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Eigenvalue bounds for transformations of solvable potentials

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Abstract. We study smooth transformations $V(r) = h_0(r) + g(h(\beta r))$ of potentials $V_0(r) = h_0(r) + h(\beta r)$ for which exact bound-state solutions of Schrödinger's equation are known. Eigenvalue approximation formulae are obtained which provide lower or upper energy bounds according to whether the transformation function g is convex or concave. Detailed results are presented for perturbed Coulomb potentials of the form $V(r) = -a/r + br + cr^2$ and $V(r) = -1/r + \mu \ln(r + r^2)$.

1. Introduction

Interesting exact solutions of Schrödinger's equation may be generated by first choosing a wavefunction ψ and then finding the corresponding potential V. This idea goes back to a paper published by Wigner [1] in 1929 and has enjoyed a considerable amount of attention since then [2, 3]. The following simple example will serve to fix ideas. If we choose the wavefunction for the bottom of the Y_l^m angular-momentum subspace to be $\psi(r) = r^l \exp(-\frac{1}{2}(r + \beta r^2))Y_l^m(\theta, \phi)$, then Schrödinger's equation $H\psi = (-\Delta + V)\psi = E\psi$ is satisfied if

$$V(r) = -\frac{1}{r} + \beta r + (\beta r)^2 \qquad \text{and} \qquad E = (3 + 2l)\beta - \tfrac{1}{4}. \tag{1}$$

Such exact eigenvalues are certainly useful but they stop short of treating, for example, the more general problem $V(r) = -a/r + br + cr^2$ in which the coefficients $\{a, b, c\}$ are *arbitrary*.

In this paper we use exact eigenvalues such as (1) to estimate the spectrum corresponding to a potential $V(r)$ of the form

$$V(r) = -\frac{1}{r} + g(\beta r + (\beta r)^2) \tag{2}$$

where g is a smooth transformation. We shall show that the bottom of the spectrum of H in the Y_l^m subspace may be approximated by the expression

$$E \approx \min_{t>0} \left\{ f(t) - h\left(\frac{t^2 f'(t)}{2l+3}\right) + tf'(t) - \frac{1}{4} \right\}$$

where

$$f(t) = g(\beta t + (\beta t)^2) \qquad h(t) = t + t^2.$$

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This formula provides a lower bound or an upper bound to the exact ground-state energy E according to whether the transformation function g is convex ($\approx = \geqslant$) or concave ($\approx = \leqslant$). This allows us, for example, to estimate the spectrum corresponding to $V(r) = -a/r + br + cr^2$ for arbitrary $\{a, b, c\}$.

At the cost of more complicated conditions on the coefficients, the collection (1) of exact eigenvalues may be extended to certain excited states including $\ell \neq 0$. In section 2 we summarize the more detailed exact results for the perturbed Coulomb case. Since similar results may be obtained for other families of potentials such as $V(r) = ar^2 + br^4 + cr^6$, we formulate the approximation theory in section 3 in a general framework suitable for application to all exact solutions of this general type. In section 4 we present numerical results for a number of specific examples some of which are compared with known results that have been obtained by other methods.

2. Perturbed Coulomb potentials

In his interesting work of solving Dirac's equations in the presence of magnetic field, Hautot [4] introduced some methods for solving certain second-order differential equations. One of these methods deals with the radial Schrödinger equation with the potential energy operator:

$$V(r) = -\frac{D}{r} + Br + Ar^2 \qquad A \neq 0. \tag{3}$$

The author obtained [5] exact solutions only for certain relations between the constants A, B, and D. He achieved this by applying the kinetic energy operator to an appropriate wavefunction and using the standard procedure of comparing the coefficients of the induced recurrence relations. More precisely, introducing

$$\psi(r) = \exp\left(-\frac{1}{2}\left(\sqrt{A}r^2 + \frac{B}{\sqrt{A}}r\right)\right)\sum_{k=0}^{n} a_k r^{k+l} \qquad n = 0, 1, 2, \ldots \tag{4}$$

into the radial Schrödinger equation (in units $\hbar = 2m = 1$)

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{2}{r}\frac{\mathrm{d}}{\mathrm{d}r} - \frac{l(l+1)}{r^2} + \left[E + \frac{D}{r} - Br - Ar^2\right]\right)\psi(r) = 0 \tag{5}$$

we obtain, after some algebra, the following three-term recursion relation between the coefficients a_k for $(k = 0, 1, 2, \ldots)$:

$$[(k+2)(k+2l+3)]a_{k+2} + \left[D - \frac{B}{\sqrt{A}}(k+2+l)\right]a_{k+1} + \left[E - \sqrt{A}(2k+2l+3) + \frac{B^2}{4A}\right]a_k = 0. \tag{6}$$

This recurrence relation terminates if $a_{n+1} = 0$, that is to say

$$E = E_{nl} = \sqrt{A}(2n+2l+3) - \frac{B^2}{4A}. \tag{7}$$

Equations (6) and (7) give the following $(n+1) \times (n+1)$ determinant which provides the relations between A, B, and D (for a given value of n) to ensure the existence of the

solutions of (5) (note that $a_{-m} = 0, m = 1, 2, \ldots$):

$$\begin{vmatrix} a_0 & b_0 & & & & & \\ c_1 & a_1 & b_1 & & & & \\ & c_2 & a_2 & b_2 & & & \\ & & . & . & . & & \\ & & & . & . & . & \\ & & & & c_{n-1} & a_{n-1} & b_{n-1} \\ & & & & & c_n & a_n \end{vmatrix} = 0 \tag{8}$$

where

$$\begin{cases} a_k = D - (B/\sqrt{A})(k + l + 1) \\ b_k = (k + 1)(k + 2l + 2) \\ c_k = E_{nl} - \sqrt{A}(2k + 2l + 1) + (B/\sqrt{A}). \end{cases}$$

Since this early work the technique of generating exact solutions for a Schrödinger operator has been widely applied [6–14], either to obtain some interesting potential functions with known eigenvalues, or to investigate the quality of perturbation theory.

3. Transformed potentials

In order to lay down a general framework for the approximation method we are about to construct, we consider a Schrödinger Hamiltonian of the form

$$H = -\triangle + h_0(r) + f(r) \tag{9}$$

where $h_0(r)$ is a fixed potential term and $f(r)$ is a smooth transformation $g(h(\beta r))$ of a second scaled potential term $h(\beta r)$, $\beta > 0$. Such a transformation always exists by the monotonicity of h. For example, when $h_0(r) = -1/r$ and $h(\beta r) = \beta r + (\beta r)^2$ and g is the identity transformation, the problem is exactly solvable for $n = 0$. Indeed, in this case, we have from (7) and (8) that E_{0l} is given by (1).

The tools required to develop our approximation theory arise from the geometric relationship between a potential shape and the set $\{\epsilon_{nl}\}$ of the energy trajectories generated by it. This technique was first introduced to analyse the spectrum of the many-body problem [15]; a more complete account and recent applications may be found in [16]. For the transformed Hamiltonian

$$H = -\triangle - \frac{l+1}{r} + g(h(\beta r)) \tag{10}$$

we have for the tangent line at $(h, g(h))$ that

$$\alpha(t) + h(\beta(t)r) = f^{(t)}(r) \tag{11}$$

where t is the point of contact between $h(\beta r)$ and $f(r) = g(h(\beta r))$. The parameters $\alpha(t)$ and $\beta(t)$ are determined as follows. Suppose that ϕ is an invertible function defined by $\phi(t\beta(t)) = tf'(t)$, where $'$ denotes differentiation with respect to t. Then, using (11), we have

$$\begin{cases} \beta(t) = (1/t)\phi^{-1}(tf'(t)) \\ \alpha(t) = f(t) - h(\phi^{-1}(tf'(t))). \end{cases} \tag{12}$$

Differentiation of (12) with respect to t gives

$$\frac{\alpha'(t)}{\beta'(t)} = -th'(t\beta(t)). \tag{13}$$

On the other hand, the energy formula (1) with (11) gives

$$\epsilon_{0l}(t) = \alpha(t) + \beta(t)(2l+3) - \tfrac{1}{4}. \tag{14}$$

By differentiating (14) with respect to t and using the extreme condition $\epsilon'_{nl}(t) = 0$, we get

$$\frac{\alpha'(t)}{\beta'(t)} = -(2l+3). \tag{15}$$

Now, since

$$\phi(t\beta(t)) = tf'(t) = t\beta(t)h'(t\beta(t)) \tag{16}$$

we have from (13), (15), and (16) that

$$\beta(t) = \frac{tf'(t)}{2l+3}. \tag{17}$$

Thus

$$th'\left(\frac{t^2 f'(t)}{2l+3}\right) = (2l+3). \tag{18}$$

Finally we obtain using (12), (17), and (14) that

$$\epsilon_{0l}(t) = f(t) - h\left(\frac{t^2 f'(t)}{2l+3}\right) + tf'(t) - \frac{1}{4}. \tag{19}$$

Equations (18) and (19) establish the energy bounds of the Hamiltonian (10). Indeed solving (18) with respect to t, for any smooth function $f(r) = g(h(\beta r))$, yields the optimal solution $\hat{t}$ then $\epsilon_{0l}(\hat{t})$ gives [16] lower bounds when the transformation g is convex and upper bounds when g is concave.

Equations (18) and (19) represent a complete recipe for a bound to the lowest eigenvalue ($n = 0$) of any Coulomb problem perturbed by a smooth transformation $g(h)$ of $h(\beta r) = \beta r + (\beta r)^2$. Although we shall not develop the more general case in detail here, the method for $n > 0$ works as follows. If we consider the Schrödinger equation (5) with $A = B^2$, we have from (7) that $E_{nl} = B(2n + 2l + 3) - \frac{1}{4}$. The parameter D is related to B through a recurrence relation which can be obtained by expanding the determinant (8) about the last row or column and using $A = B^2$:

$$\begin{aligned} &D_k = [D - (k + l + 1)]D_{k-1} - 2Bk(k + 2l + 1)D_{k-2} \\ &k = 0, 1, 2, \ldots \qquad\qquad D_{-2} = 0, \;\; D_{-1} = 1. \end{aligned} \tag{20}$$

For example, $D_0 = D - (l+1)$ which implies the condition $D = l+1$. In the same manner as we discussed above we obtain the corresponding formulae (18) and (19), but instead of $(2l + 3)$ we have, in general, $(2n + 2l + 3)$.

A case of physical interest occurs [17] when $n = 1$ and B approaches zero. In this case, we have from (20) that $D \approx l + 2$, this allows us to keep the potential $h_0(r) = -D/r$ as a fixed term. Thus, we have

$$th'\left(\frac{t^2 f'(t)}{2l+5}\right) = (2l+5)$$

$$\epsilon_{1l}(t) = f(t) - h\left(\frac{t^2 f'(t)}{2l+7}\right) + tf'(t) - \frac{1}{4}$$

which gives a bound to the first excited state of $H = -\triangle - (l+2)/r + g(h(\beta r))$, where g is any tranformation of h.

4. Numerical results and conclusion

One of the interesting points concerning the bounds we have obtained is the variety of approximations made possible by different choices of the transformation g. For example, in section 3, we can take $f(r) = g(h(\beta r)) = \mu r + \lambda r^2$ or $f(r) = g(h(r)) = \mu\{e^{\lambda(r+r^2)} - 1\}$, for arbitrary μ and λ etc, where in each case equations (18) and (19) give us a bound. A second point is the possibility of using the approximation with different base functions h. For example, if we consider $h(r) = -1/r + r$ and use an appropriate smooth transformation, the method we have discussed can easily give a bound for the eigenvalues of the harmonic oscillator Hamiltonian perturbed by $f(r) = g(h(r))$. This particular example can be discussed in terms of the theory presented in [16], but the method presented here is much simpler and more general: simpler in the sense that its derivation and the formulae it produces are simple; more general in the sense that, given an arbitrary smooth transformation g, formulae (18) and (19) provide an eigenvalue bound without any further ado.

Our first example is

$$H = -\triangle - \frac{1}{r} + \mu r + \lambda r^2$$

where μ and λ are arbitrary real parameters. That is to say, we consider $f(r) = \mu r + \lambda r^2$. It is clear that the transformation g exists for such an f. Equation (18) gives

$$4\lambda t^4 + 2\mu t^3 + (2l+3)t - (2l+3)^2 = 0 \tag{21}$$

while the energy formula (19) gives

$$\epsilon_{0l}(t) = 3\lambda t^2 + 2\mu t - \frac{\mu t^2 + 2\lambda t^3}{2l+3}\left(1 + \frac{\mu t^2 + 2\lambda t^3}{2l+3}\right) - \frac{1}{4}. \tag{22}$$

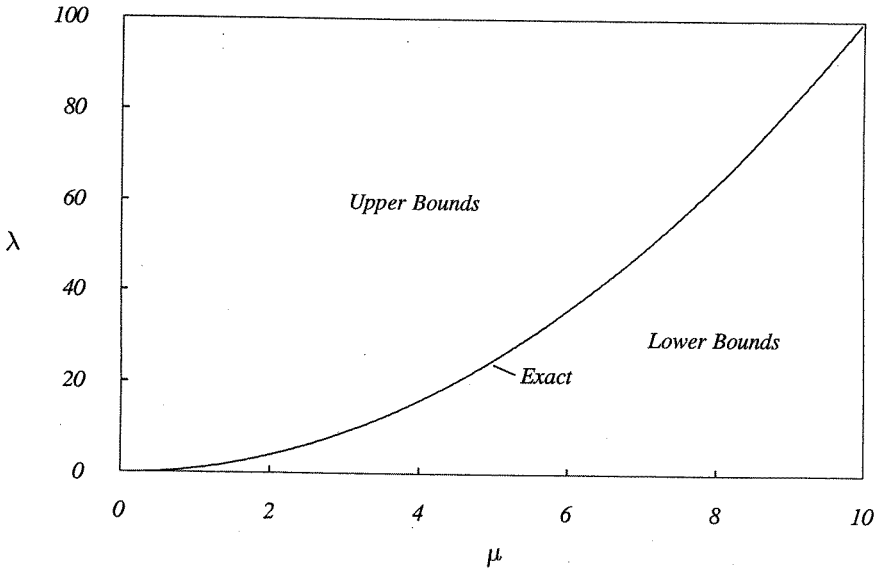

Figure 1. Two parametric regions: if $\mu < \sqrt{\lambda}$, the formulae (21) and (22) yield a lower bound for the ground-state energy of the Hamiltonian $H = -\triangle - \frac{1}{r} + \mu r + \lambda r^2$, while $\mu > \sqrt{\lambda}$ yields an upper bound.

Table 1. Eigenvalues of $H = -\frac{1}{2}\triangle - \frac{1}{r} + \mu r + \lambda r^2$ for different values of μ and λ. Comparison between results E^{B} of Bessis *et al* [13], using the moment method, and the present work which yields the lower bound E^{L}.

μ	λ	E^{B}	E^{L}
0	1	0.593 771	0.514 269
0	10	4.150 124	3.979 871
0	100	16.805 248	16.475 256
0	1000	59.375 469	58.762 742
0	5000	138.557 196	137.624 947
−2.0	1	−1.171 674	−1.431 541
−1.0	1	−0.226 187	−0.380 198
−0.5	1	0.196 002	0.081 963
0.5	1	0.971 616	0.922 717
1	1	1.332 845	1.311 628

Table 2. Eigenvalues of $H = -\triangle - \frac{1}{r} + \mu r + \lambda r^2$ for different values of μ and λ. Comparison between the lower bound E^{L} given by formulae (18) and (19) and accurate values E^{N} found by direct numerical integration.

μ	λ	E^{N}	E^{L}
0.001	0.001	−0.236	−0.238
0.001	1	1.786	1.707
0.01	0.01	−0.152	−0.153
0.01	1	1.795	1.717
0.1	0.1	0.378	0.354
0.1	1	1.885	1.814
0.5	1	2.278	2.239
1	2	3.657	3.629

Table 3. Eigenvalues of $H = -\triangle - \frac{1}{r} + \mu \ln(r + r^2)$ for different values of μ. Comparison between the upper bound E^{U} given by (23) and accurate values E^{N} found by direct numerical integration.

μ	E^{N}	E^{U}
0.0001	−0.249 78	−0.249 75
0.0005	−0.248 89	−0.248 75
0.001	−0.247 78	−0.247 52
0.005	−0.238 97	−0.237 65
0.01	−0.228 10	−0.225 45
0.05	−0.145 68	−0.132 27
0.1	−0.051 53	−0.024 56
0.5	0.520 33	0.654 13

For arbitrary λ, μ, and l, equations (21) and (22) give the required approximation. We may use any rootfinding method [18] to solve (21) for $\hat{t}$ and substitute this in (22) to yield the approximate eigenvalue. The natural question which arises now is whether $\epsilon_{0l}(\hat{t})$ is an upper or lower bound. The answer depends on the convexity of $f(r)$: the proof of this may be found in [16]. Indeed we can easily demonstrate using elementary differentiation

that if $\mu < \sqrt{\lambda}$, then $\epsilon_{0l}(\hat{t})$ is a lower bound for the Schrödinger Hamiltonian with potential $-1/r + \mu r + \lambda r^2$; and if $\sqrt{\lambda} < \mu$, then $\epsilon_{0l}(\hat{t})$ is an upper bound. In figure 1 we plot these two independent regions: along the curve $\lambda = \mu^2$ we have the exact solution. By means of a scale transformation (to remove the $\frac{1}{2}$ in front of the Laplacian) we can compare our bounds with the results of Bessis *et al* [13]: these are shown in table 1. These results show that our simple formulae can be used to obtain a satisfactory bound for a class of potentials generated by g without the lengthy derivations required in each case by the moment method [13] or the shifted $1/N$ expansion [14]. In table 2 we report our results using (18) and (19) for a range of values of μ and λ and, for comparison, the corresponding accurate results obtained by direct numerical integration of (3).

As another example of a smooth transformation $g(h(\beta r))$ we consider $f(r) = \mu \ln(r + r^2)$, where μ is arbitrary real. The Hamiltonian becomes

$$H = -\triangle - \frac{1}{r} + \mu \ln(r + r^2)$$

and the formulae (18) and (19) provide an upper bound if $\mu > 0$ or a lower bound if $\mu < 0$:

$$\begin{cases} 4\mu t^3 + (2\mu + 2l + 3)t^2 - (2l + 2)(2l + 3)t - (2l + 3)^2 = 0 \\ \epsilon_{0l}(t) = \mu \ln(t + t^2) + \mu \left(\dfrac{1 + 2t}{1 + t} \right) - \dfrac{\mu}{2l + 3} \left(\dfrac{t + 2t^2}{1 + t} \right) \left(1 + \dfrac{\mu}{2l + 3} \dfrac{t + 2t^2}{1 + t} \right) - \dfrac{1}{4}. \end{cases} \tag{23}$$

A comparison of some results obtained by this formula and the corresponding results obtained by direct numerical integration are reported in table 3.

The main point of the approach described in this paper is to provide a way to generate simple approximate formulae to be used for exploratory purposes. Once the appropriate ranges of the potential parameters are established, direct numerical methods could be used to find more accurate eigenvalues.

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