavefunction $R(r) = r^l(1 + a_1 r + a_2 r^2 + a_3 r^3 + a_4 r^4)\exp(-a_1 r)$.

ℓ	E	β	a_1	$(a_2 \times 10^{-2})$	$(a_3 \times 10^{-3})$	$(a_4 \times 10^{-5})$	State of the level
0	−1/50	1·858 230	1/5	−15·2716	15·057	−36·988	4s
		6·429 088	1/5	−2·5181	−3·671	20·558	3s
		14·327 947	1/5	0·3402	−1·174	−5·427	2s
		27·384 736	1/5	1·4494	0·454	0·523	1s
1	−1/72	2·907 805	1/6	−5·2114	2·912	−4·376	5p
		8·617 654	1/6	−0·6542	−1·137	3·522	4p
		17·574 309	1/6	0·5286	−0·302	−1·410	3p
		30·900 233	1/6	1·0194	0·272	0·268	2p
2	−1/98	3·934 422	1/7	−2·4648	0·890	−0·904	6d
		10·722 765	1/7	−0·1661	−0·484	0·951	5d
		20·698 991	1/7	0·4760	−0·097	−0·515	4d
		34·643 822	1/7	0·7538	0·175	0·150	3d
3	−1/128	4·950 722	1/8	−1·3763	0·349	−0·256	7f
		12·788 575	1/8	−0·0008	−0·244	0·332	6f
		23·773 063	1/8	0·4007	−0·032	−0·227	5f
		38·487 641	1/8	0·5794	0·118	0·090	4f

and an equation of fourth degree for β. The wavefunctions $R(r) = r^l(1 + a_1 r + a_2 r^2 + a_3 r^3 + a_4 r^4)\exp(-\nu r)$ in 3-dimensional space for $\ell = 0,1,2,3$ are given in table 3.

In this way it is possible to find all the exact solutions of the cut-off Coulomb problem. The state of the energy level is determined from the number of nodes of the wavefunction $R(r)$ for any ℓ. In general when we put $S_k = 0$ we get a determinant D_{k-1} of order $k-1$ which vanishes for certain values of β. We find that the exact bound-state energy is of the form $E = -\nu^2/2 = -2/(2k + 2\ell + N - 5)^2$ with the eigenfunction

$$R(r) = r^l \exp(-\nu r)[1 + \nu r + a_2 r^2 + a_3 r^3 + \ldots + a_{k-2} r^{k-2}]$$

for $k = 3,4,5,\ldots$

We know from (2) that 4-dimensional perturbed Coulomb problem can be reduced to 4-dimensional anharmonic oscillator problem. So it is of special interest to study the cut-off Coulomb problem in 4-dimensional space. Our method is applicable to Schrödinger equation in N-dimensional space. For any arbitrary positive value of β, one has to apply the general Hill determinant method (Biswas *et al* 1971; Chaudhuri *et al* 1987; Chaudhuri and Mondal 1991) and find the zeros of Det D_n [equation 14] as $n \to \infty$ for the eigenenergies of the problem. Equation (6) shows that the cut-off Coulomb problem in N-dimensional space is reduced to solutions of the confluent Heun equation for general values of the parameters (Exton 1991).

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