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LETTER TO THE EDITOR

On the Schrödinger equation with a Gaussian potential

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Abstract. Eigenvalues and approximate eigenfunctions of the Schrödinger equation with an attractive radial Gaussian potential are obtained from a first-order perturbation treatment based on a *scaled* harmonic oscillator model. The bound-state energies are of comparable accuracy to those obtained using high-order perturbation theory or numerical integration.

The solution of Schrödinger's equation with an attractive radial Gaussian potential, $V(r) = -A \exp(-\lambda r^2)$, has attracted a great deal of recent interest. Thus, Buck (1977 unpublished; quoted by Bessis *et al* (1982)) and Crandall (1983) have calculated bound-state eigenvalues numerically, while Stephenson (1977) used the wkb approximation. Rayleigh-Schrödinger perturbation theory based on Jacobi functions, and carried through first order only (Bessis *et al* 1982), yields fair numerical accuracy, but the comparison (zero-order) Hamiltonian adopted is rather complex so that the calculation of the first-order matrix elements is by no means straightforward. By contrast, high-order perturbation theory based on a Taylor series expansion of $V(r)$ combined with hypervirial Padé analysis (Lai 1983) yields precise energies, but not wavefunctions.

A simple alternative perturbation procedure, which yields approximate eigenfunctions as well as eigenvalues, is the following. The leading non-trivial term in the expansion of $V(r)$ is $\lambda A r^2$, suggesting that we choose as comparison Hamiltonian the operator H_0 which describes the three-dimensional isotropic harmonic oscillator. Thus, we take

$$H_0 = -\nabla^2 + k^2 r^2, \quad (1)$$

leaving k as a disposable scale parameter to be determined appropriately. The eigenvalue problem is then amenable to solution by means of conventional Rayleigh-Schrödinger perturbation theory with the perturbing operator given by

$$H_1 = -[k^2 r^2 + A \exp(-\lambda r^2)], \quad (2)$$

and different choices of k lead to representations which have been called *rescaled* (Banerjee 1979) or *renormalised* (Killingbeck 1981) perturbation series.

The spectrum of H_0 has been studied in detail (see e.g. Messiah 1961) and the eigenvalues take the form

$$E_{nl}^{(0)} = (2p+3)k = (4n+2l+3)k \quad (n, l = 0, 1, 2, \dots) \quad (3)$$

where, to each value of $p=2n+l$, there correspond $\frac{1}{2}(p+1)(p+2)$ energetically degenerate states of well defined angular momentum with quantum numbers l and m .

The corresponding eigenfunctions $\psi_{nlm}^{(0)}$ are products of normalised spherical harmonics $Y_{lm}(\theta, \phi)$ and radial functions $R_{nl}(r)$ given by

$$R_{nl}(r) = N_{nl} \exp(-\frac{1}{2}kr^2) r^l L_n^{l+1/2}(kr^2) \quad (4)$$

where $L_n^{l+1/2}(kr^2)$ denotes an associated Laguerre polynomial.

Examination of the eigenvalues computed previously (cf Lai 1983) shows that the lower levels of $H_0 + H_1$ are almost degenerate, with a degeneracy pattern identical with that of the $E_{nl}^{(0)}$, so that our choice of H_0 is sensible. It is also convenient, since matrix elements of H_1 can be calculated without great difficulty with the functions $\psi_{nlm}^{(0)}$.

Because of the orthonormality of the spherical harmonics, it is necessary to calculate only radial integrals between states of the *same* l . We find very easily that

$$\langle ml|r^2|nl\rangle = k^{-1} \{ \frac{1}{2}(4n+2l+3)\delta_{m,n} - [(n+1)(n+l+\frac{3}{2})]^{1/2}\delta_{m,n+1} \} \quad (5)$$

and (for details, see the appendix)

$$\begin{aligned} \langle ml|\exp(-\lambda r^2)|nl\rangle \\ = k^{l+3/2} \lambda^{m+n} (m!n! \Gamma(m+l+\frac{3}{2})\Gamma(n+l+\frac{3}{2}))^{1/2} / (k+\lambda)^{m+n+l+3/2} \\ \times \sum_{i=0}^{\min(m,n)} \frac{1}{\Gamma(i+l+\frac{3}{2})i!(m-i)!(n-i)!} \left(\frac{k}{\lambda}\right)^{2i} \end{aligned} \quad (6)$$

so that the matrices of H_0 and H_1 are fully determined analytically.

In particular, the lowest energy level for each l (corresponding to $n=0$) is given (correct to first order) by

$$E_{0l} = \langle \psi_{0l}^{(0)} | H_0 + H_1 | \psi_{0l}^{(0)} \rangle = (l + \frac{3}{2})k - f_l(t) \quad (7)$$

where

$$f_l(t) = At^{l+3/2}, \quad t = k/(k+\lambda). \quad (8)$$

Since equation (7) is a rigorous upper bound, we may now optimise E_{0l} with respect to k and obtain the result (valid for *all* λ, A)

$$E_{0l} = \lambda t [(l + \frac{3}{2})(1-t) - 1] / (1-t)^2, \quad (1-t)^2 t^{l+1/2} = \lambda/A. \quad (9)$$

Note that the optimised value, $k = (\lambda A)^{1/2}$, leads to $t = [1 + (\lambda/A)^{1/2}]^{-1}$ which is a fair approximation to the optimised t for low l .

Table 1 contains perturbation energies (correct to first order) calculated with $k=20$ and with optimised values of k , compared with the most accurate values available (Crandall 1983, Lai 1983). The effect of optimising k is negligible for low l , but becomes increasingly significant as l increases, and it is clear that with k optimised, $\psi_{0l}^{(0)}(k)$ provides a very satisfactory representation of these eigenfunctions.

For $n \geq 1$, the energy calculated from first-order perturbation theory is not a guaranteed upper bound unless constraints are placed on the variation of the scale parameter k . For example, for $n=1$, we find that

$$E_{1l} = (l + \frac{7}{2})k - [t^2 + (l + \frac{3}{2})(1-t)^2]f_l(t), \quad (10)$$

and unconstrained variation of this expression yields energies which are slightly too low for low l (see table 1). However, these optimised perturbation energies are clearly excellent *approximations* to the true energy levels, whereas those calculated with $k = (\lambda A)^{1/2}$ are very much less accurate. Similar results are easily obtained for the

Table 1. Calculated eigenvalues, $-E_{nl}$.

l	$n = 0$ states				$n = 1$ states		
	(1)	(2)	(3)	(4)	(1)	(2)	(3)
0	341.7715	341.8831	341.8952	341.8952	268.4722	269.6802	269.6445
1	304.0681	304.4334	304.4627	304.4628	233.1574	235.5181	235.4500
2	267.2077	268.0554	268.1104	268.1107	198.5335	202.5141	202.4313
3	231.1502	232.7840	232.8746	232.8753	164.5697	170.7122	170.6393
4	195.8573	198.6594	198.7965	198.7983	131.2361	140.1660	140.1351
5	161.2927	165.7278	165.9248	165.9282	98.5045	110.9411	110.9929
6	127.4216	134.0435	134.3164	134.3226	66.3476	83.1183	83.3060
7	94.2110	103.6719	104.0401	104.0512	34.7397	56.8013	57.1963

- (1) Perturbation results, $k = 20$.
- (2) Perturbation results, k optimised.
- (3) Variational results.
- (4) Accurate values from Crandall (1983) and Lai (1983).

more highly excited states having $n \geq 2$, and we may conclude that the functions $\psi_{nl}^{(0)}(k)$, with k optimised, are excellent first approximations to *all* the bound states.

Energy levels of greater accuracy can be obtained quite easily by using variational trial functions which consist of linear combinations of the functions $\psi_{nl}^{(0)}(k)$, since these constitute a suitable complete orthonormal set for any *fixed* k . If we solve the appropriate secular equation, each eigenvalue can be optimised in turn and still yields a rigorous upper bound to one of the energy levels (MacDonald 1933), but the choice of k is expected to be much less critical once we include a few more terms of the set $\{\psi_{nl}^{(0)}(k)\}$. It turns out that, with k chosen so as to optimise E_{0l} (equation (9) above) the off-diagonal matrix element $\langle \psi_{0l}^{(0)} | H_0 + H_1 | \psi_{1l}^{(0)} \rangle$ vanishes identically, showing that this choice of k is optimal for any linear combination of $\psi_{0l}^{(0)}$ and $\psi_{1l}^{(0)}$. To obtain greater accuracy for the $n = 0$ eigenvalues, it is sufficient to solve a 2×2 secular equation based on $\psi_{0l}^{(0)}$ and $\psi_{2l}^{(0)}$ only with k chosen to optimise E_{0l} . We then obtain the 'variational' results of table 1, and we note that Bessis *et al* (1982) obtained similar accuracy in their variational calculations based on Jacobi functions but required linear combinations of at least seven compared with just two employed here.

Appendix

The integrals $\langle ml | \exp(-\lambda r^2) | nl \rangle$ may be written conveniently

$$\langle ml | \exp(-\lambda r^2) | nl \rangle = \frac{1}{2} N_{ml} N_{nl} I(m, n; \mu) / k^{l+3/2} \tag{A1}$$

where

$$I(m, n; \mu) = \int_0^\infty e^{-(1+\mu)x} x^p L_m^p(x) L_n^p(x) dx \tag{A2}$$

and we have written

$$x = kr^2, \quad \mu = \lambda/k, \quad p = l + \frac{1}{2}. \tag{A3}$$

The normalisation constant N_{ml} is obtained easily as a special case of (A1), using the

standard result (Abramowitz and Stegun 1965, (AS) (22.2.12))

$$I(m, n; 0) = \Gamma(n + p + 1) \delta_{mn} / n!. \tag{A4}$$

When $\mu \neq 0$, we rewrite

$$I(m, n; \mu) = t^{p+1} \int_0^\infty e^{-y} y^p L_m^p(ty) L_n^p(ty) dy \tag{A5}$$

where

$$t = 1/(1 + \mu) = k/(k + \lambda). \tag{A6}$$

Now, using AS (22.12.7), we may write

$$L_m^p(ty) = (1 - t)^m \Gamma(m + p + 1) \sum_{i=0}^m \frac{1}{\Gamma(i + p + 1)(m - i)!} \left(\frac{t}{1 - t}\right)^i L_i^p(y) \tag{A7}$$

and similarly for $L_n^p(ty)$. Thus, on account of (A4), we have finally

$$I(m, n; \mu) = t^{p+1} (1 - t)^{m+n} \Gamma(m + p + 1) \Gamma(n + p + 1) \times \sum_{i=0}^{\min(m,n)} \frac{1}{\Gamma(i + p + 1) i! (m - i)! (n - i)!} \left(\frac{t}{1 - t}\right)^{2i}, \tag{A8}$$

which yields equation (6) of the text.

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