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Numerical calculation of the energy eigenvalues for a local potential†

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Abstract. A recent method, based on obtaining a first order nonlinear differential equation, to calculate the energy eigenvalues for a local potential has been improved. Two transformations which are capable of greater manoeuvrability and which reduce computational labour are suggested.

1. Introduction

Recently Kermode (1971) proposed a method for calculating S state energy eigenvalues for a local potential. It was later generalized for higher angular momentum states (Kermode and Nunn 1971). This method is essentially based on transforming the Schrödinger equation into a first order nonlinear differential equation. It is in the spirit of Calogero's variable phase approach for scattering phase shifts (Calogero 1967). Proper boundary conditions are obtained by suitably transforming the logarithmic derivative y. The technique of reducing a second order differential equation into first order equations for finding the solutions is not new and has been suggested earlier, for example, by Prüffer (Hartman 1964) for homogeneous equations and Ridley (1957) for inhomogeneous equations. But the method has never been used for finding the eigenvalues.

In this paper we have suggested two transformations. They add to the usefulness and the flexibility of the method proposed by Kermode and Nunn.

The logarithmic derivative $y_{l,\mu}(r)$ of the radial solution $u_{l,\mu}(r)$ of the Schrödinger equation for negative energies ($-\hbar^2\mu^2/2m$, where m is the reduced mass) satisfies the differential equation

$$\frac{dy_{l,\mu}(r)}{dr} = -y_{l,\mu}^2 + \frac{l(l+1)}{r^2} + V(r) + \mu^2 \tag{1}$$

with the boundary condition $y_{l,\mu}(0) = \infty$. At the energy of a bound state (say μ_B)

$$y_{l,\mu_B}(r) \xrightarrow[\text{large } r]{} \frac{h_l^{(1)}(z_B)}{h_l^{(1)}(z_B)} \equiv p_{l,\mu_B}(r), \tag{2}$$

where $z_B = i\mu_B r$ and $h_l^{(1)}(z_B)$ is the Riccati–Hankel function of the first kind. The prime denotes differentiation with respect to r.

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2. Transformations

In order to obtain a well behaved function Kermode and Nunn (1971) used the following transformation:

$$y_{l,\mu}(r) = \mu \cot f_{l,\mu}(r) + p_{l,\mu}(r)$$

giving $f_{l,\mu_B}(0) = 0$ and $f_{l,\mu_B}(\infty) = (2n+1)\pi/2$. This transformation does not have any adjustable parameter. We, instead, suggest writing $y_{l,\mu}(r)$ as

$$y_{l,\mu}(r) = q(r)p_{l,\mu}(r) \cot f_{l,\mu}(r) \equiv \chi_{l,\mu}(r) \cot f_{l,\mu}(r). \tag{3}$$

The function $f_{l,\mu}(r)$ satisfies the differential equation

$$\chi f' = \frac{\chi'}{2} \sin 2f + \chi^2 \cos^2 f - \left(V(r) + \frac{l(l+1)}{r^2} + \mu^2 \right) \sin^2 f. \tag{4}$$

The function $q(r)$ is essentially a smooth function vanishing linearly as $r \to 0$ and going to ± 1 for large r. This function should preferably have a range shorter than the range of the interaction. This will be helpful in reducing the range of integration. There can, of course, be many functions satisfying this criterion. One good choice is

$$q(r) = -\left(1 + l\frac{r-1}{r^\eta + l}\right) \qquad \eta \geqslant 2. \tag{5}$$

This leads to boundary conditions identical with those of Kermode (1971), namely, $f_{l,\mu_B}(0) = 0$ and $f_{l,\mu_B}(\infty) = (n+\frac{3}{4})\pi$. For $l = 0$, this transformation reduces to that of Kermode (1971). The parameter η can have any value greater than two.

Another choice for $q(r)$ leading to the same boundary conditions (ie $f_{l,\mu_B}(0) = 0$, $f_{l,\mu_B}(\infty) = (n+\frac{3}{4})\pi$) is

$$q(r) = -(1 - \theta(l-1)\, e^{-\eta r})$$

where

$$\begin{aligned} \theta(x) &= 1 \qquad x \geqslant 0 \\ &= 0 \qquad x < 0. \end{aligned} \tag{6}$$

The parameter η could have any value such that η^{-1} is smaller than the range of the force. For $l = 0$, this case also reduces to that of Kermode (1971).

3. Calculation and results

We have compared the method of Kermode and Nunn with our two transformations for a simple model potential of the square well type (depth 20 fm^{-2}, range 1 fm). We consider only the $l = 1$ case. This potential supports only one bound state with $\mu_B = 2{\cdot}6765526\ fm^{-1}$. The equations, in each case, were integrated by the Runge–Kutta method taking a fixed step length. The parameter η, which enters our transformations was taken equal to 3, 5 and 8.

In table 1 we give the values which the function f takes at 1 fm (beyond this the potential is zero) for the different cases. In every case μ is equal to μ_B. The last row gives the exact limiting value. Our first approximation gives five decimal place accuracy with a step length of 0·025 fm, while a step length of at least a fifth of this has to be

Table 1. Values of the function f at 1 fm for the different methods

Step length	Method of Kermode and Nunn	First transformation			Second transformation		
		$\eta = 3$	$\eta = 5$	$\eta = 8$	$\eta = 3$	$\eta = 5$	$\eta = 8$
0·025	1·571812	2·356194	2·356193	2·356193	2·381713	2·359567	2·356345
0·0125	1·570931	2·356192	2·356192	2·356192	2·381715	2·359570	2·356357
Limiting value	1·570796		2·356196			2·356196	

used with the method of Kermode and Nunn for the same accuracy (with the step length of 0·00625 fm we got the limiting value of 1·570754). Our second transformation apparently does not appear to be good. The reason is that the function $q(r)$ has not yet (at $r = 1$ fm) attained its asymptotic value. For the cases where the potential is not discrete, as is the case with our model potential, this transformation is as good as the first one.

Another point of interest is the rate of growth of $f(r)$ with r. For $\eta = 8$, $f(r)$ attains about 40 % of its limiting value at $r = 0{\cdot}5$ fm. It can be further increased by taking a larger value of η. No such parameter is available in the method of Kermode and Nunn. This is interesting because one can reduce the number of steps in the integration by taking a variable step length; fine for small r where most potentials are strong and coarse for large r.

The potentials containing a hard core (radius c) can also be handled by taking the boundary conditions $y_{l,\mu_B}(c) = \infty$ and $f_{l,\mu_B}(c) = 0$, and integrating equation (4) onwards from $r = c$.

The proposed transformations thus reduce considerably the computational labour in finding the eigenvalues compared with the procedure of Kermode and Nunn. In particular the availability of the free parameter η greatly adds to the versatility of this method.

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