Hypervirial theorems applied to the perturbation theory for screened Coulomb potentials

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By applying the hypervirial relations with the Hellman-Feynman theorem to screened Coulomb potentials, the authors derive the energy levels of atoms correct to the sixth order of the perturbation parameter λ explicitly without any calculation of perturbed wave functions. The energies of atoms up to the twentieth order of λ are also calculated by computer. In the case of the Yukawa potential, the authors demonstrate by explicit calculation that the K-shell energy converges, at least for $Z \geq 5$, with the value of $\lambda_0 = 0.85$, and that the L-shell energy converges, at least for $Z \geq 24$, with $\lambda_0 = 0.70$.

I. INTRODUCTION

The problem of screened Coulomb potentials is of great importance in the atomic phenomena. It has been treated analytically and numerically with several procedures such as the WKB method,[1] the quantum-defect method,[2] the analytic perturbation theory,[3] and the nonperturbative approach.[4] The usual Rayleigh-Schrödinger perturbation theory applied to screened Coulomb potentials is rather complicated, requiring numerical work. However, in the analytic perturbation method,[3] one can construct the screened wave functions, bound-state energies, normalizations, and phase shifts in powers of a small parameter λ characterizing the screening. In particular, one obtains the energy levels in closed form correct to the third order of λ. In the nonperturbative approach,[4] the analyticity properties of the energy levels of screened Coulomb potentials are analyzed for small values of the perturbation parameter λ, and the energy levels of the atoms are calculated in certain approximation using dispersion relations.

It is the purpose of this paper to calculate the energy levels and various expectation values of screened Coulomb potentials in powers of the perturbation parameter λ, using the hypervirial theorems[5] (HVT) and the Hellman-Feynman theorem (HFT). The HVT and HFT have been applied to the problems of anharmonic oscillators,[6] and of a hydrogen atom with perturbation λr.[7] The energy and expectation values of position coordinates can be calculated in power series of the perturbation parameter λ without any calculation of perturbed wave functions in this approach.

In this paper, we will apply the HVT and HFT to screened Coulomb potentials. Using the hypervirial properties of certain commutation relations instead of solving the perturbed wave functions, we will show that the energy and other expectation values of position coordinates of an atom with atomic number Z can be calculated, in principle, correct to any order of λ. In Sec. II we will outline the hypervirial theorems and the Hellman-Feynman theorem for screened Coulomb potentials. In Sec. III we will apply the result of Sec. II explicitly to screened Coulomb potentials and derive formulas for the energy and the expectation values $\langle r^j \rangle$ of the atom with atomic number Z up to the sixth order and the fourth order of the perturbation parameter λ, respectively. Finally in Sec. IV we evaluate the values of the energy levels of atoms up to the sixth order in λ and also up to the twentieth order in λ and demonstrate that the perturbation series for the binding energies will converge at least for some values of Z if the value of $\lambda_0 = \lambda / Z^{1/3}$ is smaller than one.

II. FORMULATION OF THE PROBLEM

The Hamiltonian for a screened Coulomb potential $V_c(r)$ can be written

$$H = -\frac{1}{2}\frac{d^2}{dr^2} - \frac{1}{r}\frac{d}{dr} + V(r), \tag{1}$$

where $V(r)$ is the sum of the centrifugal term and the screened central potential $V_c(r)$. Here we use atomic units $\hbar = e = m_e = 1$, so that distances are measured in the Bohr radius a_0, energies in units of $2R_y = 27.212$ eV. From Eq. (1) we obtain the basic commutation relations[7]

$$\left[\frac{d}{dr}, H\right] = \frac{dV}{dr} + \frac{1}{r^2}\frac{d}{dr}, \tag{2}$$

$$[r^j, H] = \tfrac{1}{2} j(j+1) r^{j-2} + j r^{j-1}\frac{d}{dr}, \tag{3}$$

where j are positive integers. The hypervirial theorems require that $\langle [r^j(d/dr), H] \rangle$ with $j \geq 0$ vanish for the eigenstates of Eq. (1). Hence we obtain the hypervirial relations between the energy E and the various expectation values of $\langle r^j \rangle$ (Ref. 7),

$$2jE\langle r^{j-1}\rangle = 2j\langle r^{j-1}V\rangle + \left\langle r^j \frac{dV}{dr}\right\rangle - \tfrac{1}{4} j(j-1)(j-2)\langle r^{j-3}\rangle, \tag{4}$$

where

$$V(r)=l(l+1)/2r^2+V_c(r)\,. \tag{5}$$

The screened central potential $V_c(r)$ is assumed to take the form[8]

$$V_c(r)=-\frac{Z}{r}\sum_{k=0}^{\infty} V_k(\lambda r)^k\,, \tag{6}$$

where Z is the charge of the nucleus and λ is a parameter characterizing the screening ($\lambda=\lambda_0 Z^{1/3}$). The coefficients V_k in Eq. (6) alternate in sign and decrease with increasing k. The Hellman-Feynman theorem states that if $H=H(\lambda)$, where λ is the perturbation parameter, then

$$\frac{\partial E}{\partial\lambda}=\left\langle\frac{\partial H}{\partial\lambda}\right\rangle=\left\langle\frac{\partial V_c(r)}{\partial\lambda}\right\rangle\,. \tag{7}$$

The HVT and HFT given by Eqs. (4) and (7) form the basic equations for our calculation of the energy and various expectation values of $\langle r^j\rangle$ of screened Coulomb potentials in Sec. III.

III. SCREENED COULOMB POTENTIALS

We consider an atom of atomic number Z with a screened Coulomb potential of the form[8]

$$V_c(r)=-\frac{Z}{r}\sum_{k=0}^{\infty} V_k(\lambda r)^k, \tag{8}$$

where λ is the perturbation parameter. For the Yukawa potential, the coefficients V_k are

$$V_k=(-1)^k/k!\,. \tag{9}$$

The term $V(r)$ in Eq. (1) is then given by

$$V(r)=l(l+1)/2r^2+V_c(r)\,. \tag{10}$$

Substituting Eqs. (8) and (10) into Eq. (4), we obtain the hypervirial relations

$$(E+ZV_1\lambda)\langle r^j\rangle =-\frac{1}{2}\left[\frac{2j+1}{j+1}Z\langle r^{j-1}\rangle+\left(-\frac{j\,l(l+1)}{j+1}+\tfrac{1}{4}j(j-1)\right)\times\langle r^{j-2}\rangle+\sum_{k=2}^{\infty}\frac{2j+k+1}{j+1}ZV_k\lambda^k\langle r^{j+k-1}\rangle\right]\,. \tag{11}$$

We assume that the energy and the expectation values of $\langle r^j\rangle$ can be expanded in power series of the perturbation parameter λ as

$$E=\sum_{k=0}^{\infty}E^{(k)}\lambda^k\,, \tag{12}$$

$$\langle r^j\rangle=\sum_{k=0}^{\infty}C_j^{(k)}\lambda^k\,, \tag{13}$$

where the energy of the unperturbed nth states $E_n^{(0)}=-Z^2/2n^2$ is known. From the condition of normalization that $\langle r^0\rangle=\langle 1\rangle=1$, we also get

$$C_k^{(0)}=\delta_{0k}\,. \tag{14}$$

Equation (11) combined with Eqs. (12) and (13) provides us a connection between the coefficients $E^{(k)}$ and the coefficients $C_j^{(k)}$. With the aid of Eqs. (7), (8), (12), and (13), the perturbed energies $E^{(k)}$ are found to be

$$kE^{(k)}=-Z\sum_{m=1}^{k}mV_mC_{m-1}^{(k-m)}\,. \tag{15}$$

To calculate explicitly the perturbed energies $E^{(k)}$ up to the sixth order of λ, we proceed by calculating the coefficients $C_j^{(k)}$ from Eq. (11). Equating the coefficients of λ^0 on both sides of Eq. (11), we obtain

$$C_j^{(0)}=\frac{n^2}{Z^2}\left[\frac{2j+1}{j+1}ZC_{j-1}^{(0)}+\left(-\frac{j\,l(l+1)}{j+1}+\tfrac{1}{4}j(j-1)\right)C_{j-2}^{(0)}\right], \tag{16}$$

where n is the principal quantum number of the atom. Here, in deriving Eq. (16), the energy $E_n^{(0)}$ of the unperturbed nth state has been used. From the condition that $C_0^{(0)}=1$, we find, from Eq. (16)

$$C_{-1}^{(0)}=Z/n^2\,. \tag{17}$$

With the known values of $C_{-1}^{(0)}$ and $C_0^{(0)}$, Eq. (16) generates the following results:

$$C_1^{(0)}=(1/2Z)[3n^2-l(l+1)]\,, \tag{18a}$$

$$C_2^{(0)}=(n^2/2Z^2)[5n^2+1-3l(l+1)]\,, \tag{18b}$$

$$C_2^{(0)}=(n^2/8Z^3)[35n^4+25n^2-30n^2l(l+1)+3l^2(l+1)-6l(l+1)]\,, \tag{18c}$$

$$C_4^{(0)}=(n^4/8Z^4)[63n^4+105n^2+12-70n^2l(l+1)+15l^2(l+1)^2-50l(l+1)]; \tag{18d}$$

$$C_5^{(0)}=(n^4/16Z^5)[231n^6+735n^4+294n^2-315n^4l(l+1)+105n^2l^2(l+1)^2-525n^2l(l+1)-5l^3(l+1)^3+40l^2(l+1)^2-60l(l+1)]\,. \tag{18e}$$

If we equate the coefficients of λ on both sides of Eq. (11), we find

$$C_k^{(1)}=0\quad\text{for } k\geqslant -1\,. \tag{19}$$

Next we consider the coefficients of λ^2 in Eq. (11). With the aid of Eq. (15), we obtain the recurrence relation for $C_j^{(2)}$,

$$C_j^{(2)}=\frac{n^2}{Z^2}\left[\frac{2j+3}{j+1}ZV_2C_{j+1}^{(0)}+\frac{2j+1}{j+1}ZC_{j-1}^{(2)}-[3n^2-l(l+1)]V_2C_j^{(0)}+\left(-\frac{jl(l+1)}{j+1}+\tfrac{1}{4}j(j-1)\right)C_{j-2}^{(2)}\right]. \tag{20}$$

Employing the condition that $C_0^{(2)}=0$, we find, from Eq. (20), the following results:

$$C_{-1}^{(2)}=-(V_2/2Z)[3n^2-l(l+1)], \tag{21a}$$

$$C_1^{(2)}=(V_2/4Z^3)n^2[7n^4+5n^2-3l^2(l+1)^2], \tag{21b}$$

$$C_2^{(2)}=(V_2/8Z^4)n^4[45n^4+63n^2-14n^2l(l+1)-15l^2(l+1)^2-10l(l+1)], \tag{21c}$$

$$C_3^{(2)}=(V_2/16Z^5)n^4[231n^6+585n^4+84n^2-135n^4l(l+1)-63n^2l^2(l+1)^2-189n^2l(l+1)+15l^3(l+1)^3-30l^2(l+1)^2]. \tag{21d}$$

Similarly, if we investigate the coefficients of λ^3 and λ^4 in Eq. (11) and employ the conditions $C_0^{(3)}=C_0^{(4)}=0$, we find the recurrence relations for $C_j^{(3)}$ and $C_j^{(4)}$,

$$C_j^{(3)}=\frac{n^2}{z^2}\left[\frac{2j+1}{j+1}ZC_{j-1}^{(3)}+\left(-\frac{jl(l+1)}{j+1}+\tfrac{1}{4}j(j-1)\right)C_{j-2}^{(3)}-\frac{V_3}{Z}n^2[5n^2+1-3l(l+1)]C_j^{(0)}+2\frac{j+2}{j+1}ZV_3C_{j+2}^{(0)}\right], \tag{22}$$

$$C_j^{(4)}=\frac{n^2}{Z^2}\left[\frac{2j+1}{j+1}ZC_{j-1}^{(4)}+\left(-\frac{jl(l+1)}{j+1}+\tfrac{1}{4}j(j-1)\right)C_{j-2}^{(4)}+\frac{2j+3}{j+1}ZV_2C_{j+1}^{(2)}+\frac{2j+5}{j+1}ZV_4C_{j+3}^{(0)}+2(E^{(2)}C_j^{(2)}+E^{(4)}C_j^{(0)})\right]. \tag{23}$$

With the help of Eq. (15), we obtain then for $C_{-1}^{(3)}$, $C_1^{(3)}$, $C_2^{(3)}$, $C_{-1}^{(4)}$, and $C_1^{(4)}$,

$$C_{-1}^{(3)}=-(V_3/2Z^2)n^2[5n^2+1-3l(l+1)], \tag{24a}$$

$$C_1^{(3)}=(V_3/8Z^4)n^4[45n^4+63n^2-14n^2l(l+1)-15l^2(l+1)^2-10l(l+1)], \tag{24b}$$

$$C_2^{(3)}=(V_3/8Z^5)n^4[143n^6+345n^4+28n^2-90n^4l(l+1)-21n^2l^2(l+1)^2-126n^2l(l+1)], \tag{24c}$$

and

$$C_{-1}^{(4)}=-(n^2/8Z^3)[(105V_4+28V_2^2)n^4+(75V_4+20V_2^2)n^2-90V_4n^2l(l+1)+(9V_4-12V_2^2)l^2(l+1)^2-18V_4l(l+1)], \tag{25a}$$

$$C_1^{(4)}=(n^4/16Z^5)\{V_4[231n^6+585n^4+84n^2-135n^4l(l+1)-63n^2l^2(l+1)^2-189n^2l(l+1)+15l^3(l+1)^3-30l^2(l+1)^2+V_2^2[99n^6+225n^4-21n^2l^2(l+1)^2-30l^3(l+1)^3]\}. \tag{25b}$$

Combining Eqs. (15), (18), (19), (21), (24), and (25), the energies of the atom with atomic number Z through the sixth order of λ are found to be

$$E_n^{(1)}=-ZV_1, \tag{26a}$$

$$E_n^{(2)}=-\tfrac{1}{2}[3n^2-l(l+1)]V_2, \tag{26b}$$

$$E_n^{(3)}=-(n^2/2Z)[5n^2+1-3l(l+1)]V_3, \tag{26c}$$

$$E_n^{(4)}=-n^2/8Z^2[(35V_4+7V_2^2)n^4+(25V_4+5V_2^2)n^2-30n^3l(l+1)V_4+(3V_4-3V_2^2)l^2(l+1)^2-6l(l+1)V_4], \tag{26d}$$

$$E_n^{(5)}=-(n^4/8Z^3)[(63V_5+45V_2V_3)n^4+(105V_5+63V_2V_3)n^2+12V_5-(70V_5+14V_2V_3)n^2l(l+1)+(15V_5-15V_2V_3)l^2(l+1)^2-(50V_5+10V_2V_3)l(l+1)], \tag{26e}$$

$$E_n^{(6)}=-(n^4/16Z^4)[(231V_6+231V_2V_4+143V_3^2+33V_2^3)n^6+(735V_6+585V_2V_4+345V_3^2+75V_2^3)n^4+(294V_6+84V_2V_4+28V_3^2)n^2-(315V_6+135V_2V_4+90V_3^2)n^4l(l+1)+(105V_6-63V_2V_4-21V_3^2-7V_2^3)n^2l^2(l+1)^2-(525V_6+189V_2V_4+126V_3^2)n^2l(l+1)+(-5V_6+15V_2V_4-10V_2^3)l^3(l+1)^3+(40V_6-30V_2V_4)l^2(l+1)^2-60V_6l(l+1)], \tag{26f}$$

where $E_n^{(k)}$ is the kth perturbed energy to the nth state of the electron. Equations (26a)–(26c) are in agreement with the result of the analytic perturbation theory.[3]

For completeness, the expectation values of $\langle r\rangle$, $\langle r^{-1}\rangle$, and $\langle r^2\rangle$ up to the fourth and third orders of λ, respectively, are given below:

$$\langle r\rangle=(1/2Z)[3n^2-l(l+1)]+(n^2/4Z^3)V_2[7n^4+5n^2-3l^2(l+1)^2]\lambda^2$$
$$+(n^4/8Z^4)V_3[45n^4+63n^2-14n^2l(l+1)-15l^2(l+1)^2-10l(l+1)]\lambda^3$$
$$+(n^4/16Z^5)\{V_4[231n^6+585n^4+84n^2-135n^4l(l+1)-63n^2l^2(l+1)^2$$
$$-189n^2l(l+1)+15l^3(l+1)^3-30l^2(l+1)^2]$$
$$+V_2^2[99n^6+225n^4-21n^2l^2(l+1)^2-30l^3(l+1)^3]\}\lambda^4+\cdots, \tag{27a}$$

$$\langle r^{-1}\rangle=Z/n-(V_2/2Z)[3n^2-l(l+1)]\lambda^2-(V_3/2Z^2)n^2[5n^2+1-3l(l+1)]\lambda^3$$
$$-(n^2/8Z^3)[(105V_4+28V_2^2)n^4+(75V_4+20V_2^2)n^2-90V_4n^2l(l+1)$$
$$+(9V_4-12V_2^2)l^2(l+1)^2-18V_4l(l+1)]\lambda^4+\cdots, \tag{27b}$$

$$\langle r^2\rangle=(n^2/2Z^2)[5n^2+1-3l(l+1)]+(V_2/8Z^4)n^4[45n^4+63n^2-14n^2l(l+1)-15l^2(l+1)^2-10l(l+1)]\lambda^2$$
$$+(V_3/8Z^5)n^4[143n^6+345n^4+28n^2-90n^4l(l+1)-21n^2l^2(l+1)^2$$
$$-126n^2l(l+1)]\lambda^3+\cdots. \tag{27c}$$

From the above calculations, we show that with the use of the hypervirial relations and the Hellman-Feynman theorem, it is, in principle, possible to derive the energy and the expectation values of $\langle r^j\rangle$ in power series of the perturbation parameter λ correct to any order of λ. The energy and $\langle r^j\rangle$ presented above are, effectively, expansions in $\lambda n^2/Z$. Since $\lambda=\lambda_0Z^{1/3}$, where λ_0 is a constant, we find that the energy and $\langle r^j\rangle$ are given as expansions in $\lambda_0 n^2Z^{-2/3}$. However, it is hard to see from Eq. (26) that the series for E is asymptotic[4] in powers of $(Z/\lambda n^2)$. Therefore we expect Eq. (26) to be valid for the K shell of all but the least-Z elements and for other low-lying levels of high-Z elements[3]. In additional to Eq. (26), one can also employ the computer to calculate the energies of atoms to higher order of λ by solving Eqs. (11)–(15).

IV. DISCUSSIONS AND CONCLUSIONS

We have derived explicitly the energy of the atom with atomic number Z correct to the sixth order of the perturbation parameter λ in the previous section. Equations (11)–(15) can also be used to calculate the energies of atoms up to higher orders of λ if the computer is employed. For simplicity, we confine ourselves, in this section, to the Yukawa potential

$$V_c(r)=-(Z/r)e^{-\lambda r}, \tag{28}$$

where the perturbation parameter λ is given by

$$\lambda=\lambda_0Z^{1/3} \tag{29}$$

corresponding to the Z dependence of the reciprocal of the Thomas-Fermi radius of the atom.[3] We note that the model potential in Eq. (28) used here is not entirely realistic, and other physical effects such as relativistic corrections are known to enter.

Using Eqs. (9) and (29), we find, from Eq. (26), for the energy E_n of the atom in the S state ($l=0$),

$$E_n=-(Z^2/2n^2)+Z^{4/3}\lambda_0-\tfrac{3}{4}n^2Z^{2/3}\lambda_0^2+\tfrac{1}{12}n^2(5n^2+1)\lambda_0^3-\tfrac{11}{192}n^4(7n^2+5)Z^{-2/3}\lambda_0^4+\tfrac{1}{320}n^4(171n^4+245n^2+4)Z^{-4/3}\lambda_0^5$$
$$-\tfrac{1}{5760}n^6(4763n^4+11580n^2+1057)Z^{-2}\lambda_0^6+\cdots, \tag{30}$$

where n is the principal quantum number of the unperturbed nth state. We note that the first four terms of Eq. (30) have been derived before,[3] and that E_n in Eq. (30) is an expansion in $\lambda_0n^2Z^{-2/3}$ and may diverge for low-Z elements. In addition to Eq. (30), we also calculate E_n up to the twentieth order of λ by solving Eqs. (11)–(15) using the computer.

Instead of comparing the results of our analytic calculation with the experiments[9] or numerical calculations with the same potential, we list in Tables I–III some values of energy levels with $n=1$, 2, and 3 for various values of Z. In this way, one is able to examine how the perturbation series converges for different values of Z and λ_0. In Table I, we list our calculated values of E_1 up to the third, sixth, eighth, twelfth, sixteenth, and twentieth orders of λ for some values of Z with $\lambda_0=0.85$. We see, from Table I, that the perturbation series of the K-shell energy begins to converge at least for $Z=5$, and that once the perturbation series converges sufficiently quickly, the first seven terms or even the first four terms of the series will give a fairly accurate value of E_1. In

TABLE I. Calculated K-shell binding energies E_1 up to the third, sixth, eighth, twelfth, sixteenth, and twentieth orders of λ for some values of Z with $\lambda_0 = 0.85$.

	E_1 (eV)					
Z	$\sim\lambda^3$	$\sim\lambda^6$	$\sim\lambda^8$	$\sim\lambda^{12}$	$\sim\lambda^{16}$	$\sim\lambda^{20}$
2	−11.2	−18.8	−24.6	−129.4	−2507.1	−88 331.2
3	−44.7	−49.2	−49.8	−56.6	−115.3	−868.0
4	−99.6	−102.9	−102.9	−103.9	−107.3	−131.4
5	−177.1	−179.9	−179.7	−179.7	−180.1	−181.6
6	−278.0	−280.3	−280.2	−280.1	−280.1	−280.3
7	−402.6	−404.7	−404.6	−404.5	−404.5	−404.5
8	−551.3	−553.3	−553.1	−553.1	−553.1	−553.1
9	−724.5	−726.3	−726.2	−726.2	−726.2	−726.2
14	−1963.6	−1965.0	−1964.9	−1964.9	−1964.9	−1 964.9
20	−4286.9	−4288.0	−4288.0	−4288.0	−4288.0	−4 288.0

TABLE II. Calculated L-shell binding energies E_2 for some values of Z with $\lambda_0 = 0.70$.

	E_2 (eV)					
Z	$\sim\lambda^3$	$\sim\lambda^6$	$\sim\lambda^8$	$\sim\lambda^{12}$	$\sim\lambda^{16}$	$\sim\lambda^{20}$
15	−238.6	−267.7	−268.6	−282.2	−352.1	−792.1
20	−555.9	−578.0	−576.9	−577.2	−580.4	−592.2
21	−635.6	−656.8	−655.6	−655.5	−657.2	−663.3
22	−720.8	−741.3	−740.0	−739.6	−740.5	−743.7
23	−811.6	−831.4	−830.1	−829.6	−830.0	−831.7
24	−908.1	−927.2	−925.9	−925.3	−925.5	−926.4
25	−1010.1	−1028.7	−1027.4	−1026.8	−1026.8	−1027.3
26	−1117.9	−1135.9	−1134.7	−1134.1	−1134.0	−1134.3
30	−1606.6	−1622.8	−1621.8	−1621.3	−1621.2	−1621.2
40	−3239.1	−3252.5	−3251.9	−3251.7	−3251.6	−3251.6

TABLE III. Calculated M-shell binding energies E_3 for some values of Z with $\lambda_0 = 0.50$.

	E_3 (eV)					
Z	$\sim\lambda^3$	$\sim\lambda^6$	$\sim\lambda^8$	$\sim\lambda^{12}$	$\sim\lambda^{16}$	$\sim\lambda^{20}$
30	−418.3	−466.2	−465.3	−473.1	−505.7	−640.9
34	−613.5	−656.1	−654.1	−655.4	−663.4	−690.1
35	−668.2	−709.7	−707.5	−708.1	−713.7	−731.7
36	−725.2	−765.8	−763.5	−763.4	−767.3	−779.6
37	−784.6	−824.2	−821.9	−821.4	−824.1	−832.5
38	−846.4	−885.2	−882.7	−882.0	−883.8	−889.5
39	−910.7	−948.6	−946.1	−945.2	−946.3	−950.2
40	−977.3	−1014.4	−1012.0	−1010.9	−1011.6	−1014.2
41	−1046.4	−1082.8	−1080.3	−1079.2	−1079.5	−1081.3
50	−1779.1	−1810.4	−1808.3	−1807.2	−1806.9	−1806.9

Table II, we present our calculated values of the L-shell energy E_2 up to various orders of λ for some values of Z with $\lambda_0 = 0.70$. It appears from Table II that the perturbation series for E_2 with $\lambda_0 = 0.70$ starts to converge at least for $Z = 24$. We note that the perturbation series E_2 will converge for somewhat larger value of Z if λ_0 is chosen to be larger than 0.70. In Table III, we present the M-shell energy E_3 up to various orders of the perturbation parameter λ for some values of Z with $\lambda_0 = 0.50$. The energy series E_3 seems to converge at least for $Z = 40$ with $\lambda_0 = 0.50$. As in the case of E_1 and E_2, the first seven terms of the perturbation series for E_3 will give a fairly accurate value of E_3 for $Z \geq 40$ and $\lambda_0 = 0.50$.

From Tables I, II, and III, we see that the K-shell energy with $\lambda_0 = 0.85$, the L-shell energy with $\lambda_0 = 0.70$, and the M-shell energy with $\lambda_0 = 0.50$ will definitely converge for $Z \geq 5$, $Z \geq 24$, and $Z \geq 40$, respectively. Our calculation also indicates that E_1 will converge at least for $Z = 6$ if $\lambda_0 = 1.00$, and E_2 will converge at least for $Z = 29$ if $\lambda_0 = 0.85$. Thus, for the Yukawa potential, the perturbation series for the binding energies seem to converge at least for some values of Z if the perturbation parameter λ_0 is smaller than one.

In conclusion, by employing the hypervirial theorems and the Hellman-Feynman theorem for the problem of screened Coulomb potentials, we have demonstrated that one can obtain, in principle, analytically the energies and $\langle r^j \rangle$ of the atoms correct to any order of the perturbation parameter λ as one wishes. In this paper, we have presented the explicit formulas for the energies of the atoms correct to the sixth order of λ. We have also calculated E_n up to the twentieth order of λ using the computer. The perturbation expansion of E_n in powers of λ seems to converge for almost all the K-shell with $\lambda_0 < 1$, for the L-shell with $Z \geq 24$ and $\lambda_0 = 0.70$, and for the M-shell with $Z \geq 40$ and $\lambda_0 = 0.50$. Compared with other approximation methods of calculation, the present method using the hypervirial relations is more straightforward. Thus, the present method of calculation using the hypervirial theorems and the Hellman-Feynman theorem may play an important role in the description of screened Coulomb potentials.

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