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1985 J. Phys. A: Math. Gen. 18 2403

(http://iopscience.iop.org/0305-4470/18/12/037)

J. Phys. A: Math. Gen. **18** (1985) 2403-2408. Printed in Great Britain

COMMENT

1/N expansion for the Gaussian potential

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Received 19 February 1985

Abstract. The method of large-N expansion has been applied to an attractive radial Gaussian potential to obtain its bound state energy levels. It has been shown that the shifted $1/N$ expansion technique provides a better approximation than the method of unshifted $1/N$ expansion and yields energy values which are in good agreement with the accurate numerical and analytic results.

The solution of the Schrödinger equation with an attractive radial Gaussian potential of the form $V(r) = -A\exp(-\lambda r^2)$, the interest in which was evoked by the work of Buck *et al* (1977) on the determination of α-α scattering phase shifts using a local Gaussian potential as a model for the nucleus-nucleus interaction, has received significant attention in recent years. The energy eigenvalues of such an attractive Gaussian potential were obtained first by Buck (1977) by direct numerical integration and then by Stephenson (1977) by the Liouville-Green uniform asymptotic method. Bessis *et al* (1982) have determined its bound state energies fairly accurately using a perturbational and variational treatment on a conveniently chosen basis of transformed Jacobi functions. More accurate values have been obtained by Lai (1983) by using higher-order perturbation theory combined with hypervirial-Padé analysis. These results are in excellent agreement with the numerical values reported later by Crandall (1983). Recently, Cohen (1984) has proposed a simple method to calculate the bound state energies of the Gaussian potential from a first-order perturbation theory based on a scaled harmonic oscillator model. This method, however, fails to yield the true upper bounds for higher particle levels.

In the interim, the semiclassical large N expansion has emerged as a very useful technique for providing energy eigenvalues for bound states of the quantal systems with surprisingly good accuracy (Mlodinow and Papanicolaou 1980, 1981, Mlodinow and Shatz 1984, Chatterjee 1985 and references therein). One palpable advantage of this scheme over the ordinary Rayleigh-Schrödinger perturbation theory is that unlike the perturbation theory which requires a partitioning of the Hamiltonian into two parts, one being so small it can be treated as a small perturbation, the method of large N expansion uses $1/k = 1/(N+2l)$ as the expansion parameter, where N is the spatial dimensionality and l, the angular momentum and hence preserves the potentiality of finding application in the strong coupling problems for which the usual perturbative treatments fail (Witten 1979). Notwithstanding the proven success of the $1/N$ expansion in dealing with a number of potential problems, the expansion is at times plagued with slow convergence, particularly for the higher excited states. To avoid this difficulty, Sukhatme and Imbo (1983) have introduced what they have called the

0305-4470/85/122403+06$02.25

shifted $1/N$ expansion which brings in an extra degree of freedom 'a' in the expansion parameter which is now given by $1/\bar{k} = 1/(N+2l-a)$. The new parameter 'a' is chosen by physical arguments and is found to depend linearly on the particle level. Consequently, the shifted $1/N$ expansion entails a drastic improvement on the convergence of the energy series.

In this comment, we do not purport to introduce any new idea. Our main goal will be to report that the energy eigenvalues of the a tractive radial Gaussian potential calculated within the framework of the shifted $1/N$ expansion are in fair agreement with the numerical and perturbative results. We furthermore show that the shifted $1/N$ expansion is a much better approximation than the unshifted one, particularly for the higher particle levels. We follow the method of Imbo *et al* (1984).

The radial part of the N-dimensional Schrödinger equation is given by

$$\left[-\frac{\hbar^2}{2m}\left(\frac{d^2}{dr^2}+\frac{N-1}{r}\frac{d}{dr}\right)+\frac{l(l+N-2)}{2r^2}+V(r)\right]R(r)=ER(r), \tag{1}$$

which on substituting $R(r)=r^{-(N-1)/2}u(r)$, reduces to the effective one-dimensional equation

$$-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}u(r)+\left(\frac{(k-1)(k-3)}{8mr^2}+V(r)\right)u(r)=Eu(r), \tag{2}$$

where $k=N+2l$. Equation (2) is the starting point in the unshifted $1/N$ expansion, whereas in the shifted $1/N$ expansion one has to introduce an additional parameter 'a' in terms of which equation (2) now reads

$$-\frac{d^2}{dr^2}u(r)+\bar{k}^2\left(\frac{[1-(1-a)/\bar{k}][1-(3-a)/\bar{k}]}{4r^2}+\tilde{V}(r)\right)u(r)=Eu(r), \tag{3}$$

where $\bar{k}=(N+2l-a)$, $\tilde{V}(r)=V(r)/\bar{k}^2$ and the units have been chosen so that $\hbar=2m=1$. In the limit of large $\bar{k}(N\to\infty)$ the energy eigenvalue to leading order is given by

$$E_\infty=\bar{k}^2(1/4r_0^2+\tilde{V}(r_0)), \tag{4}$$

where r_0 is to be obtained by minimising the effective potential $V_{\text{eff}}=(1/4r_0^2+\tilde{V}(r_0))$. Quantum fluctuations around the classical minimum can be incorporated in the higher-order corrections for which one defines $x=(\sqrt{\bar{k}}/r_0)(r-r_0)$. Then on expanding around $x=0$ and making use of the equation for r_0, equation (3) becomes, after rearranging the terms,

$$(-d^2/dx^2+\tfrac{1}{4}\omega^2x^2+\varepsilon_0+\hat{V}(x))\Psi(x)=\lambda\Psi(x), \tag{5}$$

where

$$\omega=(3+r_0V''(r_0)/V'(r_0))^{1/2}, \tag{6}$$

$$\varepsilon_0=\frac{\bar{k}}{4}-\frac{(2-a)}{2}+\frac{(1-a)(3-a)}{4\bar{k}}+\frac{r_0^2\bar{k}V(r_0)}{(N+2l-a)^2}, \tag{7}$$

$$\lambda=\frac{Er_0^2}{\bar{k}}, \tag{8}$$

and

$$\hat{V}(x)=\frac{1}{\bar{k}^{1/2}}(\varepsilon_1 x+\varepsilon_3 x^3)+\frac{1}{\bar{k}}(\varepsilon_2 x^2+\varepsilon_4 x^4)+\frac{1}{\bar{k}^{3/2}}$$
$$\times(\delta_1 x+\delta_3 x^3+\delta_5 x^5)+\frac{1}{\bar{k}^2}(\delta_2 x^2+\delta_4 x^4+\delta_6 x^6)+\ldots, \tag{9}$$

with

$$\begin{aligned}
&\varepsilon_1=(2-a), \qquad \varepsilon_2=-3(2-a)/2, \qquad \varepsilon_3=-1+\frac{r_0^5 V'''(r_0)}{6\bar{k}^2},\\
&\varepsilon_4=\tfrac{5}{4}+r_0^6 V''''(r_0)/24\bar{k}^2; \qquad \delta_1=-\tfrac{1}{2}(1-a)(3-a), \qquad \delta_2=\tfrac{3}{4}(1-a)(3-a),\\
&\delta_3=2(2-a), \qquad \delta_4=-\tfrac{5}{2}(2-a), \qquad \delta_5=-\tfrac{3}{2}+r_0^7 V'''''(r_0)/120\bar{k}^2,\\
&\delta_6=\tfrac{7}{4}+r_0^8 V''''''(r_0)/720\bar{k}^2.
\end{aligned} \tag{10}$$

Now applying the fourth-order Rayleigh-Schrödinger perturbation theory to the perturbed harmonic oscillator (6) and arranging terms in the series for E in powers of $1/\bar{k}$, we obtain, for $N=3$ (which is the dimension of interest)

$$\begin{aligned}
E=\sum_{n=-2}^{\infty}\bar{k}^{-n}E^{(n)}
&=(3+2l-a)^2\left(\frac{1}{4r_0^2}+\tilde{V}(r_0)\right)+(3+2l-a)\left(\frac{(n+\frac{1}{2})\omega}{r_0^2}-\frac{(2-a)}{2r_0^2}\right)\\
&+\left(\frac{(1-a)(3-a)}{4r_0^2}+\frac{(1+2n)}{r_0^2}\tilde{\varepsilon}_2+\frac{3(1+2n+2n^2)}{r_0^2}\tilde{\varepsilon}_4\right.\\
&\left.-\frac{1}{\omega r_0^2}[\tilde{\varepsilon}_1^2+6(1+2n)\tilde{\varepsilon}_1\tilde{\varepsilon}_3+(11+30n+30n^2)\tilde{\varepsilon}_3^2]\right)\\
&+\frac{1}{(3+2l-a)}\left(\frac{1}{r_0^2}[(1+2n)\tilde{\delta}_2+3(1+2n+2n^2)\tilde{\delta}_4+5(3+8n+6n^2+4n^3)\tilde{\delta}_6]\right.\\
&-\frac{1}{\omega r_0^2}[(1+2n)\tilde{\varepsilon}_2^2+12(1+2n+2n^2)\tilde{\varepsilon}_2\tilde{\varepsilon}_4+2(21+59n+51n^2+34n^3)\tilde{\varepsilon}_4^2\\
&+2\tilde{\varepsilon}_1\tilde{\delta}_1+6(1+2n)\tilde{\varepsilon}_1\tilde{\delta}_3+30(1+2n+2n^2)\tilde{\varepsilon}_1\tilde{\delta}_5+6(1+2n)\tilde{\varepsilon}_3\tilde{\delta}_1\\
&+2(11+30n+30n^2)\tilde{\varepsilon}_3\tilde{\delta}_3+10(13+40n+42n^2+28n^3)\tilde{\varepsilon}_3\tilde{\delta}_5]\\
&+\frac{1}{\omega^2 r_0^2}[4\tilde{\varepsilon}_1^2\tilde{\varepsilon}_2+36(1+2n)\tilde{\varepsilon}_1\tilde{\varepsilon}_2\tilde{\varepsilon}_3+8(11+30n+30n^2)\tilde{\varepsilon}_2\tilde{\varepsilon}_3^2\\
&+24(1+2n)\tilde{\varepsilon}_1^2\tilde{\varepsilon}_4+8(31+78n+78n^2)\tilde{\varepsilon}_1\tilde{\varepsilon}_3\tilde{\varepsilon}_4\\
&+12(57+189n+225n^2+150n^3)\tilde{\varepsilon}_3^2\tilde{\varepsilon}_4]-\frac{1}{\omega^3 r_0^2}[8\tilde{\varepsilon}_1^3\tilde{\varepsilon}_3+108(1+2n)\tilde{\varepsilon}_1^2\tilde{\varepsilon}_3^2\\
&\left.+48(11+30n+30n^2)\tilde{\varepsilon}_1\tilde{\varepsilon}_3^3+30(31+109n+141n^2+94n^3)\tilde{\varepsilon}_3^4]\right),
\end{aligned} \tag{11}$$

where

$$\tilde{\varepsilon}_j = \frac{\varepsilon_j}{(2m\omega/\hbar)^{j/2}}, \qquad \tilde{\delta}_j = \frac{\delta_j}{(2m\omega/\hbar)^{j/2}}.$$

The above expression with $a = 0$ gives the energy in the unshifted $1/N$ expansion, with the corresponding classical minimum r_0 given by

$$2r_0^3 V'(r_0) = (3+2l)^2. \tag{12}$$

In the shifted version of the formalism, 'a' is to be chosen from the condition

$$E^{(-1)} = 0, \tag{13}$$

which then leads to the equation for determining 'a'

$$a = 2-(2n+1)\omega. \tag{14}$$

Next substituting (14) and (6) in the equation for r_0 in the shifted $1/N$ expansion, we obtain

$$[2r_0^3 V'(r_0)]^{1/2} - (2n+1)\left(3+\frac{r_0 V''(r_0)}{V'(r_0)}\right)^{1/2} = (2l+1). \tag{15}$$

Once r_0 is determined, the rest of the calculations become quite straightforward.

The method delineated above can readily be applied to the attractive radial Gaussian potential $V(r) = -A\,e^{-\lambda r^2}$. For the purpose of comparison with the works of various authors we set $A = 400$, $\lambda = 1$. In this case (12) and (15) read respectively

$$40r_0^2 \exp(-r_0^2/2) = (3+2l), \tag{12a}$$

and

$$40r_0^2 \exp(-r_0^2/2) - (2n+1)(4-2r_0^2)^{1/2} = (2l+1). \tag{15a}$$

We have calculated the energies both in the unshifted and the shifted $1/N$ expansions (see table 1). It is apparent from the results depicted in table 1 that for $n = 0$ states the unshifted $1/N$ expansion is on par with the shifted $1/N$ expansion and proves to be an excellent approximation. However, as n increases, the accuracy of the unshifted $1/N$ expansion deteriorates appreciably. This is not a little surprising in view of the fact that while $E^{(n)}$'s involve positive powers of n, r_0 and $1/k$ in the unshifted $1/N$ expansion do not. The shifted $1/N$ expansion on the other hand is found to yield fairly accurate results even for large n and l. However, for states very close to the continuum, the shifted $1/N$ expansion too, to the order considered in this comment, cannot claim its efficacy. It fails to predict, for instance, that $n = 7$, $l = 0$ is a bound state as dictated by the accurate numerical work (Crandall 1983) and the hypervirial Padé analysis (Lai 1983). This clearly shows that as one goes up the potential well, the shape of the potential becomes increasingly important. Hence to improve the situation for the bound states lying close to the continuum one should probably include more higher-order terms in $1/\bar{k}$. This is a rather tedious, albeit straightforward, job and has not been attempted in the present work.

Table 1. Energy eigenvalues, $-E_n$. First line, shifted $1/N$ expansion; second line, unshifted $1/N$ expansion; third line, hypervirial-Padé analysis (Lai 1983); fourth line, numerical result (Crandall 1983).

n \ l	0	1	2	3	4	5	6	7
0	341.8952	304.4629	268.1108	232.8753	198.7983	165.9283	134.3227	104.0514
	341.8952	304.4628	268.1108	232.8753	198.7983	165.9283	134.3227	104.0513
	341.8952	304.4628	268.1107	232.8753	198.7983	165.9282	134.3226	104.0512
	341.8952	304.4628	268.1107	232.8753	198.7983	165.9282		
1	269.6457	235.4513	202.4324	170.6404	140.1362	110.9938	83.3068	57.1971
	269.6415	235.4465	202.4270	170.6340	140.1284	110.9840	83.2935	57.1774
	269.6445	235.4500	202.4313	170.6393	140.1351	110.9929	83.3060	57.1963
	269.6445	235.4500	202.4313	170.6393	140.1351	110.9929		
2	203.9969	173.2573	143.8212	115.7649	89.1836	64.2016	40.9905	19.8093
	203.9306	173.1802	143.7299	115.6538	89.0436	64.0163	40.7278	19.3971
	203.9835	173.2443	143.8091	115.7542	89.1750	64.1959	40.9887	19.8128
	203.9835	173.2443	143.8091	115.7542	89.1750	64.1959		
3	145.4307	118.4320	92.9186	69.0127	46.8809	26.7680	9.0798	
	145.0832	118.0224	92.4244	68.3977	46.0813	25.6609	7.3964	
	145.3779	118.3840	92.8781	68.9836	46.8681	26.7779	9.1259	
	145.3779	118.3840	92.8781	68.9836	46.8681	26.7779		
4	94.5817	71.7197	50.6231	31.5185	14.7685	1.0300		
	93.4194	70.3313	48.9152	29.3284	11.7787	−3.4467		
	94.4577	71.6236	50.5677	31.5211	14.8515	1.2949		
	94.4577	71.6236	50.5677	31.5211	14.8515			
5	52.3080	34.1785	18.3249	5.2989				
	49.2596	30.4652	13.6072	−1.0911				
	52.1436	34.1299	18.4404	5.6729				
	52.1436	34.1299	18.4404	5.6731				
6	19.8693	7.5643	−1.2014					
	12.9244	−1.2173	−13.0949					
	19.9663	8.0833	0.1841					
	19.9663	8.0833	0.2049					
7	−0.4145							
	−15.2660							
	1.3467							
	1.3473							

The author is grateful to Shri N C Deb for computational help. He also wishes to thank the CSIR, India for financial support.

References

Bessis N, Bessis G and Joulabin B 1982 *J. Phys. A: Math. Gen.* **15** 3679
Buck B 1977 unpublished
Buck B, Friedrich H and Wheatley C 1977 *Nucl. Phys.* A **275** 246
Chatterjee A 1985 *J. Phys. A: Math. Gen.* **18** 735
Cohen M 1984 *J. Phys. A: Math. Gen.* **17** L101
Crandall R E 1983 *J. Phys. A: Math. Gen.* **16** L395

Imbo T, Pagnamenta A and Sukhatme U 1984 *Phys. Rev.* D **29** 1669
Lai C S 1983 *J. Phys. A: Math. Gen.* **16** L181
Mlodinow L and Papanicolaou N 1980 *Ann. Phys., NY* **128** 314
—— 1981 *Ann. Phys., NY* **131** 1
Mlodinow L and Shatz M P 1984 *J. Math. Phys.* **25** 943
Stephenson G 1977 *J. Phys. A: Math. Gen.* **10** L229
Sukhatme U and Imbo T 1983 *Phys. Rev.* D **28** 418
Witten E 1979 *Nucl. Phys.* B **160** 57