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A Numerical Solution of Wave Equations for Real or Complex Eigenvalues

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Abstract

A simple but efficient computational procedure is given for calculating either real or complex eigenvalues of wave equations. The method is based essentially on the 'outgoing-waves-only' criterion and enables one to use both short and long range potentials. The technique is illustrated by its application to scattering states of the square well potential.

Introduction

The problem of calculating real and complex eigenvalues of the 'wave equation' is frequently encountered in theoretical physics. Though many methods are available for finding the real eigenvalues, techniques applicable to excited states and complex eigenvalues are not as well documented. In this paper a simple method for solving these problems is reported. It is based essentially on the 'outgoing-waves-only' criterion (Blatt and Weisskopf 1952) and enables one to determine the real and complex eigenvalues of the wave equation for both ground and excited states.

Theory

Consider an equation of the form

$$\frac{\mathrm{d}^2 u_l(r,k)}{\mathrm{d}r^2} + \left(k^2 - v(r) - \frac{l(l+1)}{r^2}\right) u_l(r,k) = 0, \tag{1}$$

for either real or complex k^2. Given that the potential vanishes identically for r greater than some distance a, that is,

$$v(r) = 0, \qquad r > a, \tag{2}$$

the method of defining real and complex eigenvalues k_0^2 for equation (1) is well known, and need only be stated briefly here. The radial wavefunction $u_l(r,k)$ of equation (1) satisfies

$$u_l(0,k) = 0, \tag{3}$$

and in the asymptotic region $r > a$ it may be expanded in terms of incoming I_l and outgoing O_l solutions of equation (1) for $v(r) = 0$. These solutions are related to the spherical Hankel functions of the first and second kind and have the asymptotic behaviour

$$O_l \to \exp\{\mathrm{i}(kr - \tfrac{1}{2}l\pi)\}, \quad I_l \to \exp\{-\mathrm{i}(kr - \tfrac{1}{2}l\pi)\} \qquad \text{as} \qquad r \to \infty. \tag{4}$$

For potentials satisfying equation (2), the eigenvalue condition is that the solution exhibits outgoing-waves-only behaviour; that is, for certain values of k, denoted by k_0, at large r

$$u_l(r, k_0) \equiv O_l(k_0 r) \to \exp\{\mathrm{i}(k_0 r - \tfrac{1}{2}l\pi)\} \qquad (r \to \infty). \tag{5}$$

For bound states, k_0 is purely imaginary of the form $\mathrm{i}\gamma$ with $\gamma > 0$ and the requirement (5) is simply that the wavefunction goes exponentially to zero at infinity. For resonant states, k lies in the lower half plane,

$$k_0 = \gamma_1 - \mathrm{i}\gamma_2 \qquad \text{with} \qquad \gamma_1 \geqslant 0, \quad \gamma_2 > 0, \tag{6}$$

and one requires the wavefunction to satisfy equation (5). These requirements ensure that the modulus squared of the full time-dependent wavefunction will decay exponentially with time, corresponding to the decay of the resonant state (Humblet and Rosenfeld 1961). Hence we seek a solution of equation (1) satisfying equation (3) and going asymptotically to the outgoing wave solution $O_l(k_0 r)$. To calculate the eigenvalues k_0, we have developed a simple yet general method, which has not been previously used to our knowledge. To illustrate this method, let us first rewrite equation (1) as

$$\frac{\mathrm{d}^2 u_l(r,k)}{\mathrm{d}r^2} = \left(-k^2 + v(r) + \frac{l(l+1)}{r^2}\right) u_l(r,k). \tag{1a}$$

Starting from the asymptotic solution

$$u_l = O_l \equiv \mathrm{h}_l^{(1)}(kr), \tag{7}$$

where $\mathrm{h}_l^{(1)}(z)$ is the Riccatti Hankel function (Abramowitz and Stegun 1965), equation (1a) is numerically integrated into the origin and the value of $u_l(0,k)$ is ascertained. The problem is thus reduced to finding a solution of equation (1a), with starting values given by (7) and satisfying (3). A series expansion for $\mathrm{h}_l^{(1)}(z)$ (Abramowitz and Stegun 1965) provides starting values of the integration.

Note that $\mathrm{h}_l^{(1)}(z)$ is related to the spherical Hankel function and satisfies the equation

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}r^2} + k^2 - \frac{l(l+1)}{r^2}\right) \mathrm{h}_l^{(1)}(kr) = 0.$$

For real k^2 a simple Regula Falsi calculation is sufficient to find the zeros of $u_l(0,k)$. The excited bound states of the system can also be found, with the number of nodes of the solution giving the degree of excitation.

To find the scattering state eigenvalues, we follow an analogous procedure. The problem here is to find zeros of the complex function $u_l(0,k)$. A routine CREG has been developed for this purpose which uses a combination of complex Regula Falsi procedures and Monte Carlo methods to minimize $u_l(0,k)$. Details are given in Appendix 1.

If the short range condition (2) on the potential is dropped, the procedure for scattering states becomes somewhat more difficult owing to problems of numerical stability. For complex k, as given by equation (6), the outgoing wave solution is highly oscillatory with the amplitude increasing for large radial distances. Because of this behaviour, it is extremely difficult to find a stable numerical method for integrating

equation (1a). These considerations, however, apply only to the real r axis. If we allow r to be complex, $r = x\,e^{i\theta}$ say, then the outgoing wave solution

$$u \to \exp(ikx\,e^{i\theta})$$

will decay if

$$\mathrm{Re}(ik\,e^{i\theta}) < 0, \qquad \text{that is,} \qquad \tan\theta > \gamma_2/\gamma_1 . \tag{8}$$

In many cases, θ is also bounded above by the requirement that the potential decay to zero for large x. We can then adopt the procedure as outlined above, for short ranged potentials. Starting values for the numerical integration are given by a generalized WKB approximation (see Appendix 2),

$$u_l(r,k) = h_l^{(1)}(k\bar{r})/\{1-k^{-2}v(r)\}^{\frac{1}{4}}, \tag{9}$$

where

$$\bar{r} = r - \int_r^\infty [\{1-k^{-2}v(t)\}^{\frac{1}{2}} - 1]\,dt .$$

Allowing r to be complex, we rewrite equation (1a) as,

$$\frac{d^2u_l(x,k)}{dx^2} = \left(-(k\,e^{i\theta})^2 + e^{2i\theta}v(x\,e^{i\theta}) + \frac{l(l+1)}{x^2}\right)u_l(x,k). \tag{10}$$

To minimize computer time, the following transformations are made

$$x = t/(3-2t), \qquad y_l = (3-2t)u_l, \tag{11}$$

which, on substitution into equation (10), give

$$\frac{d^2y_l(t,k)}{dt^2} = \frac{9}{(3-2t)^4}\left\{-(k\,e^{i\theta})^2 + e^{2i\theta}v\left(\frac{t\,e^{i\theta}}{3-2t}\right) + \frac{l(l+1)(3-2t)^2}{t^2}\right\}y_l(t,k). \tag{12}$$

With two starting values given by the expression (9), equation (12) is integrated into the origin by using Milne's recurrence relation (Abramowitz and Stegun 1965),

$$\xi_{n-1} = 2\xi_n + h^2F_ny_n - \xi_{n+1} + O(h^6), \tag{13}$$

where

$$\xi_n = y_n(1-\tfrac{1}{12}h^2F_n),$$

$$F_n = \frac{9}{(3-2t_n)^4}\left\{-(k\,e^{i\theta})^2 + e^{2i\theta}v\left(\frac{t_n\,e^{i\theta}}{3-2t_n}\right) + \frac{l(l+1)(3-2t_n)^2}{t_n^2}\right\}$$

and h is the step length in t. As F may be singular at the origin, a Taylor series expansion around $t = h$ is used to find $y(0,k)$. This gives

$$y(0,k) = (2+h^2F_1)y_1 - y_2 + O(h^4), \tag{14}$$

where F_1 and y_1 are the values of F and y for $t = h$, and y_2 is the value of y for $t = 2h$. The values of y_1 and y_2 are found from the recurrence relation (13).

Antibound states are outgoing wave solutions with $k_0 = i\gamma$, $\gamma < 0$. The procedures discussed above may be applied to these states by using a single parameter search along the negative imaginary k axis.

Square Well Potential Complex Eigenvalues

Although the square well potential does not exhibit long range characteristics, it does enable one to derive an exact formulation for the eigenvalues, thus permitting a simple check on the numerical procedure. Consider the potential

$$\left.\begin{aligned} v(r) &= -V_0, \quad r < a, \\ &= 0, \quad r \geqslant a. \end{aligned}\right\} \tag{15}$$

If we apply continuity of the logarithmic derivative of the wavefunction at the boundary a, and impose the outgoing-waves-only criterion, we obtain the following equation for the scattering eigenvalues

$$K\mathrm{j}_{l-1}(Ka)/\mathrm{j}_l(Ka) = k\,\mathrm{h}^{(1)}_{l-1}(ka)/\mathrm{h}^{(1)}_l(ka), \tag{16}$$

where

$$K = (k^2 + V_0)^{\frac{1}{2}}$$

and $\mathrm{j}_l(Ka)$ and $\mathrm{h}^{(1)}_l(ka)$ are respectively the Riccati Bessel and Riccati Hankel function of the first kind. The relation (16) is a transcendental equation for the complex eigenvalue k and may be solved by using CREG. Although the potential is short ranged, the procedure outlined in equations (9) to (14) is used for this illustration as a test of their validity. For $a = 1$, $l = 3$ and $V_0 = 25$, the following results are obtained: by solving equation (16)

$$k_0 = 2{\cdot}25059 - \mathrm{i}(0{\cdot}14377), \qquad k_0^2 = 5{\cdot}04456 - \mathrm{i}(0{\cdot}646269);$$

by numerical integration, using the procedure outlined here,

$$k_0 = 2{\cdot}25064 - \mathrm{i}(0{\cdot}143597), \qquad k_0^2 = 5{\cdot}04474 - \mathrm{i}(0{\cdot}646371).$$

The close agreement between these results gives confidence in the validity of the method.

Conclusions

We have outlined here a procedure for numerically calculating real and complex eigenvalues of the wave equation. This has been coded by the authors in Fortran IV for an IBM 360/50 I computer, with some inner loops for the recurrence relation (13) being coded in IBM 360 assembler language. A typical application by us would involve finding eigenvalues for a sum of three Yukawa potentials. For l values from 0 to 5 with three real and three complex eigenvalues, this would take approximately 37 s of central processing unit time. The procedure is thus sufficiently fast to enable quite ambitious calculations requiring eigenvalues to be undertaken.

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Appendix 1. CREG—A Complex Regula Falsi and Monte Carlo Method for finding Zeros of Complex Functions

Our problem is to find the values of a complex variable $z = x+iy$ for which a given analytic function $f(z)$ becomes zero. We describe here how the well-known Regula Falsi technique, so powerful for finding zeros of real functions, can be modified for calculations in the complex plane.

For a real variable, start from two approximate zeros x_1 and x_2 and predict a new approximate zero x_3 by linear interpolation:

$$x_3 = \{f(x_1)x_2 - f(x_2)x_1\}/\{f(x_1) - f(x_2)\}. \tag{A1}$$

If x_1 and x_2 are close to each other and to a simple zero, then x_3 will in general be a better approximation.

We now seek to generalize the method so as to find the simple zeros z_0 of an analytic function $f(z)$ of a complex variable z. Expanding $f(z)$ in a Taylor series around a point z near z_0, we have

$$f(z_0) = f(z) + f'(z)(z_0 - z) + \ldots \tag{A2}$$

and hence

$$z_0 = z - f(z)/f'(z). \tag{A3}$$

As in the real case, this iterative method will converge provided

$$|f(z)f''(z)/\{f'(z)\}^2| < 1.$$

If we replace the derivative in (A3) by a difference quotient, as in the secant method for real variables, we obtain from two initial approximations, the subsequent iteration

$$z_3 = \{f(z_1)z_2 - f(z_2)z_1\}/\{f(z_1) - f(z_2)\}. \tag{A4}$$

However, we cannot straddle our zero by z_1 and z_2 since points in the complex plane cannot be ordered. Instead, we need some criterion for deciding whether z_3 is an allowable next approximation. There is always a danger that z_3 may be a wild extrapolation and we must be prepared to reject it.

We adopted the following criterion: if $|f(z_3)|$ is less than both $|f(z_1)|$ and $|f(z_2)|$ and $|z_3 - z_1| < \varepsilon$, where ε is a predetermined constant, then accept z_3 and for the next 'interpolation' use z_3 and whichever of z_1 and z_2 has the lower $|f(z)|$. If these conditions are not satisfied, z_3 is rejected. A new z_3 is then selected by a Monte Carlo technique. From the points z_1, z_2 the point giving the lowest value of $|f(z)|$ is

chosen as a starting point. Call this point z_1. Function values are sampled at random points in the neighbourhood of this point until a point termed z_2 is found which has a lower value of $|f(z_2)|$ than $|f(z_1)|$. These two points are then used for the interpolation (A4).

In numerical analysis, the choice of an initial approximation can be difficult. In our application of equation (A4), we were guided by the eigenvalue condition that k_0 lies in the lower half plane

$$k_0 = \gamma_1 - i\gamma_2, \qquad \text{with} \qquad \gamma_1 \geqslant 0, \quad \gamma_2 > 0. \tag{A5}$$

Our approach was similar to that of a Regula Falsi calculation. From an initial point z_1 near the origin, function values were calculated for z values on the straight line

$$z_{i+1} = z_i + \Delta z. \tag{A6}$$

At each step, the function values were tested to see whether $\mathrm{Re}\, f(z)$ or $\mathrm{Im}\, f(z)$ had changed sign. If so, the interpolation (A4) was used to find the next point; if not, then $|f(z)|$ was tested. If we had

$$|f(z_{i+1})| < |f(z_i)| \quad \text{or} \quad |f(z_{i+1})| < |f(z_{i-1})|,$$

the next point was found from (A4); if not, then equation (A6) was used to find the next point. In no instance did this procedure fail to provide reasonable starting values for our search.

Appendix 2. Generalized WKB Technique for Large Range Starting Values

Let us write equation (1) in the form

$$\frac{d^2 u_l}{dr^2} + \left(k^2(r) - \frac{l(l+1)}{r^2}\right) u_l = 0, \tag{A7}$$

where

$$k^2(r) = k^2 - v(r).$$

We seek an approximate solution to equation (A7) for large r as starting values for numerical integration into the origin.

If $v(r)$ is strictly zero, then $u_l(r)$ reduces to $h_l^{(1)}(kr)$. For large r, $v(r)$ is small and hence we seek an expansion valid for small $v(r)$ whose zeroth-order term is $h_l^{(1)}(kr)$. We derive such an expansion by a process analogous to the standard WKB approximation for $l = 0$. The latter may be derived by seeking a solution of

$$d^2u/dr^2 + k^2(r)\, u/\lambda^2 = 0 \tag{A8}$$

in the form

$$u = \exp\{i(S_0 + \lambda S_1 + \lambda^2 S_2 + \ldots)/\lambda\}. \tag{A9}$$

On substituting equation (A9) into (A8) and equating coefficients of the parameter λ (ultimately to be set equal to unity), giving S_0 and S_1, we find

$$u_{\mathrm{WKB}} = k^{-\frac{1}{2}}(r) \exp\left\{\frac{i}{\lambda}\left(\int k(r')\, dr' + O(\lambda^2)\right)\right\}. \tag{A10}$$

Proceeding by analogy in the general case, we consider the equation

$$\frac{d^2u_l}{dr^2} + \left(\frac{k^2(r)}{\lambda^2} - \frac{l(l+1)}{r^2}\right)u_l = 0. \tag{A11}$$

Guided by the form of equation (A10) we try the expansion

$$u_l = A(r)\, h_l^{(1)}(\chi) \tag{A12}$$

with

$$\chi = (\chi_0 + \lambda\chi_1 + \lambda^2\chi_2 + \ldots)/\lambda.$$

Substituting equation (A12) into (A11) and equating coefficients of λ, we find that either $A(r)$ or χ_1 may be chosen arbitrarily. The particular choice $\chi_1 = 0$ (suggested by the form of equation A10) yields

$$A(r) \propto k^{-\frac{1}{2}}(r) \qquad \text{and} \qquad \chi_0 = \int k(r')\, dr'.$$

On then omitting terms χ_2 and beyond, setting $\lambda = 1$ and making a particular choice of the multiplicative constant in $A(r)$, we obtain equation (9) given in the text.

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