SHIFTED 1/N EXPANSION AND ENCLOSED QUANTUM SYSTEMS

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A modified version of the shifted 1/N expansion method is formulated for constrained quantum mechanical system. This method is applied to boxed-in hydrogen atom and spherical harmonic oscillator. Results from the shifted 1/N expansion method are compared with the exact numerical results in case of hydrogen atom, and with approximate analytical results in case of the spherical harmonic oscillator. Agreement between the results is found to be good in both the cases.

1. Introduction

The shifted 1/N expansion, proposed by Sukhatme and Imbo [1,2], is a powerful tool for finding the energy eigenvalues and eigenfunctions of the Schrödinger equation for spherically symmetric potentials [3-7]. In this novel approach, the calculations are carried out for states with arbitrary quantum numbers n and l, using fourth-order perturbation theory in the shifted expansion parameter $1/\overline{k}$, where $\overline{k} = N + 2l - a$. Here N is number of spatial dimensions, $l(l + N - 2)\hbar^2$ the eigenvalue of the square of the N-dimensional orbital angular momentum, and a is a suitable shift which will be discussed later. The shift a dramatically improves the

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simplicity of the analytic expressions and the convergence of the perturbation series for the energy eigenvalues. This technique is applicable to a much wider class of problem than are most other approximation methods, and has been extended successfully to relativistic potential as well [8-11].

Altough variational and other methods have been applied to constrained harmonic oscillator and hydrogen atom problems [12-17], to the best of the authors knowledge, there is no 1/N formalism to deal with constrained quantum mechanical systems.

The study of confined quantum mechanical systems has received increased attention recently [18] and is of importance in the investigation of anharmonic effect in solids, in atoms and in molecules under high pressure [12], and also in impurity binding energies in quantum wells [19].

In the present paper, we develop a formalism for the shifted 1/N expansion procedure suitable for enclosed quantum mehanical systems with radial potentials. It will be shown that the problem of constrained systems can be reduced to that of energy-dependent potentials. The shifted 1/N expansion method can then be applied in a suitable manner [20]. Explicit calculations have been done for spherical harmonic oscillator and boxed-in hydrogen atom only.

The organisation of the paper is as follows. To make the paper self-contained, we discuss the shifted 1/N formalism for an arbitrary spherically symmetric potential in Section 2. In Section 3 the shifted 1/N formalism for constrained system is developed. We apply this method to the boxed-in hydrogen atom in Section 4, and compare our results with existing exact numerical ones. It may be noted that though the wave function for a radially symmetric three dimensional oscillator can be obtained in a analytic form, the eigenvalues for a constrained system can be obtained by finding the roots of F(a, b, z) = 0, where F(a, b, z) is the confluent hypergeometric function. In general the roots can be found out by numerical analysis. In Section 5 we discuss some analytical results, both exact and approximate, for 3-D spherical harmonic oscillator and compare them with the values obtained by the shifted 1/N expansion method. Section 6 is kept for conclusion and remarks.

2. Shifted 1/N formalism for an arbitrary potential

In this Section we shall formulate the shifted 1/N expansion for an arbitrary spherically symmetric potential V(r). The radial Schrödinger equation in N spatial dimension is (in the following we follow the notations of Ref. 2)

$$\left[-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{(k-1)(k-3)\hbar^2}{8mr^2} + V(r)\right]\psi(r) = E\psi(r)$$
(2.1)

where

$$k = N + 2l. \tag{2.2}$$

In terms of the shifted variable $\overline{k} = k - a$, one has

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$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}r^2} + \overline{k}^2 \left[\frac{\hbar^2\{1 - (1-a)/\overline{k}\}\{1 - (3-a)/\overline{k}\}}{8mr^2} + \frac{V(r)}{Q}\right]\psi(r) = E\psi(r) \quad (2.3)$$

where Q is a constant which rescales the potential (in large \overline{k} limit) and will be determined below.

The leading contribution to ${\cal E}$ comes from the effective potential

$$V_{eff}(r) = \frac{\hbar^2}{8mr^2} + \frac{V(r)}{Q}$$
(2.4)

(V(r) is assumed to be well behaved so that $V_{e\!f\!f}(r)$ has a min. at r_0).

 ${\cal Q}$ is then determined from the following equation

$$4mr_0^3 V'(r_0) = \hbar^2 Q. (2.5)$$

Now the origin is shifted to r_0 by means of the definition

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$$x \equiv \frac{(\overline{k})^{1/2}}{r_0} (r - r_0). \tag{2.6}$$

Performing a series expansion in powers of x about x = 0, we obtain

$$\left\{-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{\overline{k}\hbar^2}{8m}\left[1 + \frac{3x^2}{\overline{k}} - \frac{4x^3}{\overline{k}^{3/2}} + \frac{5x^4}{\overline{k}^2} - \dots\right] - \frac{(2-a)\hbar^2}{4m}\left[1 - \frac{2x}{\overline{k}^{1/2}} + \frac{3x^2}{\overline{k}} - \dots\right] + \frac{(1-a)(3-a)\hbar^2}{\overline{k}8m}\left[1 - \frac{2x}{\overline{k}^{1/2}} + \frac{3x^2}{\overline{k}} - \dots\right] + \frac{(1-a)(3-a)\hbar^2}{\overline{k}8m}\left[1 - \frac{2x}{\overline{k}^{1/2}} + \frac{3x^2}{\overline{k}} - \dots\right] + \frac{r_0^2\overline{k}}{\overline{Q}}\left[V(r_0) + \frac{V^{(2)}(r_0)r_0^2x^2}{2\overline{k}} + \frac{V^{(3)}(r_0)r_0^3x^3}{\overline{k}^{3/2}} + \dots\right]\right\}\psi = \frac{Er_0^2}{\overline{k}}\psi.$$
(2.7)

Now the Schrödinger equation for a l-dimensional anharmonic oscillator is

$$\left[-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{1}{2}m^2\omega^2x^2 + \varepsilon_0 + P(x)\right]\phi(x) = \lambda\phi(x)$$
(2.8)

where P(x) is the perturbation term given by

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$$P(x) = g^{1/2}(\varepsilon_1 x + \varepsilon_3 x^3) + g(\varepsilon_2 x^2 + \varepsilon_4 x^4)$$

+ $g^{3/2}(\delta_1 x + \delta_3 x^3 + \delta_5 x^5) + g^2(\delta_2 x^2 + \delta_4 x^4 + \delta_6 x^6)...$ (2.9)

We compare Eqs. (2.7) and (2.8), term by term to define all the anharmonic parameters in terms of \overline{k} , Q, r_0 and the potential derivatives.

Proceeding in a straightforward way we obtain the following identifications:

$$\omega = \left[\frac{3\hbar^2}{4m^2} + \frac{r_0^4 V^{(2)}(r_0)}{mQ}\right]^{1/2} = \frac{\hbar}{2m} \left[3 + \frac{r_0 V^{(2)}(r_0)}{V'(r_0)}\right]^{1/2}$$
(2.10)

$$g = \frac{1}{\overline{k}} \tag{2.11}$$

$$\lambda = \frac{Er_0^2}{\overline{k}} \tag{2.12}$$

$$\varepsilon_0 = \frac{\hbar^2 \overline{k}}{2m} - (2-a)\frac{\hbar^2}{4m} + (1-a)(3-a)\frac{\hbar^2}{8m\overline{k}} + \frac{r_0^2 \overline{k}}{Q}V(r_0)$$
(2.13)

$$\varepsilon_1 = \frac{\hbar^2}{2m}(2-a) \tag{2.14}$$

$$\varepsilon_2 = -\frac{3\hbar^2}{4m}(2-a) \tag{2.15}$$

$$\varepsilon_3 = -\frac{\hbar^2}{2m} + r_0 \frac{V^{(3)}(r_0)}{6Q} \tag{2.16}$$

$$\varepsilon_4 = \frac{5\hbar^2}{8m} + r_0^6 \frac{V^{(4)}(r_0)}{24Q} \tag{2.17}$$

$$\delta_1 = -\frac{(1-a)(3-a)\hbar^2}{4m} \tag{2.18}$$

$$\delta_2 = \frac{3(1-a)(3-a)\hbar^2}{8m} \tag{2.19}$$

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$$\delta_3 = \frac{(2-a)\hbar^2}{m} \tag{2.20}$$

$$\delta_4 = -\frac{5(2-a)\hbar^2}{4m}$$
(2.21)

$$\delta_5 = -\frac{3\hbar^2}{4m} + r_0^7 \frac{V^{(5)}(r_0)}{120Q} \tag{2.22}$$

$$\delta_6 = \frac{7\hbar^2}{8m} + r_0^8 \frac{V^{(6)}(r_0)}{720Q}.$$
(2.23)

For any value of the radial quantum number n and for any value of l, the energy $E_{n,l}$ is given by an expansion in powers of $1/\overline{k}$

$$E_{n,l} = E_0 + E_1 + E_2 + E_3 + \dots$$

where

$$E_0 = \overline{k}^2 \left[\frac{\hbar^2}{8mr_0^2} + \frac{V(r_0)}{Q} \right]$$
(2.24)

$$E_{1} = \frac{\bar{k}}{r_{0}^{2}} \left[(n + \frac{1}{2})\hbar\omega - (2 - a)\frac{\hbar^{2}}{4m} \right]$$
(2.25)

$$E_{2} = \frac{1}{r_{0}^{2}} \left[\frac{\hbar^{2}}{8m} (1-a)(3-a) + \{(1+2n)\tilde{\varepsilon}_{2} + 3\tilde{\varepsilon}_{4}(1+2n+2n^{2})\} - \frac{1}{\hbar\omega} \{\tilde{\varepsilon}_{1}^{2} + 6(1+2n)\tilde{\varepsilon}_{1}\tilde{\varepsilon}_{3} + (11+30n+30n^{2})\tilde{\varepsilon}_{3}^{2}\} \right]$$
(2.26)

$$E_{3} = \frac{1}{\bar{k}r_{0}^{2}} \left[\{ (1+2n)\tilde{\delta}_{2} + 3(1+2n+2n^{2})\tilde{\delta}_{4} + 5(3+8n+6n^{2}+4n^{3})\tilde{\delta}_{6} \} - \frac{1}{\hbar\omega} \{ (1+2n)\tilde{\varepsilon}_{2}^{2} + 12(1+2n+2n^{2})\tilde{\varepsilon}_{2}\tilde{\varepsilon}_{4} + 2(21+59n+51n^{2}+34n^{3})\tilde{\varepsilon}_{4}^{2} + 2\tilde{\varepsilon}_{1}\tilde{\delta}_{1} + 6(1+2n)\tilde{\varepsilon}_{1}\tilde{\delta}_{3} \right]$$

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$$+30(1+2n+2n^{2})\tilde{\varepsilon}_{1}\tilde{\delta}_{5}+6(1+2n)\tilde{\varepsilon}_{3}\tilde{\delta}_{1}$$

$$+2(11+30n+30n^{2})\tilde{\varepsilon}_{3}\tilde{\delta}_{3}+10(13+40n+42n^{2}+28n^{3})\tilde{\varepsilon}_{3}\tilde{\delta}_{5}\}$$

$$+\frac{1}{\hbar^{2}\omega^{2}}\{4\tilde{\varepsilon}_{1}^{2}\tilde{\varepsilon}_{2}+36(1+2n)\tilde{\varepsilon}_{1}\tilde{\varepsilon}_{2}\tilde{\varepsilon}_{3}+8(11+30n+30n^{2})\tilde{\varepsilon}_{2}\tilde{\varepsilon}_{3}^{2}$$

$$+24(1+2n)\tilde{\varepsilon}_{1}^{2}\tilde{\varepsilon}_{4}+8(31+78n+78n^{2})\tilde{\varepsilon}_{1}\tilde{\varepsilon}_{3}\tilde{\varepsilon}_{4}$$

$$12(57+183n+225n^{2}+150n^{3})\tilde{\varepsilon}_{3}^{2}\tilde{\varepsilon}_{4}\}$$

$$-\frac{1}{\hbar^{3}\omega^{3}}\{8\tilde{\varepsilon}_{1}^{2}\tilde{\varepsilon}_{3}+108(1+2n)\tilde{\varepsilon}_{1}^{2}\tilde{\varepsilon}_{3}^{2}+48(11+30n+30n^{2})\tilde{\varepsilon}_{1}\tilde{\varepsilon}_{3}^{3}$$

$$+30(31+109n+141n^2+94n^3)\tilde{\varepsilon}_3^4\}]$$
(2.27)

where

$$\tilde{\varepsilon}_j = \frac{\varepsilon_j}{(2m\omega/\hbar)^{j/2}} \tag{2.28}$$

$$\tilde{\delta}_j = \frac{\delta_j}{(2m\omega/\hbar)^{j/2}}, \quad j = 1, 2, 3, \dots$$
(2.29)

Now the shift parameter is fixed from the requirement that the term E_1 vanishes. Therefore,

$$a = 2 - 2(2n+1)\frac{m\omega}{\hbar}.$$
 (2.30)

For any specific choise of n, l, N, the constant Q should be such as to make Eqs. (2.1) and (2.3) identical. Hence,

$$\overline{k} = \sqrt{Q}.\tag{2.31}$$

Using this in Eqs. (2.5), (2.10) and (2.30), we obtain an explicit equation for determining r_0 , viz.

$$N + 2l - 2 + (2n+1) \left[3 + \frac{r_0 V^{(2)}(r_0)}{V^{(1)}(r_0)} \right]^{1/2} = \left(\frac{4m r_0^3 V^{(1)}(r_0)}{\hbar^2} \right)^{1/2}.$$
 (2.32)

Having determined r_0 , all the energy eigenvalues and eigenfunctions can be computed in a straightforward way. Excellent results have been obtained by this method (for large values of n) for a wide class of spherically symmetric potentials [3-11]. The shift improves the convergence of the perturbation series for the energy eigenvalues.

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3. Shifted 1/N formalism for constrained quantum mechanical system

In this Section we develop a formalism for the shifted 1/N expansion procedure for enclosed quantum mechanical system with spherically symmetric potential. The method can be applied to any quantum mechanical system confined within a hard spherical box.

We start with the 3-dimensional radial Schrödinger equation for a spherically symmetric potential V(r) (units are $\hbar = m = 1$)

$$-\frac{1}{2}\frac{\mathrm{d}^2\psi_r}{\mathrm{d}r^2} + \left[V(r) + \frac{l(l+1)}{2r^2} - E\right]\psi_r = 0.$$
(3.1)

Confinement can be imposed on this system by demanding $\psi_r(b) = 0$, where b is the radius of the confining spherical box. We make the coordinate transformation

$$r = f(\zeta, b) \tag{3.2}$$

which maps the domain of definition of ψ_r from (0, b) in r space to $(0, \infty)$ in ζ space.

Redefining the wave function as

$$\psi_{\zeta} \equiv \sqrt{f'(\zeta, b)\phi(\zeta)} \tag{3.3}$$

where the prime denotes differentiation with respect to the variable ζ , Eq. (3.1) is transformed into

$$-\frac{1}{2}\frac{\mathrm{d}^{2}}{\mathrm{d}\zeta^{2}} + \{f'(\zeta,b)\}^{2}\left\{V(\zeta) - E + \frac{l(l+1)}{2\{f(\zeta,b)\}^{2}}\right\} + \frac{3}{8}\{\frac{f''(\zeta,b)}{f'(\zeta,b)}\}^{2} - \frac{1}{4}\frac{f''(\zeta,b)}{f'(\zeta,b)}\right]\phi = 0,$$
(3.4)

 ζ being a dimensionless variable, we can make the following scaling transformation

$$y = b\zeta. \tag{3.5}$$

Eq. (3.4) can then be cast formally into an eigenvalue equation

$$-\frac{1}{2}\frac{\mathrm{d}^2\phi}{\mathrm{d}y^2} + \left[V_S(y) + \frac{l(l+1)}{2y^2} - E_S\right]\phi = 0.$$
(3.6)

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where

$$V_{S}(y) = \frac{1}{b^{2}} \{ [V(\zeta) - E] [f'(\zeta, b)]^{2} + \frac{l(l+1)}{2} \left[\frac{f'(\zeta, b)}{f(\zeta, b)} \right]^{2} + \frac{3}{8} \left[\frac{f''(\zeta, b)}{f'(\zeta, b)} \right]^{2} - \frac{1}{4} \frac{f'''(\zeta, b)}{f'(\zeta, b)} \} - \frac{l(l+1)}{2y^{2}}.$$
(3.7)

Equation (3.6) is the Schrödinger equation with an energy-dependent potential $V_S(y)$, and the energy value E can be obtained following Papp [20]. This equation resembles equation (2.1) if we impose the condition $E_S \to 0$. The usual shifted 1/N expansion method, as discussed in Section 2 earlier, can then be applied to Eq. (3.6). The lowest order approximation to energy is given by

$$E_{S}^{0} = \overline{k}^{2} V_{eff}(y_{0}) = \overline{k}^{2} \left[\frac{1}{8y_{0}^{2}} + \frac{V_{S}(y_{0})}{Q} \right]$$
(3.8)

with

$$\frac{\mathrm{d}V_{eff}(y)}{\mathrm{d}y}\Big|_{y=y_0} = 0.$$
(3.9)

 y_0 is obtained by the standard technique of shifted 1/N expansion, and is the solution of the equation

$$N + 2l - 2 + (2n+1) \left[3 + \frac{y_0 V_S^{(2)}(y_0)}{V_S^{(1)}(y_0)} \right]^{1/2} = \left[4y_0^3 V_S^{(1)}(y_0) \right]^{1/2}.$$
 (3.10)

Energy, up to the third order, is obtained from

$$E_S = E_S^0 + E_S^2 + E_S^3 \tag{3.11}$$

where E_S^2 and E_S^3 can be calculated using Eqs. (2.26) and (2.27), respectively.

4. Boxed-in hydrogen atom

In this Section we apply our formalism to the constrained Coulomb problem and compare our results with those of existing exact numerical ones.

The potential for this problem is

$$V(r) = -\frac{1}{r}.\tag{4.1}$$

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We make the coordinate transformation

$$r = f(\zeta, b) = \frac{b}{\zeta + 1} \tag{4.2}$$

so that

$$\zeta = \frac{b-r}{r}.\tag{4.3}$$

Thus $\psi_r(b) = 0$ in r space goes over to $\psi(\zeta = 0)$ in ζ space. $V_S(y)$ then takes the form

$$V_S(y) = -\frac{1}{b(1+y/b)^3} - \frac{E}{(1+y/b)^4} + \frac{l(l+1)}{2b^2(1+y/b)^2} - \frac{l(l+1)}{2y^2}.$$
 (4.4)

Energy up to the third order is then given by Eq. (3.11) where E_S^0 , E_S^2 and E_S^3 are calculated using Eqs. (3.8), (2.6) and (2.7), respectively.

In Tables 1, 2 and 3, we compare the exact results of Marin and Cruz [18] with those obtained by our method (i.e. shifted 1/N expansion method for constrained quantum mechanical system). Table 1 is for the ground state (1s) whereas Tables 2 and 3 are for the 2p and 3d exited states, respectively.

TABLE 1.

b	E(shifted 1/N)	E(exact)
0.5	15.2941	14.748
0.81	4.5359	4.39165
1.15	1.5170	1.48625
1.5	0.4365	0.4370
1.711	0.1230	0.12625
2.0	-0.1270	-0.125
2.2005	-0.2335	-0.2322
2.807	-0.4000	-0.3978
3.192	-0.450	-0.4432
3.5	-0.467	-0. 46435
5.0	-0.50	-0.4964
6.0	-0.50	-0.49925

Comparison of energy eigenvalues for the boxed-in hydrogen atom obtained from shifted 1/N method with the exact results for l = 0.

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b	E(shifted 1/N)	E(exact)
1.41	3.9104	3.74345
1.68	2.5612	2.45315
2.0	1.6447	1.5760
2.698	0.7075	0.6777
3.0	0.5030	0.48125
3.5	0.2847	0.2712
4.11	0.1307	0.12245
4.77	0.0345	0.02995
5.528	-0.0273	-0.03125
6.0	-0.0520	-0.05555
6.497	-0.0708	-0.07395
7.0	-0.0845	-0.08745
8.54	-0.1080	-0.11015
10.235	-0.1195	-0.1197
12.0	-0.1250	-0.1241

TABLE 2.Comparison of energy eigenvalues for the boxed-in hydrogen atom obtained from
shifted 1/N method with the exact results for l = 1.



Comparison of the exact energy eigenvalues for the constrained Coulomb problem with those obtained from shifted 1/N method for l = 2.

b	E(shifted 1/N)	E(exact)
7.0	0.0941	0.0966
7.5	0.0661	0.0683
8.0	0.04405	0.0461
10.0	-0.0083	-0.0071
12.0	-0.032	-0.0312
14.0	-0.0436	-0.0432
16.0	-0.0497	-0.0492
18.0	-0.0534	-0.0533

In all three cases, energies are in Rydbergs (1 Ry = 13.6 eV) and radii (of the confining spherical box), in Bohr units (1 B.u. = 0.0529 nm).

5. Constrained spherical harmonic oscillator

The potential for the spherical harmonic oscillator is

$$V(r) = \frac{r^2}{2}.$$
 (5.1)

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If we take the coordinate to transform as

$$r = f(\zeta, b) = \frac{b\zeta}{\zeta + 1} \tag{5.2}$$

so that

$$\zeta = \frac{r}{b-r} \tag{5.3}$$

and $\psi_r(b) = 0$ goes over to $\psi(\zeta = \infty) = 0$, then $V_S(y)$ turns out to be

$$V_S(y) = \frac{y^2}{2(1+y/b)^6} - \frac{E}{(1+y/b)^4} + \frac{l(l+1)}{2y^2(1+y/b)^2} - \frac{l(l+1)}{2y^2}.$$
 (5.4)

With this value of $V_S(y)$, energy is calculated using Eqs. (3.11), (3.8), (2.6) and (2.7) as described earlier.

To compare our results numerically we find an approximate analytical formula to find the energy values of the constrained harmonic oscillator. This is done as no numerical results exist for values of orbital angular momentum l greater than 1, whereas shifted 1/N expansion procedure is expected to give good results for relatively large values of l.

The reduced radial Schrödinger equation for the 3-dimensional harmonic oscillator is given by

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}r^2} + \left[\frac{l(l+1)}{r^2} + 2E - r^2\right]\psi = 0, \tag{5.5}$$

whose solution is

$$\psi(r) = Ar^{l+1}e^{-r^2/2} {}_lF_l\left(\frac{l}{2} + \frac{3}{4} - \frac{E}{2}, l + \frac{3}{2}, r^2\right).$$
(5.6)

Here A is a normalisation constant and $_{l}F_{l}(\alpha,\beta,z)$ is the confluent hypergeometric function written in a power series in z as [21]

$${}_{l}F_{l}(\alpha,\beta,z) = 1 + \frac{\alpha z}{\beta} + \frac{\alpha(\alpha+1)}{\beta(\beta+1)}\frac{z^{2}}{2!} + \frac{\alpha(\alpha+1)(\alpha+2)}{\beta(\beta+1)(\beta+2)}\frac{z^{3}}{3!} + \dots$$
(5.7)

Imposing the boundary condition

$$\psi(r=b)=0$$

energy E is obtained by solving the equation

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$${}_{l}F_{l}\left(\frac{l}{2}+\frac{3}{4}-\frac{E}{2},l+\frac{3}{2},b^{2}\right)=0.$$
(5.8)

Thus $\beta = l + \frac{3}{2}$, $\alpha = \frac{l}{2} + \frac{3}{4} - \frac{E}{2}$ and hence $\beta/2 - \alpha = E/2$. Some exact results for l = 0 and l = 1 can be obtained by using the numerical values of zeroes of ${}_{l}F_{l}(\alpha, \beta, z)$ compiled by Slater [22]. However, when $\beta/2 - \alpha$ is large, but β not too large, a good approximation for ${}_{l}F_{l}(\alpha, \beta, z)$ has been found by Tricomi [23], viz.

$${}_{l}F_{l}(\alpha,\beta,z) \approx \Gamma(\beta) \frac{\exp\left(2k\cos^{2}\Theta\right)}{(\pi k\sin 2\Theta)^{1/2}} (2k\cos\Theta)^{1-\beta} \\ \left[\sin(\overline{\Theta}+\alpha\pi) - A_{1}(\Theta) \frac{\cos(\overline{\Theta}+\alpha\pi)}{k\sin 2\Theta} + O(k^{-2})\right]$$
(5.9)

where

$$\Theta = \cos^{-1} \frac{z}{4k} \tag{5.10}$$

$$\overline{\Theta} = k(2\Theta - \sin 2\Theta) + \frac{\pi}{4} \tag{5.11}$$

$$A_1(\Theta) = \frac{1}{12} \left[\frac{5}{4\sin^2 \Theta} + (3\beta^2 - 6\beta + 2)\sin^2 \Theta - 1 \right]$$
(5.12)

and

$$k = \frac{\beta}{2} - \alpha = \frac{E}{2}.$$
(5.13)

The roots of $_{l}F_{l}(\alpha,\beta,z)$ are given by (up to $O(1/k^{2})$)

$$\sin(\overline{\Theta} + \alpha \pi) - \frac{A_1(\Theta)\cos(\overline{\Theta} + \alpha \pi)}{k \sin 2\Theta} = 0.$$
 (5.14)

We have obtained the energy eigenvalue E by this method (the confinement parameter b is given). It is seen that this approximate analytical formula reproduces the exact results for l = 0, 1 when $b \leq 2.5$.

In Table 4 numerical results by the shifted 1/N method are given for l = 0and 1. Values marked * are obtained by utilizing the numerical results for zeros of $_lF_l(\alpha, \beta, z)$ as given by Slater. Other symbols are expressed in the table itself. In Table 5, 1/N results have been compared with those obtained from Eq. (5.14) for l = 2 and 3.

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TABLE 4.***

Energy levels of the enclosed harmonic oscillator as a function of the radius of the box b. E is in units of $\hbar\omega$ and b in units of $\hbar/(m\omega)^{1/2}$. n = 0

E(exact)

40.42578**

 10.5^{*}

 8.30^{*}

4.9036

 4.5^{*}

8.675

5.128

4.705

10.2822

1.7018	2.1968	2.10^{*}			
2.0	1.8658	1.7648	3.4005	3.2469	
3.0	1.536	1.5061	2.63	2.5313	
5.0	1.5	1.5000	2.5	2.4999	

 4.10^{*}

2.5050

* Results obtained from the roots of $_{l}F_{l}(\alpha, \beta, z) = 0$ given in Ref. 22.

** Results obtained from Eq. (5.14).

⁺ Result taken from Ref. 13.

b

0.5

1.0

1.5

0.77504

0.9892

1.1187

1.1215

1.5811

*** The unmarked exact results are taken from Ref. 18.

4.2486

2.6068

TABLE 5. Energy eigenvalues for large l values. E^+ are the results obtained from solving Eq. (5.14).

b	$l = 2$ $E(1/N) = E^+$		$l = 3$ $E(1/N) = E^+$	
0.5	69.705	67.47284	102.405	102.4668
1.0	17.634	17.06677	25.824	25.8133
$1.0 \\ 1.5$	8.238	7.9643	11.930	11.86031

6. Conclusion and remarks

We have developed a formalism for shifted 1/N expansion method for confined or constrained quantum mechanical system with radial potentials. We have applied our method to find the energy values of the boxed-in hydrogen atom and the constrained harmonic oscillator. For the latter problem, one can obtain approximate analytical results. However, for the constrained hydrogen atom even this is not possible to obtain. Hence the shifted 1/N expansion technique can be useful in calculating

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the eigenvalues of such system. As is well known, the degree of accuracy of the shifted 1/N method increases with increasing l. However, even for low values of l, the shifted 1/N results agree fairly well with those of the exact numerical ones. However, for E numerically very small in the Coulomb case (near the transition zone from positive to negative values), the shifted 1/N expansion method is not very accurate. As $b \to \infty$, the exact Coulomb results $E = -1/2n^2$ is reproduced by the shifted 1/N method, providing a check on our formalism. As for the constrained harmonic oscillator, the agreement between our result and Tricomi's approximate formula is excellent for l = 3, when b is relatively small ($b \le 2$).

References

- 1) U. Sukhatme and T. Imbo, Phys. Rev. D28 (1983) 418;
- 2) T. Imbo, A. Pagnamenta and U. Sukhatme, Phys. Rev. D29 (1984) 1669;
- 3) R. Dutta, U. Mukherjee and Y. P. Varshni, Phys. Rev. D34 (1986) 777;
- 4) B. Roy and R. K. Roychoudhury, J. Phys. A, Math. Gen. 20 (1987) 3051;
- 5) R. K. Roychoudhury and Y. P. Varshni, Phys. Rev. A37 (1988) 2309;
- 6) A. Chatterjee, Phys. Rep. 186 (1990) 249 and references therein;
- 7) E. Papp, Phys. Rev. A38 (1988) 2158; see also E. Papp, Phys. Rep. 4 (1988) 171;
- 8) R. K. Roychoudhury and Y. P. Varshni, a) J. Phys. A, Math. Gen. 20 (1987) L 1083;
 b) Phys. Rev. A39 (1989) 5523;
- 9) O. Mustafa and R. Sever, Phys. Rev. A44 (1991) 4142;
- 10) B. Roy and R. K. Roychoudhury, J. Phys. A, Math. Gen. 23 (1990) 3555;
- 11) M. M. Panja and R. Dutta, Phys. Rev. A38 (1988) 3937;
- 12) A. Michels, J. De Boer and A. Bijl, Physica 4 (1937) 981; P. Dean, Proc. Camb. Phil. Soc. 62 (1966) 277;
- 13) V. C. Aguilera-Navarro, E. Ley Koo and A. H. Zimerman, J. Phys. A, Math. Gen. 13 (1980) 3585;
 U. Larsen, J. Phys. A, Math. Gen. 16 (1983) 2137;

A. Consortini and B. R. Frieden, Il Nuovo Cim. 35 (1976) 153;

- 14) J. L. Marin and S. A. Cruz, J. Phys. B, At. Mol. Opt. Phys. 24 (1991) 2899;
- 15) G. Barton, A. J. Bray and A. J. McKane, Am. J. Phys. 58 (1990) 751;
- 16) F. M. Martinez, J. Phys. A, Math. Gen. 24 (1991) 1351;
- 17) J. Groecki and W. Byers Brown, J. Phys. B, Al. Mol. Opt. Phys. 22 (1989) 2659;
- 18) J. L. Marin and S. A. Cruz, Am. J. Phys. 59 (1991) 931;
- 19) G. Bastard, Phys. Rev. B24 (1981) 4714;
 A. D' Andrea and R. Del Sole, Phys. Rev. B32 (1985) 2337; see also Ref. 14 for earlier works;
- 20) E. Papp, J. Math. Phys. 32 (1991) 967;
- M. Abramowitz and I. A. Stegun, Handbook of Mathematical Functions, Dover, N. Y. (1970);

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22) L. J. Slater, Hypergeometric Functions, Cambridge Univ. Press, (1960);

23) F. G. Tricomi, Ann. Mat. (4) 28 (1949) 263.

POMAKNUTI 1/N RAZVOJ I OGRANIČENI KVANTNI SISTEMI

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Za ograničene kvantno mehaničke sisteme formulirana je modificirana verzija pomaknutog 1/N razvoja. Metoda je primjenjena na vodikov atom i sferni harmonički oscilator koji se nalazi u kutiji. Rezultati pomaknutog 1/N razvoja uspoređeni su s egzaktnim numeričkim rezultatima za vodikov atom, te približnim analitičkim rezultatima za sferni harmonički oscilator. Slaganje rezultata je dobro u oba slučaja.

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