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A note on the Schrödinger equation for the potential $A\exp(-x^2)-l(l+1)/x^2$

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Abstract. The bound states energies and eigenfunctions of the Schrödinger equation with a radial gaussian potential are obtained using a perturbational and also a variational treatment on a conveniently chosen basis of transformed Jacobi functions. The accuracy of the results is fairly good.

Recently, special interest has been drawn to the resolution of the eigenequation

$$\left(\frac{d^2}{dx^2}+A\exp(-x^2)-\frac{l(l+1)}{x^2}+E\right)\psi(x)=0 \tag{1}$$

with the associated boundary conditions $\psi(0)=\psi(\infty)=0$.

In particular, the attractive radial gaussian potential has been used as a potential model in the theory of nucleon–nucleon scattering (Buck 1977) and eigenvalues of the wave equation (1) have been computed by direct numerical integration by Buck and have also been obtained by Stephenson (1977) using the Liouville–Green asymptotic method.

In the present paper, it is shown that the traditional Rayleigh–Schrödinger method can lead to analytical approximations of the energies with a fairly good accuracy.

It is clear that the gaussian potential $\exp(-x^2)$ behaves as $(\cosh x)^{-2}$ and that the rotational term $1/x^2$ closely resembles $(\sinh x)^{-2}$. Hence a suitable and exactly soluble unperturbed wave equation is

$$\left(\frac{d^2}{dx^2}+\frac{A}{(\cosh x)^2}-\frac{l(l+1)}{(\sinh x)^2}+E^{(0)}\right)\psi^{(0)}(x)=0. \tag{2}$$

When setting $A=\mu^2-\frac{1}{4}$, equation (2) is just the transformed Jacobi eigenfunction. Its solutions can be obtained either by the factorisation method (Infeld and Hull 1951, Hadinger *et al* 1974) or more classically (see, for instance, Szegö 1978). The eigenvalues are

$$E_{nl}^{(0)}=-(2n+\mu+l+\tfrac{3}{2})^2. \tag{3}$$

The square integrable eigenfunctions are

$$\psi_{nl}^{(0)}(x)=N_{nl}(\sinh x)^{l+1}(\cosh x)^{\mu+1/2}P_n^{(l+1/2,\mu)}(\cosh 2x) \tag{4}$$

where $P_n^{(l+1/2,\mu)}$ is a Jacobi polynomial and N_{nl} is the normalisation constant.

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In order to satisfy the boundary conditions (1), the condition $\mu \leqslant -(n+l+1)$ must hold. Hence, one has to choose the negative solution of $\mu^2 - \frac{1}{4} = A$, i.e. $\mu = -(A+\frac{1}{4})^{1/2}$.

Following from the choice (2) of the unperturbed wave equation, the perturbation to be considered is

$$V(x) = A[\exp(-x^2) - (\cosh x)^{-2}] - l(l+1)(x^{-2} - (\sinh x)^{-2}). \tag{5}$$

Matrix elements of $V(x)$ on the basis of the functions $\psi_{nl}^{(0)}(x)$ are not at all easy to calculate in closed form. Therefore a simple expedient is to expand the first term of (5) in a Taylor series in $u(x) = (\cosh x)^{-2}$ near $x = 0$, i.e. in a series of $((\cosh x)^{-2} - 1)^j = (-1)^j (\tanh x)^{2j}$. One gets

$$\exp(-x^2) - (\cosh x)^{-2} = \sum_{j=2} a_j (\tanh x)^{2j}. \tag{6}$$

An appropriate expansion for the second term of (5) could be

$$x^{-2} - (\sinh x)^{-2} = \tfrac{1}{3}(\cosh x)^{-2/5} + \sum_{j=2} b_j (\tanh x)^{2j} \tag{7}$$

where the first term has been found by noting that its expansion in powers of x reproduces the first two terms of the expansion in x^{2j} of the left-hand side, i.e. $x^{-2} - (\sinh x)^{-2} \simeq \frac{1}{3} - \frac{1}{15}x^2 + \ldots$. Values of the a_j and b_j coefficients can be found easily, for instance, by noting that

$$\begin{aligned} a_n &= \lim_{x \to 0^+} \left((\coth x)^{2n} (\exp(-x^2) - 1) + (\coth x)^{2n-2} - \sum_{j=2}^{n-1} a_j (\coth x)^{2(n-j)} \right) \\ b_n &= \lim_{x \to 0^+} \left((\coth x)^{2n} [x^{-2} + 1 - (\coth x)^2 - \tfrac{1}{3}(\cosh x)^{-2/5}] - \sum_{j=2}^{n-1} b_j (\coth x)^{2(n-j)} \right) \end{aligned} \tag{8}$$

and the use of the expansion of the functions in series of x^{2j}. One finds

$$\begin{aligned} &a_2 = -1/6 \qquad a_3 = -1/90 \qquad a_4 = 57/2520 \qquad a_5 = 1033/37800 \\ &a_6 = 0.024667708 \qquad a_7 = 0.020542460 \qquad a_8 = 0.016622222 \\ &a_9 = 0.013314561 \qquad a_{10} = 0.010640834 \qquad a_{11} = 0.008514754 \\ &a_{12} = 0.006832858 \qquad a_{13} = 0.005502169 \qquad a_{14} = 0.004446471 \\ &a_{15} = 0.003605590 \\ &b_2 = -34/4725 \qquad b_3 = -386/70875 \qquad b_4 = -0.003986789 \\ &b_5 = -0.002244698. \end{aligned} \tag{9}$$

Only the first fifteen a_j and the first five b_j have been reproduced since they are sufficient to yield numerically stable results.

Finally, the perturbation (5) can be written

$$V(x) = \tfrac{1}{3} l(l+1) (\cosh x)^{-2/5} + \sum_{j=2} (A a_j - l(l+1) b_j)(\tanh x)^{2j}. \tag{10}$$

Such an expansion (10) of $V(x)$ leads to matrix elements which can be merely expressed in terms of Euler Γ functions. Indeed, let us consider the current matrix elements

$$\left\langle nl \left| \frac{(\sinh x)^{2u}}{(\cosh x)^{2v}} \right| ml \right\rangle = (N_{nl} N_{ml})^{-1} \int_0^\infty \psi_{nl}^{(0)}(x) \frac{(\sinh x)^{2u}}{(\cosh x)^{2v}} \psi_{ml}^{(0)}(x)\, \mathrm{d}x. \tag{11}$$

Setting $y = \cosh(2x)$, the wavefunctions $\psi_{nl}^{(0)}(x)$ can be written (see equation (4))

$$\psi_{nl}^{(0)} = N_{nl} 2^{-(\alpha+\beta+1)/2} (y-1)^{(2\alpha+1)/4} (y+1)^{(2\beta+1)/4} P_n^{(\alpha,\beta)}(y) \tag{12}$$

where $\alpha = l + \frac{1}{2}$ and $\beta = \mu$.

The matrix element (11) becomes

$$\left\langle nl \left| \frac{(\sinh x)^{2u}}{(\cosh x)^{2v}} \right| ml \right\rangle = 2^{-(\alpha+\beta+u-v+2)} \int_1^\infty (y-1)^{\alpha+u} (y+1)^{\beta-v} P_n^{(\alpha,\beta)}(y) P_m^{(\alpha,\beta)}(y)\, dy. \tag{13}$$

In order to take advantage of the orthogonality property of the wavefunctions (12), one can expand the $P_n^{(\alpha,\beta)}(y)$ on the finite basis of the $P_k^{(\alpha+u,\beta-v)}(y)$

$$P_n^{(\alpha,\beta)}(y) = \sum_{k=0}^{n} C_k^{(n)}(u,v) P_k^{(\alpha+u,\beta-v)}(y). \tag{14}$$

A general expression of the coefficients $C_k^{(n)}$, which involves ratios of Γ functions, has been given by Miller (see Miller 1968, formula (3.2) p 1178); for brevity's sake it is not reproduced here. Hence, one gets

$$\left\langle nl \left| \frac{(\sinh x)^{2u}}{(\cosh x)^{2v}} \right| ml \right\rangle = 2^{-(\alpha+\beta+u-v+2)} \sum_{k=0}^{n} \sum_{t=0}^{m} C_k^{(n)}(u,v) C_t^{(m)}(u,v)$$
$$\times \int_1^\infty (y-1)^{\alpha+u} (y+1)^{\beta-v} P_k^{(\alpha+u,\beta-v)}(y) P_t^{(\alpha+u,\beta-v)}(y)\, dy. \tag{15}$$

Now, owing to the orthogonality property of the wavefunctions (12), the expression (15) can be rewritten

$$\left\langle nl \left| \frac{(\sinh x)^{2u}}{(\cosh x)^{2v}} \right| ml \right\rangle = \sum_{k=0}^{k_M} C_k^{(n)}(u,v) C_k^{(m)}(u,v) I_k^{(\alpha+u,\beta-v)} \tag{16}$$

where $k_M = \min(n, m)$ and

$$I_k^{(a,b)} = 2^{-(a+b+2)} \int_1^\infty (y-1)^a (y+1)^b |P_k^{(a,b)}(y)|^2\, dy. \tag{17}$$

A closed form expression of the above integral is obtained easily by using successively the orthogonality property of the Jacobi polynomials, then Rodrigues formula and integrating the result by parts k times (see, for instance, Szegö 1978). Indeed, one can write

$$\begin{aligned} I_k^{(a,b)} &= 2^{-(a+b+2)} \int_1^\infty (y-1)^a (y+1)^b P_k^{(a,b)} l_{kk}^{(a,b)} y^k\, dy \\ &= 2^{-(a+b+k+2)} \frac{l_{kk}^{(a,b)}}{k!} \int_1^\infty y^k \left(\frac{d}{dy}\right)^k [(y-1)^{k+a}(y+1)^{k+b}]\, dy \\ &= 2^{-(a+b+k+2)} (-1)^k l_{kk}^{(a,b)} \int_1^\infty (y-1)^{k+a}(y+1)^{k+b}\, dy \end{aligned} \tag{18}$$

where

$$l_{kk}^{(a,b)} = 2^{-k} \binom{2k+a+b}{k}$$

is the coefficient of y^k in the Jacobi polynomial $P_k^{(a,b)}(y)$.

The last integral in (18) is found in tables (see, for instance, Gradshteyn and Ryzhik 1980) and one gets

$$I_k^{(a,b)} = \tfrac{1}{2}\frac{\Gamma(k+a+1)\Gamma(-k-a-b)}{\Gamma(k+1)\Gamma(-k-b)(2k+a+b+1)}. \tag{19}$$

Finally, the required matrix element between normalised wavefunctions can be written (see equations (11), (15), (17) and (19))

$$\int_0^\infty \psi_{nl}^{(0)}(x)\frac{(\sinh x)^{2u}}{(\cosh x)^{2v}}\psi_{ml}^{(0)}(x)\,\mathrm{d}x = \sum_{k=0}^{k_M} X_k^{(n)}(u,v)\,X_k^{(m)}(u,v) \tag{20}$$

with

$$X_k^{(n)}(u,v) = C_k^{(n)}(u,v)\,(I_k^{(\alpha+u,\beta-v)}/I_k^{(\alpha,\beta)})^{1/2}.$$

The energy at the first order of the perturbation is

$$E_{nl}^{(1)} = -(2n+\mu+l+\tfrac{3}{2})^2 - \sum_{k=0}^{n}\Big(\tfrac{1}{3}l(l+1)\,|X_k^{(n)}(0,\tfrac{2}{5})|^2$$

$$+\sum_{j=2}(Aa_j - l(l+1)b_j)\,|X_k^{(n)}(j,j)|^2\Big). \tag{21}$$

An improvement of the technique can be obtained by expanding $\exp(-x^2)$ in a Taylor series in $u(x)=(\cosh x)^{-2}$ near the maximum x_0 of the electronic density function $|\psi_{nl}^{(0)}(x)|^2$, or, more crudely, for sake of simplicity, near the maximum x_0 of the density of the $n=0$ state. In that case, it is defined by the condition $(\tanh x_0)^2 = -(l+1)/(\mu+\frac{1}{2})$. This last choice of x_0 is found to be acceptable on average for all states and has been used when defining the unperturbed functions.

When truncating the expansion of $\exp(-x^2)$ after the first two terms, one gets

$$\exp(-x^2) \simeq d_0 + d_1(\cosh x)^{-2} \tag{22}$$

where

$$d_0 = \exp(-x_0^2)(1 - x_0\coth x_0) \qquad d_1 = \exp(-x_0^2)x_0\,(\cosh x_0)^3/\sinh x_0.$$

Then, instead of the unperturbed eigenequation (2), one considers the Jacobi eigenequation

$$\Big(\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{Ad_1}{(\cosh x)^2} + d_0 - \frac{l(l+1)}{(\sinh x)^2} + \mathscr{E}^{(0)}\Big)\phi^{(0)}(x) = 0. \tag{23}$$

The associated eigenvalues are

$$\mathscr{E}_{nl}^{(0)} = -(2n+\mu'+l+\tfrac{3}{2})^2 - Ad_0 \tag{24}$$

with $\mu' = -(Ad_1+\frac{1}{4})^{1/2}$.

The perturbation to be considered is

$$\mathscr{V}(x) = V(x) + \frac{A(1-d_1)}{(\cosh x)^2} - Ad_0. \tag{25}$$

The energy, at the first order of the perturbation, is

$$\mathscr{E}_{nl}^{(1)} = \mathscr{E}_{nl}^{(0)} - \langle\phi_{nl}^{(0)}|\mathscr{V}(x)|\phi_{nl}^{(0)}\rangle \tag{26}$$

where the calculation of matrix elements of $\mathcal{V}(x)$ in the basis of the $\phi_{nl}^{(0)}$ is the same (with μ' instead of μ) as that of $V(x)$ in the basis of the $\psi_{nl}^{(0)}$.

It is shown in table 1 that, for the case $A = 400$ and the states n and $l = 0$–7, the above expression for $\mathscr{E}_{nl}^{(1)}$ leads to results which compare well with those obtained by direct integration of the Schrödinger equation (Buck 1977). These results are corroborated by a variational calculation on a truncated basis of $\phi_{nl}^{(0)}$ functions (7–10 basis functions). The coefficients of the eigenvectors have been obtained by diagonalisation of the variational matrix but are not reproduced here. By inspection, one can see

Table 1. Bound states eigenvalues. First line, perturbational calculation; second line, variational calculation; third line, numerical integration (Buck 1977); fourth line, Liouville–Green method (Stephenson 1977).

n \ l	0	1	2	3	4	5	6	7
0	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
	341.9	304.5	268.1	232.9	198.8	165.9	134.3	104.1
	341.6	304.2	267.9	232.6	198.5	165.7	134.1	103.9
1	269.646	235.453	202.434	170.640	140.128	110.970	83.255	57.099
	269.644	235.450	202.431	170.639	140.134	110.989	83.295	57.171
	269.7	235.5	202.4	170.6	140.1	111.0	83.3	57.2
	269.4	235.2	202.2	170.4	139.9	110.7	83.0	56.9
2	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
	204.0	173.3	143.8	115.8	89.2	64.2	41.0	19.8
	203.7	173.0	143.6	115.5	88.9	63.9	40.7	19.5
3	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	
	145.4	118.4	92.9	69.0	46.9	26.8	9.1	
	145.1	118.1	92.6	68.7	46.6	26.5	8.8	
4	94.344	71.595	50.564	31.375	14.187	−0.797		
	94.454	71.617	50.557	31.499	14.794	(1.1)		
	94.5	71.6	50.6	31.5	14.9	—		
	94.2	71.4	50.3	31.3	14.6	—		
5	52.131	34.130	18.120	4.257				
	52.139	34.119	18.419	5.6				
	52.2	34.2	18.5	—				
	51.9	33.9	18.2	—				
6	19.920	7.269	−3.117					
	19.921	8.045	(0.2)					
	20.0	8.1	—					
	19.7	7.8	—					
7	−0.919							
	1.463							
	1.4							
	1.1							

that, in all cases, there is a predominant coefficient and that the mixing of the unperturbed $\phi_{nl}^{(0)}$ states is small and, naturally, increases with the values of n and l. This trend is followed by the value δ of the third finite difference in n of the eigenvalues $\mathscr{E}_{nl}$:

$$\Delta_n^3(\mathscr{E}_{nl}) = 3(\mathscr{E}_{n+1,l} - \mathscr{E}_{n+2,l}) - (\mathscr{E}_{nl} - \mathscr{E}_{n+3,l}) = \delta.$$

It is easily verified (equation (24) or (3)) that for the unperturbed eigenvalues $\mathscr{E}_{nl}^{(0)}$ the value of δ is exactly zero for any n and l. In table 1, the value of δ ranges from 0.5 to 2.3 as n and l increase.

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