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A simple iterative method for resonance calculation

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Abstract. A recently developed procedure for solving the stationary Schrödinger equation in matrix representation form is proved to be useful in calculating quasibound energy levels. Results for a simple quantum mechanical model with potential energy function $V=-r^{-1}+\lambda r$ ($\lambda<0$) are shown to be very accurate.

Burrows and Core (1984) showed that a technique for solving non-linear operator equations iteratively may be promising in obtaining bound-state energy eigenvalues from the stationary Schrödinger equation. The method was then modified by Fernández *et al* (1985a, b) who obtained very accurate results for one-dimensional and central-field problems (Fernández *et al* 1985a) and for two-dimensional anharmonic oscillators (Fernández *et al* 1985b).

The iterative procedure has not been applied to continuum states because it is expected to be divergent. In spite of this, it may be useful in resonance calculations provided an appropriate truncation criterion is used. This fact is illustrated in the present paper by means of the model Hamiltonian

$$H=\tfrac{1}{2}p^2-r^{-1}+\lambda r \qquad p=-\mathrm{i}\nabla \tag{1}$$

which was studied by several authors (see, for example, Quigg and Rosner 1979 and references therein, Austin 1981, Gerry and Silverman 1983) for positive and negative λ values. The most accurate bound-state eigenvalues ($\lambda>0$) were obtained by Fernández *et al* (1985a) using the iterative procedure.

The Hamiltonian operator (1) has no bound states for negative λ values and the resonance positions were accurately calculated by numerical integration of the Schrödinger equation and through rearrangement of the Rayleigh-Schrödinger perturbation series as Padé approximants (Austin 1981). Therefore, it is a good test problem.

In order to show how to calculate the quasibound energy levels of model (1) let us consider the more general eigenvalue problem

$$A|\psi_n\rangle=E_nB|\psi_n\rangle \tag{2}$$

where A and B are Hermitian operators. If $|\psi_n\rangle$ is expanded in an appropriate basis set of vectors $|i\rangle$, $|\psi_n\rangle=C_{0n}|0\rangle+C_{1n}|1\rangle+\ldots$, and the coefficient C_{nn} is arbitrarily chosen to be equal to unity, then the secular equation for the remaining expansion coefficients

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is found to be

$$E_n = \left(B_{nn} + \sum_{i \neq n} B_{ni} C_{in} \right)^{-1} \left(A_{nn} + \sum_{i \neq n} A_{ni} C_{in} \right) \tag{3a}$$

$$C_{jn} = (A_{jj} - E_n B_{jj})^{-1} \sum_{i \neq j} (E_n B_{ji} - A_{ji}) C_{in} \qquad j \neq n \tag{3b}$$

where $A_{ij} = \langle i|A|j\rangle$ and $B_{ij} = \langle i|B|j\rangle$. This equation is easily solved by means of the Gauss-Seidel iterative method (Kuo 1965):

$$E_n^{(s)} = \left(B_{nn} + \sum_{i \neq n} B_{ni} C_{in}^{(s)} \right)^{-1} \left(A_{nn} + \sum_{i \neq n} A_{ni} C_{in}^{(s)} \right) \tag{4a}$$

$$C_{jn}^{(s+1)} = (A_{jj} - E_n^{(s)} B_{jj})^{-1} \left(\sum_{i<j} (E_n^{(s)} B_{ji} - A_{ji}) C_{in}^{(s+1)} + \sum_{i>j} (E_n^{(s)} B_{ji} - A_{ji}) C_{in}^{(s)} \right) \qquad j \neq n \tag{4b}$$

provided $E_n^{(s)} \neq A_{jj}/B_{jj}$ for all $s = 0, 1, \ldots$, and $j \neq n$. An appropriate starting point is $C_{in}^{(0)} = \delta_{in}$.

The Schrödinger equation for H is easily shown to be a particular case of (2) where $A = \frac{1}{2}rp^2 - 1 + \lambda r^2$ and $B = r$. These operators can be written in terms of the three generators of the SO(2, 1) Lie algebra that is realised as $K_0 = \frac{1}{2}(g^{-1}rp^2 + gr)$, $K_1 = \frac{1}{2}(g^{-1}rp^2 - gr)$ and $K_2 = \boldsymbol{r} \cdot \boldsymbol{p} - \mathrm{i}$ (Gerry and Silverman 1983, Fernández *et al* 1985a), where the real positive parameter g plays an important role as shown below. Owing to this, the matrix elements of A and B in the basis set of eigenvectors of K_0 can be easily calculated.

For negative λ values the iterative procedure is divergent, disregarding the convergence-accelerating algorithm used, because the Hamiltonian operator (1) has no bound states. However, numerical calculation shows that for each g value an integer M exists so that $D_s > D_{s+1}$ ($D_s = |E_n^{(s)} - E_n^{(s-1)}|$) if $s < M$ and $D_s < D_{s+1}$ if $s > M$. It is therefore not unreasonable to think that $E_n^{(M)}$ may be the closest approximation to E_n and that D_M is approximately the error of the calculation. The g value is set so that M is as large as possible.

Results for the ground state of (1) are shown in table 1 together with the corresponding g and M values. The present method seems to be more accurate than the Padé approximant built from the Rayleigh-Schrödinger perturbation series (Austin 1981).

In closing, further comments about the present method appear to be necessary. When the quantum mechanical problem studied has bound states the convergence of the iterative procedure may probably be accelerated by the Newton-Raphson method or another appropriate algorithm. However, it is our aim to keep the method as simple as possible and to avoid manipulating large matrices. It is clear that the Gauss-Seidel technique fulfils this requirement completely.

Table 1. Ground-state energy level of $H = \frac{1}{2}p^2 - r^{-1} + \lambda r$.

λ	Present	g	M	Padé approximants†	Exact†
−0.02	$-0.530\,663\,983\,5318 \pm 6 \times 10^{-13}$	0.90	12	$-0.530\,663\,984 \pm 5 \times 10^{-10}$	−0.530 664
−0.03	$-0.546\,591\,51 \pm 2 \times 10^{-8}$	0.812	11	$-0.546\,59 \pm 5 \times 10^{-6}$	−0.546 592
−0.04	$-0.563\,07 \pm 2 \times 10^{-5}$	0.76	9	$-0.5631 \pm 5 \times 10^{-5}$	−0.563 098

†Austin (1981).

We do not actually know whether our choice of the adjustable parameter has been tried previously with regard to iterative procedures. We have certainly found it very useful in dealing with asymptotic perturbation series (Fernández *et al* 1984). Besides, g may have equally well been set so that $D_s = 0$, but this leads to similar results provided a solution exists.

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