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LETTER TO THE EDITOR

Fast eigenvalue algorithm for central potentials

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Abstract. An algorithm is described that seeks out Schrödinger eigenvalues E_{nl} for a given central potential $V(r)$. The algorithm has, in principle, arbitrary precision. A particular implementation has absolute error $|E-E_{nl}|$ decreasing as T^{-3}, where T is machine computing time. The method is tested on the central Gaussian potential $V(r)=-A\exp(-\lambda r^2)$ of recent interest.

Herein is described an algorithm for efficient integration of the radial Schrödinger equation ($\hbar = 2m = 1$):

$$-\psi'' + [V(r) + l(l+1)/r^2]\psi = E\psi, \tag{1}$$

yielding arbitrary-precision eigenvalues E_{nl}. Such an algorithm is useful for assessing errors associated with various approximation theories. A good example of a potential that has received much theoretical attention along these lines is the central Gaussian

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

having been used in models of nucleon–nucleon scattering (Buck *et al* 1977). Approximation schemes for this potential have included Liouville–Green asymptotic methods (Stephenson 1977), Rayleigh–Schrödinger perturbation methods and Jacobi basis variational methods (Bessis *et al* 1982), and hypervirial-Padé methods (Lai 1983). The latter reference contains a table summarising much of the recent work.

The standard method of integrating the second-order equation (1) suffers from possible machine instabilities and from inherent difficulty of establishing a good boundary condition criterion for halting computation when a test E is not a bound state value. The present method has the key advantages of (a) being a first-order differential method, and (b) having clear boundary criteria. The method is highly stable and reliable by virtue of (a), and easy to automate by virtue of (b). The computation algorithm described presently has experimental error in the calculated E value behaving as

$$|E - E_{nl}| \sim CT^{-3} \tag{3}$$

where T is the machine time used in getting E, and the constant C depends on the form of $V(r)$, the quantum numbers n, l, and of course on the machine used. The present method was implemented on a DEC PDP 11/70 with the result that the ground state eigenvalue E_{00} for the Gaussian (2), $A = 400$, $\lambda = 1$, computes to eleven significant figures in one second of CPU time. This eigenvalue and others are tabulated in table 2, in the same format used in the references (Lai 1983).

The key idea is to invoke a Prüfer transformation (Tricomi 1961, Hasova *et al* 1979) defining the trajectory function

$$\gamma(z) = \cot^{-1}[\psi'(z/F)/F\psi(z/F)], \tag{4}$$

where $F = (|E|)^{1/2}$. We assume that the potential satisfies $V(\infty) = 0$ and $r^2 V(r) \to 0$ as $r \to 0$. Then the transformed Schrödinger equation (1) and boundary condition at $z = 0$ are written simply as

$$\mathrm{d}\gamma/\mathrm{d}z = 1 - U(z)\sin^2\gamma, \qquad \gamma(0) = 0, \tag{5}$$

where the function U is given by

$$U(z) = V(z/F)F^{-2} + l(l+1)z^{-2} + 1 - \mathrm{sgn}(E). \tag{6}$$

This transformation provides rapid algorithms for *rigorous* bounds on one-dimensional ground states (Crandall and Reno 1982). Though the angular momentum term in (6) makes it difficult to establish rigorous bounds for the radial problem, transformation (4) does yield a fast algorithm for converging on correct values of E. These will be special values such that the trajectory γ has certain asymptotic properties. The arc cotangent in (4) is to be interpreted in such a way that γ is continuous, passing through the appropriate number of intercepts $\gamma = j\pi$; $j = 1, 2, \ldots$ as z increases. There is to be one such intercept for each zero of ψ on $r \in (0, \infty)$. Intercepts $\gamma = (j + \frac{1}{2})\pi$ correspond to critical points ($\mathrm{d}\psi/\mathrm{d}r = 0$). The ground state trajectory, for example, will pass through the value $\gamma = \frac{1}{2}\pi$, but not the value $\gamma = \pi$ since the ground state wavefunction has no positive zeros. A bound state is distinguished by the property that γ approaches the appropriate asymptote from below, as $z \to \infty$. This asymptote is determined by a given number $(n-1)$ of positive zeros of γ, together with the condition

$$\lim_{z\to\infty} \mathrm{cosec}^2\,\gamma(z) = 2, \tag{7}$$

which states the appropriate boundary condition at $z = \infty$. Thus the bound state eigenvalue E_{nl} is that E for which the differential equation with boundary condition (5) yields a trajectory having upper asymptote

$$a = \sup_z \gamma(z) = \pi(n - \tfrac{1}{4}). \tag{8}$$

Note that a convention common in the literature, that n denotes one plus the number of positive zeros of ψ, is used here.

The trajectory γ can be thought of as the 'phase' of the wavefunction, for example if $\psi(r) = \sin(Fr)$ as in the free particle problem then γ is just the argument z, and there are no bound states since there are no natural asymptotes of the type (8). For the Coulomb potential $V(r) = -2/r$, on the other hand, there is a ground state trajectory $\gamma(z) = \cot^{-1}(1/r - 1)$, with asymptotic phase $\gamma(\infty) = \frac{3}{4}\pi$, consistent with (8). The general effect of the angular momentum number l is to alter the initial slope of the trajectory. In machine implementations it is a convenient fact that:

$$\mathrm{d}\gamma/\mathrm{d}z|_{z=0} = 1/(l+1). \tag{9}$$

This condition is normally used only at the beginning of a trajectory interaction, whence the number l appears only in the function (6) during computation. This is to say that all necessary effects of l on the boundary conditions of the radial problem are taken care of by assignment (9).

The computation algorithm can be put into a convenient stepwise form:

(1) Choose n (one plus number of positive zeros) and l.

(2) Choose a trial energy pair $e_1 < e_2$ for which E_{nl} must be an intermediate value; e.g. $e_1 = -A$, $e_2 = 0$ for the Gaussian (2).

(3) Set $E = \frac{1}{2}(e_1 + e_2)$, $z = 0$, $\gamma = 0$, and iterate the first-order equation (5) until either $\gamma' < 0$ or $\gamma > a$ (of equation (8)).

(4) If $\gamma' < 0$ then set $e_1 = E$, or set $e_2 = E$. Then go to step (3).

This algorithm automatically seeks out the correct value of E_{nl} as the limiting value of the variable E in the loop comprised of steps (3)–(4). In our implementation, a fourth-order Runge–Kutta formula was used (Abramowitz and Stegun 1965) to iterate equation (5). It is this particular fourth-order accuracy that gives the exponent -3 in the experimental behaviour of accuracy with respect to computing time (3). Certainly, higher-order algorithms would improve the temporal convergence even further.

The above algorithm was first tested on a known case, similar to the Gaussian problem. Consider the potential

$$V(r) = -420\,\mathrm{sech}^2 r, \tag{10}$$

having ground state energy $E_{00} = -361 = -19^2$. For various values of the increment dz for the Runge–Kutta solution in step (3) the convergent value of E was obtained. Table 1 shows the effect of decreasing dz, which improves accuracy at the expense

Table 1. Ground state convergence for the potential $V(r) = -420\,\mathrm{sech}^2 r$ using the algorithm of the text with fourth-order Runge–Kutta. The exact eigenvalue is $-19^2 = -361$.

Runge–Kutta dz	Output E	T (CPU seconds)
1	−361.001 6	0.15
2^{-1}	−361.000 007	0.4
2^{-2}	−361.000 000 4	0.9
2^{-3}	−361.000 000 02	2.4
2^{-4}	−361.000 000 001	5.9
2^{-5}	−361.000 000 000 06	13.9
2^{-6}	−361.000 000 000 003	28.9

of more computing time. The data are closely fitted by the estimate (3). Indeed, it is evident that halving the increment dz essentially doubles the total convergence time T while improving absolute error by more than one decade of magnitude. A second check on accuracy behaviour was performed on the ground state of the Gaussian (2) with $A = 400$, $\lambda = 1$ as customary choices (Lai 1983). The algorithm was repeated with successively smaller increments dz until the 16th figure did not change. The result is:

$$E_{00} = -341.895\,214\,561\,2383, \tag{11}$$

a result that consumed 60 seconds of CPU time for $dz = 0.002$ in the automated algorithm. A final check was performed on the ground state problem for the one-dimensional potential $V(x) = x^4$, with slightly different equations (5), (6) for the even-parity condition (Crandall and Reno 1982). The result agrees completely with

'Penk's number':

$$E_0^{(x^4)} = 1.060\,362\,090\,484\,1820, \tag{12}$$

again consuming about 60 seconds of CPU time with $dz = 0.002$.

Table 2 shows values for the Gaussian potential (2) obtained systematically with the algorithm. Parentheses indicate those digits not in agreement with Lai (1983).

Table 2. Results of fast algorithm for eigenvalues $-E_{nl}$ of the potential $V = -400\exp(-r^2)$. Agreement with previous work (Lai 1983) is to four digits except where indicated by ( ).

n \ l	0	1	2	3	4	5
1	341.895 214 561 2383	304.462 838 52	268.110 735 27	232.875 300 61	198.798 2702	165.928 199
2	269.644 459 39	235.450 042 38	202.431 257 3	170.639 314	140.135 139	110.992 946
3	203.983 528 80	173.244 320 48	143.809 144 2	115.754 199	89.174 956	64.195 877
4	145.377 898 02	118.383 981 2	92.878 069 7	68.983 554	46.868 114	26.777 853
5	94.457 747 55	71.623 551 4	50.567 690	31.521 076	14.851 4875	1.29(699)
6	52.143 586 4	34.129 934 9	18.440 44	5.67(3144)	—	—
7	19.966 318	8.083 33	0.(2049)			
8	1.34(73)					

There is no implication that Lai's numbers are in error—these digits should be considered unresolved at present. The algorithm has apparent difficulties with energies lying near the continuum, and to a lesser extent for higher l values. The entries of table 2 are terminated at that digit not changing when initial increment dz is halved. The accuracy of an entry can be taken to be ± 2 in the final digit, on the basis of canonical experiments with known potentials (such as (10)). However, the parenthesised entries, that are out of agreement with previous results, are naturally suspect. One possible explanation of discrepancy is that the $\sin^2$ calculation in differential equation (5) is not perfect on the machine used, although this has not been determined.

It should be remarked that a *global* eigenvalue-seeking algorithm can be written out. Whereas the algorithm described herein allows a program that asks for input values of n, l, it is simple to extend the approach so that only the potential need be specified while the new program seeks out *all* E_{nl} bound energies. The most direct way to do this is to note that the number of bound states for a given l is just the number of zero crossings of the zero-energy solution of the Schrödinger equation for that l. In this way, potentials such as the Gaussian with finitely many bound states can be globally analysed.

A further improvement on the general approach would be to extend the rigorous upper–lower bounding theorems of Crandall and Reno (1982) for the present three-dimensional cases. Using such new results, one could then resolve issues such as the digits of table 2 in the eigenvalues near the continuum.

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