On large-*N* expansions

2002 J. Phys. A: Math. Gen. 35 10663

(http://iopscience.iop.org/0305-4470/35/49/313)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND GENERAL

J. Phys. A: Math. Gen. **35** (2002) 10663–10667 PII: S0305-4470(02)38624-4

COMMENT

On large-*N* expansions

Francisco M Fernández

Cequinor (Conicet), Facultad de Ciencias Exactas, Universidad Nacional de La Plata, Calle 47 y 115, Casilla de Correo 962, 1900 La Plata, Argentina

E-mail: framfer@isis.unlp.edu.ar

Received 24 June 2002
Published 28 November 2002
Online at stacks.iop.org/JPhysA/35/10663

Abstract
We show that a recently proposed shifted large-*l* expansion is exactly the well-known shifted large-*N* expansion. Results for truncated Coulomb potentials cast doubts on previous conclusions drawn from shifted large-*l* calculations.

PACS number: 03.65.Ge

Large-*N* expansions prove to be a simple and sufficiently accurate way of calculating energies of one-dimensional and central-field quantum-mechanical models. Such approaches are extremely popular and have therefore been discussed by many authors. Despite such popularity, there still seems to be a good deal of misunderstanding about them. For example, the authors of two recent papers propose a variant of the well-known shifted large-*N* expansion technique (SLNT) [1–3] that they call the pseudoperturbative shifted-*l* expansion technique (PSLET) [4, 5]. They state, 'the difficulty in calculating high-order corrections in SLNT through Rayleigh–Schrödinger perturbation theory results in loss in accuracy. PSLET makes it possible to calculate high-order corrections, which improves the accuracy', and 'the outstanding feature of the attendant PSLET is that it avoids troublesome questions such as those pertaining to the nature of small-parameter expansions, . . .' [5].

We believe that such statements are at least misleading, and for that reason here we discuss and compare the SLNT and the PSLET. The SLNT is an expansion in powers of $\bar{k}^{-1/2}, \bar{k} = k - a, k = N + 2l$, where N, l and a stand for the number of dimensions, the angular momentum quantum number and a properly chosen shift, respectively. On the other hand, the PSLET is an expansion in powers of $\bar{l}^{-1/2}$, where $\bar{l} = l - \beta$, and β is a shift. After expanding the potential-energy function and the centrifugal term in Taylor series about an appropriate point r_0 one is left with the Hamiltonian operator for a harmonic oscillator plus a polynomial perturbation. Then one applies perturbation theory and obtains the perturbation series for the eigenfunctions and eigenvalues.

Up to this point, the PSLET and the SLNT are similar; however, Odeh and Mustafa [4, 5] seem to believe that the SLNT is somehow tied to a particular way of calculation of the perturbation corrections, which restricts systematic improvement to low order. They appear to be unaware of earlier SLNT calculations of much greater orders [6–9] than those considered

in their papers. Moreover, the method used in those earlier papers for the calculation of the perturbation corrections for excited states is much more efficient than that used by Odeh and Mustafa.

The convergence properties of the SLNT and the PSLET perturbation series depend on the form of the potential-energy function and on the value of the shift parameter [6–11]. Therefore, it is not true that one can bypass questions regarding the 'smallness of the perturbation'.

In order to make all those points clear, here we apply the SLNT to some truncated Coulomb potentials and carry out a perturbation calculation of order greater than those considered by Odeh and Mustafa [5], and try to find out whether the PSLET is in any way different to, or offers any advantage over, the well-known SLNT.

For brevity, we consider the dimensionless radial eigenvalue equation $\hat{H}\Phi = E\Phi$, where $\hat{H} = -\frac{1}{2}\frac{d^2}{r^2} + \frac{(k-1)(k-3)}{8r^2} + V(r)$, $V(r)$ is the potential-energy function, $k = N + 2l$, N is the space dimension and $l = 0, 1, \ldots$ is the angular momentum quantum number. The radial part of the eigenfunction satisfies the boundary conditions $\Phi(0) = \Phi(\infty) = 0$ for bound states.

We define $\bar{k} = k - a$, where a is an appropriate shift (see below), introduce a perturbation parameter $\lambda = \bar{k}^{-1/2}$ and expand the potential-energy function and the centrifugal term in Taylor series about $r = r_0$; for example, $V(r) = \sum_{j=0}^{\infty} V_j(r_0)(r - r_0)^j$, $V_j(r) = \frac{1}{j!}\frac{\mathrm{d}^j}{\mathrm{d}r^j}V(r)$. Choosing the expansion point r_0 to satisfy $4r_0^3 V_1(r_0) = \bar{k}^2$ we obtain a new Hamiltonian operator [11]

$$\begin{aligned}\hat{h} &= r_0^2\lambda^2\hat{H} - \frac{(k-1)(k-3)\lambda^2}{8} - r_0^2\lambda^2 V_0 \\ &= -\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}q^2} + \frac{\omega^2}{2}q^2 + \sum_{j=1}^{\infty}(a_j q^{j+2} + b_j q^j)\lambda^j + \sum_{j=1}^{\infty} c_j q^j \lambda^{j+2}\end{aligned} \tag{1}$$

where $q = \frac{r-r_0}{\lambda r_0}$, $\omega^2 = \frac{3}{4} + \frac{2r_0^4 V_2}{k^2}$, $a_j = \frac{(-1)^j(j+3)}{8} + \frac{V_{j+2}}{k^2}r_0^{j+4}$, $b_j = \frac{(-1)^j(2-a)(j+1)}{4}$, and $c_j = \frac{(-1)^j(a-1)(a-3)(j+1)}{8}$.

The Hamiltonian $\hat{h}$ is a dimensionless harmonic oscillator with frequency ω plus a polynomial perturbation. Therefore, we can apply perturbation theory to $\hat{h}\chi = \varepsilon\chi$ and obtain λ-power series for the eigenvalue ε and the eigenfunction χ. From the perturbation series for ε we easily obtain the eigenvalue of the original equation

$$E = V_0 + \frac{1}{8r_0^2\lambda^2} + \frac{2a - 4 + 8\varepsilon_0}{8r_0^2\lambda^2} + \frac{(a-1)(a-3) + 8\varepsilon_2}{8r_0^2} + \frac{1}{r_0^2}\sum_{j=2}^{\infty}\varepsilon_{2j}\lambda^{2j-2} \tag{2}$$

where $\varepsilon_0 = \left(\nu + \frac{1}{2}\right)\omega$ and $\nu = 0, 1, \ldots$ is the harmonic-oscillator quantum number. One can easily prove that the perturbation corrections of odd order ε_{2j+1} vanish for all j [11].

The purpose of the shift parameter a is the improvement of the convergence properties of the perturbation series. It is customary to choose a in order to remove the third term on the right-hand side of equation (2): $a = 2 - 4\varepsilon_0 = 2 - 2(2\nu + 1)\omega$. In this way, the SLNT gives the correct answer for the harmonic oscillator and the hydrogen atom to all orders [1–3, 9]. However, there are difficult cases in which this simple choice is insufficient and it is necessary to select an order-dependent value of a according to minimal sensitivity or any other appropriate criterion [6–11].

It follows from the equations given above that r_0 depends on k and ν:

$$2 - 2(2\nu + 1)\sqrt{\frac{3V_1 + 2r_0V_2}{4V_1}} = k - 2\sqrt{r_0^3 V_1}. \tag{3}$$

At this point, it is appropriate to compare the SLNT with the PSLET. First, one easily convinces oneself that equation (3) is equivalent to that derived by Odeh and Mustafa [4, 5].

Second, note that $\frac{\bar{k}}{2} = \bar{l} = l - \beta$ for $N = 3$ if $\beta = \frac{a-3}{2}$. Therefore, if the shift parameters a and β are chosen according to the same criterion, then the SLNT and the PSLET give exactly the same result. In other words, the PSLET is nothing but a disguised SLNT. The only advantage of the method proposed by Mustafa and Odeh [4, 5] appears to be a claimed improved calculation of the perturbation corrections. However, as we have already noted in the introduction, there are earlier calculations [6–9] of much larger order than those considered by Mustafa and Odeh, and, consequently, their claim seems to lack support.

In addition to what we have just mentioned, Mustafa and Odeh state that the accuracy of the PSLET results increases with the number of radial nodes (ν in the equations above); however, their approach based on logarithmic perturbation theory is impractical for highly oscillatory wavefunctions. In fact, they appear to draw that conclusion from results for at most one nodal surface [5]. Moreover, they first suggest that the PSLET series are asymptotic divergent and then conclude, 'the PSLET results show a good converging trend to the exact values as the truncation parameter becomes larger ... ' [5]. It is well known that in some cases one does not appreciate the divergence of the perturbation series if one does not take into account terms of sufficiently large order. We show some results below.

Following Odeh and Mustafa [5] we consider the truncated Coulomb potentials $V(r) = -\frac{1}{(r^b+\alpha^b)^{1/b}}$, $\alpha, b > 0$. In order to calculate the perturbation coefficients ε_{2j} we make use of the method of Swenson and Danforth that combines perturbation theory with the hypervirial and Hellmann–Feynman theorems [11]. Although this method does not give the eigenfunction explicitly, it is most convenient for our present purposes because it is easily programmable and yields perturbation corrections of any order in terms of the quantum numbers of the unperturbed Hamiltonian operator (the harmonic oscillator in the present case). Therefore, the calculation of the energy of highly oscillatory states offers no more difficulty than the ground state. This is not the case for the logarithmic perturbation theory that becomes increasingly cumbersome as the number of nodes increases [5].

We carry out the calculation by means of Maple [12] in the following way: first, we obtain the perturbation coefficients ε_j exactly in terms of unevaluated $\varepsilon_0, \omega, a_j, b_j$ and c_j; second, we substitute the symbolic values of those variables according to the equations shown above; third, we solve equation (3) for r_0 numerically for the chosen values of α and b and convert the result to a fraction; fourth, we obtain the sum (2) in floating-point arithmetic with a sufficient number of digits. In this way, we hope to avoid round-off errors. We truncate the divergent series $S = t_0 + t_1 + t_2 + \cdots$ according to a well-known criterion based on the assumption that the error of $S_M = t_0 + t_1 + \cdots + t_M$ is proportional to $|t_{M+1}|$ [11, 13]. In this communication $E = S$ and t_j is the term corresponding to the perturbation coefficient ε_{2j}.

We expect the accuracy of the approach to decrease with α because the potential-energy function is singular at $r = (-1)^{1/b}\alpha$. In what follows, we consider the case $b = 1$ as a benchmark. We are aware that one can solve this simple model more efficiently in other ways. For example, one can transform the Schrödinger equation for the s states into a hypergeometric equation, or into a three-term recurrence relation for any state by means of a straightforward power-series expansion with an appropriate exponential factor [14]. In this way, one may easily obtain much more accurate results for such particular example. On the other hand, the SLNT and PSLET apply to real and rational values of b which the power-series method may not be suitable for.

Table 1 shows S_M, $\log|t_M|$ and $\log|t_M/S_M|$ for $\alpha = 0.1, l = \nu = 0$; $\alpha = 0.1$ being the most unfavourable case considered by Odeh and Mustafa [5]. Note that the logarithmic error decreases from $M = 0$ to $M = 12$ and then it appears to increase as expected for an asymptotic divergent series. Although Maple enables one to use floating-point arithmetic of arbitrary precision, the RAM of our computer was insufficient to perform calculations of larger order

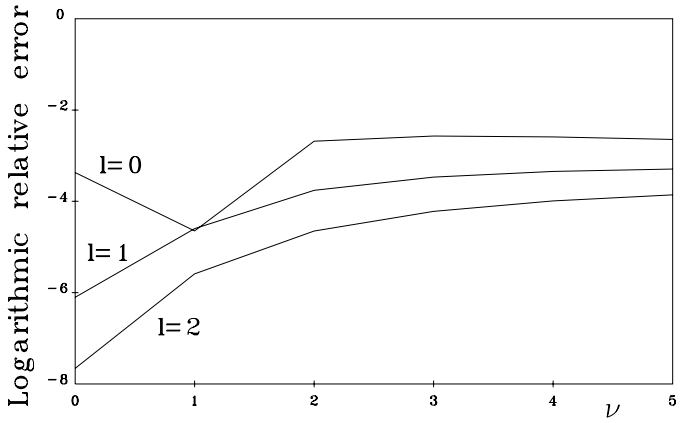

Figure 1. Logarithmic relative error for the energies supported by the potential-energy function $V(r) = -1/(r + 0.1)$ for several values of l and ν.

Table 1. Shifted large-N expansion for the ground-state eigenvalue ($l = 0$, $\nu = 0$) of the potential $V(r) = -1/(r + 0.1)$.

M	S_M	$\log \lvert t_M \rvert$	$\log \lvert t_M / S_M \rvert$
0	−0.386	−0.45	−0.04
2	−0.389	−2.54	−2.13
4	−0.3865	−2.68	−2.27
6	−0.3869	−3.37	−2.96
8	−0.3876	−3.14	−2.73
10	−0.3879	−3.52	−3.11
12	−0.3878	−3.78	−3.37
14	−0.3874	−3.42	−3.00

with sufficient accuracy. According to the present calculation (and the truncation criterion mentioned above) the SLNT approximate energy is $E = -0.3879$ with a logarithmic relative error $\log |t_M/S_M| = -3.37$. This result agrees with the corresponding Padé approximant constructed by Odeh and Mustafa [5], and our estimate of the logarithmic error is consistent with the difference between the perturbation and exact energies [5].

As already stated above, our perturbation series is valid for any radial quantum number ν. This generality comes from an appropriate implementation of Rayleigh–Schrödinger perturbation theory already discussed above, and enables us to study the accuracy of the SLNT (or PSLET) in terms of ν. Figure 1 shows the logarithmic relative error for $l = 0$, $l = 1$ and $l = 2$, as a function of ν. We clearly appreciate that the error decreases with l and slowly increases with ν, except for misleading oscillations at low values of ν that may mask the overall trend. The former behaviour is explained by the obvious fact that the perturbation parameter decreases with l. On the other hand, as ν increases, the energy approaches the rim of the well and is increasingly affected by the anharmonic part of the potential. Odeh and Mustafa [5] concluded, 'The accuracy of the PSLET results increases with increasing l and/or n_r'. However, they did not really monitor the sole effect of n_r on the accuracy because they allowed l to increase with n_r (ν in present notation) as they considered states 1s, 3p and 4d. The apparent reason for the choice of that sequence of states was that they were unable to

apply their perturbation algorithm to eigenfunctions with more than one node. Figure 1, on the other hand, shows the effect of v on the accuracy for fixed values of l.

We have tried to prove the following facts. First, the PSLET is just a version of the SLNT for three dimensions. Second, it is not true that the PSLET enables one to obtain more perturbation corrections than the SLNT. In fact, here we have obtained more perturbation corrections and for more states than those ever considered by Odeh and Mustafa [5] because we resorted to a more efficient implementation of perturbation theory. Third, it seems that the SLNT (and, consequently, also the PSLET) is divergent. As expected, the accuracy of properly truncated series increases with the angular quantum number and decreases with the radial quantum number. We agree with Odeh and Mustafa [5] in that the SLNT yields acceptable eigenvalues for truncated Coulomb potentials over a wide range of quantum numbers, and for that reason we do not believe it necessary to resort to more sophisticated choices of the shift parameter a [9–11].

References

[1] Sukhatme U and Imbo T 1983 *Phys. Rev.* D **28** 418
[2] Imbo T, Pagnamenta A and Sukhatme U 1984 *Phys. Rev.* D **29** 1669
[3] Imbo T, Pagnamenta A and Sukhatme U 1984 *Phys. Lett.* A **105** 183
[4] Mustafa O and Odeh M 2000 *J. Phys. A: Math. Gen.* **33** 5207
[5] Odeh M and Mustafa O 2000 *J. Phys. A: Math. Gen.* **33** 7013
[6] Maluendes S A, Fernández F M, Mesón A M and Castro E A 1986 *Phys. Rev.* D **34** 1835
[7] Maluendes S A, Fernández F M and Castro E A 1987 *Phys. Rev.* A **36** 1452
[8] Maluendes S A, Fernández F M and Castro E A 1987 *Phys. Lett.* A **124** 215
[9] Chaterjee A 1990 *Phys. Rep.* **186** 249
[10] Njock M G K, Nsangou M and Bona Z 2000 *Phys. Rev.* A **61** 042105
[11] Fernández F M 2000 *Introduction to Perturbation Theory in Quantum Mechanics* (Boca Raton, FL: CRC Press)
[12] Maple 7 2000 (Waterloo Maple Inc.)
[13] Bender C M and Orszag S A 1978 *Advanced Mathematical Methods for Scientists and Engineers* (New York: McGraw-Hill)
[14] Fernández F M 1991 *J. Phys. A: Math. Gen.* **61** 1351