PHYSICAL REVIEW A VOLUME 38, NUMBER 3 AUGUST 1, 1988

Comparison of $1/N$ expansion and shifted $1/N$ expansion for eigenenergies of an atomic potential

Y. P. Varshni

Ottawa-Carleton Institute for Physics, University of Ottawa, Ottawa, Canada K1N 6N5

(Received 11 December 1987)

Eigenenergies are calculated for the potential $V(r)=-(a/r)[1+(1+br)e^{-2br}]$ by the shifted $1/N$ expansion method and the results are compared with those obtained by Sever and Tezcan for the same potential by the $1/N$ method. The shifted $1/N$ expansion results show a large improvement over the $1/N$ expansion results.

The large-N expansion, where N is the number of spatial dimensions, has been applied by a number of authors for solving the Schrödinger equation.[1-9] For spherically symmetric potentials, the method has been improved by Sukhatme *et al.*[10,11] by using the quantity $1/\bar{k}$ as an expansion parameter, where $\bar{k}=N+2l-a$, l being the orbital angular momentum quantum number and "a" is a suitable shift. This modified method is known as the shifted $1/N$ expansion and has proved to be useful for a number of potentials.[12-18] A modified $1/N$ expansion has also been proposed.[19]

Recently Sever and Tezcan[9] (ST) have applied the large-N expansion to the following potential:

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

With appropriate values of a and b, Eq. (1) represents the potential experienced by the second electron in a helium atom, due to the nucleus and the first electron. Earlier Gerry and Laub[20] had studied this potential by the dynamical-group method. Besides its importance for the helium problem, the potential (1) is of special interest being the prototype of more general potentials used in atomic problems.[20-25] Potential (1) is a special case of the corresponding potential in the case of heliumlike ions:[26]

$$V(r)=-\frac{(Z-1)}{r}+\frac{1}{r}(1+Zr)e^{-2Zr} , \tag{2}$$

where Z is the nuclear charge.

In the present note we present the eigenvalue results obtained from the shifted $1/N$ expansion method for the potential (1) and compare them with those obtained by the $1/N$ expansion method. This enables us to draw inferences as to the improvement possible by the shifted $1/N$ expansion as also the limitations of the two methods.

ST have expressed their results in terms of β, where $\beta=b/a$. As we wish to compare our results with those of ST, we shall find it convenient to express the potential (1) in terms of β:

$$U(x)=\frac{V(r)}{a^2}=-(1/x)[1+(1+\beta x)e^{-2\beta x}] , \tag{3}$$

where $x=ar$.

Imbo *et al.*[11] have discussed the method for obtaining eigenvalues by the shifted $1/N$ expansion. Here we only quote the final expressions obtained using their method. We shall use atomic units ($\hbar=m=1$) in obtaining the formulas.

The potential is replaced by an effective potential and the energy eigenvalues are obtained in terms of the position of the minimum of this potential, x_0. The expression which determines x_0 is as follows:

$$(2l+1)+(2n_r+1)\left[\frac{1+y+2\beta x_0 y+2\beta^2 x_0^2 y-4\beta^3 x_0^3 y}{1+y+2\beta x_0 y+2\beta^2 x_0^2 y}\right]^{1/2}=2[x_0(1+y+2\beta x_0 y+2\beta^2 x_0^2 y)]^{1/2} , \tag{4}$$

where n_r is the radial quantum number and $y=e^{-2\beta x_0}$.

The energy is given by an expansion in powers of $1/\bar{k}$, where

$$\bar{k}=2[x_0(1+y+2\beta x_0 y+2\beta^2 x_0^2 y)]^{1/2} . \tag{5}$$

Thus we have

$$\frac{E}{a^2}=\frac{\bar{k}^2}{x_0^2}\left[\frac{1}{8}-\frac{1+y+\beta x_0 y}{4(1+y+2\beta x_0 y+2\beta^2 x_0^2 y)}+\frac{\gamma^{(1)}}{\bar{k}^2}+\frac{\gamma^{(2)}}{\bar{k}^3}+O(1/\bar{k}^4)\right] . \tag{6}$$

The expressions for $\gamma^{(1)}$ and $\gamma^{(2)}$ appearing in the corrections to the leading order of the energy expansion are given in Ref. 18. The various quantities occurring in these expressions can be expressed as follows for the potential (1):

$$\tilde{\epsilon}_j=\epsilon_j/(2\omega)^{j/2}, \quad \tilde{\delta}_j=\delta_j/(2\omega)^{j/2} ,$$

$$\omega=\frac{1}{2}\left[\frac{1+y+2\beta x_0 y+2\beta^2 x_0^2 y-4\beta^3 x_0^3 y}{1+y+2\beta x_0 y+2\beta^2 x_0^2 y}\right]^{1/2} ,$$

$$a=2-2(2n_r+1)\omega \ ,$$

$$\delta_1=-\tfrac{2}{3}\delta_2=-(1-a)(3-a)/4 \ ,$$

$$\delta_3=-\tfrac{4}{5}\delta_4=2\epsilon_1=-\tfrac{4}{3}\epsilon_2=2-a \ ,$$

$$\epsilon_3=-\frac{1}{2}+\frac{3+3y+6\beta x_0y+6\beta^2x_0^2y+4\beta^3x_0^3y+4\beta^4x_0^4y}{12(1+y+2\beta x_0y+2\beta^2x_0^2y)} \ ,$$

$$\epsilon_4=\frac{5}{8}-\frac{3+3y+6\beta x_0y+6\beta^2x_0^2y+4\beta^3x_0^3y+2\beta^4x_0^4y+2\beta^5x_0^5y}{12(1+y+2\beta x_0y+2\beta^2x_0^2y)} \ ,$$

$$\delta_5=-\frac{3}{4}+\frac{15+15y+30\beta x_0y+30\beta^2x_0^2y+20\beta^3x_0^3y+10\beta^4x_0^4y+4\beta^5x_0^5y+4\beta^6x_0^6y}{60(1+y+2\beta x_0y+2\beta^2x_0^2y)} \ ,$$

$$\delta_6=\frac{7}{8}-\frac{45+45y+90\beta x_0y+90\beta^2x_0^2y+60\beta^3x_0^3y+30\beta^4x_0^4y+12\beta^5x_0^5y+4\beta^6x_0^6y+4\beta^7x_0^7y}{180(1+y+2\beta x_0y+2\beta^2x_0^2y)} \ .$$

The calculated values of E/a^2 by the shifted $1/N$ expansion are compared with those obtained by $1/N$ expansion and also with the "exact" values obtained from a numerical intergration of the Schrödinger equation in Tables I and II for 1*s* and 2*s* states, respectively. ST have given expressions for E/a^2 to the order β^4 for both the states. In order to see the effect of higher-order terms, the coefficients of β^5 and β^6 terms were calculated for the 1*s* state from the equations given by ST. The final result to the order β^6 for the 1*s* state (by the $1/N$ expansion) is as follows:

$$E/a^2=-2+\beta-\tfrac{1}{2}\beta^3+5\beta^4/8-1781\beta^5/10\,240$$
$$+74\,879\beta^6/163\,840 \ .$$

We may note here one minor misprint in one of the relevant equations in ST's paper: In Eq. (21), in the expression for $E_0^{(7)}$, the second term should be $36D^3/\tilde{a}$. We further note that the calculations of ST were carried out with the correct expression[27] and their numerical results are correct.

ST have given eigenvalues obtained from a numerical solution of the Schrödinger equation for $\beta \le 1$. As we wanted to go to higher values of β and also to improve the accuracy of some of the values for $\beta \le 1$, new calculations were carried out and the results obtained are shown in Tables I and II. Numerov's method with a logarithmic mesh was used.

Next we consider the individual states in detail. The

TABLE I. Comparison of energy eigenvalues for the 1*s* state of potential (1) as calculated from the $1/N$ expansion method, the shifted $1/N$ expansion method, and numerical intergration of the Schrödinger equation.

β	E/a^2 $1/N$ expansion (to order β^4)	E/a^2 $1/N$ expansion (to order β^6)	E/a^2 Shifted $1/N$ expansion	E/a^2 Exact
0.02	−1.980 00	−1.980 00	−1.980 00	−1.980 00
0.04	−1.960 03	−1.960 03	−1.960 03	−1.960 03
0.06	−1.940 10	−1.940 10	−1.940 10	−1.940 10
0.08	−1.920 23	−1.920 23	−1.920 23	−1.920 23
0.1	−1.900 44	−1.900 44	−1.900 44	−1.900 44
0.3	−1.708 44	−1.708 53	−1.709 56	−1.709 59
0.5	−1.5234	−1.5217	−1.5363	−1.536 55
0.7	−1.3214	−1.2969	−1.3836	−1.384 22
1.0	−0.8750	−0.5919	−1.1921	−1.194 20
1.2	−0.3680	+0.5639	−1.0871	−1.091 00
1.4	0.4290	2.9348	−0.9978	−1.004 20
1.6	1.648	7.492	−0.9230	−0.931 61
1.8	3.445	15.70	−0.8636	−0.871 09
2.0	6.000	29.68	−0.8244	−0.820 70
2.2	9.517	52.37	−0.8163	−0.778 70
2.4	14.224	87.71	−0.8564	−0.743 61
2.6			−0.9598	−0.714 19
2.8			−1.1114	−0.689 42
3.0			−1.1952	−0.668 46
3.2			−0.9032	−0.650 62

TABLE II. Comparison of energy eigenvalues for the 2*s* state of potential (1) as calculated from the $1/N$ expansion method, the shifted $1/N$ expansion method, and numerical integration of the Schrödinger equation.

β	E/a^2 $1/N$ expansion (to order β^4)	E/a^2 Shifted $1/N$ expansion	E/a^2 Exact
0.02	−0.480 05	−0.480 05	−0.480 05
0.04	−0.460 38	−0.460 38	−0.460 38
0.06	−0.441 16	−0.441 21	−0.441 21
0.08	−0.422 46	−0.422 67	−0.422 67
0.1	−0.404 25	−0.404 88	−0.404 87
0.3	−0.166 25	−0.275 46	−0.273 83
0.5	0.8437	−0.2295	−0.212 94
0.7	4.4017	−0.2735	−0.187 53
1.0	21.000	−0.3164	−0.172 17
1.2	45.628	−0.2156	−0.166 75
1.4	87.336	−0.1734	−0.162 61
1.6	152.65	−0.1501	−0.159 08
1.8		−0.1370	−0.155 93
2.0		−0.1303	−0.153 06
2.2		−0.1272	−0.150 45
2.4		−0.1258	−0.148 09

$1/N$ expansion technique that has been used by ST is based on the series expansion in terms of β in the calculation. It is convergent for $\beta \leq 1$. The agreement between the $1/N$ expansion values and the exact values is quite good for both the states when β is close to zero. Next we consider the individual states in detail. First the 1*s* state. For the $1/N$ expansion, the calculated values are shown, both to order β^4 and to β^6. It will be noticed from Table I that for the $1/N$ expansion the results to order β^6 are equal to or better than those to order β^4 for $\beta \leq 0.3$ but above this the situation is reversed and the β^6 results become rapidly much poorer than the β^4 results. The shifted $1/N$ expansion results show a significant improvement over the $1/N$ expansion results for $\beta \geq 0.3$. However, a comparison of the shifted $1/N$ expansion results with the exact values shows that the former values show an increasing error with increase in β. At $\beta = 2.0$, the error has reached 0.45% and above this value of β the error increases rather rapidly, reaching 79% at $\beta = 3$. In this region the correction terms (involving $\gamma^{(1)}$ and $\gamma^{(2)}$) are rather large, and of opposite sign.

Next we consider the 2*s* state. The $1/N$ expansion results show a rapid divergence from the exact results for $\beta > 0.1$. The shifted $1/N$ expansion results start showing an improvement over the $1/N$ expansion results from a much smaller value of β, as compared to the 1*s* case. However, as compared to the exact results, the shifted $1/N$ results show substantial errors as β increases beyond 0.5. The error continues to increase to $\beta = 1$ but, interestingly enough, then it drops. The numerical magnitude of the calculated energy from the shifted $1/N$ expansion remains greater than the exact value to about $\beta \simeq 1.5$, but then it becomes smaller. Beyond this point the error increases at first rapidly but then it settles at about 15%. For simple screened potentials, like the Yukawa potential, the results from the shifted $1/N$ expansion[12] show a slow and monotonous increase in error with the increase in the screening parameter. Potential (2) consists of three types of terms: a Coulomb term, a screened Coulomb term, and an exponential term, and the foregoing results show that for such a potential a much more complicated pattern is observed in the errors.

For the helium atom, $\beta = 2$ and for this value of β the agreement between the calculated value by the shifted $1/N$ expansion and the exact value for the 1*s* state is quite satisfactory, but for the 2*s* state, the error is rather large, being 14.9%. The $1/N$ expansion values are of the wrong sign and have very large errors.

In conclusion, we find that the shifted $1/N$ expansion offers a large improvement over the $1/N$ expansion for eigenvalues of the potential (2). It is highly likely that a similar situation will exist for other similar potentials. However, even with the shifted $1/N$ expansion, caution is necessary, and large errors are possible.

This work was supported in part by a research grant from the Natural Sciences and Engineering Research Council of Canada.

---

[1] L. Mlodinow and N. Papanicolaou, Ann. Phys. N.Y. **128**, 314 (1980); **131**, 1 (1981).

[2] L. Mlodinow and M. P. Shatz, J. Math. Phys. **25**, 943 (1984).

[3] G. Moreno and A. Zepeda, J. Phys. B **17**, 21 (1984).

[4] A. Chatterjee, J. Phys. A **18**, 1193 (1985); **18**, 2403 (1985); **19**, 3707 (1986).

[5] A. Chaterjee, Phys. Rev. A **34**, 2470 (1986); **35**, 2722 (1987).

[6] S. Erkoç and R. Sever, Phys. Rev. D **33**, 588 (1986).

[7] M. Jameel, J. Phys. A **19**, 1967 (1986).

[8] R. Sever and C. Tezcan, Phys. Rev. A **35**, 2725 (1987).

[9] R. Sever and C. Tezcan, Phys. Rev. A **36**, 1045 (1987).

[10] U. Sukhatme and T. Imbo, Phys. Rev. D **28**, 418 (1983).

[11] T. Imbo, A. Pagnamenta, and U. Sukhatme, Phys. Rev. D **29**, 1669 (1984).

[12] T. Imbo, A. Pagnamenta, and U. Sukhatme, Phys. Lett. **105A**, 183 (1984).

[13] R. Dutt, U. Mukherji, and Y. P. Varshni, Phys. Rev. A **34**, 777 (1986).

[14] R. Dutt, U. Mukherji, and Y. P. Varshni, J. Phys. B **19**, 3411 (1986).

[15] B. Roy, Phys. Rev. A **34**, 5108 (1986).

[16] B. Roy and R. Roychoudhury, J. Phys. A **20**, 3051 (1987).

[17] A. Z. Tang and F. T. Chan, Phys. Rev. A **35**, 911 (1987).

[18] Y. P. Varshni, Phys. Rev. A **36**, 3009 (1987).

[19] S. A. Maluendes, F. M. Fernandez, and E. A. Castro, Phys. Lett. **124A**, 215 (1987).

[20] C. C. Gerry and J. Laub, Phys. Rev. A **30**, 1229 (1984).

[21] J. Yunta, E. R. Mayquez, and C. Sanchez del Rio, Phys. Rev. A **9**, 1483 (1974).

[22] M. Berrondo, J. P. Daudey, and O. Goscinski, Chem. Phys.

Lett. **62**, 34 (1979).
[23]A. Hibbert, Adv. Atomic Mol. Phys. **18**, 309 (1982).
[24]L. Szasz, *Pseudopotential Theory of Atoms and Molecules* (Wiley, New York, 1986).
[25]F. Salvat, J. D. Martinez, R. Mayol, and J. Parellada, Phys. Rev. A **36**, 467 (1987).
[26]A. K. Bhatia and R. N. Madan, Phys. Rev. A **7**, 523 (1973).
[27]R. Sever and C. Tezcan (private communication).