Hypervirial $1/N$ expansion for a more general screened Coulomb potential

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By employing the N-dimensional hypervirial equations with the Hellman-Feynman theorem to the more general case of a screened Coulomb potential, $V(r)=-(a/r)[1+(1+br)e^{-2br}]$, the entire bound-state energy spectrum is obtained.

I. INTRODUCTION

Screened Coulomb potentials are known to adequately describe the effective interaction in many-body atomic phenomena. Since the Schrödinger equation for such potentials does not admit exact solutions, they have been treated analytically[1-14] and numerically[15-28] by employing various approximate methods. The potential $V(r)=-(a/r)[1+(1+br)e^{-2br}]$, defined for an electron of the helium in the field of the other electron and the nucleus, has been first studied by Gerry and Laub[9] and us[14] by obtaining the energy eigenvalues of the ground state and the first excited state and the corresponding wave functions.

In the present work we extend our previous work by using the hypervirial theorem[29] and the Hellman-Feynman theorem. These theorems have been applied to some problems[7,13,30,31] to obtain the energy and expectation values of position coordinates. We follow the method of Grant and Lai[7] and use an N-dimensional generalization of the hypervirial equations and the Hellman-Feynman theorem to obtain the entire bound-state energy spectrum.

II. METHOD AND CALCULATIONS

The potential to be solved is

$$V(r)=-(a/r)[1+(1+br)e^{-2br}] . \tag{1}$$

The Schrödinger equation in N dimensions (with $m=\hbar=1$) for a particle in a spherically symmetric potential $V(r)$ is given by

$$[-\tfrac{1}{2}\nabla_N^2+V_N(r)]\Psi(\mathbf{r})=E\Psi(\mathbf{r}) , \tag{2}$$

where $\mathbf{r}$ is an N-dimensional vector of magnitude r and ∇_N^2 can be written in spherical polar coordinates as

$$\nabla_N^2=\frac{\partial^2}{\partial r^2}+\frac{N-1}{r}\frac{\partial}{\partial r}-\frac{L^2}{r^2} , \tag{3}$$

L being the angular momentum operator in N dimensions having the eigenvalue $l(l+N-2)$ and $V_N(r)$ is the N-dimensional generalization of $V(r)$. Substituting

$$\Psi(\mathbf{r})=r^{-(N-1)/2}U(r)Y_{lm}(\Omega) \tag{4}$$

into Eq. (2), we obtain

$$HU(r)=EU(r) , \tag{5}$$

where the Hamiltonian H is given by

$$H=-\frac{1}{2}\frac{d^2}{dr^2}+k^2\left[\frac{(1-1/k)(1-3/k)}{8r^2}+\tilde{V}_N(r)\right] , \tag{6}$$

with $k=N+2l$ and $\tilde{V}_N(r)=V_N(r)/k^2$. Now we may use the hypervirial theorem

$$\left\langle u(r)\left|\left[r^j\frac{d}{dr},H\right]\right|u(r)\right\rangle=0 \tag{7}$$

to obtain

$$E\langle r^j\rangle=k^2\langle r^j\tilde{V}(r)\rangle+\tfrac{1}{2}(j+1)^{-1}k^2\left\langle r^{j+1}\frac{d\tilde{V}(r)}{dr}\right\rangle-\tfrac{1}{8}j(j+1)^{-1}[j^2-(k-2)^2]\langle r^{j-2}\rangle \tag{8}$$

or

$$E\langle r^j\rangle=\langle r^jV(r)\rangle+\tfrac{1}{2}(j+1)^{-1}\left\langle r^{j+1}\frac{dV(r)}{dr}\right\rangle-\tfrac{1}{8}j(j+1)^{-1}[j^2-(k-2)^2]\langle r^{j-2}\rangle . \tag{9}$$

Using the following form of the expansion of the potential:

$$V(r)=-\frac{a}{r}[1+(1+\tilde{b}r/k^2)\exp(-2\tilde{b}r/k^2)]=\sum_{n=0}^{\infty}V_{1n}\tilde{b}^{\,n}r^{n-1}+\sum_{n=0}^{\infty}V_{2n}\tilde{b}^{\,n+1}r^n , \tag{10}$$

where $b=\tilde{b}/k^2$ and

$$V_{1n}=-a[\delta_{n0}+(-1)^n]\frac{2^n}{n!k^{2n}} ,\qquad V_{2n}=-a(-1)^n\frac{2^n}{n!k^{2n}} , \tag{11}$$

Eq. (8) reduces to

$$\left[E - a\frac{\tilde{b}}{k^2}\right]\langle r^j\rangle = -\frac{2j+1}{j+1}a\langle r^{j-1}\rangle + \frac{2j+3}{j+1}a\frac{\tilde{b}^2}{k^4}\langle r^{j+1}\rangle + \sum_{n=2}^{\infty}\frac{2j+n+1}{2(j+1)}V_{1n}\tilde{b}^{\,n}\langle r^{j+n-1}\rangle + \sum_{n=2}^{\infty}\frac{2j+n+2}{2(j+1)}V_{2n}\tilde{b}^{\,n+1}\langle r^{j+n}\rangle - \frac{j}{8(j+1)}[j^2-(k-2)^2]\langle r^{j-2}\rangle . \quad (12)$$

We introduce the expansions

$$\langle r^j\rangle = \sum_{n'=0}^{\infty} C_j^{(n')}\tilde{b}^{\,n'} \quad (13)$$

and

$$E_n = \sum_{n''=0}^{\infty} E_n^{(n'')}\tilde{b}^{\,n''} , \quad (14)$$

where the energy of the unperturbed nth states in 3-space $E_n^{(0)} = -2a^2/n^2$ with $Z=2$ may be written in N dimensions as

$$E_n^{(0)} = -\frac{8a^2}{(N+2n-3)^2} , \quad n=1,2,3,\ldots , \quad (15)$$

so that Eq. (12) becomes

$$\sum_{n'=0}^{\infty}\sum_{n''=0}^{\infty} E_n^{(n'')}c_j^{(n')}\tilde{b}^{(n'+n'')} - \frac{a\tilde{b}}{k^2}\sum_{n'=0}^{\infty} C_j^{(n')}\tilde{b}^{\,n'} = -\frac{2j+1}{j+1}a\sum_{n'=0} C_{j-1}^{(n')}\tilde{b}^{\,n'} + \frac{2j+3}{j+1}\frac{a\tilde{b}^2}{k^4}\sum_{n'=0}^{\infty} C_{j+1}^{(n')}\tilde{b}^{\,n'} + \sum_{n''=2}^{\infty}\sum_{n'=0}^{\infty}\frac{(2j+n''+1)}{2(j+1)}V_{1n}C_{j+n''-1}^{(n')}\tilde{b}^{(n'+n'')} + \sum_{n''=2}^{\infty}\sum_{n'=0}^{\infty}\frac{(2j+n''+2)}{2(j+1)}V_{2n}C_{j+n}^{(n')}\tilde{b}^{(n'+n''+1)} - \frac{j}{8(j+1)}[j^2-(k-2)^2]\sum_{n'=0}^{\infty} C_{j-2}^{(n')}\tilde{b}^{\,n'} . \quad (16)$$

Combining the terms of the same order in $\tilde{b}^{\,0}$, we obtain a recurrence relation

$$C_j^{(0)} = \frac{1}{E_n^{(0)}}\left[-\frac{2j+1}{j+1}aC_{j-1}^{(0)} - \frac{j[j^2-(k-2)^2]}{8(j+1)}C_{j-2}^{(0)}\right] . \quad (17)$$

From (13), it is obvious that

$$C_0^{(n')} = \delta_{0n'} \quad (18)$$

Setting $j=0$ in Eq. (17), we get

$$C_{-1}^{(0)} = -E_n^{(0)}/a \quad (19)$$

and

$$C_1^{(0)} = -3a/2E_n^{(0)} - (k^2-4k+3)/16a , \quad (20a)$$

$$C_2^{(0)} = 5a/2E_n^{(0)^2} + (3k^2-12k+5)/16E_n^{(0)} , \quad (20b)$$

$$C_3^{(0)} = -35a^3/8E_n^{(0)^3} - 7a(3k^2-12k+5)/64E_n^{(0)^2} + 9a(5-k)(1+k)/64E_n^{(0)^2} + 3(5-k)(1+k)(k^2-4k+3)/512aE_n^{(0)} . \quad (20c)$$

Next we use the Hellman-Feynman theorem

$$\left\langle\frac{dH}{d\tilde{b}}\right\rangle = \frac{dE}{d\tilde{b}} \quad (21)$$

to obtain

TABLE I. Comparison of the energy for $0<\beta<0.1$ as calculated from the numerical solution of the Schrödinger equation with those to order β^4 of the present work.

	E_{nl}/a^2	$E_{\text{numerical}}$	E_{nl}/a^2	$E_{\text{numerical}}$
	$\beta=0.02$		$\beta=0.04$	
1s	−1.980 00	−1.980 00	−1.960 03	−1.960 00
2s	−0.480 05	−0.480 05	−0.460 38	−0.460 38
2p	−0.480 04	−0.480 04	−0.460 28	−0.460 38
3s	−0.202 45	−0.202 46	−0.1837	−0.1838
3p	−0.202 42	−0.202 43	−0.1835	−0.1836
3d	−0.202	−0.2024	−0.1832	−0.1833
4s	−0.105 61	−0.105 65	−0.0879	−0.0891
4p	−0.105 58	−0.105 61	−0.0878	−0.0889
4d	−0.105 50	−0.105 52	−0.0876	−0.0884
4f	−0.105 37	−0.105 39	−0.0872	−0.0876
	$\beta=0.06$		$\beta=0.08$	
1s	−1.9401	−1.9400	−1.9202	−1.9201
2s	−0.4412	−0.4412	−0.4225	−0.4227
2p	−0.4409	−0.4409	−0.4218	−0.4220
3s	−0.1660	−0.1670	−0.1481	−0.1520
3p	−0.1656	−0.1664	−0.1479	−0.1510
3d	−0.1649	−0.1654	−0.1472	−0.1489
4s	−0.0681	−0.0761	−0.036	−0.0664
4p	−0.0685	−0.0755	−0.039	−0.0654
4d	−0.0690	−0.0743	−0.043	−0.0634
4f	−0.0694	−0.0723	−0.049	−0.0601

$$PE_n^{(p)} = \sum_{q=1}^{P} qV_q C_{q-1}^{(p-q)} \ . \tag{22}$$

Then equating the coefficients of $\tilde{b}$ on both sides of Eq. (16) and using Eq. (22) we obtain

$$C_j^{(1)} = \frac{1}{E_n^{(0)}} \left[-\frac{2j+1}{j+1} a C_{j-1}^{(1)} - \frac{j}{8(j+1)} [j^2 - (k-2)^2] C_{j-2}^{(1)} \right] , \tag{23}$$

which simply leads to

$$C_p^{(1)} = 0 \ , \quad p \geq -1 \ . \tag{24}$$

Similarly equating the coefficients of $\tilde{b}^2$, $\tilde{b}^3$, $\tilde{b}^4$, etc. on both sides of Eq. (16) and using Eq. (22), we can find the values of $C_j^{(2)}$, $C_j^{(3)}$, $C_j^{(4)}$, etc., respectively, for $j \geq -1$. Finally, using Eq. (14) we obtain the bound-state energy spectrum in the powers of screening parameter b,

$$\begin{aligned} E_{nl} = {} & E_n^{(0)} + ab - \{(2a/3)[5a^2/2E_n^{(0)^2} + (3k^2 - 12k + 5)/16E_n^{(0)}]\} b^3 \\ & + \{(2a/3E_n^{(0)})[-35a^3/8E_n^{(0)^2} - 7a(3k^2 - 12k + 5)/64E_n^{(0)} + 9a(5-k)(1+k)/64E_n^{(0)} \\ & + 3(5-k)(1+k)(k^2 - 4k + 3)/512a]\} b^4 \ . \end{aligned} \tag{25}$$

TABLE II. Improvement in energy with respect to orders of β.

β		$(E_{nl}/a^2)_0$	$(E_{nl}/a^2)_1$	$(E_{nl}/a^2)_3$	$(E_{nl}/a^2)_4$
0.02	1s	−2.0	−1.98	1.980 00	−1.980 00
	2s	−0.5	−0.48	−0.480 06	−0.480 05
	2p	−0.5	−0.48	−0.480 04	−0.480 04
	3s	−0.222	−0.202	−0.202 50	−0.202 45
	3p	−0.222	−0.202	−0.202 46	−0.202 42
	3d	−0.222	−0.202	−0.202 39	−0.202 37
	4s	−0.125	−0.105	−0.105 86	−0.105 61
	4p	−0.125	−0.105	−0.1058	−0.1056
	4d	−0.125	−0.105	−0.1057	−0.1055
	4f	−0.125	−0.105	−0.1055	−0.1054
0.05	1s	−2.0	−1.95	−1.950 06	−1.950 06
	2s	−0.5	−0.45	−0.4509	−0.4507
	2p	−0.5	−0.45	−0.4506	−0.4505
	3s	−0.222	−0.172	−0.1765	−0.1747
	3p	−0.222	−0.172	−0.1760	−0.1745
	3d	−0.222	−0.172	−0.1749	−0.1740
	4s	−0.125	−0.075	−0.089	−0.079
	4p	−0.125	−0.075	−0.088	−0.079
	4d	−0.125	−0.075	−0.085	−0.079
	4f	−0.125	−0.075	−0.083	−0.078
0.08	1s	−2.0	−1.92	−1.9203	−1.9202
	2s	−0.5	−0.42	−0.424	−0.423
	2p	−0.5	−0.42	−0.423	−0.422
	3s	−0.222	−0.142	−0.160	−0.148
	3p	−0.222	−0.142	−0.158	−0.148
	3d	−0.222	−0.142	−0.153	−0.147
	4s	−0.125	−0.045	−0.100	−0.036
	4p	−0.125	−0.045	−0.096	−0.039
	4d	−0.125	−0.045	−0.088	−0.043
	4f	−0.125	−0.045	−0.076	−0.049

Substituting $k = N + 2l$ with $N = 3$ for 3-space in Eq. (25) and defining $\beta = b/a$, we simply get

$$E_{nl}/a^2 = -2/(n-l)^2 + \beta - \{[5(n-l)^4 + (n-l)^2]/12a\}\beta^3 + \{5[7(n-l)^6 + 5(n-l)^4]/96a^2\}b^4 . \quad (26)$$

III. RESULTS AND CONCLUSIONS

We have derived the bound-state energy spectrum of the more general screened Coulomb potential $V(r) = -(a/r)[1+(1+br)e^{-2br}]$ in the powers of the screening parameter b. The expression (26) exactly gives the same results for the ground state and the first excited energies which are obtained in our earlier paper[14] by using the large-N expansion technique of Mlodinow and Shatz.

Some numerical values of energies of the first four states for different values of β are compared with those which are obtained by solving the Schrödinger equation numerically (see Table I). Numerov's method is used. For the energy eigenvalues a total of 5000 steps are taken with the step size $\Delta r = 0.003$ and tolerance 1.0×10^{-8}. Results are in good agreement for small values of β and for the first three states. We have also illustrated the improvement of the energy with respect to orders of β in the Table II.

To conclude, we have investigated the hypervirial $1/N$ expansion for a particle bound in a more general screened Coulomb potential. The method provides the entire energy spectrum and may have some advantage over the large-N expansion technique of Mlodinow and Shatz if one does not need to calculate the corresponding wave functions simultaneously.

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