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LETTER TO THE EDITOR

On the application of continued fractions to bound-state problems

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Abstract. We point out that the eigenvalue condition used by Biswas and Vidhani in a recent paper gives incorrect results for bound-state energies in two of the examples with which they illustrate their method. The error in the first of these applications is traced to the fact that their representations of bound-state radial functions do not necessarily vanish at the origin. In the second example in question, the bound states are not properly distinguished from the anti-bound states. In both cases, the defective results arise from neglect of boundary conditions.

Biswas and Vidhani (1973, to be referred to as BV) have revived a method of Ince (1926) and used it to investigate solutions of the radial Schrödinger equation for several simple potentials. Their procedure generates a continued-fraction representation of the logarithmic derivative of one of the two independent solutions of a transformed radial equation. They claim that the bound-state energies can be found from the condition that the resulting continued fractions terminate. This criterion is not derived by them from properties of bound-state radial functions; rather, they seem to infer its general validity from the circumstance that it is true for the one-dimensional harmonic oscillator. The results they obtain for the s wave bound states of the exponential potential demonstrate that their conjecture must in general be false.

The equation for the s wave radial function $U(E,r)$ for an attractive exponential potential is written by BV as (equation (2.10) of their paper)

$$\frac{d^2U}{dr^2}+\left[E+A\exp\left(-\frac{r}{a}\right)\right]U=0. \tag{1}$$

This is transformed into

$$x\frac{d^2X}{dx^2}+(b-x)\frac{dX}{dx}-\frac{b}{2}X=0 \tag{2}$$

by the substitutions $\chi=\surd(-E)$, $\rho=\chi r$, $U=\exp(-\rho)v(\rho)$, $\xi=\exp(-\rho/2\chi a)$, $x=2ic\xi$, $X=\exp(ic\xi)v(\xi)$. Here $b=1+4\chi a$ and $c^2=4a^2A$. Following Ince (1926), they conclude that

$$\frac{X'}{X}=\cfrac{\frac{1}{2}b}{(b-x)+\cfrac{x(\frac{1}{2}b+1)}{(b-x+1)+\ddots}} \tag{3}$$

where the prime denotes differentiation with respect to x. They note that the continued fraction on the right-hand side of (3) terminates when $\frac{1}{2}b = -n$, $n = 0,1,2,\ldots$. Since $b = 1+4a\surd(-E)$, their assumption that the continued fraction should indeed terminate when it represents the logarithmic derivative of a transformed bound-state radial function leads them to assert that the bound-state energies for the exponential potential in (1) are given by

$$E = -\frac{(2n+1)^2}{16a^2}, \qquad n = 0,1,2,\ldots \tag{4}$$

Equation (4) suffers from two obvious faults: (i) the energies it yields are independent of the potential strength A (and also of the sign of A); and (ii) it defines an infinite sequence of bound-state energies, in direct contradiction to the Bargmann (1952) inequality (see, eg, Newton 1966, p 357).

These defects are directly attributable to the fact that the boundary conditions on $U(E,r)$ were not specified by BV. In fact, examination of equation (3) when $b = 0$ and $b = -2$ shows that the resulting radial functions are neither normalizable nor real and do not vanish at $r = 0$, so they cannot represent bound states. Explicitly, we find for $n = 0$ ($b = 0$)

$$U_0(r) = N_0 \exp(+r/4a)\exp[-2ia\surd(A)\exp(-r/2a)],$$

and for $n = 1$ ($b = -2$)

$$U_1(r) = N_1 \exp(+3r/4a)\exp[-2ia\surd(A)\exp(-r/2a)]2[1+ic\exp(-r/2a)].$$

Thus, it is clear that in this example the termination of the continued fraction does *not* correspond to the location of bound-state energies. (We note parenthetically that the energies specified by (4) cannot be identified with the 'redundant poles' either, as may be seen by referring to Newton (1966, p 420).) Because they neglected to specify the branch of the square root in their definition $\chi = \surd(-E)$, Biswas and Vidhani give us no way of determining the sheet of the energy Riemann surface on which the energies given by (4) are defined.

It is possible to extract bound-state energies from equation (3) if one recognizes the right-hand side as the continued-fraction expansion of $\mathrm{d}/\mathrm{d}x(\ln{}_1F_1(\frac{1}{2}b,b;x))$ (an expansion which does not terminate in general) and transforms the hypergeometric function ${}_1F_1$ into a Bessel function whose argument depends on the strength of the potential. One then searches for energies such that the Bessel function vanishes at $r = 0$ (see, eg, Newton 1966, p 420)—these are the bound-state energies. However, there appears to be no advantage in obtaining the continued fraction as an intermediate step, since the form of the solution may be recognized from the transformed differential equation directly.

Following the above example, BV apply their method to the Hulthén potential, for which they write the s wave radial equation as

$$\frac{\mathrm{d}^2U}{\mathrm{d}r^2}+\left(k^2+\frac{\lambda\mu\mathrm{e}^{-\mu r}}{1-\mathrm{e}^{-\mu r}}\right)U = 0. \tag{5}$$

With the substitutions $U = \exp(-ikr)g$ and $z = \exp(-\mu r)$, they obtain

$$\frac{g'}{g} = \cfrac{ab}{[c-(a+b+1)z]+\cfrac{z(1-z)[ab+(a+b+1)]}{[c+1-(a+b+3)z]+\cdots}}, \tag{6}$$

where the prime denotes differentiation with respect to z,

$$a = \frac{ik}{\mu} + \frac{\sqrt{(-k^2+\lambda\mu)}}{\mu}, \qquad b = \frac{ik}{\mu} - \frac{\sqrt{(-k^2+\lambda\mu)}}{\mu}, \qquad c = 1 + \frac{2ik}{\mu}.$$

Again, demanding that the continued fraction (6) terminate at each bound-state energy, they claim that the bound-state wavenumbers are given by the conditions $a = -n$ or $b = -n$, $n = 0,1,2,\ldots$. From this they conclude that the bound-state energies are

$$E = k^2 = \frac{-1}{4n^2}(\lambda - n^2\mu)^2, \qquad n = 0, 1, 2, \ldots. \tag{7}$$

Once more, we are confronted by an infinity of bound states for attractive or repulsive potentials of any strength, even if we discard the entry with $n = 0$, which is clearly spurious. In this case also the Bargmann inequality is violated. The difficulty here again arises from neglect of boundary conditions. The energy sheet on which (7) holds has not been clearly defined by BV. Comparison of equation (7) with the formulae of Newton (1966, p 422), shows that all but at most a finite number of the energies in this sequence correspond to anti-bound states and thus belong on the unphysical sheet of the energy Riemann surface. If $\lambda > 0$, then those terms on the right-hand side of (7) with $n = 1,2,\ldots < \mu^{-1/2}|\lambda|^{1/2}$ represent genuine bound states.

It thus appears that the eigenvalue condition employed by BV is incorrect in general. In those particular instances for which it happens to work as for the Hulthén potential above, care is required to insure the observance of physical boundary conditions. A continued-fraction algorithm for bound-state energies which is free of these deficiencies has been given by Lovelace and Masson (1962).

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