COMMENT

The shifted $1/N$ expansion and the energy eigenvalues of the Hulthen potential for $l \neq 0$

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Abstract. The shifted $1/N$ expansion has been used to obtain the energy values of the Hulthen potential for non-zero values of the orbital angular momentum. The analytic expression for the energies $E_{n,l}$ yield fairly accurate results for a wide range of values of n, l and the screening parameter λ. The energy values obtained by this method have been compared and found to be in excellent agreement with Padé approximation calculations.

Recently, a great deal of interest has been shown in the application of the shifted $1/N$ expansion (Sukhatme and Imbo 1983, Imbo *et al* 1984a) to a class of screened Coulomb potentials which have wide applications in various branches of physics (Imbo *et al* 1984b, Roy 1986). Amongst the various screened Coulomb potentials, the Hulthen potential which, in atomic units, is given by

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

(λ being the screening parameter and Z being the charge of the nucleus) has a special status because it yields closed analytic solutions for S waves (Flügge 1974) and therefore is often used as an approximation for the screened Coulomb potentials. However, one does not have such nice solutions for higher partial waves. Amongst various methods for obtaining the energy values of the Hulthen potential for $l \neq 0$ (Dutt and Mukherji 1982, Patil 1984, Popov and Weinberg 1985) the Padé approximation method yields fairly accurate results (Lai and Lin 1980). However, it is an iterative procedure and the other works mentioned earlier involve elaborate calculations.

In the present comment we shall study the non-zero angular momentum states of the Hulthen potential by using the shifted $1/N$ expansion.

The shifted $1/N$ expansion differs from the ordinary large-N expansion (Mlodinow and Papanicolaou 1980, 1981) in the expression for the expansion parameter. In the former, the expansion parameter is $1/\bar{k}$, where $\bar{k} = N + 2l - a$, whereas in the latter it is $1/k$ where $k = N + 2l$, N being the number of spatial dimensions, $l(l + N - 2)\hbar^2$ is the eigenvalue of the square of the N-dimensional orbital angular momentum and a is the shift chosen by requiring agreement between the $1/\bar{k}$ expansions and the exact analytic results for the harmonic oscillator and Coulomb potentials (Sukhatme and Imbo 1983). Since the shifted $1/N$ expansion is not an expansion in powers of the potential, it can be used for problems which do not necessarily involve small coupling constants for perturbation theory.

The radial Schrödinger equation in N spatial dimensions in terms of the shifted variable $\bar{k} = N + 2l - a$ is (Mlodinow and Shatz 1984)

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

where $V(r)$ is given by equation (1).

In order to get useful results from a $1/\bar{k}$ expansion, the large-E limit of the potential must be suitably defined (Imbo *et al* 1984a). Since the angular momentum barrier term behaves like $\bar{k}^2$ at large $\bar{k}$, so should the potential $V(r)$. This will give rise to an effective potential which does not vary with $\bar{k}$ at large values of $\bar{k}$, resulting in a sensible zeroth-order classical result. Hence we consider the following equation (Imbo *et al* 1984a):

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

where Q is a constant to be specified later.

The shifted $1/N$ expansion method consists in solving equation (3) systematically in terms of the expansion parameter $1/\bar{k}$. The leading contribution to the energy comes from the effective potential

$$V_{\text{eff}}(r) = \frac{\hbar^2}{8mr^2} + \frac{V(r)}{Q}. \tag{4}$$

Now if we assume that $V(r)$ is sufficiently well behaved so that $V_{\text{eff}}(r)$ has a minimum at $r = r_0$ and there are well defined bound states, then the following relationship is valid:

$$4mr_0^3 V'(r_0) = \hbar^2 Q \tag{5}$$

where r_0 is the root of the equation

$$N + 2l - 2 + (2n+1)\left(3 + \frac{r_0 V''(r_0)}{V'(r_0)} \right)^{1/2} = \left(\frac{4mr_0^3 V'(r_0)}{\hbar^2} \right)^{1/2}. \tag{6}$$

For the derivation of equation (6) we refer the reader to the paper by Imbo *et al* (1984a).

Once r_0 is determined, the leading term in E is given by

$$\bar{k}^2 V_{\text{eff}}(r_0) = \frac{\bar{k}^2}{r_0^2}\left(\frac{\hbar^2}{8m} + \frac{r_0^2 V(r_0)}{Q} \right). \tag{7}$$

The next contribution is of order $\bar{k}$ and is (Imbo *et al* 1984a)

$$\frac{\bar{k}}{r_0^2}\left((n + \tfrac{1}{2})\hbar w - \frac{(2-a)\hbar^2}{4m} \right). \tag{8}$$

The shift a is chosen so that this contribution vanishes. Therefore we obtain

$$a = 2 - 2(2n+1)mw/\hbar. \tag{9}$$

The successive contributions to the energy are determined by the substitution

$$x = (\bar{k}^{1/2}/r_0)(r - r_0) \tag{10}$$

in equation (3) and expanding about $x = 0$ in powers of x. Since the algorithm for the shifted $1/N$ expansion has been developed previously (Imbo *et al* 1984a), we present only the essential steps here.

The energy eigenvalues are given by an expansion in powers of $1/\bar{k}$, where $\bar{k} = N = 2l - a$, as

$$E_{n,l} = \frac{\bar{k}}{r_0^2}\left[\frac{\hbar^2\bar{k}}{8m} + \frac{r_0^2\bar{k}V(r_0)}{Q} + \frac{\beta^{(1)}}{\bar{k}} + \frac{\beta^{(2)}}{\bar{k}^2} + O\left(\frac{1}{\bar{k}^3}\right)\right] \tag{11}$$

where

$$\beta^{(1)} = \frac{\hbar^2(1-a)(3-a)}{8m} + (1+2n)\tilde{\varepsilon}_2 + 3(1+2n+2n^2)\tilde{\varepsilon}_4$$

$$- \frac{1}{\hbar w}[\tilde{\varepsilon}_1^2 + 6(1+2n)\tilde{\varepsilon}_1\tilde{\varepsilon}_3 + (11+30n+30n^2)\tilde{\varepsilon}_3^2] \tag{12}$$

$$\beta^{(2)} = (1+2n)\tilde{\delta}_2 + 3(1+2n+2n^2)\tilde{\delta}_4 + 5(3+8n+6n^2+4n^3)\tilde{\delta}_6$$

$$- \frac{1}{\hbar w}[(1+2n)\tilde{\varepsilon}_2^2 + 12(1+2n+2n^2)\tilde{\varepsilon}_2\tilde{\varepsilon}_4 + 2(21+59n+51n^2$$

$$+ 34n^3)\tilde{\varepsilon}_4^2 + 2\tilde{\varepsilon}_1\tilde{\delta}_1 + 6(1+2n)\tilde{\varepsilon}_1\tilde{\delta}_3 + 30(1+2n+2n^2)\tilde{\varepsilon}_1\tilde{\delta}_5$$

$$+ 6(1+2n)\tilde{\varepsilon}_3\tilde{\delta}_1 + 2(11+30n+30n^2)\tilde{\varepsilon}_3\tilde{\delta}_3 + 10(13+40n+42n^2$$

$$+ 28n^3)\tilde{\varepsilon}_3\tilde{\delta}_5] + \frac{1}{(\hbar w)^2}[4\tilde{\varepsilon}_1^2\tilde{\varepsilon}_2 + 36(1+2n)\tilde{\varepsilon}_1\tilde{\varepsilon}_2\tilde{\varepsilon}_3$$

$$+ 8(11+30n+30n^2)\tilde{\varepsilon}_2\tilde{\varepsilon}_3^2 + 24(1+2n)\tilde{\varepsilon}_1^2\tilde{\varepsilon}_4 + 8(31+78n$$

$$+ 78n^2)\tilde{\varepsilon}_1\tilde{\varepsilon}_3\tilde{\varepsilon}_4 + 12(57+189n+225n^2+150n^3)\tilde{\varepsilon}_3^2\tilde{\varepsilon}_4]$$

$$- \frac{1}{(\hbar w)^3}[8\tilde{\varepsilon}_1^3\tilde{\varepsilon}_3 + 108(1+2n)\tilde{\varepsilon}_1^2\tilde{\varepsilon}_3^2 + 48(11+30n+30n^2)$$

$$\times \tilde{\varepsilon}_1\tilde{\varepsilon}_3^3 + 30(31+109n+141n^2+94n^3)\tilde{\varepsilon}_3^4] \tag{13}$$

$$\tilde{\varepsilon}_j = \frac{\varepsilon_j}{(2mw/\hbar)^{j/2}} \qquad \tilde{\delta}_j = \frac{\delta_j}{(2mw/\hbar)^{j/2}} \qquad j = 1, 2, \ldots. \tag{14}$$

$$w = \frac{\hbar}{2m}\left(3 + \frac{r_0 V''(r_0)}{V'(r_0)}\right)^{1/2} \tag{15}$$

$$\varepsilon_1 = (2-a)\hbar^2/2m \tag{16}$$

$$\varepsilon_2 = -3\hbar^2(2-a)/4m \tag{17}$$

$$\varepsilon_3 = -\frac{\hbar^2}{2m} + \frac{r_0^5 V''(r_0)}{6Q} \tag{18}$$

$$\varepsilon_4 = \frac{5\hbar^2}{8m} + \frac{r_0^6 V''''(r_0)}{24Q} \tag{19}$$

$$\delta_1 = -(1-a)(3-a)\hbar^2/4m \tag{20}$$

$$\delta_2 = 3(1-a)(3-a)\hbar^2/8m \tag{21}$$

$$\delta_3 = (2-a)\hbar^2/m \tag{22}$$

$$\delta_4 = -5(2-a)\hbar^2/4m \tag{23}$$

$$\delta_5 = -\frac{3\hbar^2}{4m} + \frac{r_0^7 V''''(r_0)}{120Q} \tag{24}$$

$$\delta_6 = \frac{7\hbar^2}{8m} + \frac{r_0^8 V''''''(r_0)}{720Q}. \tag{25}$$

For any given choice of n and l, equation (6) becomes a transcendental equation which can be solved numerically to obtain r_0. Substitution of r_0 into equations (5) and (11)-(25) immediately gives the energy eigenvalues. In all our calculations, we have used atomic units so that $\hbar = m = 1$. We list our energy values for the various states in tables 1 and 2 and compare them with Padé approximation calculations (Lai and Lin 1980). It is clear from table 1 that, for $\lambda \geq 0.35$, the successive contributions from the perturbation series are substantial and one needs to consider higher-order terms in the $1/\bar{k}$ expansion to obtain better accuracy. However, it should be noted that our first-order correction in $1/\bar{k}$, i.e. $E_{n,l}^{(1)}$, has been compared with the twelfth-order correction in λ, i.e. $E_{n,l}^{(12)}$ (Lai and Lin 1980), and as is evident from the tables the agreement is fairly good.

Therefore the shifted $1/N$ expansion has proved to be an efficient method for studying the Hulthen potential for $l \neq 0$.

Table 1. Energy eigenvalues $E_{n,l}$ in atomic units as a function of the screening parameter λ for 2p-3d states. The results of the Padé approximation calculations (given in parentheses) and our calculations, which include one correction in $1/\bar{k}$, are shown.

Screening parameter	2p	3p	3d
0.025		−0.043 707	−0.043 603
		(−0.043 707)	(−0.043 603)
0.050	−0.101 045	−0.033 159	−0.032 753
	(−0.101 043)	(−0.033 165)	(−0.032 753)
0.100	−0.079 180	−0.015 982	−0.014 489
	(−0.079 179)	(−0.016 054)	(−0.014 484)
0.150		−0.004 276	−0.001 469
		(−0.004 466)	(−0.001 391)
0.200	−0.041 908		
	(−0.041 886)		
0.300	−0.014 009		
	(−0.013 790)		
0.350	−0.004 437		
	(−0.003 779)		

Table 2. Energy eigenvalues $E_{n,l}$ in atomic units as a function of the screening parameter λ for 4p-4f states. The results of Padé approximation calculations (given in parentheses) and our calculation for $E_{n,l}$, which includes one correction in $1/\bar{k}$, are shown.

Screening parameter	4p	4d	4f
0.025	−0.019 945	−0.091 845	0.019 691
	(−0.019 949)	(−0.019 846)	(−0.019 691)
0.050	−0.011 002	−0.010 656	−0.010 062
	(−0.011 058)	(−0.010 667)	(−0.010 062)
0.075	−0.004 398	−0.003 793	−0.002 564
	(−0.004 622)	(−0.003 834)	(−0.002 556)

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