

Shifted large- N expansion for the bound states of the Hellmann potential

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The method of shifted large- N expansion, where N is the number of spatial dimensions, is applied to study the bound states of the Hellmann potential, which represents the superposition of the attractive Coulomb potential $(-A/r)$ and the Yukawa potential $B \exp(-Cr)/r$ of arbitrary strength B and screening parameter C . It emerges that although the analytic expressions for the energy eigenvalues $E_{n,l}$ yield quite accurate results for a wide range of n, l in the limit of very weak screening, the results become gradually worse as the strength B and the screening coefficient C increase. This happens due to the fact that the effective large- N potential becomes quite shallow in comparison to the true potential and the expansion parameter is not sufficiently small enough to guarantee the convergence of the expansion series for the energy levels. Furthermore, the present analysis reveals an intrinsic limitation of the technique in case of specific superposition of potentials: For certain choices of $B, C, n,$ and l , the structure of the effective potential becomes such that it does not possess a local minimum and consequently the method turns out to be inapplicable to determining the corresponding bound-state energies. However, such a limitation does not persist for a simple screened Coulomb potential and reasonably accurate energy eigenvalues and bound-state normalizations are obtained for the neutral atoms. It is expected that the normalized bound-state wave functions obtained through the shifted large- N formalism may be useful in calculating the oscillator strength, bound-bound dipole transition matrix elements, etc. which have significant importance in atomic processes.

I. INTRODUCTION

Recently Adamowski¹ has presented a study of the systematics of the energy eigenvalues of the two-particles interacting through the potential

$$V(r) = -A/r + B e^{-Cr}/r, \quad (1)$$

where A and B are the strengths of the Coulomb and the Yukawa potentials, respectively, and C is the screening parameter. It is assumed that A and C are positive whereas B can be positive or negative. The potential in (1) with B positive was first suggested by Hellmann^{2,3} many years ago and henceforth this potential will be referred to as the Hellmann potential irrespectively of the sign of B . The Hellmann potential has been used by various workers to represent the electron-core^{4,5} or the electron-ion^{6,7} interaction. Varshni and Shukla⁸ used this model potential for alkali hydride molecules. Das and Chakravarty⁹ have recently proposed that such a potential is suitable for the study of inner-shell ionization problems.

The bound-state energies of the Hellmann potential for various sets of values of B and C have been studied elaborately by Adamowski in a variational framework using ten variational parameters. The energy eigenvalues have been predicted very accurately but the calculations involve extensive computational time and effort. Moreover, compact analytic expressions for the energy eigenvalues are not obtainable.

In this paper, we propose to investigate the bound-state

properties of the Hellmann potential using the large- N expansion technique which has been claimed to be very powerful for solving the Schrödinger equation to obtain the bound-state energies as well as the wave functions in potential problems.¹⁰⁻²¹ For our work we follow the shifted $1/N$ expansion method first suggested by Sukhatme and Imbo.¹⁶ These authors modified the standard $1/N$ method through the introduction of a shift parameter so as to restore the exact Coulomb results in the leading order of the expansion. The accuracy of the shifted large- N expansion has been tested for many smoothly changing spherically symmetric potentials, e.g., the power-law potentials, logarithmic, anharmonic oscillator, Yukawa, Gaussian, etc. Although the accuracy of the energy eigenvalues is in general extremely good for such smooth potentials, it is not *a priori* guaranteed that the approach will work equally well for the superposition of simple potentials such as the Hellmann potential. On the contrary, it has been conjectured¹⁹ that the technique may not be suitable for rapidly varying potentials which cannot be adequately described by a few leading terms in the $1/N$ expansion series. However, to our knowledge, no explicit case study has been undertaken to substantiate this conjecture.

One of the prime motivations of the present study is to explore the regions of validity of the large- N technique for the superposition of potentials such as the one in (1) which manifests different structures for various range of values of B and C . Our calculations reveal that the de-

gree of accuracy of the predicted energy eigenvalues varies appreciably for different range of values of B and C and for different quantum states. These observations have relevance in the context of applications of the shifted $1/N$ expansion technique to realistic problems of atomic physics. We pursue this work with a view to compute bound-state normalizations and energy levels of neutral atoms, which have been studied in recent time using various analytic techniques.²²⁻²⁴ The static screened Coulomb potential (SSCP)

$$V(r) = -(\alpha Z)e^{-\delta r}/r \quad (2)$$

which emerges as a special case of the Hellmann potential in (1) with $A=0$, $B=-\alpha Z$, and $C=\delta$, where $\alpha=(137.037)^{-1}$ is the fine-structure constant and Z is the atomic number, is often used for the description of the energy levels of neutral atoms. It is known that SSCP yields reasonable results only for the innermost states when Z is large. However, for the outermost and middle atomic states, it gives rather poor results. Although the bound-state energies for the SSCP with $Z=1$ have been studied¹⁸ in the light of the shifted large- N method, it is perhaps reasonable to investigate whether the method is useful in predicting bound-state energy levels and bound-state nor-

TABLE I. Energy eigenvalues ($-E$) in atomic units of states $1s-4f$ for the Hellmann potential as functions of the screening parameter C for $B=\pm 5$. The variational results of Adamowski (Ref. 1) converted to our scale of units are given in parentheses. The blanks correspond to divergent results and the abbreviations (n.a) indicate nonapplicability of the present method.

C	0.05	0.1	0.2	0.5	2	10
$B = +5$						
State						
$1s$	0.01098 (0.01099)	0.02078 (0.02083)	0.03845 (0.03858)	0.08238 (0.08280)	0.22011 (0.21877)	0.29851 (0.42197)
$2s$	0.00848 (0.00857)	0.01452 (0.01481)	0.02363 (0.02432)	0.04165 (0.04263)	0.02724 (0.07959)	0.12500 (0.11464)
$2p$	0.01075 (0.01075)	0.01992 (0.01993)	0.03536 (0.03538)	0.06737 (0.06736)	0.11296 (0.11563)	0.12500 (0.12492)
$3s$	0.00661 (0.00670)	0.01045 (0.01090)	0.01575 (0.01645)	0.02183 (0.02564)	0.05491 (0.04069)	0.05555 (0.05238)
$3p$	0.00835 (0.00838)	0.01410 (0.01421)	0.02232 (0.02249)	0.03578 (0.03610)	0.05538 (0.05246)	0.05555 (0.05552)
$3d$	0.01029 (0.01029)	0.01829 (0.01830)	0.03001 (0.03001)	0.04700 (0.04694)	0.05554 (0.05543)	0.05555 (0.05555)
$4s$	0.00524 (0.00503)	0.00788 (0.00807)	0.01112 (0.01182)	0.01112 (0.01706)	0.03125 (0.02463)	0.03125 (0.02987)
$4p$	0.00656 (0.00655)	0.01032 (0.01035)	0.01518 (0.01537)	0.01578 (0.02241)	0.03125 (0.02989)	0.03125 (0.03123)
$4d$	0.00803 (0.00803)	0.01307 (0.01311)	0.01942 (0.01943)	0.02598 (0.02723)	0.03125 (0.03118)	0.03125 (0.03125)
$4f$	0.00965 (0.00965)	0.01617 (0.01617)	0.02388 (0.02387)	0.03030 (0.03185)	0.03125 (0.03125)	0.03125 (0.03125)
$B = -5$						
$1s$	17.7515 (17.7515)	17.5062 (17.5062)	17.0244 (17.0244)	15.6483 (15.6483)	10.0929 (10.0930)	0.9788 (0.9788)
$2s$	4.2561 (4.2561)	4.0241 (4.0241)	3.5931 (3.5931)	2.5306 (2.5308)	0.6375 (0.4583)	0.1250 (0.1668)
$2p$	4.2551 (4.2551)	4.0202 (4.0202)	3.5784 (3.5784)	2.4552 (2.4552)	0.2203 (0.1910)	0.1250 (0.1251)
$3s$	1.7635 (1.7635)	1.5520 (1.5520)	1.1949 (1.1943)	0.5253 (0.5226)	0.1129 (0.1129)	0.0556 (0.0667)
$3p$	1.7625 (1.7625)	1.5484 (1.5484)	1.1819 (1.1819)	0.4788 (0.4753)	0.0727 (0.0727)	0.0556 (0.0556)
$3d$	1.7606 (1.7606)	1.5412 (1.5412)	1.1568 (1.1568)	0.3757 (0.3758)	n.a (0.0557)	0.0555 (0.0555)
$4s$	0.8983 (0.8983)	0.7095 (0.7127)	0.4438 (0.4400)	0.2498 (0.1215)	0.0516 (0.0516)	0.0313 (0.0356)
$4p$	0.8974 (0.8974)	0.7095 (0.7095)	0.4314 (0.4303)	0.1310 (0.1031)	0.0381 (0.0381)	0.0312 (0.0312)
$4d$	0.8956 (0.8956)	0.7030 (0.7030)	0.4107 (0.4105)	0.0446 (0.0692)	n.a (0.0313)	0.0312 (0.0312)
$4f$	0.8928 (0.8928)	0.6933 (0.6933)	0.3799 (0.3799)	n.a (0.0340)	n.a (0.0312)	0.0312 (0.0312)

malizations of light to heavy neutral atoms.

The relevant steps of the shifted large- N expansion scheme for obtaining the analytic expressions for the bound-state energy levels, eigenfunctions, and normalization constants are presented in Secs. II and III. In Sec. IV we discuss the numerical results. The bound-state energies of the Hellmann potential have been computed for $1s$ to $4f$ states as functions of C and for various positive and negative values of B . To assess the accuracy of our results we compare the predicted energy eigenvalues with those obtained by Adamowski through his variational method.¹ To be more informative and compact we present in Table I only those cases for which discrepancies are appreciable for certain values of C . A few interesting features of our results are observed: In certain regions of values of B and C , excellent agreement is observed between the variational solutions and the results of the shifted $1/N$ calculation. As expected, for a given quantum number n , the results improve as l increases. However,

for certain combinations of B , C , n_r , and l , it seems that the method is not at all workable as the effective potential becomes very shallow and does not possess a local minimum. A few interesting regularities of the energy levels with respect to B and l emerge: For $l > l'$, the observed spacing of the energy levels $E_{n,l} > E_{n,l'}$ for $B < 0$ or $E_{n,l} < E_{n,l'}$ for $B > 0$ is found to be consistent with the level ordering theorem of Grosse and Martin.²⁵ In Sec. V, we compare our calculations for the bound-state energies and normalizations of neutral atoms with those obtained by analytic perturbation theory²² and also by numerical method. The accuracy of the shifted large- N calculations for the energy levels is found to be extremely good. However, the normalization factors are not obtained so accurately due to the fact that we have considered only the leading order term in the expansion series for the wave function. In the concluding section, we briefly discuss the scope of extending the method to other areas of atomic physics.

II. SHIFTED $1/N$ EXPANSION FORMULAS FOR ENERGY EIGENVALUES

In N spatial dimensions, the radial Schrödinger equation for the Hellmann potential in atomic units ($\hbar = m = e = 1$) is

$$\left[-\frac{1}{2} \frac{d^2}{dr^2} + \frac{(\bar{k} + a - 1)(\bar{k} + a - 3)}{8r^2} - \frac{A}{r} + B \frac{e^{-Cr}}{r} \right] \chi_{n,l}(r) = E_{n,l} \chi_{n,l}(r), \quad (3)$$

where $\bar{k} = N + 2l - a$, a is the so called shift parameter. We follow the prescription of the shifted $1/N$ discussed in detail by Imbo *et al.*¹⁷ and present here only the analytic expressions which are required to evaluate the bound-state energies. The energy eigenvalues are given by an expansion in powers of $1/\bar{k}$. The relevant analytic formulas in physical $N = 3$ space are obtained as follows:

$$E_{n,l} = \frac{\bar{k}^2}{r_0^2} \left[\left[\frac{1}{8} - \frac{(A - B e^{-Cr_0})}{4(A - B e^{-Cr_0} - BC e^{-Cr_0})} \right] + \frac{\gamma^{(1)}}{\bar{k}^2} + \frac{\gamma^{(2)}}{\bar{k}^3} + O\left[\frac{1}{\bar{k}^4}\right] \right] \quad (4)$$

in which the quantity r_0 satisfies the equation

$$(2l + 1) + (2n_r + 1) \left[\frac{A - B e^{-Cr_0}(1 + Cr_0 - C^2 r_0^2)}{A - B e^{-Cr_0}(1 + Cr_0)} \right]^{1/2} = 2\{r_0[A - B e^{-Cr_0}(1 + Cr_0)]\}^{1/2}. \quad (5)$$

In Eqs. (4) and (5), n_r and $n = (n_r + l + 1)$ are the radial and principal quantum numbers, respectively. The quantities $\gamma^{(1)}$ and $\gamma^{(2)}$ appearing in the corrections to the leading order of the energy expansion are

$$\gamma^{(1)} = \frac{1}{8}(1 - a)(3 - a) + (1 + 2n_r)\bar{\epsilon}_2 + 3(1 + 2n_r + 2n_r^2)\bar{\epsilon}_4 - \omega^{-1}[\bar{\epsilon}_1^2 + 6(1 + 2n_r)\bar{\epsilon}_1\bar{\epsilon}_3 + (11 + 30n_r + 30n_r^2)\bar{\epsilon}_3^2], \quad (6)$$

$$\begin{aligned} \gamma^{(2)} = & (1 + 2n_r)\bar{\delta}_2 + 3(1 + 2n_r + 2n_r^2)\bar{\delta}_4 + 5(3 + 8n_r + 6n_r^2 + 4n_r^3)\bar{\delta}_6 \\ & - \omega^{-1}[(1 + 2n_r)\bar{\epsilon}_2^2 + 12(1 + 2n_r + 2n_r^2)\bar{\epsilon}_2\bar{\epsilon}_4 + 2(21 + 59n_r + 51n_r^2 + 34n_r^3)\bar{\epsilon}_4^2 + 2\bar{\epsilon}_1\bar{\delta}_1 \\ & + 6(1 + 2n_r)\bar{\epsilon}_1\bar{\delta}_3 + 30(1 + 2n_r + 2n_r^2)\bar{\epsilon}_1\bar{\delta}_5 + 6(1 + 2n_r)\bar{\epsilon}_3\bar{\delta}_1 + 2(11 + 30n_r + 30n_r^2)\bar{\epsilon}_3\bar{\delta}_3 \\ & + 10(13 + 40n_r + 42n_r^2 + 28n_r^3)\bar{\epsilon}_3\bar{\delta}_5] \\ & + \omega^{-2}[4\bar{\epsilon}_1^2\bar{\epsilon}_2 + 36(1 + 2n_r)\bar{\epsilon}_1\bar{\epsilon}_2\bar{\epsilon}_3 + 8(11 + 30n_r + 30n_r^2)\bar{\epsilon}_2\bar{\epsilon}_3^2 + 24(1 + 2n_r)\bar{\epsilon}_1^2\bar{\epsilon}_4 \\ & + 8(31 + 78n_r + 78n_r^2)\bar{\epsilon}_1\bar{\epsilon}_3\bar{\epsilon}_4 + 12(57 + 189n_r + 225n_r^2 + 150n_r^3)\bar{\epsilon}_3^2\bar{\epsilon}_4] \\ & - \omega^{-3}[8\bar{\epsilon}_1^3\bar{\epsilon}_3 + 108(1 + 2n_r)\bar{\epsilon}_1^2\bar{\epsilon}_3^2 + 48(11 + 30n_r + 30n_r^2)\bar{\epsilon}_1\bar{\epsilon}_3^3 + 30(31 + 109n_r + 141n_r^2 + 94n_r^3)\bar{\epsilon}_3^4], \quad (7) \end{aligned}$$

in which

$$\begin{aligned} \bar{\epsilon}_j &= \epsilon_j / \bar{\omega}^{j/2}, \quad \bar{\delta}_j = \delta_j / \bar{\omega}^{j/2}, \quad \bar{\omega} = 2\omega, \quad \omega = \frac{1}{2} \left[\frac{A - B e^{-Cr_0}(1 + Cr_0 - C^2 r_0^2)}{A - B e^{-Cr_0}(1 + Cr_0)} \right]^{1/2}, \quad a = 2 - (2n_r + 1)\bar{\omega}, \\ \delta_1 &= -\frac{2}{3}\delta_2 = -(1-a)(3-a)/4, \quad \delta_3 = -\frac{4}{3}\delta_4 = 2\epsilon_1 = -\frac{4}{3}\epsilon_2 = (2-a), \\ \epsilon_3 &= -\frac{1}{2} + \frac{r_0}{\bar{k}^2} [A - B e^{-Cr_0}(1 + Cr_0 + \frac{1}{2}C^2 r_0^2 + \frac{1}{6}C^3 r_0^3)], \\ \epsilon_4 &= \frac{5}{8} + \frac{r_0}{\bar{k}^2} [-A + B e^{-Cr_0}(1 + Cr_0 + \frac{1}{2}C^2 r_0^2 + \frac{1}{6}C^3 r_0^3 + \frac{1}{24}C^4 r_0^4)], \\ \delta_5 &= -\frac{3}{4} + \frac{r_0}{\bar{k}^2} [A - B e^{-Cr_0}(1 + Cr_0 + \frac{1}{2}C^2 r_0^2 + \frac{1}{6}C^3 r_0^3 + \frac{1}{24}C^4 r_0^4 + \frac{1}{120}C^5 r_0^5)], \\ \delta_6 &= \frac{7}{8} + \frac{r_0}{\bar{k}^2} [-A + B e^{-Cr_0}(1 + Cr_0 + \frac{1}{2}C^2 r_0^2 + \frac{1}{6}C^3 r_0^3 + \frac{1}{24}C^4 r_0^4 + \frac{1}{120}C^5 r_0^5 + \frac{1}{720}C^6 r_0^6)]. \end{aligned} \tag{8}$$

For any given choice of the quantum numbers, n_r and l , Eq. (5) can in principle be solved for r_0 for a set of values of A , B , and C . Only in some special cases (to be discussed in Sec. IV), a real solution is not obtainable and the method fails to predict the corresponding bound-state energies. Once r_0 is determined, the task of obtaining the energy eigenvalues from the algebraic expressions Eqs. (4) and (6)–(8) becomes relatively simple and straightforward. One may easily check that in the Coulomb limit, i.e., $A=1$, $C \rightarrow \infty$ and/or $B \rightarrow 0$, $\gamma^{(1)}$ and $\gamma^{(2)}$ vanish identically. Consequently, one recovers from Eq. (4) the well-known Coulomb result

$$E_{n,l}^C = -1/2n^2. \tag{9}$$

III. NORMALIZED EIGENFUNCTIONS IN THE SHIFTED LARGE- N EXPANSION

The conventional large- N expansion technique yields the radial wave functions, $\chi_{n,l}(r)$ which are accurate only near the minimum of the effective potential. Very recently, Imbo and Sukhatme²⁰ have obtained improved wave functions which are accurate for all r and any choice of the quantum numbers. Following their prescription, we thus write the leading order bound-state wave functions

$$\chi_{n,l}(r) = C_{n,l} r^{(k-1)/2} e^{-\lambda(r/r_0)^{\bar{\omega}}} L_{n_r}^{(k-2)/\bar{\omega}}(2\lambda(r/r_0)^{\bar{\omega}}) \tag{10}$$

in which

$$\lambda = \bar{k}/2\bar{\omega}, \tag{11}$$

L_n^m is the Laguerre function²⁶

$$L_n^m(x) = \frac{e^x x^{-m}}{n!} \frac{d^n}{dx^n} (e^{-x} x^{n+m}) \tag{12}$$

and $C_{n,l}$ is a constant. For screened Coulomb problems, the usual practice is to express the bound-state wave functions in terms of the confluent hypergeometric functions.

Using the connecting formula²⁶

$$L_n^m(x) = \frac{(n+m)!}{n!m!} {}_1F_1(-n, m+1; x), \tag{13}$$

Eq. (10) becomes

$$\begin{aligned} \chi_{n,l}(r) &= N_{n,l} r^{(k-1)/2} e^{-\lambda(r/r_0)^{\bar{\omega}}} \\ &\quad \times {}_1F_1(-n+l+1, (k-2)/\bar{\omega}+1; 2\lambda(r/r_0)^{\bar{\omega}}), \end{aligned} \tag{14}$$

where the normalization constant $N_{n,l}$ is given by

$$N_{n,l} = \frac{\left[\frac{k-2}{\bar{\omega}} + n_r \right]!}{n_r! \left[\frac{k-2}{\bar{\omega}} \right]!} C_{n,l}. \tag{15}$$

The constant $C_{n,l}$ may easily be determined from the normalization integral for $\chi_{n,l}(r)$. Changing the variable

$$x = 2\lambda(r/r_0)^{\bar{\omega}} \tag{16}$$

one gets from Eq. (10)

$$C_{n,l}^2 \frac{r_0^k}{\bar{\omega}} (2\lambda)^{-k/\bar{\omega}} \int_0^\infty x^{(k/\bar{\omega}-1)} e^{-x} [L_{n_r}^{(k-2)/\bar{\omega}}(x)]^2 dx = 1. \tag{17}$$

Using the relations²⁶

$$L_n^\alpha(x) = \sum_{m=0}^n (-1)^m \frac{(n+\alpha)!}{(n-m)!(\alpha+m)!m!} x^m, \tag{18}$$

$$\int_0^\infty e^{-x} x^{\gamma-1} L_n^\alpha(x) dx = \frac{\Gamma(\gamma)\Gamma(1+\alpha+n-\gamma)}{n!\Gamma(1+\alpha-\gamma)}, \quad \text{Re } \gamma > 0, \tag{19}$$

in Eq. (17), we obtain finally

$$C_{n,l}^2 \frac{r_0^k}{\tilde{\omega}} (2\lambda)^{-k/\tilde{\omega}} \sum_{m=0}^{n_r} \frac{(-1)^m \left[n_r + \frac{k-2}{\tilde{\omega}} \right]! \Gamma \left[\frac{k}{\tilde{\omega}} + m \right] \Gamma \left[1 + n_r - m - \frac{2}{\tilde{\omega}} \right]}{(n_r - m)! m! n_r! \left[\frac{k-2}{\tilde{\omega}} + m \right]! \Gamma \left[1 - m - \frac{2}{\tilde{\omega}} \right]} = 1. \quad (20)$$

From Eqs. (15) and (20), one can determine the normalization constant for any bound quantum state. In the limit of the nonrelativistic point Coulomb potential, one retrieves from Eqs. (14), (15), and (20), the Coulomb bound-state wave function²⁷

$$\chi_{n,l}(r) = N_{n,l}^C r^{l+1} e^{-r/n} {}_1F_1(-n+l+1, 2l+2; 2r/n) \quad (21)$$

with

$$N_{n,l}^C = (2/n)^{l+3/2} \frac{1}{(2l+1)!} \left[\frac{(n+l)!}{2n(n-l-1)!} \right]^{1/2}. \quad (22)$$

IV. NUMERICAL RESULTS

For the numerical work, we take $A=1$ and thus our B is to be identified with half of the corresponding rescaled parameter in Adamowski's paper. Consequently, our energy eigenvalues are half of those obtained by Adamowski. We compute the binding energies ($-E_{n,l}$) of the lowest-lying states, $1s$ to $4f$, for various values of B and C obtained from the analytic expressions given in Eqs. (4)–(8). The predicted results are then compared with the accurate energy eigenvalues²⁸ obtained by Adamowski using a high precision variational technique. However, for brevity, we display results in Table I only for those sets of values of B and C for which appreciable discrepancies are observed. Although we do not present here all the energy eigenvalues considered by Adamowski, our calculation reveals certain interesting features of the shifted large- N expansion method of approximation.

(i) For low strength of B , the energy eigenvalues obtained from the shifted $1/N$ expansion are in good agreement with the variational results for low values of the screening parameter C . Obviously, when C is small the Coulomb field character prevails and the shifted large- N method has been adjusted to that. However, the results become gradually worse as B and/or C are large. Appreciable discrepancy of our results from the variational calculations occurs particularly for the s states and for large $B \sim \pm 5$. Even for the ground state, the error shoots up to 29% for $B=+5$, $C=10$ (see Table I). We suspect that this happens because the large- N effective potential becomes shallow and its minimum (r_0) shifts appreciably from the minimum of the true potential. This may be seen clearly from Fig. 1 in which we depict the gap between the minima of the true and the effective potentials for the ground state for $B=+5$, $C=10$. For certain values of C , the large- N effective potentials for some states becomes so shallow that the expansion for the energy series becomes divergent in the sense that $\gamma^{(1)}$ and $\gamma^{(2)}$ terms in (4) dominate over the leading term and consequently one gets anomalous results. In Table I, the space

for the predicted energy eigenvalues is kept blank for such a situation.

(ii) For certain negative B , it is not possible to determine r_0 , the most crucial parameter without the knowledge of which the calculation cannot proceed. For peculiar combinations of B , C , n_r , and l , the quantity within the square root sign on the left-hand side of Eq. (5) becomes negative before r_0 attains the value necessary for the matching condition to be satisfied. One such case is $B=-5$, $C=0.5$, $n_r=0$, and $l=3$, i.e., for the $4f$ state. For this set of values, the variations of the left-hand side (LHS) as well as of the right-hand side (RHS) of Eq. (5) with r_0 are shown in Fig. 2. The LHS becomes imaginary at $r_0=4.61$. Absence of crossing of the curves indicates that no real solution of Eq. (5) exists. Several such combinations have been observed and as a result, the method is not applicable (abbreviated as n.a in Table I), to determine the corresponding bound-state energies. Clearly, this implies that the large- N expansion has limitations for potentials having varied structure in different domains of the potential parameters.

(iii) The results presented in Table I indicate the level ordering:¹ $l > l'$, $E_{n,l} \geq E_{n,l'}$ for $B \leq 0$. We show that this can be interpreted from the criterion obtained by Grosse and Martin.²⁵ It was shown that for the potential

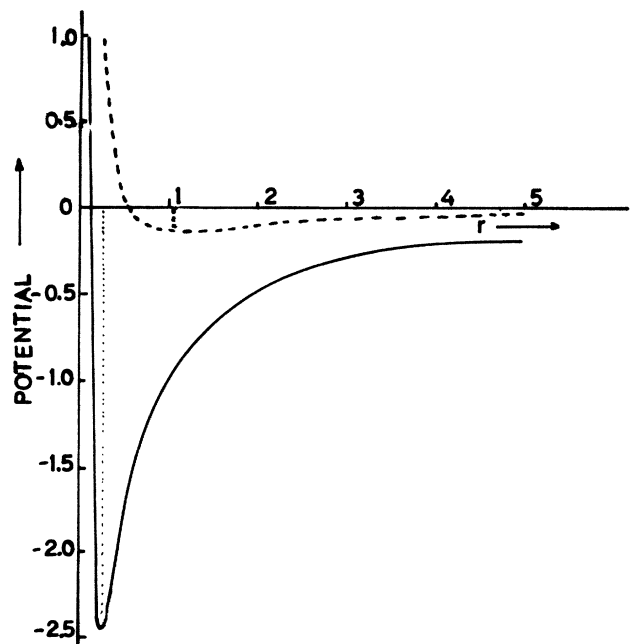


FIG. 1. Schematic diagrams of the behavior of the Hellmann potential, $V(r) = -1/r + 5\exp(-10r)/r$ (solid curve) and the large- N effective potential for the ground state (dashed curve) as a function of r . The locations of the minima of the potentials are shown by dotted lines.

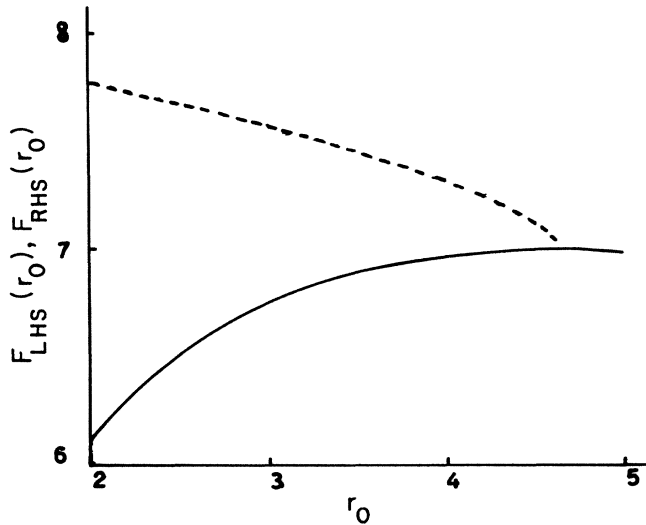


FIG. 2. Variations of $F_{RHS}(r_0)$ and $F_{LHS}(r_0)$, the RHS (solid line) and the LHS (dashed line) of Eq. (5), respectively with r_0 for $B = -5$, $C = 0.5$, $n_r = 0$, $l = 3$. Before crossing occurs, $F_{LHS}(r_0)$ becomes complex at $r_0 = 4.61$.

$$V(r) = -1/r + U(r), \quad \frac{d}{dr} \left[r^2 \frac{dU}{dr} \right] \leq 0 \quad (23)$$

the energy levels satisfy the inequality

$$E_{n,l} \geq E_{n,l'} \quad \text{for } l > l'. \quad (24)$$

Comparing the Hellmann potential in (1) with that in (23), we find

$$U(r) = B e^{-Cr}/r$$

and

$$\frac{d}{dr} \left[r^2 \frac{dU}{dr} \right] = BC^2 r e^{-Cr}. \quad (25)$$

All other quantities except B remaining positive, lead to the condition

$$\frac{d}{dr} \left[r^2 \frac{dU}{dr} \right] \leq 0 \quad \text{for } B \leq 0 \quad (26)$$

which corroborates with the observed level ordering for the Hellmann potential.

V. ENERGY LEVELS AND BOUND-STATE NORMALIZATIONS FOR NEUTRAL ATOMS

Recently McEnnan *et al.*²² developed an analytic perturbation theory in which the energy levels and the bound-state normalizations of neutral atoms were obtained using the SSCP given in (2). To assess the effectiveness of the present nonperturbative approach in this context, we carry out calculation for the energy eigenvalues and normalizations for the neutral atoms. For the energy levels, one needs simply to make appropriate changes in Eqs. (4)–(8) for the potential (2). The explicit forms of the normalization factors for the first three levels obtained from Eqs. (15) and (20) are given as

$$N_{10} = \left[\frac{\tilde{\omega} (2\lambda)^{3/\tilde{\omega}}}{r_0^3 \Gamma(3/\tilde{\omega})} \right]^{1/2},$$

$$N_{20} = \left[\frac{1}{\tilde{\omega}} + 1 \right] \left[\frac{\tilde{\omega} (2\lambda)^{3/\tilde{\omega}}}{r_0^3 \Gamma(3/\tilde{\omega}) \left[1 - \frac{1}{\tilde{\omega}} + \frac{4}{\tilde{\omega}^2} \right]} \right]^{1/2}, \quad (27)$$

$$N_{21} = \left[\frac{\tilde{\omega} (2\lambda)^{5/\tilde{\omega}}}{r_0^5 \Gamma(5/\tilde{\omega})} \right]^{1/2}.$$

A comparison of our expressions for the bound-state energies and normalizations with analytic perturbation calculations of McEnnan *et al.*²² and exact numerical results is given in Table II. We consider $Z = 13, 36, 79$ in order to cover the range of low to high atomic numbers. It is found that the difference between the shifted $1/N$ expansion results and the exact values for the K shell is somewhat less than 1% for low Z and improves as Z increases. Maximum discrepancy occurs for the L shell, the predicted normalizations are in error up to 15% for $Z = 36$. This indicates that only the leading-order term of the wave function as given in Eq. (10) does not yield adequate screening effect on the normalization constant. For better results, one requires to incorporate the contribution due to the nonleading terms in the $1/N$ expansion for the wave functions.

TABLE II. Bound-state energies (in keV) and bound-state normalizations for neutral atoms. The numbers in parentheses indicate powers of 1D by which the values are to be multiplied; e.g., $-1.424(-1) = -1.424 \times 10^1$.

Z	n	l	Bound-state energy (keV)			Bound-state normalization		
			Present (shifted $1/N$)	Analytic Perturbation (Ref. 22)	Numerical	Present (shifted $1/N$)	Analytic perturbation (Ref. 22)	Numerical
13	1	0	$-1.488(0)^a$	$-1.484(0)$	$-1.488(0)$	$5.810(-2)$	$5.711(-2)$	$5.692(-2)$
36	1	0	$-1.424(1)$	$-1.424(1)$	$-1.424(1)$	$2.691(-1)$	$2.674(-1)$	$2.674(-1)$
	2	0	$-1.676(0)$	$-1.615(0)$	$-1.692(0)$	$9.910(-2)$	$8.933(-2)$	$8.618(-2)$
	2	1	$-1.567(0)$	$-1.504(0)$	$-1.566(0)$	$6.900(-3)$	$6.582(-3)$	$6.306(-3)$
79	1	0	$-7.491(1)$	$-7.495(1)$	$-7.495(1)$	$8.749(-1)$	$8.731(-1)$	$8.731(-1)$
	2	0	$-1.249(1)$	$-1.245(1)$	$-1.250(1)$	$3.162(-1)$	$2.999(-1)$	$2.982(-1)$
	2	1	$-1.225(1)$	$-1.221(1)$	$-1.225(1)$	$5.110(-2)$	$4.937(-2)$	$4.905(-2)$

VI. CONCLUDING REMARKS

The detailed analysis of the results in terms of various domains of parameters B and C of the Hellmann potential reveals a few important facts concerning the applicability of the shifted large- N expansion method. It appears that for certain regions of values of these parameters, convergence of the series expansion for the energy eigenvalues is in serious trouble for certain quantum states. This is an indication that the Taylor series expansion around the large- N minimum is not adequately reproducing the correct potential, i.e., six derivatives¹⁷ which go into the calculations of the first two nonleading terms $\gamma^{(1)}$ and $\gamma^{(2)}$ in Eq. (4) are not sufficient to describe a potential with too much structure. Once this happens, one should not trust results for values of n_r higher than the value at which the expansion ceases to converge. To circumvent the convergence problem, an elegant prescription based on large- N expansion in supersymmetric (SUSY) quantum mechanics has been proposed very recently by Imbo and Sukhatme.²⁹ It has been shown that faster convergence of the series expansion for the energy eigenvalues can be achieved using a supersymmetric partner potential of a given potential in $(N+2)$ -dimensional space. This approach has been shown to work for simple potentials only. Since SUSY partner potentials are narrower, it might well be that this technique with $N=5$ will have improved convergence for potentials which have trouble using $N=3$.

In a few circumstances, it is observed that even the location of the minimum of the effective potential cannot be ascertained and as a result the method seems to be inapplicable to these cases. This is clearly a limitation of the large- N method which has not been mentioned earlier.

However, this fact should not diminish the utility of this method as the problem arises only in case of superposition of two potentials of widely different ranges. So far it did not occur in the case of simple potentials. The method being algebraic in nature, leads to calculational simplicity to a great extent without sacrificing the accuracy of the predicted numerical results. In order to obtain similar accurate results by direct numerical integration of the Schrödinger equation, one needs to invoke quadrupole precision technique. Furthermore, one has to take precaution to avoid truncation error.

To conclude, we like to mention that the normalized wave functions obtained in the shifted large- N expansion technique may be quite useful in obtaining analytic expressions for several important quantities such as the oscillator strength^{27,30} and nonrelativistic single-electron $(nl;n'l')$ dipole transition matrix elements for screened central atomic potentials. Results for various bound-bound transitions from atomic inner shells have been obtained by Wang and Pratt³¹ using a nonrelativistic analytic perturbation theory. Study of these parameters from the standpoint of the present nonperturbative approach may have significance as far as the applications of the large- N technique to atomic physics is concerned. Work in this direction is in progress at present.

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