

$1/N$ expansions for central potentials revisited in the light of hypervirial and Hellmann-Feynman theorems and the principle of minimal sensitivity

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The hypervirial and Hellmann-Feynman theorems are used in the methods of $1/N$ expansion to construct Rayleigh-Schrödinger perturbation expansion for bound-state energy eigenvalues of spherical symmetric potentials. An iteration procedure of calculating correction terms of arbitrarily high orders is obtained for any kind of $1/N$ expansion. The recurrence formulas for three variants of the $1/N$ expansion are considered in this work, namely, the $1/n$ expansion and the shifted and unshifted $1/N$ expansions which are applied to the Gaussian and Patil potentials. As a result, their credibility could be reliably judged when account is taken of high-order terms of the eigenenergies. It is also found that there is a distinct advantage in using the shifted $1/N$ expansion over the two other versions. However, the shifted $1/N$ expansion diverges for s states and in certain cases is not applicable as far as complicated potentials are concerned. In an effort to solve these problems we have incorporated the principle of minimal sensitivity in the shifted $1/N$ expansion as a first step toward extending the scope of applicability of that technique, and then we have tested the obtained approach to some unfavorable cases of the Patil and Hellmann potentials. The agreement between our numerical calculations and reference data is quite satisfactory.

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I. INTRODUCTION

A large number of important physical problems in various branches of physics require using spherically symmetric potentials. To be specific, many theoretical calculations have been carried out by various workers with the Hellmann potential [1,2] to study the electron-core [3–5] or the electron-ion [6,7] interactions, atomic inner-shell ionization problems [8], alkali hydride molecules [9], other molecular [10], and solid-state physics [2,11–14] problems. The Hulthén potential [15], one of the most important short-range potentials, has been the subject matter of many studies in nuclear and particle physics [16–20], atomic physics [21,22], and solid-state physics [23]. The exponential cosine screened Coulomb potential and the celebrated Morse potential [24] have attracted considerable attention in solid-state physics [25] and chemical physics [26], respectively. The problem of accurately determining the energy eigenvalues and eigenfunctions for spherically symmetric potentials is, therefore, of considerable interest.

Since only a handful of potentials are solvable analytically, one has to resort to direct numerical techniques [22,25,27–30] or approximation methods. The most widely investigated schemes involve the Rayleigh-Schrödinger

(coupling constant) perturbation theory [23,31–39] and the Rayleigh-Ritz variational method [22,23,40–44] techniques. Accurate results for physical observables have been obtained from these two predominant perturbative and variational methods. Because of their successes in quantum mechanics, they have also been extensively developed for application to the more complicated problems of phase transitions and quantum field theory. However, one of the shortcomings of these approaches is that they involve, in general, quite elaborate algebraic manipulations and require considerable computational time and effort. Furthermore, their applications become restricted due to nonavailability of compact analytic expressions of energy levels and bound-state wave functions. The limitations of these methods (in particular the coupling constant perturbation theory) have become increasingly apparent, for instance for solving the problems of critical phenomena and quantum chronodynamics. Thus, the development of new computational methods (analytical approximation schemes) that provide at least the same order of accuracy has become an important enterprise. A large number of attempts in this direction have already been made in the past. The so-called $1/N$ expansions (with N referring to different objects in different theories) are one class of methods that have emerged in recent years as a very useful and powerful technique of attack in nonrelativistic quantum mechanics [45–58], multicomponent model problems in quantum field theory [59–62], solid-state physics [63,64], and statistical physics [65–69]. In quantum mechanics this approach, which was physically motivated for power-law potentials, has spawned a strong debate. For details see Ref. [70] in which the history of the development of $1/N$ expansions is reflected. It should be noted that although the large- N tech-

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nique is itself a kind of perturbation theory, it can be used for problems which do not manifestly involve a small coupling constant for performing the perturbation theory.

Because of the nonuniqueness of the passage to classical mechanics different versions of this method resulting from different choices of the expansion parameter $1/\Lambda$ have been suggested in the context of Schrödinger quantum mechanics. Three of them, namely $1/n$ expansion, the unshifted expansion, and the shifted $1/N$ expansion (denoted PINE, ULNE, SLNE, respectively), on which we focus our attention in this paper, have been worked out in detail for problems with spherical or axial symmetries (e.g., hydrogen atom in magnetic and electric fields): $\Lambda = 2n$, where n is principal quantum number [71–78]; $\Lambda = D + 2l$, D and l are the spatial dimensionality and the orbital quantum number, respectively [46]; $\Lambda = D + 2l - a$, where a is a suitable shift so as to restore exact results for the harmonic oscillator and Coulomb potentials in the leading-order of the expansion [59,79–82]. This simple modification gives rise to dramatic consequences. In particular it considerably improves the analytic simplicity and the convergence of the perturbation series for the energy eigenvalues in comparison with the unshifted $1/N$ expansion. The procedure of the above-mentioned versions consists of assuming $D \rightarrow \infty$ or $l \rightarrow \infty$ (for a fixed radial quantum number) which is equivalent in quantum mechanics to $\hbar \rightarrow 0$ or $M \rightarrow \infty$. Then incorporating the finite N corrections by taking into account the effects of quantum fluctuations and anharmonicity leads to a systematic expansion in powers of $1/\Lambda$. The physical values of D and l are substituted in the final formula. The Rayleigh-Schrödinger and the logarithmic perturbation schemes (referred to as RSPT and LPT, respectively) have been used for the calculation of these corrections. But their applications are restricted by serious difficulties. In the first case it is extremely laborious to advance beyond the first few terms. In this connection, it should be mentioned that calculating and rearranging the sixth order in power of $1/\Lambda$, we have obtained the next term for the energy spectrum to order $1/\Lambda^3$. It should be noted that the previous expression of the energy spectrum to order $1/\Lambda^2$, i.e., the first four terms of the expansion, was derived by Imbo Paanamenta, and Sukhatme [81]. We have proceeded efficiently by employing MATHEMATICA. However, the derivation is tediously long. The second case [34,46,72,82–85] gives energy corrections for the ground state but complications arise for excited states due to the separation of the zeros of the wave function in the form of an individual factor. The original study by Bender and Wu [87] on the anharmonic oscillator gave rise to an entire industry of large-order perturbation theory [72,88] which led, in recent years, to considerable progress in the calculations of higher perturbation orders in quantum mechanics. Some algebraic recursion methods, allowing one to evaluate high orders, were proposed in the past, each order getting progressively much more complicated [47,52,54,86]. In particular, Maluendes *et al.* reported a powerful approach in which the coefficients of the shifted $1/N$ expansion of arbitrarily high orders could be generated by means of the hypervirial (HV) and the Hellmann-Feynman (HF) theorems [89], thereby providing an excellent check for the convergence of the method. How-

ever, the previous authors did not give explicit expressions of their algorithm. We have completed that work on one hand in deriving in detail the recurrence relations for the quantities of interest and on the other hand by comparing these formulas with those obtained from the RSPT given in Appendix A. These formulas, which are given subsequently, are convenient for numerical calculations. Recently Stepanov and Tutik [90] have constructed a remarkable approach based on a semiclassical interpretation of the $1/N$ expansion. The proposed technique, which explicitly uses expansion in terms of Planck's constant \hbar , clarifies the complementarity of the $1/N$ approach and the WKB approximation and leads to simple recursion relations for the discrete energy spectrum through Zwaan-Dunham quantization conditions [91,92]. We have compared our analytical results with the later ones and found that they are identical. The RSPT formulas available (e.g., up to order $1/\Lambda^2$) are also reproduced. Thus it seems that the Rayleigh-Schrödinger series is generated by our set of recursion relations, which is also quite universal in the sense that the passage to any variant of the $1/N$ expansion is implemented in its formulation [90]. Our procedure, which is equivalent to the version of Stepanov and Tutik as far as the recurrence relations are concerned, provides a satisfactory and simple way of avoiding the cumbersome sums over intermediate unperturbed states, and involves only simple algebraic equations which are easier to handle.

The SLNE has already generated immense activities by proving its efficacy in quantum mechanics. The energy spectrum obtained by Imbo, Pagnamenta, and Sukhatme [81] has been discussed extensively and successfully applied to numerous simple and smooth potentials, e.g., Yukawa [54,55,81,93], rotating harmonic oscillator [52,94,95], exponential cosine screened Coulomb [96–98], Morse oscillator [99], Gaussian [55], power-law, and logarithmic [52,53,81,100]. Applications have been made to deal with laser-atom interactions [101]. It has also been shown [102] that the SLNE is equally effective in the scattering domain. The method is very useful in predicting low-energy scattering lengths and phase shifts by spherically symmetric short-range potentials. However, the approximation used by these authors is of too low order, so that the convergence of the method could not be reliably judged. Dutt, Mukherji, and Varshni [103] pointed out that although the accuracy of the results is in general extremely good for these smooth potentials, it is not *a priori* guaranteed that SLNE will work equally well for the superposition of simple potentials. They investigated the case of the Hellmann potential which is the superposition of two simple potentials of widely different ranges. The detailed analysis of the results reveals that for certain regions of values of parameters, not only is the convergence of the series expansion for the energy eigenvalues in serious trouble for certain quantum states, but the location of the minimum of the effective potential also cannot be ascertained. Tang and Chan [104] also observed that the expansion series is not valid in a certain region of the screening parameter for the Hulthén potential. Using the Coulomb potential perturbed by a polynomial in r , Roychoudhury, Varshni, and Sengupta [105] also concluded that for complicated potential shapes, SLNE can give poor or erroneous

results. Varshni [106] and Sever and Tezcan [58] obtained from ULNE and SLNE eigenenergies of an atomic potential which represents the interaction experienced by the second electron in a helium atom due to the nucleus and the first electron. That potential is of special interest being the prototype of more general potentials used in atomic problems. They found that the SLNE offers a large improvement over ULNE. However, they stressed that even with SLNE, caution is necessary since large errors are possible. On the other hand, these recurrence relations have been applied hitherto only to a narrow class of simple potentials [86,90]. To the best of our knowledge, such investigations with more complicated potentials have not been reported in the literature. Moreover, the SLNE and PINE have not been compared so far, even for simple potentials. In this paper we undertake this study to show which of these two approaches is more accurate for the bound states of central potentials. For this purpose we have extended the above-mentioned works to take into account large orders so as to assess their effects on the accuracy of the SLNE, PINE, ULNE energy spectra. As a result it is found that SLNE surpasses the PINE, but exhibits limitations concerning particularly the s states. Clearly in that case it leads to asymptotically divergent series. The choice of the physically motivated order-independent shift parameter is reexamined in the light of the numerical results. In an effort to improve the results obtained from the SLNE algorithm we have applied the prescriptions for the choice of an order-dependent shift parameter that has been claimed to be very powerful by Maluendes *et al.* [86]. Moreover, it is logical and meaningful to probe whether the range of applicability of the modified SLNE (denoted HVHP-PMS) may be widened by the incorporation of the principle of minimal sensitivity (PMS). More details concerning that principle can be seen in Ref. [107].

The organization of this paper is as follows. Section II describes the essentials of the HVHF method. We establish the hierarchy of equations for the corrections to the energy to all orders and underline their reduction to RSPT and Stepanov-Tutik general expressions included in appendixes A and B, respectively. The modified SLNE is presented. In Sec. III we carry out a detailed numerical study of the different theoretical schemes. The calculations of the first 11–21 partial sums of the perturbation series for the energy are displayed, using one simple and two more complicated potentials. Only the states which are unfavorable with the Imbo *et al.* formulas [81] are considered in the context of the HVHF-PMS. Finally, in Sec. IV we make some concluding remarks.

II. METHODS AND CALCULATIONS

The nonrelativistic formalism described in this section is a follow up to the work undertaken by Maluendes *et al.* [86]. For the sake of brevity, we only report the essential steps here. Unless otherwise indicated we use throughout this paper atomic units in which $\hbar = m = e = 1$. For simplicity of notation, quantum number indices will be suppressed.

The radial part of the time-independent Schrödinger equa-

tion for a central-field model in terms of the expansion parameter Λ is given by [90]

$$\left\{ -\frac{1}{2} \frac{d^2}{dr^2} + \frac{\Lambda^2}{8r^2} \left(1 + \frac{2A}{\Lambda} + \frac{4B}{\Lambda^2} \right) + V(r) \right\} \chi(r) = E\chi(r), \quad (1)$$

with

$$\frac{1}{4} \Lambda^2 + \frac{A}{2} \Lambda + B = l(l+1). \quad (2)$$

Because of the nonuniqueness of passage to classical mechanics, the specific variant of the $1/N$ expansion is determined by the choice of parameters Λ , A , and B . This enables one to describe within the same formalism any kind of the $1/N$ expansion. In this paper we are interested in three of them.

(i) $1/n$ expansion (PINE)

$$\Lambda = 2n, \quad A = -(2n_r + 1), \quad B = n_r(n_r + 1), \\ n = n_r + l + 1, \quad (3)$$

where n_r is the radial quantum number.

(ii) Shifted $1/N$ expansion (SLNE)

$$\Lambda = 2l + D - a, \quad A = 1 - D + a, \quad B = \frac{(D-a)(D-a-2)}{4}, \quad (4)$$

a is the so-called shift parameter.

(iii) The unshifted $1/N$ expansion can be deduced from the SLNE delineated above in setting $a = 0$. The leading contribution to the energy comes from the effective potential in the limit of large Λ

$$V_{\text{eff}}^{\infty}(r) \equiv V_{\text{eff}}(r) = V(r) + \frac{\Lambda^2}{8r^2}. \quad (5)$$

One assumes $V(r)$ to be sufficiently well behaved so that $V_{\text{eff}}(r)$ has a minimum at r_0 and there are well-defined bound states. Once r_0 is determined from the equation

$$\Lambda^2 - 4r_0^3 V_0' = 0, \quad V_0 = V(r_0), \quad V_0' = \frac{d}{dr_0} V_0, \quad (6)$$

the leading term is given by

$$E_0 = V_{\text{eff}}(r_0) = V_0 + \frac{\Lambda^2}{8r_0^2}. \quad (7)$$

Quantum fluctuations around the minimum r_0 are defined by

$$x = \frac{1}{g} (r/r_0 - 1), \quad g = 1/\Lambda^{1/2}. \quad (8)$$

Then on expanding around $x = 0$ and making use of Eq. (6) for r , Eq. (1) becomes

$$\left\{ -\frac{d^2}{dx^2} + \sum_{i=0}^{\infty} (\alpha_i g^i x^{i+2} + \beta_i g^i x^i + \xi_i g^{i+2} x^i) \right\} \chi(x) = \tilde{E} \chi(x), \quad (9)$$

where we have introduced the following notations:

$$\tilde{E} = 2r_0^2 g^2 (E - E_0), \quad \alpha_i = (-1)^i \frac{i+3}{4} + \frac{r_0^{i+1}}{2(i+2)!} \frac{V_0^{(i+2)}}{V_0'}, \quad (10)$$

$$\beta_i = (-1)^i \frac{i+1}{2} A, \quad \xi_i = (-1)^i (i+1) B. \quad (11)$$

It should be noted that there are some misprints in the corresponding formula in Ref. [86].

Following the prescription of Maluendes *et al.*, a dummy perturbation parameter λ is introduced in Eq. (9) as shown below and is set equal to unity at the end of the calculation

$$H \chi(x) = \tilde{E} \chi(x), \quad H = -\frac{d^2}{dx^2} + U, \quad (12)$$

where

$$U = \sum_{i=0}^{\infty} \alpha_i g^i \lambda^i x^{i+2} + \beta_i g^i \lambda^i x^i + \xi_i g^{i+2} \lambda^{i+2} x^i. \quad (13)$$

The use of quantum-mechanical HV and HF theorems to generate perturbation expansions is well known [36,39,108–116]. It should be noted that McRae and Vrscaj [117] have exploited the classical versions of these useful quantum-mechanical theorems to construct a classical perturbation theory without Fourier series for separable classical Hamiltonians. For a comprehensive review of the above theorems and their applications in both classical and quantum mechanics, see Ref. [118]. The HV and HF theorems provide the relationships between \tilde{E} and the various expectation values of $\langle x^m \rangle$ through the following equations:

$$\frac{1}{2} m(m-1)(m-2) \langle x^{m-3} \rangle + 2m \tilde{E} \langle x^{m-1} \rangle - 2m \langle x^{m-1} U \rangle - \langle x^m U' \rangle = 0, \quad (14)$$

$$\frac{\partial \tilde{E}}{\partial \lambda} = \left\langle \frac{\partial U}{\partial \lambda} \right\rangle. \quad (15)$$

The essence of the HVHF perturbative method is to assume that the energy and the expectation values of position coordinates can be expanded in power series of the perturbation parameter λ as

$$\tilde{E} = \sum_{k=0}^{\infty} \tilde{E}^{(k)} \lambda^k, \quad (16)$$

$$\langle x^m \rangle = \sum_{k=0}^{\infty} x_m^{(k)} \lambda^k, \quad (17)$$

whose coefficients can be calculated recursively. They carry significant information about the behavior of bound-state energies. The large-order behavior as well as the summability of these series will be of interest. It is clear from the foregoing that the starting point is the normalization condition and the harmonic-oscillator eigenvalues which write

$$x_0^{(0)} = 1, \quad x_0^{(k)} = 0, \quad k \geq 1, \quad (18)$$

$$\tilde{E}^{(0)} = (1 + 2n_r) \omega + \beta_0, \quad (19)$$

$\omega = \alpha_0^{1/2}$ is the frequency of small vibrations about the equilibrium orbit. By equating like powers of λ on both sides of Eqs. (14) and (15) after substitution of the expansions (16) and (17), we readily find a set of coupled relations involving the terms $\tilde{E}^{(k)}$ and $x_m^{(k)}$

$$\begin{aligned} & \frac{1}{2} m(m-1)(m-2) x_{m-3}^{(k)} + 2m \sum_{i=0}^k \tilde{E}^{(i)} x_{m-1}^{(k-i)} \\ & - \sum_{i=0}^k [(2m+i+2) \alpha_i g^i x_{i+m+1}^{(k-i)} + (2m+i) \beta_i g^i x_{m-1}^{(k-i)}] \\ & - \sum_{i=0}^k (2m+i) \xi_i g^{i+2} x_{i+m-1}^{(k-i)} = 0, \end{aligned} \quad (20)$$

$$\begin{aligned} (k+1) \tilde{E}^{(k+1)} &= \sum_{i=0}^k (i+1) [\alpha_{i+1} x_{i+3}^{(k-i)} + \beta_{i+1} x_{i+1}^{(k-i)}] g^{i+1} \\ & + \theta(k-1) \sum_{i=0}^{k-1} (i+2) \xi_i g^{i+2} x_i^{(k-i-1)}, \end{aligned} \quad (21)$$

where $\theta(x)$ is the Heaviside function.

To calculate explicitly the perturbed energies in a hierarchical manner, we proceed by giving to k various integer values starting with $k=0$. For example, we get $[k=0,1]$ in Eq. (20) the following expressions by setting

(i) $k=0$,

$$x_0^{(0)} = 1, \quad x_1^{(0)} = 0, \quad x_2^{(0)} = 2\bar{E}^{(0)}, \quad x_3^{(0)} = 0, \quad (22a)$$

$$\begin{aligned} x_m^{(0)} &= \frac{1}{2m \alpha_0} \left[\frac{1}{2} (m-1)(m-2)(m-3) x_{m-2}^{(0)} \right. \\ & \left. + 2(m-1) \bar{E}^{(0)} x_{m-2}^{(0)} \right], \end{aligned}$$

$$\bar{E}^{(0)} = \tilde{E}^{(0)} - \beta_0, \quad m \geq 4. \quad (22b)$$

(ii) $k=1$

$$x_0^{(1)} = 0, \quad x_1^{(1)} = -2g(\beta_1 + 3\alpha_1 x_2^{(0)}), \quad x_2^{(1)} = 0, \quad (23a)$$

$$x_3^{(1)} = \frac{1}{6\alpha_0} [4\bar{E}_0 x_1^{(1)} - 5\beta_1 g x_2^{(0)} - 7\alpha_1 g x_4^{(0)}], \quad (23b)$$

$$\begin{aligned}
x_m^{(1)} = & \frac{1}{4m\alpha_0} [(m-1)(m-2)(m-3)x_{m-4}^{(1)} \\
& + 4(m-1)\bar{E}^{(0)}x_{m-2}^{(1)} - 2(2m+1)\alpha_1 g x_{m+1}^{(0)} \\
& - 2(2m-1)\beta_1 g x_{m-1}^{(0)}], \quad m \geq 4. \quad (23c)
\end{aligned}$$

For $k \geq 2$ a straightforward algebraic manipulation shows that

$$x_0^{(k)} = 0,$$

$$\begin{aligned}
x_1^{(k)} = & -\frac{1}{2\alpha_0} \left\{ \sum_{i=1}^k (i+2) [\alpha_i x_{i+1}^{(k-i)} + i\beta_i x_{i-1}^{(k-1)}] g^i \right. \\
& \left. + \theta(k-3) \sum_{i=0}^{k-2} i \xi_i g^{i+2} x_{i-1}^{(k-i-2)} \right\}, \quad (24a)
\end{aligned}$$

$$\begin{aligned}
x_2^{(k)} = & \frac{1}{4\alpha_0} \left\{ 2\bar{E}^{(k)} - \sum_{i=1}^k (i+4) [\alpha_i x_{i+2}^{(k-i)} + (i+2)\beta_i x_i^{(k-i)}] g^i \right. \\
& \left. - \sum_{i=0}^{k-2} (i+2) \xi_i g^{i+2} x_i^{(k-i-2)} \right\}, \quad (24b)
\end{aligned}$$

$$\begin{aligned}
x_3^{(k)} = & \frac{1}{6\alpha_0} \left\{ \sum_{i=1}^k [4\bar{E}^{(i)} x_1^{(k-i)} - (i+4)\beta_i g^i x_{i+1}^{(k-i)}] \right. \\
& \left. - \sum_{i=1}^k (i+6)\alpha_i g^i x_{i+3}^{(k-i)} - \sum_{i=0}^{k-2} (i+4)\xi_i g^{i+2} x_{i+1}^{(k-i-2)} \right\}, \quad (24c)
\end{aligned}$$

$$\begin{aligned}
x_m^{(k)} = & \frac{1}{2m\alpha_0} \left\{ \frac{1}{2}(m-1)(m-2)(m-3)x_{m-4}^{(k)} \right. \\
& + \sum_{i=0}^k [2(m-1)\bar{E}^{(i)} x_{m-2}^{(k-i)} - (2m+i-2)\beta_i g^i x_{i+m-2}^{(k-i)}] \\
& - \sum_{i=1}^k (2m+i)\alpha_i g^i x_{i+m}^{(k-i)} - \sum_{i=0}^{k-2} (2m+i-2) \\
& \left. \times \xi_i g^{i+2} x_{i+m-2}^{(k-i-2)} \right\}, \quad m \geq 4. \quad (24d)
\end{aligned}$$

The HF relation provides the following connection between the coefficients for the energy and expectation values,

$$\begin{aligned}
\bar{E}^{(k)} = & \frac{1}{k} \left\{ \sum_{i=0}^{k-1} (i+1) [\alpha_{i+1} x_{i+3}^{(k-i-1)} + \beta_{i+1} x_{i+1}^{(k-i-1)}] g^{i+1} \right. \\
& \left. + \theta(k-2) \sum_{i=0}^{k-2} (i+2) \xi_i g^{i+2} x_i^{(k-i-2)} \right\}, \quad k \geq 1. \quad (25)
\end{aligned}$$

Thus we can calculate the k th perturbed energy $\bar{E}^{(k)}$ from the knowledge of $x_m^{(j)}$ and $\bar{E}^{(j)}$ with $0 \leq j \leq k-1$, $0 \leq m \leq k-j+2$. From Eqs. (22)–(25) it is obvious that in general

$$x_m^{(j)} = 0, \quad m \neq 0, \quad (26)$$

if the parities of j and m are different. As a result $\bar{E}^{(1)}, \bar{E}^{(3)}, \bar{E}^{(5)}, \dots$ vanish, that is,

$$\bar{E}^{(k)} = 0, \quad k \text{ odd}. \quad (27)$$

Finally we obtain for the bound-state energy

$$E = \sum_{k=0}^{\infty} E_k, \quad (28a)$$

with

$$E_k = \frac{1}{2r_0^2 g^2} \bar{E}^{(2k-2)}, \quad k \geq 1. \quad (28b)$$

It is convenient to note that the calculation of $\bar{E}^{(2k-2)}$ involves the derivatives $V_0^{(i)}$, $1 \leq i \leq 2k$ which is also the case for the term E_k in the semiclassical formalism of Stepanov and Tutik. The algorithm for calculation of any order of perturbed energy is thus fully described. Making use of MATHEMATICA, one can check without any difficulty that the different terms E_k are exactly those derived by Stepanov and Tutik (see Appendix B). The expressions derived by Mlodinow and Shatz [100] for the ground and first excited states are also reproduced. Again with the help of a system with symbolic manipulation capabilities, it is easy to see that Eq. (28) up to fourth order coincide with the analytic results \bar{E}_k of the RSPT listed in Appendix A (i.e., $E_k = \bar{E}_k$). Therefore the HVHF perturbation method generates the Rayleigh-Schrödinger perturbation expansions. This procedure thus eliminates the usual tedious calculations of sums over intermediate states products of matrix elements which arise in the n th order of RSPT and makes it a simple matter to calculate high orders for energy levels. It is noteworthy that our scheme of calculating is quite simple and straightforward in comparison with the \hbar -expansion method.

The large- N expansion method gives rise to one of the most elegant analytic approximations for obtaining eigenvalues. Unfortunately, in certain cases (e.g., ULNE) the large- N is asymptotically divergent, particularly for s states. To overcome this difficulty, Sukhatme and Imbo proposed the SLNE in which a proper order-independent shift is considered. This extra degree of freedom is chosen so as to make the first-order contribution

$$E_1 = \frac{1}{2r_0^2 g^2} \bar{E}^{(0)} = \frac{\Lambda}{2r_0^2} [(1+2n_r)\omega + \beta_0] \quad (29)$$

in Eq. (28a) vanish, which means

$$a = 2 - 2(1+2n_r)\omega. \quad (30)$$

This simple choice yields the exact eigenvalues for the harmonic oscillator and Coulomb potentials in the leading term E_0 . We have checked numerically and with the aid of MATHEMATICA that higher-order corrections E_i ($i \geq 2$) vanish identically in these two cases.

Maluendes *et al.* showed that SLNE could be improved provided the shift value is properly set. They suggested an alternative prescription for the choice of a , which in their method becomes order dependent. In Sukhatme and Imbo's approach, one sets $E_1(a)=0$ in the infinite series (28a) which can be evaluated to arbitrary order, using our set of recurrence relations, whereas Maluendes *et al.* have chosen a to be a root of

$$E_M(a)=0, \quad (31)$$

and the eigenvalues are approximated by sequences of partial sums

$$E(a)=\sum_{i=0}^M E_i(a)=\sum_{i=0}^{M-1} E_i(a). \quad (32)$$

Since the energy is independent of the shift, the appropriated $a=a_M$ which depends on M leads to the smallest value of $|\partial E/\partial a|$. We omit the technical details of the calculations referring the reader to Ref. [121]. This criterion is an example of the principle of minimal sensitivity discussed by Stevenson [107]. In practice we proceed in determining r_0 from Eq. (31) in which the following equations are substituted:

$$\Lambda=2\sqrt{r_0^3 V'_0}, \quad a=3+2l-\Lambda. \quad (33)$$

Clearly, Eq. (31) becomes

$$E_M(r_0)=0. \quad (34)$$

We have applied the methods described above to four physically interesting potentials that have been investigated by a number of workers. Among these are one simple potential and three others that are a superposition of simple potentials.

(i) The Gaussian potential [55]

$$V(r)=-Ae^{-r^2}. \quad (35)$$

(ii) The Patil potential [119]

$$V(r)=V^{cop}(r)+V^{exc}(r)+V^{pol}(r), \quad (36)$$

in which $V^{cop}(r)$ is the Coulomb-penetration potential

$$V^{cop}(r)=\frac{2-Z}{r}-\left(\frac{2}{r}+\beta\right)e^{-\beta r}, \quad (37)$$

$V^{exc}(r)$ is the exchange potential

$$V_{l=0}^{exc}(r)=\beta\left\{\left[\frac{1}{2}-\frac{9}{2}\beta r-3\beta^2 r^2+2Z(\beta^2 r^2-\beta r-1)\right]e^{-\beta r}+\left(\frac{5}{2}+\frac{3}{2}\beta r\right)e^{-\beta r}\right\}, \quad (38)$$

$$V_{l \neq 0}^{exc}(r)=\frac{2\beta}{(2l+1)(l+2)}\times\left(2l^2+11l+\beta r\frac{4l^2+20l+27}{2l+3}\right)e^{-\beta r}, \quad (39)$$

$V^{pol}(r)$ is the polarizability potential

$$V^{pol}(r)=\frac{\tilde{\alpha}}{2}\left\{\frac{1}{r^4}\left[1-e^{-\beta r}\sum_{n=0}^3\frac{(\beta r)^n}{n!}\right]-\frac{\beta^4}{24}(0.8e^{-1.3\beta r}+0.2e^{-4.8\beta r})\right\}, \quad (40)$$

$\beta=2(Z-5/16)$, Z is the nuclear charge, and $\tilde{\alpha}$ the dipolar polarizability. The leading Coulomb penetration part of this potential is of the same type as the interaction used by Sever and Tezcan [58] and Varshni [106]. It consists of a Coulomb term, a screened Coulomb term, and an exponential term.

(iii) The Coulomb perturbed by a polynomial in r [120]

$$V(r)=\frac{\alpha}{r}+\sum_{i=1}^4 p_i r^i. \quad (41)$$

(iv) The Hellmann potential [103]

$$V(r)=-\frac{A}{r}+\frac{B}{r}e^{-Cr}. \quad (42)$$

III. NUMERICAL RESULTS AND DISCUSSION

As discussed in the Introduction, one of the prime motivations of the present study is to explore the credibility of the SLNE, PINE, and ULNE versions when account is taken of high orders of perturbation theory in the calculation of the energy eigenvalues. The fact that we are able to evaluate them using the recurrence relations presented above provides us with the possibility to examine the applicability of these schemes for a wide range of quantum numbers n and l . For the sake of discussing this important point we consider by way of examples two simple and three more complicated potentials defined in Eqs. (36)–(43). For any given choice of n and l , Eq. (6) becomes a transcendental equation which can, in principle, be easily solved numerically [121] to obtain r_0 . We have searched with great care this most crucial parameter for the different energy levels of the five potentials investigated in this paper. It has turned out that in several circumstances Eq. (6) leads to more than one minimum. In Table I are displayed several such cases concerning the Coulomb potential perturbed by a polynomial in r for which we have found two roots. Curiously the energy eigenvalues given by Roychoudhury *et al.* [105] (see column 9, first entry) correspond to the smallest value of the two roots and are seriously in error. We suspect that this happened because these authors did not advance beyond the first root encountered in the search of the minima of the large- N effective potential. It is clear that unless great care is exercised, the search of r_0 can lead to erroneous conclusions. It is impor-

TABLE I. Minima of the effective potential (column 8) and corresponding energy eigenvalues (column 9) calculated from the shifted $1/N$ expansion [81]. Data sets for the Coulomb perturbed by a polynomial in r are listed in columns 3–7. In the last column are given the exact supersymmetric values. The asterisks denote the values of roots used by Roychoudhury *et al.* (Ref. [119]).

State	α	p_1	p_2	p_3	p_4	r_0	E^a	Ref. data
1s	-1	-2.846 05	2.816 23	-1.0	0.1	1.374 84*	-121.807 18	-4.993 42
						5.004 47	-5.005 74	
1s	-5	-9.170 61	4.081 14	-1.0	0.1	0.392 00*	-23.443 23	-10.993 42
						3.583 54	-10.717 33	
2p	-1	-4.743 42	10.158 11	-2.0	0.1	1.026 82*	8.514 29	-9.096 09
						10.092 77	-28.522 68	
3d	-1	-6.008 33	44.205 41	-4.2	0.1	0.758 45*	38.860 42	-73.076 39
						21.021 62	-73.075 65	
4f	-1	-7.273 24	129.679 06	-7.2	0.1	0.641 69*	94.294 26	-148.010 22
						36.007 36	-148.006 13	
2p	-1	-15.000 00	100.500 00	-20.0	1.0	0.536 71*	37.345 10	-90.062 50
						10.029 92	-90.060 78	
3d	-1	-19.000 00	441.333 33	-42.0	1.0	0.418 03*	133.516 83	-231.027 78
						21.006 83	-231.035 80	
4f	-1	-23.000 00	1296.250 00	-72.0	1.0	0.357 56*	309.515 96	-468.015 62
						36.002 32	-468.015 44	

$$^a E = E_0 + E_2 + E_3 (E_1 = 0).$$

tant to mention at this point that the three schemes SLNE, PINE, and ULNE in their formulations do not give a criterion for choosing the appropriate root among the both in each case. This problem has not been pointed out so far owing to the fact that the above situation did not occur in the previous works reported. It should be noted that for each energy level presented in Tables II–VII we have searched for a possible second root r_0 value, but the result was negative. Once this most crucial parameter is determined, the task of obtaining energies becomes fairly straightforward.

We compare in Tables II–VII our predicted values calculated from the SLNE, PINE, and ULNE schemes to those obtained from high-precision numerical techniques by Crandall [30] and Lindgård and Nielsen [28,29] concerning, respectively, the Gaussian and Patil potentials. The progression of the energy series is shown in the tables so as to see the convergence of the three $1/N$ expansion series. In order to illustrate how closely our results agree with the reference data (RD) and be more informative, we have plotted the percent errors ($|E_{RD} - E|/|E_{RD}|$) of our computations in the three schemes in Figs. 1–7. The following clearly arises from these figures. It is obvious from Fig. 1 that SLNE results are always superior to those of PINE (i.e., SLNE > PINE) and these latter are substantially better than the ULNE corresponding ones (PINE > ULNE). One observes that SLNE and PINE converge rapidly and the degree of agreement with RD is striking. In the case of the Gaussian potential the first four terms of the eigenenergies [i.e., the limit of previous work $N=4$ (denoted LPW)] are not sufficient to guarantee the convergence of the SLNE and PINE expansion series. For the $6p$ and $8d$ states it seems that there exists an overlap region ($N > 21$) in which the two methods agree with each other quite closely. For the $4s$ state, they are stabilized in the domain $N \geq 15$. The percent errors in the

unshifted $1/N$ expansion start decreasing but then increase rather rapidly especially for the $4s$ state. The successive contributions from the perturbation series become substantial and the perturbation expansion breaks down. Figure 2 shows that SLNE > ULNE > PINE for the Patil potential. However, PINE and ULNE are not at all workable. The energy values have very large errors and are of the wrong sign for some s and p states (see, e.g., Tables VI and VII). The correction terms dominate over the leading term E_0 . SLNE yields good results only for the $7f$ state for which the percent error values become stabilized for $N \geq 15$ within 0.002–0.006 %.

Now we examine the states in detail for three specific cases.

(a) First of all we consider the case for which the principal quantum number is fixed, i.e., $n=8$ for the Gaussian potential and $n=6$ for the Patil potential. Figures 3 and 4 clearly depict the features and tendencies mentioned above, respectively, for these two potentials. A few other relevant features become apparent. Figure 3 shows that for SLNE and PINE the limit of previous works $N=4$ is insufficient for low values of l . Higher-order terms are needed to get better accuracy. In this connection Chatterjee [55] underlined that when only the terms up to $N=4$ are kept in the energy series, the shifted $1/N$ expansion predicts wrongly that the $8s$ state for instance is a continuum state. As shown in Table II, if higher-order terms are included in the calculation the SLNE treatment yields that the $8s$ state close to the continuum is a bound state and the numerical result obtained is good. Hence to improve the situation for the bound states lying close to the continuum one should include higher-order terms. Thus, caution is necessary in using the formalism based on a four-term recurrence relation [81]. These two procedures seem to converge whatever l . As expected for SLNE and ULNE, for a given principal quantum number n , the results improve as l

TABLE II. Predicted partial sums of energy eigenvalues in atomic units (Gaussian potential) of the $4s$ to $8s$ states for the $l=0$ fixed value. First entry, SLNE; second entry, P1NE; third entry, ULNE. In the last column are given the values obtained by Crandall (Ref. [30]). The numbers in square brackets indicate the powers of 10 by which the values are to be multiplied, e.g., $7.2689[+1]=7.2689\times 10^{+1}$.

State	N^a										Ref. data	
	3	5	7	9	11	13	15	17	19	21		
$4s$	$-7.2689[+1]$	$-7.2689[+1]$	$-7.2689[+1]$	$-7.2689[+1]$	$-7.2689[+1]$	$-7.2689[+1]$	$-7.2689[+1]$	$-7.2689[+1]$	$-7.2689[+1]$	$-7.2689[+1]$	$-7.2689[+1]$	$-7.2689[+1]$
	$-7.2689[+1]$	$-7.2689[+1]$	$-7.2689[+1]$	$-7.2689[+1]$	$-7.2689[+1]$	$-7.2689[+1]$	$-7.2689[+1]$	$-7.2689[+1]$	$-7.2689[+1]$	$-7.2689[+1]$	$-7.2689[+1]$	
	$7.1824[+1]$	$-7.2657[+1]$	$-7.2687[+1]$	$-7.2689[+1]$	$-7.2689[+1]$	$-7.2689[+1]$	$-7.2689[+1]$	$-7.2689[+1]$	$-7.3696[+1]$	$-7.3171[+1]$	$-1.0180[+2]$	
$5s$	$-4.6985[+1]$	$-4.7228[+1]$	$-4.7229[+1]$	$-4.7229[+1]$	$-4.7229[+1]$	$-4.7229[+1]$	$-4.7229[+1]$	$-4.7229[+1]$	$-4.7229[+1]$	$-4.7229[+1]$	$-4.7229[+1]$	$-4.7229[+1]$
	$-4.6731[+1]$	$-4.7206[+1]$	$-4.7227[+1]$	$-4.7229[+1]$	$-4.7229[+1]$	$-4.7229[+1]$	$-4.7229[+1]$	$-4.7229[+1]$	$-4.7229[+1]$	$-4.7229[+1]$	$-4.7229[+1]$	
	$-4.5005[+1]$	$-4.7073[+1]$	$-4.7209[+1]$	$-4.7226[+1]$	$-4.7228[+1]$	$-4.7229[+1]$	$-4.7229[+1]$	$-4.7229[+1]$	$-4.7327[+1]$	$-5.6679[+1]$	$-8.5780[+2]$	
$6s$	$-2.5503[+1]$	$-2.6067[+1]$	$-2.6072[+1]$	$-2.6072[+1]$	$-2.6072[+1]$	$-2.6072[+1]$	$-2.6072[+1]$	$-2.6072[+1]$	$-2.6072[+1]$	$-2.6072[+1]$	$-2.6072[+1]$	$-2.6072[+1]$
	$-2.4905[+1]$	$-2.5977[+1]$	$-2.6059[+1]$	$-2.6070[+1]$	$-2.6071[+1]$	$-2.6072[+1]$	$-2.6072[+1]$	$-2.6072[+1]$	$-2.6072[+1]$	$-2.6072[+1]$	$-2.6072[+1]$	
	$-2.1297[+1]$	$-2.5519[+1]$	$-2.5960[+1]$	$-2.6043[+1]$	$-2.6064[+1]$	$-2.6069[+1]$	$-2.6072[+1]$	$-2.7117[+1]$	$-1.4550[+2]$	$-1.2070[+4]$	$-1.2070[+4]$	
$7s$	$-8.7740[+0]$	$-9.9274[0]$	$-9.9726[+0]$	$-9.9805[+0]$	$-9.9825[+0]$	$-9.9830[+0]$	$-9.9831[0]$	$-9.9831[0]$	$-9.9831[+0]$	$-9.9831[+0]$	$-9.9831[+0]$	$-9.9832[+0]$
	$-7.3887[+0]$	$-9.6134[0]$	$-9.8966[+0]$	$-9.9583[+0]$	$-9.9751[+0]$	$-9.9804[+0]$	$-9.9821[0]$	$-9.9828[+0]$	$-9.9830[+0]$	$-9.9831[+0]$	$-9.9831[+0]$	
	$-7.0060[-1]$	$-8.3064[0]$	$-9.4679[+0]$	$-9.7882[+0]$	$-9.9003[+0]$	$-9.9441[+0]$	$-9.9625[0]$	$-1.8415[+1]$	$-1.2226[+3]$	$-1.8723[+5]$	$-1.8723[+5]$	
$8s$	$2.1538[+0]$	$-1.7280[-1]$	$-4.9010[-1]$	$-5.9497[-1]$	$-6.1987[-1]$	$-6.5410[-1]$	$-6.5497[-1]$	$-6.6768[-1]$	$-6.7014[-1]$	$-6.7130[-1]$	$-6.7130[-1]$	$-6.7365[-1]$
	$5.3190[+0]$	$9.0007[-1]$	$-2.6478[-2]$	$-3.5440[-1]$	$-4.9951[-1]$	$-5.7251[-1]$	$-6.1241[-1]$	$-6.3547[-1]$	$-6.4935[-1]$	$-6.5794[-1]$	$-6.5794[-1]$	
	$1.6785[+1]$	$4.2152[+0]$	$1.5655[+0]$	$5.6491[-1]$	$0.8596[+0]$	$-1.7082[-1]$	$-0.2295[+0]$	$-4.9132[+1]$	$-1.0311[+4]$	$-1.8431[+6]$	$-1.8431[+6]$	

^a $E = \sum_{i=0}^N E_i$.

TABLE III. Predicted partial sums of energy eigenvalues in atomic units (Gaussian potential) of the $4s$ to $8g$ states for the $n_r=3$ fixed value. First entry, SLNE; second entry, P1NE; third entry, ULNE. In the last column are given the values obtained by Crandall (Ref. [30]). The numbers in square brackets indicate the powers of 10 by which the values are to be multiplied.

State	N^a										Ref. data	
	3	5	7	9	11	13	15	17	19	21		
$4s$	-7.2689[+1]	-7.2689[+1]	-7.2689[+1]	-7.2689[+1]	-7.2689[+1]	-7.2689[+1]	-7.2689[+1]	-7.2689[+1]	-7.2689[+1]	-7.2689[+1]	-7.2689[+1]	-7.2689[+1]
	-7.2689[+1]	-7.2689[+1]	-7.2689[+1]	-7.2689[+1]	-7.2689[+1]	-7.2689[+1]	-7.2689[+1]	-7.2689[+1]	-7.2689[+1]	-7.2689[+1]	-7.2689[+1]	
	7.1824[+1]	-7.2657[+1]	-7.2687[+1]	-7.2689[+1]	-7.2689[+1]	-7.2689[+1]	-7.2689[+1]	-7.2689[+1]	-7.3696[+1]	-7.3171[+1]	-1.0180[+2]	
$5p$	-5.9087[+1]	-5.9192[+1]	-5.9192[+1]	-5.9192[+1]	-5.9192[+1]	-5.9192[+1]	-5.9192[+1]	-5.9192[+1]	-5.9192[+1]	-5.9192[+1]	-5.9192[+1]	-5.9192[+1]
	-5.8970[+1]	-5.9186[+1]	-5.9192[+1]	-5.9192[+1]	-5.9192[+1]	-5.9192[+1]	-5.9192[+1]	-5.9192[+1]	-5.9192[+1]	-5.9192[+1]	-5.9192[+1]	
	-5.8208[+1]	-5.9149[+1]	-5.9187[+1]	-5.9192[+1]	-5.9192[+1]	-5.9192[+1]	-5.9192[+1]	-5.9192[+1]	-5.9192[+1]	-5.9192[+1]	-5.9214[+1]	
$6d$	-4.6315[+1]	-4.6439[+1]	-4.6439[+1]	-4.6439[+1]	-4.6439[+1]	-4.6439[+1]	-4.6439[+1]	-4.6439[+1]	-4.6439[+1]	-4.6439[+1]	-4.6439[+1]	-4.6439[+1]
	-4.6175[+1]	-4.6431[+1]	-4.6439[+1]	-4.6439[+1]	-4.6439[+1]	-4.6439[+1]	-4.6439[+1]	-4.6439[+1]	-4.6439[+1]	-4.6439[+1]	-4.6439[+1]	
	-4.5306[+1]	-4.6381[+1]	-4.6434[+1]	-4.6438[+1]	-4.6439[+1]	-4.6439[+1]	-4.6439[+1]	-4.6439[+1]	-4.6439[+1]	-4.6439[+1]	-4.6439[+1]	
$7f$	-3.4349[+1]	-3.4491[+1]	-3.4492[+1]	-3.4492[+1]	-3.4492[+1]	-3.4492[+1]	-3.4492[+1]	-3.4492[+1]	-3.4492[+1]	-3.4492[+1]	-3.4492[+1]	-3.4492[+1]
	-3.4171[+1]	-3.4480[+1]	-3.4491[+1]	-3.4492[+1]	-3.4492[+1]	-3.4492[+1]	-3.4492[+1]	-3.4492[+1]	-3.4492[+1]	-3.4492[+1]	-3.4492[+1]	
	-3.3163[+1]	-3.4409[+1]	-3.4482[+1]	-3.4490[+1]	-3.4492[+1]	-3.4492[+1]	-3.4492[+1]	-3.4492[+1]	-3.4492[+1]	-3.4492[+1]	-3.4492[+1]	
$8g$	-2.3274[+1]	-2.3433[+1]	-2.3434[+1]	-2.3434[+1]	-2.3434[+1]	-2.3434[+1]	-2.3434[+1]	-2.3434[+1]	-2.3434[+1]	-2.3434[+1]	-2.3434[+1]	-2.3434[+1]
	-2.3035[+1]	-2.3417[+1]	-2.3433[+1]	-2.3434[+1]	-2.3434[+1]	-2.3434[+1]	-2.3434[+1]	-2.3434[+1]	-2.3434[+1]	-2.3434[+1]	-2.3434[+1]	
	-2.1840[+1]	-2.3310[+1]	-2.3417[+1]	-2.3431[+1]	-2.3434[+1]	-2.3434[+1]	-2.3434[+1]	-2.3434[+1]	-2.3434[+1]	-2.3434[+1]	-2.3434[+1]	

^a $E = \sum_{i=0}^N E_i$.

TABLE IV. Predicted partial sums of energy eigenvalues in atomic units (Gaussian potential) of the $8s$ to $8f$ states for the $n=8$ fixed values. First entry, SLNE; second entry, P1NE; third entry, ULNE. In the last column are given the values obtained by Crandall (Ref. [30]). The numbers in square brackets indicate the powers of 10 by which the values are to be multiplied.

State	N^a										Ref. data
	3	5	7	9	11	13	15	17	19	21	
$8s$	2.1538[+0]	-1.7280[-1]	-4.9010[-1]	-5.9497[-1]	-6.1987[-1]	-6.5410[-1]	-6.5497[-1]	-6.6768[-1]	-6.7014[-1]	-6.7130[-1]	
	5.3190[+0]	9.0007[-1]	-2.6478[-2]	-3.5440[-1]	-4.9951[-1]	-5.7251[-1]	-6.1241[-1]	-6.3547[-1]	-6.4935[-1]	-6.5794[-1]	-6.7365[-1]
	1.6785[+1]	4.2152[+0]	1.5655[+0]	5.6491[-1]	0.8596[+0]	-1.7082[-1]	-0.2295[+0]	-4.9132[+1]	-1.0311[+4]	-1.8431[+6]	
	-2.5733[+0]	-3.9116[+0]	-4.0108[+0]	-4.0329[+0]	-4.0389[+0]	-4.0407[+0]	-4.0413[+0]	-4.0415[+0]	-4.0416[+0]	-4.0416[+0]	
$8p$	-6.6617[-1]	-3.4356[+0]	-3.8664[+0]	-3.9801[+0]	-4.0176[+0]	-4.0316[+0]	-4.0373[+0]	-4.0397[+0]	-4.0408[+0]	-4.0412[+0]	-4.0417[+0]
	7.0523[+0]	-1.6101[+0]	-3.1486[+0]	-3.6400[+0]	-3.8395[+0]	-3.9322[+0]	-3.3790[+0]	-3.9961[+0]	-3.9014[+0]	-5.9941[+1]	
$8d$	-8.4549[+0]	-9.1882[+0]	-9.2154[+0]	-9.2193[+0]	-9.2200[+0]	-9.2202[+0]	-9.2202[+0]	-9.2202[+0]	-9.2202[+0]	-9.2202[+0]	-9.2202[+0]
	-7.3870[+0]	-8.9995[+0]	-9.1766[+0]	-9.2097[+0]	-9.2174[+0]	-9.2194[+0]	-9.2200[+0]	-9.2201[+0]	-9.2202[+0]	-9.2202[+0]	-9.2202[+0]
	-2.5944[+0]	-8.1115[+0]	-8.9017[+0]	-9.1067[+0]	-9.1745[+0]	-9.2003[+0]	-9.2110[+0]	-9.2158[+0]	-9.2177[+0]	-9.2325[+0]	
	-1.5385[+1]	-1.5754[+1]	-1.5760[+1]	-1.5760[+1]	-1.5761[+1]	-1.5761[+1]	-1.5761[+1]	-1.5761[+1]	-1.5761[+1]	-1.5761[+1]	
$8f$	-1.4843[+1]	-1.5690[+1]	-1.5752[+1]	-1.5759[+1]	-1.5760[+1]	-1.5760[+1]	-1.5761[+1]	-1.5761[+1]	-1.5761[+1]	-1.5761[+1]	-1.5761[+1]
	-1.2204[+1]	-1.5332[+1]	-1.5670[+1]	-1.5736[+1]	-1.5753[+1]	-1.5758[+1]	-1.5760[+1]	-1.5760[+1]	-1.5760[+1]	-1.5670[+1]	
	-2.3274[+1]	-2.3433[+1]	-2.3434[+1]	-2.3434[+1]	-2.3434[+1]	-2.3434[+1]	-2.3434[+1]	-2.3434[+1]	-2.3434[+1]	-2.3434[+1]	
$8g$	-2.3035[+1]	-2.3417[+1]	-2.3433[+1]	-2.3434[+1]	-2.3434[+1]	-2.3434[+1]	-2.3434[+1]	-2.3434[+1]	-2.3434[+1]	-2.3434[+1]	-2.3434[+1]
	-2.1840[+1]	-2.3310[+1]	-2.3417[+1]	-2.3431[+1]	-2.3434[+1]	-2.3434[+1]	-2.3434[+1]	-2.3434[+1]	-2.3434[+1]	-2.3434[+1]	

^a $E = \sum_{i=0}^N E_i$.

TABLE V. Predicted partial sums of energy eigenvalues in atomic units (Patil potential) of the $2s$ to $6s$ states for the $l=0$ fixed values. First entry, SLNE; second entry, P1NE; third entry, ULNE. In the last column are given the values obtained by Lingård and Nielsen (Ref. [29]). The numbers in square brackets indicate the powers of 10 by which the values are to be multiplied.

State	N^a										Ref. data
	3	5	7	9	11	13	15	17	19	21	
$2s$	-1.1369[-1]	1.5265[+0]	-6.3929[+1]	3.1698[+3]	-1.8233[+5]	8.2696[+6]	1.1181[+9]	-7.5700[+1]	-3.3161[+14]	-1.4579[+17]	-1.9814[-1]
	-1.1594[-1]	1.4458[+0]	-5.4747[+1]	2.2589[+3]	-8.1944[+4]	-4.0300[+6]	2.6848[+9]	-9.0319[+11]	-2.9895[+14]	-1.0579[+17]	
	-0.3008[+0]	-6.9586[+0]	-3.5054[-2]	-1.8919[+5]	-1.0884[+6]	-5.6310[+7]	6.8032[+9]	7.8271[+12]	-5.5895[+15]	4.1091[+1]	
	-5.5846[-2]	-5.7026[-2]	-6.0062[-2]	-4.0984[-2]	3.1421[0]	8.2991[+1]	-1.5994[+3]	2.2645[+4]	-4.6883[+5]	8.8346[+6]	
$3s$	-5.5845[-2]	-5.7020[-2]	-6.0048[-2]	-4.1917[-2]	3.0502[0]	8.2341[+1]	-1.5181[+3]	2.1652[+4]	-4.4631[+5]	8.5242[+6]	-7.4182[-2]
	-1.7680[+0]	-1.0022[+2]	-2.9831[+3]	7.7236[+5]	1.1477[+8]	-5.3169[+9]	-4.1293[+12]	-7.1612[+14]	-1.31103[+17]	-8.1298[+19]	
	-3.1281[-2]	-3.1416[-2]	-3.1780[-2]	-3.2541[-2]	-3.3929[-2]	-3.6270[-2]	-3.9924[-2]	7.6835[-3]	9.7561[+0]	7.9801[+2]	
$4s$	-3.1281[-2]	-3.1416[-2]	-3.1779[-2]	3.2540[-2]	-3.3927[-2]	-3.6266[-2]	-3.9920[-2]	7.0364[-3]	6.6540[+0]	7.9182[+2]	-3.8615[-2]
	-4.5159[+0]	-4.5844[+2]	1.0719[+3]	1.6211[+7]	-2.4188[+8]	-1.4864[+12]	-3.1695[+13]	1.8264[+17]	2.3537[+19]	-2.0012[+22]	
	-2.0005[-2]	-2.0030[-2]	2.0099[-2]	-2.0245[-2]	-2.0513[-2]	-2.0995[-2]	-2.1641[-2]	-2.2664[-2]	-2.4157[-2]	-2.6301[-2]	
$5s$	-2.0005[-2]	-2.0030[-2]	2.0099[-2]	-2.0245[-2]	-2.0513[-2]	-2.0995[-2]	-2.1641[-2]	-2.2663[-2]	-2.4156[-2]	-2.6310[-2]	-2.3637[-2]
	-8.5445[+0]	-1.3635[+3]	7.0151[+4]	-1.2805[+8]	-3.0831[+10]	-2.7943[+13]	1.3219[+16]	8.4287[+18]	-5.7718[+21]	-3.1400[+24]	
	1.3890[-2]	-1.3896[-2]	-1.3914[-2]	-1.3952[-2]	-1.4021[-2]	-1.4137[-2]	-1.4317[-2]	-1.4580[-2]	-1.4952[-2]	-1.5466[-2]	
$6s$	-1.3890[-2]	-1.3896[-2]	-1.3914[-2]	-1.3952[-2]	-1.4021[-2]	-1.4137[-2]	-1.4317[-2]	-1.4580[-2]	-1.4952[-2]	-1.5465[-2]	-1.5945[-2]
	-1.3854[+1]	-3.2002[+3]	3.7823[+6]	6.3944[+8]	-3.5738[+11]	-2.4322[+14]	3.3695[+17]	7.7586[+19]	-3.2322[+23]	2.6029[+25]	

^a $E = \sum E_i$.

TABLE VI. Predicted partial sums of energy eigenvalues in atomic units (Patil potential) of the $2s$ to $6g$ states for the $n_r=1$ fixed values. First entry, SLNE; second entry, P1NE; third entry, ULNE. In the last column are given the values obtained by Lingård and Nielsen (Ref. [29]). The numbers in square brackets indicate the powers of 10 by which the values are to be multiplied.

State	E^a										Ref. data
	3	5	7	9	11	13	15	17	19	21	
$4s$	-3.1281[-2]	-3.1416[-2]	-3.1780[-2]	-3.2541[-2]	-3.3929[-2]	-3.6270[-2]	-3.9924[-2]	7.6835[-3]	9.7561[+0]	7.9801[+2]	-3.8615[-2]
	-3.1281[-2]	-3.1416[-2]	-3.1779[-2]	-3.2540[-2]	-3.3927[-2]	-3.6266[-2]	-3.9920[-2]	7.0364[-3]	6.6540[+0]	7.9182[+2]	
	-4.5159[0]	-4.5844[+2]	1.0719[+3]	1.6211[+7]	-2.4188[+8]	-1.4864[+12]	-3.1695[+13]	1.8264[+17]	2.3537[+19]	-2.0012[+22]	
	-2.0004[-2]	-2.0014[-2]	-2.0031[-2]	-2.0054[-2]	-2.0081[-2]	-2.0109[-2]	-2.0137[-2]	-2.0164[-2]	-2.0189[-2]	-2.0213[-2]	
$5p$	-2.0004[-2]	-2.0014[-2]	-2.0031[-2]	-2.0054[-2]	-2.0081[-2]	-2.0109[-2]	-2.0137[-2]	-2.0164[-2]	-2.0189[-2]	-2.0211[-2]	-2.0373[-2]
	-1.6002[-1]	-2.3969[-1]	-3.2364[-1]	-3.3723[-1]	-1.3187[+0]	6.5883[+0]	9.0122[+1]	3.8741[+3]	8.8073[+4]	-4.2055[+6]	
	-1.3890[-2]	-1.3891[-2]	-1.3892[-2]	-1.3894[-2]	-1.3895[-2]	-1.3895[-2]	-1.3896[-2]	-1.3896[-2]	-1.3897[-2]	-1.3897[-2]	
$6d$	-1.3890[-2]	-1.3891[-2]	-1.3892[-2]	-1.3894[-2]	-1.3895[-2]	-1.3895[-2]	-1.3896[-2]	-1.3896[-2]	-1.3897[-2]	-1.3897[-2]	-1.3896[-2]
	-4.4984[-2]	-3.8605[-2]	-3.1011[-2]	-2.4924[-2]	-2.0691[-2]	-1.7983[-2]	-1.6852[-2]	1.2175[-3]	-3.5582[-1]	6.2833[+0]	
	-1.0204[-2]	-1.0204[-2]	-1.0205[-2]	-1.0205[-2]	-1.0205[-2]	-1.0205[-2]	-1.0205[-2]	-1.0205[-2]	-1.0205[-2]	-1.0205[-2]	
$7f$	-1.0204[-2]	-1.0204[-2]	-1.0205[-2]	-1.0205[-2]	-1.0205[-2]	-1.0205[-2]	-1.0205[-2]	-1.0205[-2]	-1.0205[-2]	-1.0205[-2]	-1.0204[-2]
	-2.0119[-2]	-1.4945[-2]	-1.2186[-2]	-1.0976[-2]	-1.0492[-2]	-1.0309[-2]	-1.0242[-2]	-1.0218[-2]	-1.0137[-2]	4.6453[-3]	
	-7.8125[-3]	-7.8126[-3]	-7.8126[-3]	-7.8126[-3]	-7.8126[-3]	-7.8126[-3]	-7.8126[-3]	-7.8126[-3]	-7.8126[-3]	-7.8126[-3]	
$8g$	-7.8125[-3]	-7.8126[-3]	-7.8126[-3]	-7.8126[-3]	-7.8126[-3]	-7.8126[-3]	-7.8126[-3]	-7.8126[-3]	-7.8126[-3]	-7.8126[-3]	-7.8125[-3]
	-1.1748[-2]	-9.0667[-3]	-8.1628[-3]	-7.9038[-3]	-7.8354[-3]	-7.8181[-3]	-7.8139[-3]	-7.8128[-3]	-7.8096[-3]	-7.6871[-3]	

$$^a E = \sum_{i=0}^N E_i.$$

TABLE VII. Predicted partial sums of energy eigenvalues in atomic units (Patil potential) of the $6s$ to $6g$ states for the $n=6$ fixed values. First entry, SLNE; second entry, P1NE; third entry, ULNE. In the last column are given the values obtained by Lingård and Nielsen (Ref. [29]). The numbers in square brackets indicate the powers of 10 by which the values are to be multiplied.

State	E^a										Ref. data
	3	5	7	9	11	13	15	17	19	21	
$6s$	1.3890[-2]	-1.3896[-2]	-1.3914[-2]	-1.3952[-2]	-1.4021[-2]	-1.4137[-2]	-1.4317[-2]	-1.4580[-2]	-1.4952[-2]	-1.5466[-2]	
	-1.3890[-2]	-1.3896[-2]	-1.3914[-2]	-1.3952[-2]	-1.4021[-2]	-1.4137[-2]	-1.4317[-2]	-1.4580[-2]	-1.4952[-2]	-1.5465[-2]	-1.5945[-2]
	-1.3854[+1]	-3.2002[+3]	3.7823[+6]	6.3944[+8]	-3.5738[+11]	-2.4322[+14]	3.3695[+17]	7.7586[+19]	-3.2322[+23]	2.6029[+25]	
$6p$	-1.3889[-2]	-1.3893[-2]	-1.3899[-2]	-1.3907[-2]	-1.3819[-2]	-1.3930[-2]	-1.3943[-2]	-1.3957[-2]	-1.3970[-2]	-1.3983[-2]	
	-1.3890[-2]	-1.3893[-2]	-1.3899[-2]	-1.3907[-2]	-1.3918[-2]	-1.3930[-2]	-1.3943[-2]	-1.3956[-2]	-1.3970[-2]	-1.3982[-2]	-1.4106[-2]
	-3.2630[-1]	-9.8261[-1]	-2.6073[+0]	-6.3825[+0]	-1.5060[+1]	-4.2156[+1]	-2.6876[+1]	-4.1786[+2]	4.6992[+4]	2.4542[+5]	
$6d$	-1.3890[-2]	-1.3891[-2]	-1.3892[-2]	-1.3894[-2]	-1.3895[-2]	-1.3895[-2]	-1.3896[-2]	-1.3896[-2]	-1.3897[-2]	-1.3897[-2]	-1.3896[-2]
	-4.4984[-2]	-3.8605[-2]	-3.1011[-2]	-2.4924[-2]	-2.0691[-2]	-1.7983[-2]	-1.6852[-2]	1.2175[-3]	-3.5582[-1]	-6.2833[0]	
	-1.3889[-2]	-1.3890[-2]	-1.3890[-2]	-1.3890[-2]	-1.3890[-2]	-1.3890[-2]	-1.3890[-2]	-1.3890[-2]	-1.3890[-2]	-1.3890[-2]	
$6f$	-1.3889[-2]	-1.3890[-2]	-1.3890[-2]	-1.3890[-2]	-1.3890[-2]	-1.3890[-2]	-1.3890[-2]	-1.3890[-2]	-1.3890[-2]	-1.3890[-2]	-1.3889[-2]
	-1.6462[-2]	-1.4328[-2]	-1.3956[-2]	-1.3899[-2]	-1.3891[-2]	-1.3890[-2]	-1.3890[-2]	-1.3890[-2]	-1.3888[-2]	-1.3612[-2]	
	-1.3889[-2]	-1.3889[-2]	-1.3889[-2]	-1.3889[-2]	-1.3889[-2]	-1.3889[-2]	-1.3889[-2]	-1.3889[-2]	-1.3889[-2]	-1.3889[-2]	
$6g$	-1.3889[-2]	-1.3889[-2]	-1.3889[-2]	-1.3889[-2]	-1.3889[-2]	-1.3889[-2]	-1.3889[-2]	-1.3889[-2]	-1.3889[-2]	-1.3889[-2]	-1.3889[-2]
	-1.3934[-2]	-1.3890[-2]	-1.3889[-2]	-1.3889[-2]	-1.3889[-2]	-1.3889[-2]	-1.3889[-2]	-1.3889[-2]	-1.3889[-2]	-1.3889[-2]	

$$^a E = \sum_{i=0}^N E_i.$$

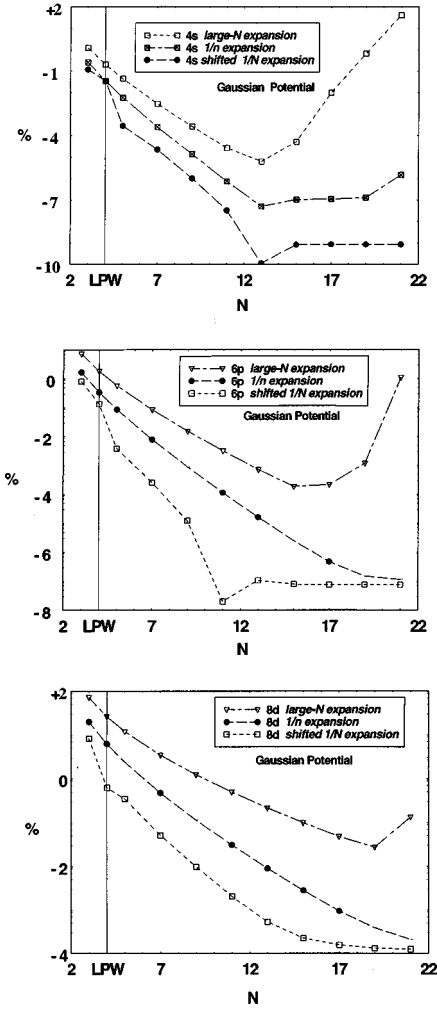


FIG. 1. Plot of the percentage difference between our shifted $1/N$ expansion (SLNE), large- N expansion (ULNE), $1/n$ expansion (PINE) eigenenergies, and Crandall reference data (Ref. [30]) vs the number of first N terms of the perturbation series for various values of quantum numbers n for l in the case of the Gaussian potential. LPW denotes the limit of previous works and curves are drawn to guide the eye. The numbers on % axis are powers of 10, i.e., for example $-3 \equiv 10^{-3}$.

increases since the expansion parameter decreases. The usefulness of SLNE is brought out more clearly for f and g levels. One sees in Fig. 3 that for higher angular-momentum states the energy values of our shifted large- N computations match the relative difference (RD) extremely well (the RD is less than $10^{-5}\%$ in the domain $N \geq 17$) with a nice convergence of the series expansion. In fact, the series expansion converges so quickly that the correction terms could be neglected. Given N , the $1/n$ expansion gets worse when l decreases despite the fact that $n=8$ is relatively high. The ULNE method asymptotically diverges. A perusal of the different curves reveals that the starting point of the divergence (i.e., the threshold order N_{\max} beyond which the expansion ceases to converge) increases with l . Switching our attention to Fig. 4, one sees that the percent errors increase in general beyond $N=20$; in other words, the expansion diverges for any kind of $1/N$ expansion.

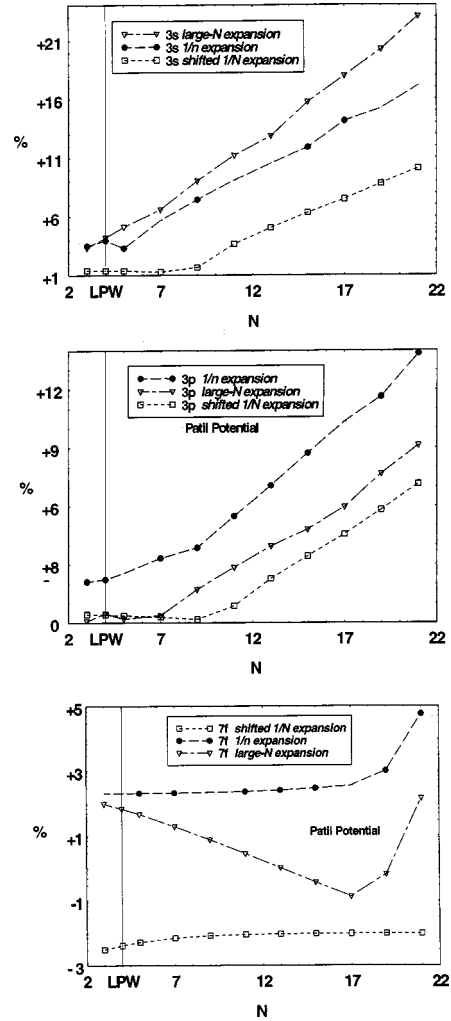


FIG. 2. Plot of the percentage difference between our shifted $1/N$ expansion (SLNE), large- N expansion (ULNE), $1/n$ expansion (PINE) eigenenergies, and Lingård and Nielsen reference data (Ref. [29]) vs the number of first N terms of the perturbation series for various values of quantum numbers n for l in the case of the Patil potential. LPW denotes the limit of previous works and curves are drawn to guide the eye. The numbers on % axis are powers of 10, i.e., for example $-3 \equiv 10^{-3}$.

(b) Let us now consider the case for which the orbital quantum number is fixed at $l=0$, for the two potentials. Figures 5 and 6 show in general the same trends as previously with, however, some marked differences. As evident for the ULNE scheme, the energies get worse when n increases since all partial sums contain terms which, for large n , behave at least like n . Λ has no n dependence to diminish the effects of the powers of n in the numerator of the partial sums. This large deviation indicates that we are out of the limit of applicability of ULNE. Likewise, the $1/n$ expansion becomes less accurate as n increases. The observations seem to confirm the study of asymptotic of large orders of the $1/n$ expansion in Ref. [78]. As a result Popov and Sergeev found that the large orders increases as factorials which explains why in many quantum-mechanical problems (e.g., the Patil potential) a divergence occurs in the summation of the en-

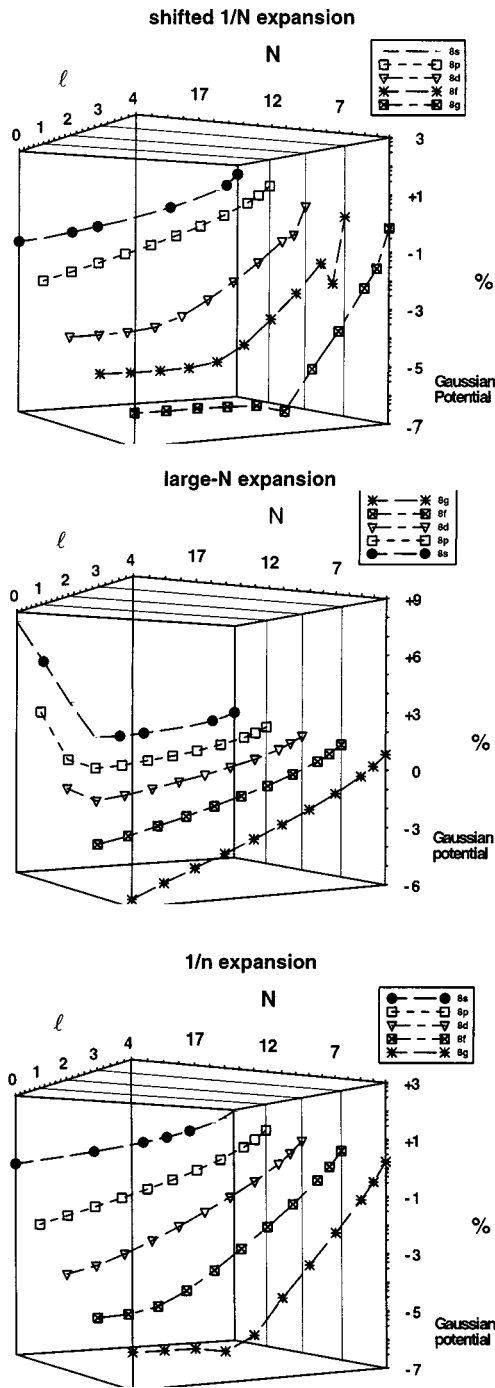


FIG. 3. An illustration of the behavior of the percentage difference between our SLNE, ULNE, and P1NE eigenenergies and Crandall reference data (Ref. [30]) as a function of the orbital quantum number l and the number of first N terms of the perturbation series for the fixed $n=8$ principal quantum number in the case of the Gaussian potential. Curves are drawn to guide the eye. The numbers on % axis are powers of 10, i.e., for example $-3 \equiv 10^{-3}$.

ergy series. From Figs. 5 and 6 we can see that, unlike the Patil potential, the percent errors for the Gaussian potential increase with n in the shifted expansion. Hence, it seems that the effects of the shift parameter in Λ , for s states particularly, depend on the potential considered. The shifted $1/N$

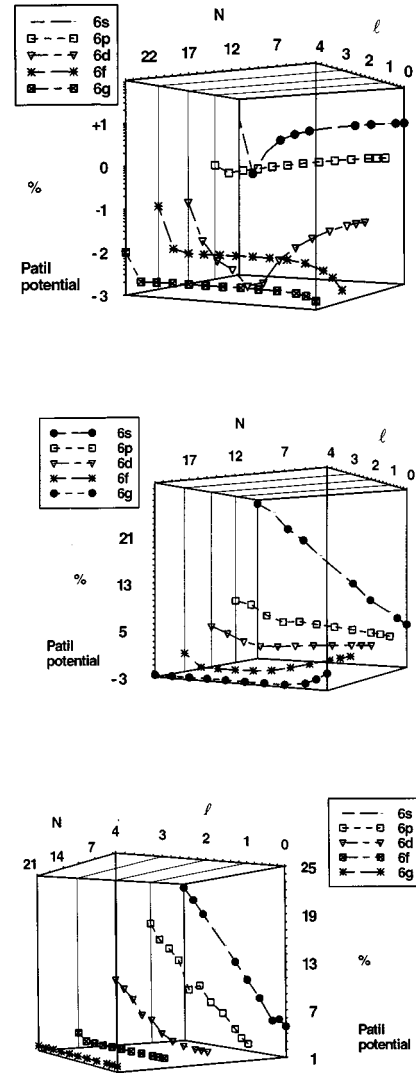


FIG. 4. An illustration of the behavior of the percentage difference between our SLNE, ULNE, and P1NE eigenenergies and Linsgård and Nielsen reference data (Ref. [29]) as a function of the orbital quantum number l and the number of first N terms of the perturbation series for the fixed $n=6$ principal quantum number in the case of the Gaussian potential. Curves are drawn to guide the eye. The numbers on % axis are powers of 10, i.e., for example $-3 \equiv 10^{-3}$.

expansion still predicts superior results.

(c) We turn to the case for which the radial quantum number is fixed at $n_r=3$ when n and l increase simultaneously. Comparing our computations for SLNE and P1NE with reference data, it clearly appears in Fig. 7 that given N , the results are more and more inaccurate with growing n and l , i.e., n effects are superior to those of l . However, the corrections improve the accuracy of the energy. On the other hand, for ULNE n effects manifest themselves gradually with the increase of N and the decrease of l . As already described above, ULNE ceases to converge beyond the limit N_{\max} .

From what precedes, it is observed that the SLNE expansion always shows an improvement over P1NE and ULNE.

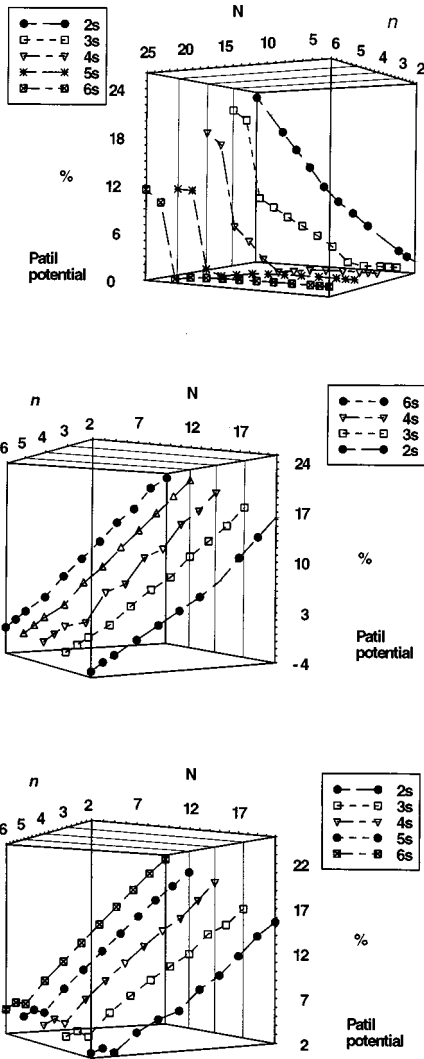


FIG. 5. An illustration of the behavior of the percentage difference between our SLNE, ULNE, and PINE eigenenergies and Linaard and Nielsen reference data (Ref. [29]) as a function of the principal quantum number n and the number of first N terms of the perturbation series for the fixed $l=0$ principal quantum number in the case of the Patil potential. Curves are drawn to guide the eye. The numbers on % axis are powers of 10, i.e., for example $-3 \equiv 10^{-3}$.

As far as the Patil potential is concerned the former approach in the case of s and p states is in trouble for low- N values and fails completely when N increases, whereas PINE and ULNE are inapplicable. This explains that in what follows, we confine ourselves to a modification of the SLNE technique to solve the problem of divergence for such unfavorable states. It is known that one could make use of appropriate methods of divergent series such as Padé approximants [36,109,111,113,114], and Padé-Hermite approximants [122] to increase the precision of the results. In this paper we resort to the order-dependent HVHF-PMS method described in some detail in Sec. II. Our aim here is to test the claim by Maluendes *et al.* [86] of the accuracy and utility of this approach for complicated potentials that are a superposition of smoothly changing spherically potentials. To this end, we

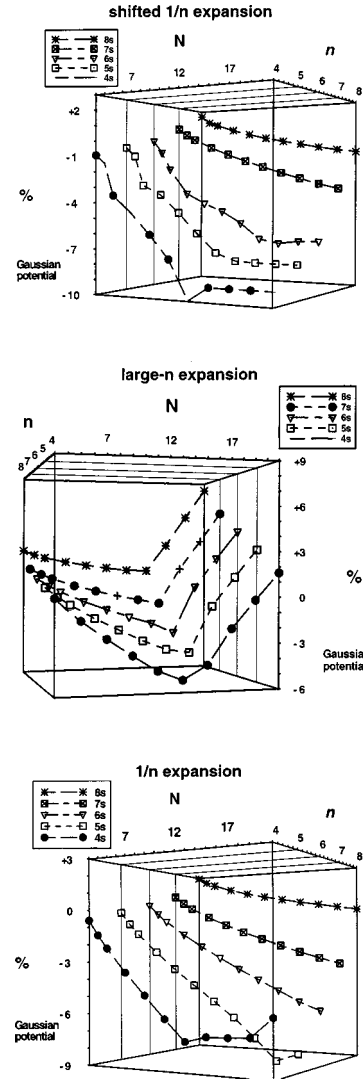


FIG. 6. An illustration of the behavior of the percentage difference between our SLNE, ULNE, and PINE eigenenergies and Crandall reference data (Ref. [30]) as a function of the principal quantum number n and the number of first N terms of the perturbation series for the fixed $l=0$ principal quantum number in the case of the Gaussian potential. Curves are drawn to guide the eye. The numbers on % axis are powers of 10, i.e., for example $-3 \equiv 10^{-3}$.

have applied for concreteness to the Patil and Hellmann potentials the shifted $1/N$ expansion in which the principle of minimal sensitivity (PMS) is incorporated. More precisely, we have restricted ourselves to bound states that cannot be adequately described by the SLNE scheme, i.e., the most unfavorable cases. To our knowledge, no explicit case study of this type has been undertaken to substantiate this claim. It should be noted that one of the shortcomings of the HVHF-PMS method is that the computation time rapidly increases with increasing the number of terms. The calculation of E_k involves the derivatives $V_0^{(i)}$ with $1 \leq i \leq 2k$. Thus, it is obvious that if one is not careful significant roundoff errors can occur, for instance as early as the eighth term in the case of the Patil potential. We have employed MATHEMATICA to

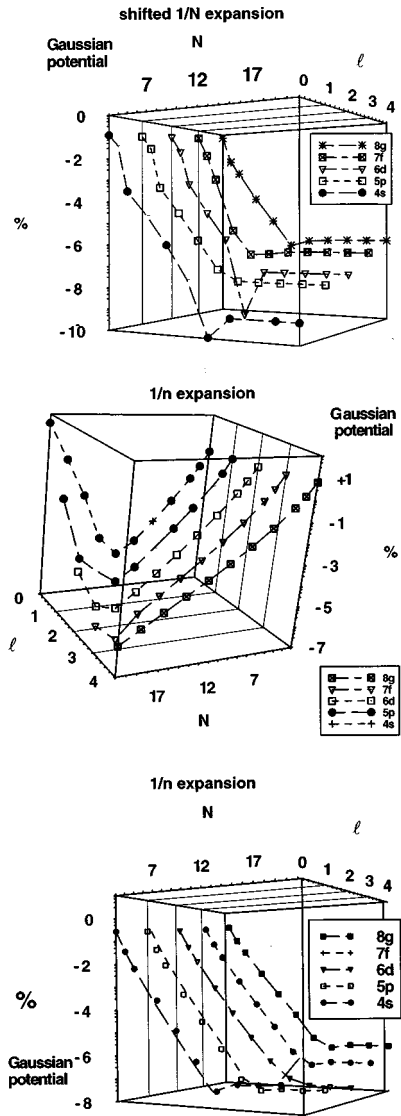


FIG. 7. An illustration of the behavior of the percentage difference between our SLNE, ULNE, and P1NE eigenenergies and Crandall reference data (Ref. [30]) as a function of the orbital quantum number l and the number of first N terms of the perturbation series for the fixed $n_r=3$ radial quantum number in the case of the Gaussian potential. Curves are drawn to guide the eye. The numbers on % axis are powers of 10, i.e., for example $-3 \equiv 10^{-3}$.

avoid roundoff errors. Only the first several terms that are not affected by roundoff errors are quoted in Tables VIII and IX. From the sequences so obtained one sees that the larger the order the more accurate our results and the less accurate those of SLNE if this latter is applicable. The numerical magnitude of the HVHF-PMS calculated energies are quite satisfactory. Clearly, the order-dependent shift considerably enhances the accuracy of the energy eigenvalues. Finally, it would be instructive to check if, as suspected by Dutt *et al.* [103], the discrepancies happen because the large- N effective potential becomes shallow and its minimum shifts appreciably from the minimum of the through potential. To see it more clearly, we have plotted in Fig. 8 the large- N effective potential for the $2s$ ground state of the Patil potential for

TABLE VIII. Predicted partial sums of energy eigenvalues in atomic units (Patil potential). First entry, HVHF-PMS; second entry, SLNE. In the last column are given the values obtained by Lingård and Nielsen (Ref. [29]). The numbers in square brackets indicate the powers of 10 by which the values are to be multiplied.

State	N^a										Ref. data
	5	7	9	11	13	15	17	19	21		
2s	-1.3050[-1]	-1.3520[-1]	-1.4112[-1]	-1.4837[-1]	-1.5704[-1]	-1.6723[-1]	-1.7910[-1]	-1.9277[-1]	-2.0844[-1]	-1.9814[-1]	
	1.5265[+0]	-6.3929[+1]	3.1698[+3]	-1.8233[+5]	8.2696[+6]	1.1181[+9]	7.5700[+11]	3.3161[+14]	-1.4579[+17]		
3s	-5.8413[-2]	-6.0305[-2]	-6.2703[-2]	-6.5624[-2]	-6.9104[-2]	-7.3184[-2]	-7.7921[-2]	-8.346[+6]	-7.4182[-2]		
	-5.8253[-2]	-6.0063[-2]	-4.0984[-2]	3.1421[+0]	8.2991[+1]	-1.5594[+4]	2.2645[+4]	-4.6883[+5]	8.8346[+6]		
4s	-3.2445[-2]	-3.3771[-2]	-3.4853[-2]	-3.6260[-2]	-3.7933[-2]	-3.9894[-2]	-3.9924[-2]	7.6835[-1]	8.7561[+0]	-3.8615[-2]	
	-3.1416[-2]	-3.1780[-2]	-3.2541[-2]	-3.3929[-2]	-3.6270[-2]	-3.9924[-2]	-3.9924[-2]	7.6835[-1]	8.7561[+0]	-2.3637[-2]	
5s	-2.0166[-2]	-2.0834[-2]	-2.2232[-2]	-2.2790[-2]	-2.3578[-2]	-2.4164[-2]	-2.4164[-2]	-2.2664[-2]	-2.4157[-2]	-2.6301[-2]	
	-2.0014[-2]	-2.0099[-2]	-2.0245[-2]	-2.0513[-2]	-2.0985[-2]	-2.1641[-2]	-2.2664[-2]	-2.4157[-2]	-2.4157[-2]	-2.6301[-2]	
6s	-1.3923[-2]	-1.4063[-2]	-1.4473[-2]	-1.5417[-2]	-1.6180[-2]	-1.4317[-2]	-1.4580[-2]	-1.4952[-2]	-1.4952[-2]	-1.5945[-2]	
	-1.3896[-2]	-1.3914[-2]	-1.3952[-2]	-1.4021[-2]	-1.4137[-2]	-1.4317[-2]	-1.4580[-2]	-1.4952[-2]	-1.4952[-2]	-1.5466[-2]	

^a $E = \sum_{l=0}^N E_l$.

TABLE IX. Predicted partial sums of energy eigenvalues in atomic units (Hellmann potential) as a function of the screening parameter C for $B = -5$. First entry, HVHF-PMS; second entry, SLNE. In the last column are given the variational results of Adamowski (Ref. [43]) converted to our scale of units. Asterisks in the second entry correspond to divergent results and the abbreviations (n.a.) indicate nonapplicability of the SLNE method.

C	State	N^a						Ref. data
		4	6	8	10	12	14	
0.5	4s	-0.3232	-0.0238	-0.0851	-0.1077	-0.1184	-0.1208	-0.1215
		-0.2498	-0.3521	-0.6607	-1.5740	-4.3660	-13.1900	
	4p	0.3812	0.6287	-0.4808	-0.8708	-0.9919	-0.1021	-0.1031
		-0.1311	-0.1375	-0.1420	-0.1733	-0.1771	-0.3658	
	4f	-0.0316	-0.0326	-0.0332	-0.0335	-0.0338	-0.0340	-0.0340
		n.a	n.a	n.a	n.a	n.a	n.a	
2	2p	0.8750	0.0743	-1.0250	-0.1204	-0.1373	-0.1939	-0.1910
		*	*	*	*	*	*	
	3p	-0.0537	-0.0553	-0.0555	-0.0557	-0.0584	-0.0764	-0.0727
		*	*	*	*	*	*	
	3d	-0.0534	-0.0553	-0.0555	-0.0556	-0.0556	-0.0559	-0.0557
		n.a	n.a	n.a	n.a	n.a	n.a	
	4d	-0.0311	-0.0313	-0.0314	-0.0311	-0.0317	-0.0318	-0.0313
		n.a	n.a	n.a	n.a	n.a	n.a	
	4f	-0.0311	-0.0312	-0.0313	-0.0313	-0.0312	-0.0312	-0.0312
		n.a	n.a	n.a	n.a	n.a	n.a	

$$^a E = \sum_{i=0}^N E_i.$$

several values of M corresponding to $E_M(r_0) = 0$. The behavior of the diagrams seems to indicate that the poor results may not be attributed to that situation contrary to what was suspected in Ref. [103].

IV. CONCLUDING REMARKS

The purpose of this work was first to explore the credibility of the three schemes SLNE, PINE, and ULNE when high

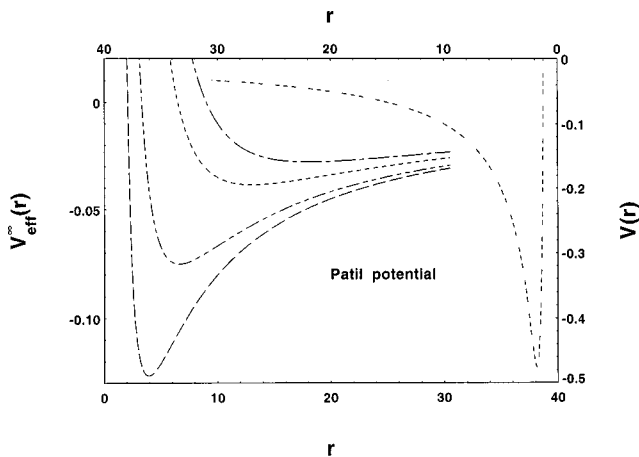


FIG. 8. Schematic diagrams of the behavior of the Patil potential (right-hand scale) and the large- N effective potential (left-hand side) corresponding to the appropriated roots of $E_M(r_0) = 0$ ($M = 2, 5, 13, 19$) for the ground state $2s$. Both $V(r)$ and r are in atomic units.

orders of the perturbation theory are taken into account, and second to test the effectiveness of the HVHF-PMS approach. To this end, we have derived explicitly algebraic recursion relations for the coefficients E by applying the hypervirial $1/N$ expansion together with the Hellmann-Feynman theorem. These recurrence formulas, convenient for computer calculations, make it possible to evaluate E for arbitrarily high orders for any kind of $1/N$ expansion. The analytic expressions for these coefficients coincide with those obtained by Stepanov and Tutik from a method based on a semiclassical interpretation of the $1/N$ expansion. Then we have used these formulas to study the applicability of each scheme concerning the Gaussian and Patil potentials, which are a smoothly changing potential and a superposition of simple potentials, respectively. Owing to limited computational facilities and order increasing roundoff errors, we have been able to handle no more than 21 perturbation corrections. We find that the shifted $1/N$ expansion offers in general a large improvement over PINE and ULNE for energy eigenvalues. In other words, there is a distinct advantage in using SLNE over the latter. The $1/n$ expansion is found to be useful only for the simple Gaussian potential. The iteration procedure converges and the correction terms improve considerably the numerical results. In the case of the Patil potential, the coefficients E_k grow sharply and PINE is not applicable. This apparently raises doubt about the applicability of that technique to complicated potentials. It also emerges from the computations that ULNE diverges whatever the type of potential considered—however, less strongly than PINE for the Patil potential. Large-order cal-

culations here are useless unless an appropriate resummation technique is used. SLNE results compare remarkably well with those of Crandall. The situation is reversed and appreciable discrepancy of the SLNE results occurs for the s and p states. Particularly for the s states, SLNE fails completely, from which it follows that caution is necessary in using SLNE. To solve the problem of divergence, we have incorporated in the shifted $1/N$ expansion the principle of minimal sensitivity as suggested by Maluendes *et al.* In order to bring out the improvement of this approach, we have applied the formulas thus derived to the Patil and Hellmann potentials, leaving the other cases for later investigations. The energy values obtained are in good agreement with reference data which proves the usefulness of the HVHF-PMS approach for such unfavorable cases. These results are quite encouraging. We are at present using that modified shifted $1/N$ expansion for extensive applications to central potentials especially for low-lying states. We are also performing the summability studies of the expansions presented in this paper as well as the acceleration of their convergence [123]. This work will be reported later in a forthcoming paper.

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APPENDIX A

For purposes of comparison with the analytical results derived from our HVHF method, we apply the conventional

Rayleigh-Schrödinger perturbation theory to Eq. (9) truncated to calculate the energy eigenvalues to $O(g^4)$. In as much as the formulas up to and including $O(g^6)$ have long been known [81], we present explicitly only the next additional terms. We consider the Schrödinger equation

$$\left\{ -\frac{1}{2} \frac{d^2}{dx^2} + \frac{1}{2} \omega^2 x^2 + \varepsilon_0 + W(x) \right\} \chi(x) = \hat{E} \chi(x), \quad (\text{A1})$$

where terms of order g^i ($i \leq 6$) are retained in the perturbation potential,

$$\begin{aligned} W(x) = & g(\varepsilon_1 x + \varepsilon_3 x^3) + g^2(\varepsilon_2 x^2 + \varepsilon_4 x^4) \\ & + g^3(\delta_1 x + \delta_3 x^3 + \delta_5 x^5) + g^4(\delta_2 x^2 + \delta_4 x^4 + \delta_6 x^6) \\ & + g^5(\gamma_3 x^3 + \gamma_5 x^5 + \gamma_7 x^7) + g^6(\gamma_4 x^4 + \gamma_6 x^6 + \gamma_8 x^8), \end{aligned} \quad (\text{A2})$$

with the following notations:

$$\varepsilon_0 = \frac{1}{2} \beta_0 + b^{(0)}, \quad b^{(0)} = \frac{1}{2} \xi_0, \quad \varepsilon_1 = \frac{1}{2} \beta_1, \quad \varepsilon_2 = \frac{1}{2} \beta_2, \quad (\text{A3})$$

$$\begin{aligned} \varepsilon_3 = \frac{1}{2} \alpha_1, \quad \varepsilon_4 = \frac{1}{2} \alpha_2, \\ \delta_1 = \frac{1}{2} \xi_1, \quad \delta_2 = \frac{1}{2} \xi_2, \quad \delta_3 = \frac{1}{2} \beta_3, \quad \delta_4 = \frac{1}{2} \beta_4, \\ \delta_5 = \frac{1}{2} \alpha_3, \quad \delta_6 = \frac{1}{2} \alpha_4, \end{aligned} \quad (\text{A4})$$

$$\begin{aligned} \gamma_3 = \frac{1}{2} \xi_3, \quad \gamma_4 = \frac{1}{2} \xi_4, \quad \gamma_5 = \frac{1}{2} \beta_5, \quad \gamma_6 = \frac{1}{2} \beta_6, \\ \gamma_7 = \frac{1}{2} \alpha_5, \quad \gamma_8 = \frac{1}{2} \alpha_6, \end{aligned} \quad (\text{A5})$$

$$\hat{E} = r_0^2 g^2 (\bar{E} - E_0) \approx \sum_{k=1}^6 \hat{E}^{(k)}. \quad (\text{A6})$$

The calculation which is carried out to sixth order in the potential, using the general formulas, yields

$$\hat{E}^{(0)} = \varepsilon_0 + (n_r + 1/2) \omega, \quad (\text{A7})$$

$$\hat{E}^{(1)} = W_{nn} = g^2 b^{(1)} + g^4 c^{(1)} + g^6 d^{(1)}, \quad (\text{A8})$$

$$\hat{E}^{(2)} = \sum_{i \neq n} \frac{W_{ni} W_{in}}{\lambda_{ni}} = g^2 b^{(2)} + g^4 c^{(2)} + g^6 d^{(2)}, \quad (\text{A9})$$

$$\hat{E}^{(3)} = \sum_{i, j \neq n} \frac{W_{ni} W_{ij} W_{jn}}{\lambda_{ni} \lambda_{nj}} - \hat{E}^{(1)} \sum_{i \neq n} \frac{W_{ni} W_{in}}{(\lambda_{ni})^2} = g^4 c^{(3)} + g^6 d^{(3)}, \quad (\text{A10})$$

$$\hat{E}^{(4)} = \sum_{i, j, k \neq n} \frac{W_{ni} W_{ij} W_{jk} W_{kn}}{\lambda_{ni} \lambda_{nj} \lambda_{nk}} - 2 \hat{E}^{(1)} \sum_{i, j \neq n} \frac{W_{ni} W_{ij} W_{jn}}{(\lambda_{ni})^2 \lambda_{nj}} - (\hat{E}^{(1)})^2 \sum_{i \neq n} \frac{W_{ni} W_{in}}{(\lambda_{ni})^3} - \hat{E}^{(2)} \sum_{i \neq n} \frac{W_{ni} W_{in}}{(\lambda_{ni})^2} = g^4 c^{(4)} + g^6 d^{(4)}, \quad (\text{A11})$$

$$\begin{aligned}
\hat{E}^{(5)} &= \sum_{i,j,k,l \neq n} \frac{W_{ni}W_{ij}W_{jk}W_{kl}W_{ln}}{\lambda_{ni}\lambda_{nj}\lambda_{nk}\lambda_{nl}} - \hat{E}^{(1)} \sum_{i,j,k \neq n} \frac{W_{ni}W_{ij}W_{jk}W_{kn}}{\lambda_{ni}\lambda_{nj}\lambda_{nk}} \left(\frac{2}{\lambda_{ni}} + \frac{1}{\lambda_{nj}} \right) \\
&\quad - \hat{E}^{(3)} \sum_{i \neq n} \frac{W_{ni}W_{in}}{(\lambda_{ni})^2} - \hat{E}^{(2)} \sum_{i,j \neq n} \frac{W_{ni}W_{ij}W_{jn}}{\lambda_{ni}\lambda_{nj}} \left(\frac{1}{\lambda_{ni}} + \frac{1}{\lambda_{nj}} \right) + (\hat{E}^{(1)})^2 \sum_{i,j \neq n} \frac{W_{ni}W_{ij}W_{jn}}{\lambda_{ni}\lambda_{nj}} \left(\frac{2}{(\lambda_{ni})^2} + \frac{1}{(\lambda_{nj})^2} \right) \\
&\quad + 2\hat{E}^{(1)}\hat{E}^{(2)} \sum_{i \neq n} \frac{W_{ni}W_{in}}{(\lambda_{ni})^2} - (\hat{E}^{(1)})^3 \sum_{i \neq n} \frac{W_{ni}W_{in}}{(\lambda_{ni})^4} \\
&= g^6 d^{(5)}, \tag{A12}
\end{aligned}$$

$$\begin{aligned}
\hat{E}^{(6)} &= \sum_{i,j,k,l,m \neq n} \frac{W_{ni}W_{ij}W_{jk}W_{kl}W_{lm}W_{mn}}{\lambda_{ni}\lambda_{nj}\lambda_{nk}\lambda_{nl}\lambda_{nm}} - \hat{E}^{(1)} \sum_{i,j,k,l \neq n} \frac{W_{ni}W_{ij}W_{jk}W_{kl}W_{lm}}{\lambda_{ni}\lambda_{nj}\lambda_{nk}\lambda_{nl}} \left(\frac{1}{\lambda_{ni}} + \frac{2}{\lambda_{nj}} + \frac{1}{\lambda_{nk}} \right) \\
&\quad - \hat{E}^{(2)} \sum_{i,j,k \neq n} \frac{W_{ni}W_{ij}W_{jk}W_{kn}}{\lambda_{ni}\lambda_{nj}\lambda_{nk}} \left(\frac{1}{\lambda_{ni}} + \frac{1}{\lambda_{nj}} + \frac{1}{\lambda_{nk}} \right) - \hat{E}^{(4)} \sum_{i \neq n} \frac{W_{ni}W_{in}}{(\lambda_{ni})^2} - (\hat{E}^{(1)})^2 \sum_{i \neq n} \frac{W_{ni}W_{in}}{(\lambda_{ni})^5} \\
&\quad - \hat{E}^{(3)} \sum_{i,j \neq n} \frac{W_{ni}W_{ij}W_{jn}}{\lambda_{ni}\lambda_{nj}} \left(\frac{1}{\lambda_{ni}} + \frac{1}{\lambda_{nj}} \right) + (\hat{E}^{(1)})^2 \sum_{i,j,k \neq n} \frac{W_{ni}W_{ij}W_{jk}W_{kn}}{\lambda_{ni}\lambda_{nj}\lambda_{nk}} \left(\frac{2}{(\lambda_{ni})^2} + \frac{2}{(\lambda_{nj})^2} + \frac{1}{(\lambda_{nk})^2} + \frac{1}{\lambda_{ni}\lambda_{nj}} \right) \\
&\quad + (\hat{E}^{(2)})^2 \sum_{i \neq n} \frac{W_{ni}W_{in}}{(\lambda_{ni})^3} + \hat{E}^{(1)}\hat{E}^{(2)} \sum_{i,j \neq n} \frac{W_{ni}W_{ij}W_{jn}}{\lambda_{ni}\lambda_{nj}} \left(\frac{2}{(\lambda_{ni})^3} + \frac{2}{(\lambda_{nj})^2} + \frac{1}{\lambda_{ni}\lambda_{nj}} \right) + 2\hat{E}^{(1)}\hat{E}^{(3)} \sum_{i \neq n} \frac{W_{ni}W_{in}}{(\lambda_{ni})^3} \\
&\quad - (\hat{E}^{(1)})^3 \sum_{i,j \neq n} \frac{W_{ni}W_{ij}W_{jn}}{\lambda_{ni}\lambda_{nj}} \left(\frac{2}{(\lambda_{ni})^3} + \frac{1}{(\lambda_{nj})^3} + \frac{1}{(\lambda_{nj})^2\lambda_{ni}} \right) - 3(\hat{E}^{(1)})^2\hat{E}^{(2)} \sum_{i \neq n} \frac{W_{ni}W_{in}}{(\lambda_{ni})^4} \\
&= g^6 d^{(6)}, \tag{A13}
\end{aligned}$$

with $\lambda_{ij} = \hat{E}_i^{(0)} - \hat{E}_j^{(0)}$, $W_{ij} = \langle i|W|j \rangle$. Substituting these expressions in Eq. (A6) and rearranging in powers of g we arrive at

$$\bar{E} = \sum_{k=0}^4 \bar{E}_k, \tag{A14}$$

where

$$\bar{E}_0 = E_0, \quad \bar{E}_1 = \frac{1}{2r_0^2 g^2} [(1 + 2n_r)\omega + \beta_0], \tag{A15}$$

$$\bar{E}_2 = \frac{1}{r_0^2} \sum_{i=0}^2 b^{(i)}, \quad \bar{E}_3 = \frac{g^2}{r_0^2} \sum_{i=0}^4 c^{(i)}, \quad \bar{E}_4 = \frac{g^4}{r_0^2} \sum_{i=0}^6 d^{(i)}. \tag{A16}$$

The coefficients $b^{(i)}$ and $c^{(i)}$ ($i \geq 1$) are listed in Ref. [124]. Omitting the algebraic complexities the sought new coefficients in the contribution \bar{E}_4 are

$$d^{(1)} = 3(1 + 2n_r + 2n_r^2) \tilde{\gamma}_4 + 5(3 + 8n_r + 6n_r^2 + 4n_r^3) \tilde{\gamma}_6 + 35(3 + 8n_r + 10n_r^2 + 4n_r^3 + 2n_r^4) \tilde{\gamma}_8, \tag{A17}$$

$$\begin{aligned}
d^{(2)} &= \frac{1}{\omega} [210(5 + 16n_r + 22n_r^2 + 12n_r^3 + 6n_r^4) \tilde{\epsilon}_3 \tilde{\gamma}_7 + 10(1 + 2n_r)(13 + 14n_r + 14n_r^2) \tilde{\epsilon}_3 \tilde{\gamma}_5 \\
&\quad + 6(1 + 2n_r) \tilde{\delta}_1 \tilde{\delta}_3 + 2(11 + 30n_r + 30n_r^2) \tilde{\epsilon}_3 \tilde{\gamma}_3 + 12(1 + 2n_r + 2n_r^2) \tilde{\epsilon}_4 \tilde{\delta}_2 + 2 \tilde{\delta}_1^2 \\
&\quad + 70(1 + 2n_r)(3 + 2n_r + 2n_r^2) \tilde{\epsilon}_1 \tilde{\gamma}_7 + 2(1 + 2n_r) \tilde{\epsilon}_2 \tilde{\delta}_2 + 30(1 + 2n_r + 2n_r^2) \tilde{\epsilon}_1 \tilde{\gamma}_5 \\
&\quad + 12(1 + 2n_r + 2n_r^2) \tilde{\epsilon}_2 \tilde{\delta}_4 + 6(1 + 2n_r) \tilde{\epsilon}_1 \tilde{\gamma}_3 + 30(1 + 2n_r)(3 + 2n_r + 2n_r^2) \tilde{\epsilon}_2 \tilde{\delta}_6 \\
&\quad + 4(1 + 2n_r)(21 + 17n_r + 17n_r^2) \tilde{\epsilon}_4 \tilde{\delta}_4 + 60(12 + 35n_r + 46n_r^2 + 22n_r^3 + 11n_r^4) \tilde{\epsilon}_4 \tilde{\delta}_4 \\
&\quad + 30(1 + 2n_r + 2n_r^2) \tilde{\delta}_1 \tilde{\delta}_5 + (11 + 30n_r + 30n_r^2) \tilde{\delta}_3^2 + 10(1 + 2n_r)(13 + 14n_r + 14n_r^2) \tilde{\delta}_3 \tilde{\delta}_5 \\
&\quad + (449 + 1400n_r + 2030n_r^2 + 1260n_r^3 + 630n_r^4) \tilde{\delta}_5], \tag{A18}
\end{aligned}$$

$$\begin{aligned}
d^{(3)} = & \frac{1}{\omega^2} [4\tilde{\varepsilon}_1^2 \tilde{\delta}_2 + 8\tilde{\varepsilon}_1 \tilde{\varepsilon}_2 \tilde{\delta}_1 + 24(1+2n_r)\tilde{\varepsilon}_1^4 \tilde{\delta}_4 + 36(1+2n_r)\tilde{\varepsilon}_1 \tilde{\varepsilon}_2 \tilde{\delta}_2 + 2(1+2n_r)\tilde{\varepsilon}_2^3 + 36(1+2n_r)\tilde{\varepsilon}_1 \tilde{\varepsilon}_3 \tilde{\delta}_2 \\
& + 36(1+2n_r)\tilde{\varepsilon}_2 \tilde{\varepsilon}_3 \tilde{\delta}_1 + 48(1+2n_r)\tilde{\varepsilon}_1 \tilde{\varepsilon}_4 \tilde{\delta}_1 + 180(1+2n_r+2n_r^2)\tilde{\varepsilon}_1^2 \tilde{\delta}_6 \\
& + 240(1+2n_r+2n_r^2)\tilde{\varepsilon}_1 \tilde{\varepsilon}_2 \tilde{\delta}_5 + 48(1+2n_r+2n_r^2)\tilde{\varepsilon}_2^2 \tilde{\varepsilon}_4 + 16(11+30n_r+30n_r^2)\tilde{\varepsilon}_2 \tilde{\varepsilon}_3 \tilde{\delta}_3 \\
& + 8(11+30n_r+30n_r^2)\tilde{\varepsilon}_3^2 \tilde{\delta}_2 + 8(31+78n_r+78n_r^2)\tilde{\varepsilon}_1 \tilde{\varepsilon}_3 \tilde{\delta}_4 + 8(31+78n_r+78n_r^2)\tilde{\varepsilon}_1 \tilde{\varepsilon}_4 \tilde{\delta}_3 \\
& + 8(31+78n_r+78n_r^2)\tilde{\varepsilon}_3 \tilde{\varepsilon}_4 \tilde{\delta}_1 + 100(1+2n_r)(13+14n_r+14n_r^2)\tilde{\varepsilon}_2 \tilde{\varepsilon}_3 \tilde{\delta}_5 \\
& + 20(1+2n_r)(21+17n_r+17n_r^2)\tilde{\varepsilon}_2 \tilde{\varepsilon}_4^2 + 36(1+2n_r)(19+25n_r+25n_r^2)\tilde{\varepsilon}_3^2 \tilde{\delta}_4 \\
& + 72(1+2n_r)(19+25n_r+25n_r^2)\tilde{\varepsilon}_3 \tilde{\varepsilon}_4 \tilde{\delta}_3 + 60(1+2n_r)(35+34n_r+34n_r^2)\tilde{\varepsilon}_1 \tilde{\varepsilon}_3 \tilde{\delta}_6 \\
& + 12(111+347n_r+472n_r^2+250n_r^3+125n_r^4)\tilde{\varepsilon}_4^3 + 40(1+2n_r)(47+45n_r+45n_r^2)\tilde{\varepsilon}_1 \tilde{\varepsilon}_4 \tilde{\delta}_5 \\
& + 20(323+1125n_r+1668n_r^2+1086n_r^3+543n_r^4)\tilde{\varepsilon}_3^2 \tilde{\delta}_6 + 24(474+1625n_r+2430n_r^2+1610n_r^3+805n_r^4)\tilde{\varepsilon}_3 \tilde{\varepsilon}_4 \tilde{\delta}_5],
\end{aligned} \tag{A19}$$

$$\begin{aligned}
d^{(4)} = & -\frac{1}{\omega^3} [144(11+30n_r+30n_r^2)\tilde{\varepsilon}_1 \tilde{\varepsilon}_3^2 \tilde{\delta}_3 + 16\tilde{\varepsilon}_1^2 \tilde{\varepsilon}_2^2 + 24(1+2n_r)(561+685n_r+685n_r^2)\tilde{\varepsilon}_1 \tilde{\varepsilon}_3 \tilde{\varepsilon}_4^2 \\
& + 32(31+78n_r+78n_r^2)\tilde{\varepsilon}_1^2 \tilde{\varepsilon}_4^2 + 80(1+2n_r)\tilde{\varepsilon}_1^3 \tilde{\delta}_5 + 216(1+2n_r)\tilde{\varepsilon}_1^2 \tilde{\varepsilon}_3 \tilde{\delta}_3 + 180(1+2n_r)\tilde{\varepsilon}_1 \tilde{\varepsilon}_2^2 \tilde{\varepsilon}_3 \\
& + 8\tilde{\varepsilon}_1^3 \tilde{\delta}_3 + 216(1+2n_r)\tilde{\varepsilon}_1 \tilde{\varepsilon}_3^2 \tilde{\delta}_1 + 48(11+30n_r+30n_r^2)\tilde{\varepsilon}_2^2 \tilde{\varepsilon}_3^2 + 240(1+2n_r)\tilde{\varepsilon}_1^2 \tilde{\varepsilon}_2 \tilde{\varepsilon}_4 \\
& + 40(49+114n_r+114n_r^2)\tilde{\varepsilon}_1^2 \tilde{\varepsilon}_3 \tilde{\delta}_5 + 96(31+78n_r+78n_r^2)\tilde{\varepsilon}_1 \tilde{\varepsilon}_2 \tilde{\varepsilon}_3 \tilde{\varepsilon}_4 + 24\tilde{\varepsilon}_1^2 \tilde{\varepsilon}_3 \tilde{\delta}_1 \\
& + 120(1+2n_r)(122+145n_r+145n_r^2)\tilde{\varepsilon}_1 \tilde{\varepsilon}_3^2 \tilde{\delta}_5 + 48(11+30n_r+30n_r^2)\tilde{\varepsilon}_3^3 \tilde{\delta}_1 \\
& + 504(1+2n_r)(19+25n_r+25n_r^2)\tilde{\varepsilon}_2 \tilde{\varepsilon}_3^2 \tilde{\varepsilon}_4 + 120(1+2n_r)(31+47n_r+47n_r^2)\tilde{\varepsilon}_3^3 \tilde{\delta}_3 \\
& + 4(11\,827+43\,479n_r+68\,424n_r^2+49\,890n_r^3+24\,945n_r^4)\tilde{\varepsilon}_3^2 \tilde{\varepsilon}_4^2 \\
& + 8(4517+16\,815n_r+26\,580n_r^2+19\,530n_r^3+9\,765n_r^4)\tilde{\varepsilon}_3^3 \tilde{\delta}_5],
\end{aligned} \tag{A20}$$

$$\begin{aligned}
d^{(5)} = & \frac{1}{\omega^4} [96\tilde{\varepsilon}_1^3 \tilde{\varepsilon}_2 \tilde{\varepsilon}_3 + 768(11+30n_r+30n_r^2)\tilde{\varepsilon}_1 \tilde{\varepsilon}_2 \tilde{\varepsilon}_3^3 + 1056(1+2n_r)\tilde{\varepsilon}_1^3 \tilde{\varepsilon}_3 \tilde{\varepsilon}_4 + 16\tilde{\varepsilon}_1^4 \tilde{\varepsilon}_4 \\
& + 288(53+138n_r+138n_r^2)\tilde{\varepsilon}_1^2 \tilde{\varepsilon}_3^2 \tilde{\varepsilon}_4 + 48(1+2n_r)(1817+2515n_r+2515n_r^2)\tilde{\varepsilon}_1 \tilde{\varepsilon}_3^3 \tilde{\varepsilon}_4 \\
& + 48(1+2n_r)(1817+2515n_r+2515n_r^2)\tilde{\varepsilon}_1 \tilde{\varepsilon}_3^3 \tilde{\varepsilon}_4 + 540(1+2n_r)(31+47n_r+47n_r^2)\tilde{\varepsilon}_2 \tilde{\varepsilon}_4^4 \\
& + 1512(1+2n_r)\tilde{\varepsilon}_1^2 \tilde{\varepsilon}_2 \tilde{\varepsilon}_3^2 + 12(15\,169+59\,385n_r+98\,160n_r^2+77\,550n_r^3+38\,775n_r^4)\tilde{\varepsilon}_3^4 \tilde{\varepsilon}_4],
\end{aligned} \tag{A21}$$

$$\begin{aligned}
d^{(6)} = & -\frac{1}{\omega^5} [144\tilde{\varepsilon}_1^4 \tilde{\varepsilon}_3^2 + 3024(1+2n_r)\tilde{\varepsilon}_1^3 \tilde{\varepsilon}_3^3 + 2304(11+30n_r+30n_r^2)\tilde{\varepsilon}_1^2 \tilde{\varepsilon}_3^4 \\
& + 3240(1+2n_r)(31+47n_r+47n_r^2)\tilde{\varepsilon}_1 \tilde{\varepsilon}_3^5 + 4(39\,709+16\,2405n_r+27\,8160n_r^2 \\
& + 23\,1510n_r^3+11\,5755n_r^4)\tilde{\varepsilon}_3^6],
\end{aligned} \tag{A22}$$

where

$$\tilde{\varepsilon}_j = \frac{\varepsilon_j}{(2\omega)^{j/2}}, \quad \tilde{\delta}_j = \frac{\delta_j}{(2\omega)^{j/2}}, \quad \tilde{\gamma}_j = \frac{\gamma_j}{(2\omega)^{j/2}}.$$

As an illustration with the class of power-law potentials Ar^v , we display below the result of the foregoing equation (A14) in the case of the shifted $1/N$ expansion

$$\begin{aligned}
\bar{E} = & \bar{k}^{(\nu-2)/(\nu+2)} (4\nu A)^{2/(\nu+2)} \left\{ \frac{\bar{k}(\nu+2)}{8\nu} - \frac{(\nu+1)(\nu-2)}{12^3 \bar{k}^2 \sqrt{\nu+2}} \left(12(1+6n_r+6n_r^2) \sqrt{\nu+2} \bar{k} - (\nu+1)(\nu-2) \right. \right. \\
& - (7\nu^2 - 31\nu - 62)n_r - (5\nu^2 - 29\nu - 58)(3+2n_r)n_r^2 - \frac{12}{\bar{k}\sqrt{\nu+2}} \left[\frac{1}{32400} (317\nu^4 - 166\nu^3 \right. \\
& - 1923\nu^2 - 15364\nu - 17164) + \frac{1}{48} (\nu+1)(\nu-2)(3\nu^2 - 19\nu - 6)n_r \\
& + \frac{1}{580} (74\nu^4 - 1147\nu^3 + 1839\nu^2 + 9332\nu + 7892)n_r^2 + \frac{1}{2160} (161\nu^4 - 3598\nu^3 + 7041\nu^2 \\
& \left. \left. + 35348\nu + 31028)(2+n_r)n_r^3 \right] \right) + O\left(\frac{1}{\bar{k}^4}\right) \left. \right\}. \tag{A23}
\end{aligned}$$

APPENDIX B

For the sake of comparison with the formulas of our HVHF method and those of the RSPT, we recall here the set of recursion relations derived by Stepanov and Tutik [90] in the framework of their semiclassical approach for the computation of the energy eigenvalues. We set here $m=1$. The \hbar expansion for the bound energy is represented in the form

$$E = \sum_{k=0}^{\infty} E_k \hbar^k, \tag{B1}$$

where

$$E_0 = V_0 + \frac{\Lambda^2}{8r_0^2}, \quad E_1 = \frac{1}{2} \left\{ \tilde{\gamma}_1 + (1+2n_r) \frac{\omega_0}{r_0} \right\}, \tag{B2}$$

$$E_k = \frac{1}{2} \left\{ \tilde{\gamma}_k + \frac{1}{r_0} C_{2k-2}^{k-1} - \sum_{i=1}^{k-1} \sum_{j=0}^{2k-2} C_j^i C_{2k-2-j}^{k-i} - 2 \sum_{j=1}^{2k-2} C_j^0 C_{2k-2-j}^{k-i} \right\}, \quad k \geq 2 \tag{B3}$$

where the coefficients C_j^i are expressed as follows:

$$C_0^0 = -\omega_0, \quad C_1^0 = -\frac{\omega_0 a_1}{2}, \tag{B4a}$$

$$C_i^0 = \begin{cases} -\frac{1}{2C_0^0} \left(2 \sum_{j=1}^p C_j^0 C_{i-j}^0 - (C_p^0)^2 - \omega_0^2 a_i \right), & i=2p \\ -\frac{1}{2C_0^0} \left(2 \sum_{j=1}^p C_j^0 C_{i-j}^0 - \omega_0^2 a_i \right), & i=2p+1, \quad p=1,2,\dots \end{cases} \tag{B4b}$$

It should be noted that in their paper Stepanov and Tutik [90] have omitted the global factor 1/2 in Eq. (23) which corresponds to Eq. (B4b),

$$C_0^1 = \frac{n_r}{r_0}, \quad C_i^1 = \frac{1}{2C_0^0} \left\{ (1+i) \left[(-1)^i \tilde{\gamma}_1 - \frac{1}{r_0} C_i^0 \right] - 2 \sum_{j=1}^i C_j^0 C_{i-j}^1 \right\}, \quad i=1,2,3,\dots \tag{B5a}$$

$$C_i^0 = \begin{cases} \frac{1}{2C_0^0} \left(\frac{2i-3}{r_0} C_0^{i-1} - 2 \sum_{j=1}^p C_0^j C_0^{i-j} + (C_0^p)^2 \right), & i=2p \\ \frac{1}{2C_0^0} \left(\frac{2i-3}{r_0} C_0^{i-1} - 2 \sum_{j=1}^p C_0^j C_0^{i-j} \right), & i=2p+1, \quad p=1,2,\dots \end{cases} \tag{B5b}$$

Finally

$$C_{2i-2}^i = 0, \quad (\text{B6a})$$

$$C_j^i = \frac{1}{2C_0^0} \left\{ (3+j-2i) \left[(-1)^j \theta(j-2i+2) \tilde{\gamma}_i - \frac{1}{r_0} C_j^{i-1} \right] - 2 \sum_{s=1}^i C_s^0 C_{j-s}^1 - \sum_{q=1}^{i-1} \sum_{s=0}^j C_s^0 C_{j-s}^{i-q} \right\}, \quad i \geq 2, \quad j = 1, 2, 3, \dots \quad (\text{B6b})$$

The quantities $\tilde{\gamma}_i$, ω_0 , and a_k are written as follows:

$$\tilde{\gamma}_1 = \frac{A\Lambda}{2r_0^2}, \quad \tilde{\gamma}_2 = \frac{B}{r_0^2}, \quad \tilde{\gamma}_i = 0, \quad i \geq 3, \quad (\text{B7a})$$

$$\omega_0^2 = 2V_2 + 3V_1 = \frac{4\Lambda^2}{r_0^2} \omega^2, \quad (\text{B7b})$$

$$a_k = \frac{2}{\omega_0^2} \left(V_{k+2} + (-1)^k \frac{k+3}{2} V_1 \right), \quad V_k = \frac{r_0^k V_0^{(k)}}{k!}, \quad k = 1, 2, \dots \quad (\text{B7c})$$

In Ref. [90] there is a misprint in the expression of a_k , i.e., V_k should be replaced by V_1 . The first coefficients a_k are related to the parameter ϵ_k , δ_k , and γ_k by

$$a_1 = \eta \epsilon_3, \quad a_2 = \eta \epsilon_4, \quad a_3 = \eta \delta_5, \quad a_4 = \eta \delta_6, \quad a_5 = \eta \gamma_7, \quad a_6 = \eta \gamma_8, \quad \eta = \frac{1}{4\Lambda \omega^2}. \quad (\text{B8})$$

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