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LETTER TO THE EDITOR

On the Schrödinger equation for the gaussian potential $-A\exp(-\lambda r^2)$

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Abstract. The energy eigenvalues of the attractive radial gaussian potential for various eigenstates are very accurately determined within the framework of the hypervirial–Padé scheme.

The attractive radial gaussian potential of the form

$$V(r) = -A\exp(-\lambda r^2) \tag{1}$$

is of importance in nuclear physics. It has been used as a potential model in the theory of nucleon–nucleon scattering (Buck *et al* 1977). The bound-state energies of the gaussian potential were first computed by Buck (1977) using direct numerical integration, and by Stephenson (1977) using the Liouville–Green asymptotic method. Recently, Bessis *et al* (1982) have obtained the bound-state energies of the potential (1) for $\lambda = 1$ using a perturbational and also a variational treatment on a conveniently chosen basis of transformed Jacobi functions. It is shown that the traditional Rayleigh–Schrödinger method on the chosen basis can yield fairly accurate results.

Meanwhile, it has been shown that many problems of screened potentials (Lai 1981, 1982, Lai and Lin 1982) can be solved to a very high accuracy by using the hypervirial relations (Hirschfelder 1960, Swenson and Danforth 1972) and the Padé approximant method (Baker 1965, Killingbeck 1978). In the present paper, we would like to report that the bound-state energies of the gaussian potential (1) for various eigenstates can be accurately calculated within the framework of this hypervirial–Padé scheme.

Let us study the Schrödinger equation for the attractive radial gaussian potential (1)

$$-\frac{1}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2\frac{\mathrm{d}R}{\mathrm{d}r}\right)+\frac{l(l+1)}{r^2}R - A\exp(-\lambda r^2)R = ER, \tag{2}$$

where the units $2m = \hbar = 1$ are used. If we introduce the function $u(r) = rR(r)$, and expand the exponential $\exp(-\lambda r^2)$ in powers of r^2, we find from equation (2)

$$\left(-\frac{\mathrm{d}^2}{\mathrm{d}r^2}+\frac{l(l+1)}{r^2}+\sum_{k=0}^{\infty}\lambda^k V_k r^{2k+2}\right)u = E'u, \tag{3}$$

where $E' = E + A$, and the potential $V'(r)$ in the above one-dimensional Schrödinger

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equation can be written as

$$V'(r)=\frac{l(l+1)}{r^2}+\sum_{k=0}^{\infty}\lambda^k V_k r^{2k+2}, \tag{4}$$

with the potential coefficients V_k given by

$$V_0=A\lambda=\omega^2, \qquad V_k=(-1)^k\omega^2/(k+1)!, \qquad k\neq 0. \tag{5}$$

We note that, in (3), $u(r)$ must vanish at $r=0$, and that the energy series E' obtained from (3) will be asymptotic for large λ.

We now proceed to solve (3) with the use of the hypervirial–Padé scheme (Killingbeck 1978, Lai 1981). Corresponding to the energy $E'=E+A$ for the Schrödinger equation (3), the Hamiltonian H' is given by

$$H'=-\mathrm{d}^2/\mathrm{d}r^2+V'(r), \tag{6}$$

where $V'(r)$ is defined by (4). If we now apply the hypervirial theorems to the Hamiltonian H', we obtain the following hypervirial relations (Swenson and Danforth 1972):

$$E'\langle r^N\rangle=\tfrac{1}{2}(N+1)^{-1}\langle r^{N+1}\,\mathrm{d}V'/\mathrm{d}r\rangle+\langle r^N V'\rangle-\tfrac{1}{4}N(N-1)\langle r^{N-2}\rangle. \tag{7}$$

Let us assume that the energy E' and the expectation values $\langle r^N\rangle$ can be expanded in power series of the perturbation parameter λ as

$$E'_j=\sum_{k=0}^{\infty}E_j^{(k)}\lambda^k, \tag{8}$$

$$\langle r^N\rangle=\sum_{k=0}^{\infty}C_N^{(k)}\lambda^k, \tag{9}$$

where $C_0^{(k)}=\delta_{0k}$. The unperturbed value of $E_j'^{(0)}$ in (8) is given by

$$E_j'^{(0)}=\omega(2j+1), \qquad j\neq 0, \tag{10}$$

where j is the quantum number for the harmonic oscillator and $j\neq 0$ as required by the condition $u(r=0)=0$ (Landau and Lifshitz 1963). The unperturbed values of $C_N^{(0)}$ can be derived from the hypervirial relations (7).

From the Hellman–Feynman theorem, we obtain the relation (Lai 1981)

$$E^{(k)}=\frac{1}{k}\sum_{m=0}^{k}mV_mC_{2m+2}^{(k-m)}, \qquad k\neq 0. \tag{11}$$

Substituting (8) and (9) into (7), we obtain also the following relations between the coefficients $C_N^{(k)}$ and the energy coefficients $E^{(k)}$:

$$\begin{aligned}C_{N+2}^{(k)}=\frac{N+1}{(n+2)\omega^2}\Big[&E^{(0)}C_N^{(k)}+E^{(1)}C_N^{(k-1)}+E^{(2)}C_N^{(k-2)}+\ldots+E^{(k)}C_N^{(0)}\\&-\left(\frac{Nl(l+1)}{N+1}-\frac{N(N-1)}{4}\right)C_{N-2}^{(k)}-\frac{N+3}{N+1}V_1C_{N+4}^{(k-1)}-\frac{N+4}{N+1}V_2C_{N+6}^{(k-2)}-\ldots\\&-\frac{N+k+2}{N+1}V_kC_{N+2k+2}^{(0)}\Big], \qquad N\geq 0,\end{aligned} \tag{12}$$

Table 1. Calculated energy eigenvalues E_{nl} for $\lambda = 1$. First line, the present calculation; second line, numerical integration (Buck 1977); third line, perturbation calculation (Bessis *et al* 1982); fourth line, variational calculation (Bessis *et al* 1982).

n \ l	0	1	2	3	4	5	6	7
0	341.8952	304.4628	268.1107	232.8753	198.7983	165.9282	134.3226	104.0512
	341.9	304.5	268.1	232.9	198.8	165.9	134.3	104.1
	341.888	304.449	268.089	232.843	198.755	165.875	134.260	103.986
	341.895	304.463	268.111	232.875	198.797	165.925	134.317	104.040
1	269.6445	235.4500	202.4313	170.6393	140.1351	110.9929	83.3060	57.1963
	269.7	235.5	202.4	170.6	140.1	111.0	83.3	57.2
	269.646	235.453	202.434	170.640	140.128	110.970	83.225	67.099
	269.644	235.450	202.431	170.639	140.134	110.989	83.295	57.171
2	203.9835	173.2443	143.8091	115.7542	89.1750	64.1959	40.9887	19.8128
	204.0	173.3	143.8	115.8	89.2	64.2	41.0	19.8
	203.955	173.226	143.803	115.755	89.167	64.141	40.814	19.371
	203.983	173.244	143.808	115.752	89.169	64.180	40.950	19.721
3	145.3779	118.3840	92.8781	68.9836	46.8681	26.7779	9.1259	
	145.4	118.4	92.9	69.0	46.9	26.8	9.1	
	145.285	118.331	92.864	68.977	46.788	26.446	8.152	
	145.377	118.381	92.873	68.973	46.846	26.727	8.995	
4	94.4577	71.6236	50.5677	31.5211	14.8515	1.2949		
	94.5	71.6	50.6	31.5	14.9	—		
	94.344	71.595	50.564	31.375	14.187	−0.797		
	94.454	71.617	50.557	31.499	14.794	(1.1)		
5	52.1436	34.1299	18.4404	5.6729				
	52.2	34.2	18.5	—				
	52.131	34.130	18.120	4.257				
	52.139	34.119	18.419	5.6				
6	19.9663	8.0833	0.1841					
	20.0	8.1	—					
	19.920	7.269	−3.117					
	19.921	8.045	(0.2)					
7	1.3467							
	1.4							
	−0.919							
	1.463							

where N are even numbers, and the potential coefficients V_k are given by (5). The recurrence relations (11) and (12) can be used to evaluate the energy coefficients $E^{(k)}$ from a knowledge of $C_N^{(m)}$ and $E^{(m)}$ with $m \leqslant k-2$ in a hierarchical manner (Lai 1982). For example, the energy eigenvalues of equation (2), up to the third order of λ, are found as

$$E = -A + 2\omega a - \tfrac{3}{4}[a^2 - \tfrac{1}{3}l(l+1) + \tfrac{1}{4}]\lambda - (a/96\omega)[11a^2 - 3l(l+1) + \tfrac{1}{4}]\lambda^2 - (1/1536\omega^2)[85a^4 + \tfrac{1}{2}a^2 - \tfrac{423}{16} - 6a^2 l(l+1) - 15l^2(l+1)^2 + \tfrac{93}{2}l(l+1)]\lambda^3 + \ldots, \tag{13}$$

where $\omega = (A\lambda)^{1/2}$, $l < j$, and $a = j + \frac{1}{2}$ with $j = 1, 2, 3, \ldots$. We note that l takes the values $0, 2, 4, \ldots$ for odd j and $1, 3, 5, \ldots$ for even j (Landau and Lifshitz 1963).

The energy series (13) is asymptotic for large λ. However, we can calculate the bound-state energies E to a very high accuracy by forming the Padé approximant to the energy series (Killingbeck 1978, Lai 1981). We confine ouselves to the calculation of the [10, 10] Padé approximant to the energy series (Baker 1965)

$$E[10,10] = E^{(0)} + \lambda E^{(1)} \frac{1 + \lambda p_1 + \lambda^2 p_2 + \ldots + \lambda^9 p_9}{1 + \lambda q_1 + \lambda^2 q_2 + \ldots + \lambda^{10} q_{10}} = E^{(0)} + \lambda E^{(1)} + \lambda^2 E^{(2)} + \ldots + \lambda^{20} E^{(20)}, \tag{14}$$

where $E^0 = -A + \omega(2j+1)$ as defined by (3).

Our calculated energy values of the [10, 10] Padé approximant for the states n and $l = 0$–7 with $\lambda = 1$ are shown in table 1. Instead of using the quantum number j of the unperturbed harmonic oscillator, we use here the customary quantum number n for the particle levels in the nucleus. Our results are compared with those obtained from numerical integration (Buck 1977), and those calculated by Bessis *et al* (1982) using the perturbational and variational treatment on a conveniently chosen basis of the transformed Jacobi functions. It appears from table 1 that the results of the present calculation are in total agreement with those of numerical integration (Buck 1977).

In conclusion, we have shown that the bound-state energies of the attractive radial gaussian potential can be accurately determined within the simple framework of the hypervirial–Padé scheme. With the introduction of the screening parameter λ in the gaussian potential $V(r) = -A \exp(-\lambda r^2)$, the present method of calculation is therefore more general than the perturbational and variational calculations of Bessis *et al* (1982).

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