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The perturbation of some exactly soluble problems in wave mechanics by the method of potential envelopes

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Abstract. Suppose the function $\varepsilon_k(v)$ which represents the kth bound-state eigenvalue of the Hamiltonian $\hat{h} = \{-\Delta + v\phi(r) + U(r)\}$ is known exactly for all allowed values of $v \geqslant 0$. This article concerns the corresponding eigenvalue $E_k(v)$ of the Hamiltonian $H = \{-\Delta + vf(\phi(r)) + U(r)\}$, where $f(\phi)$ is a smooth, increasing, and either convex or concave transformation of the potential $\phi(r)$. An application of the *method of potential envelopes* yields a simple formula for an upper or lower bound to $E_k(v)$ according to whether the transformation $f(\phi)$ is concave or convex. The example $\phi(r) = (-r^{-1} + \omega r)$, $U(r) = \omega^2 r^2$, and $f(\phi) = \lambda^{-1}\{e^{\lambda\phi} - 1\}$ for $\lambda > 0$ is discussed in detail.

1. Introduction

Interesting examples of exactly soluble problems in non-relativistic wave mechanics may be obtained by first choosing the wavefunction and then finding the corresponding potential (Wigner 1929, Reed and Simon 1978, p 223, Killingbeck 1977b, p 985, 1980). Suppose, for example, we consider wavefunctions with the form $\psi(\boldsymbol{r}) = Y_l^m(\theta, \phi) r^l \exp\{-g(r)\}$, $l = 0, 1, 2, \ldots$; then Schrödinger's equation

$$(-\Delta + V(r))\psi(\boldsymbol{r}) = \varepsilon\psi(\boldsymbol{r}) \tag{1}$$

becomes

$$(\varepsilon - V(r))r = rg''(r) + 2(l+1)g'(r) - r(g'(r))^2. \tag{2}$$

If we now choose g to have the form $g(r) = \frac{1}{2}(vr + \omega r^2)$, then we can obtain an exact solution of equation (2) by setting

$$V(r) = v\{-(l+1)/r + \omega r\} + \omega^2 r^2 \tag{3}$$

and

$$\varepsilon = (3 + 2l)\omega - v^2/4. \tag{4}$$

The special cases $l = 0$ and $\omega = 0$ or $v = 0$ correspond respectively to the familiar hydrogen-like and harmonic-oscillator ground-state problems. Unfortunately it is not possible to extend this collection of soluble potentials (say by scaling arguments) to include the potential $V(r) = (-A/r + Br + Cr^2)$ for *arbitrary* A, B and $C \geqslant 0$ because the function g which generates the problem has only *two* parameters: if the potential in equation (3) is simply multiplied by a constant, the corresponding exact ground-state

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energy remains unknown. We have recently developed a general approximation theory for *sums* of soluble potentials (Hall 1981) and this can be used to treat those (A, B, C) combinations which have no known exact solutions.

In the present article we use the *method of potential envelopes* (Hall 1980) to show how one can make use of exactly soluble problems such as those arising from equation (2) to approximate the eigenvalues of problems which are 'nearby' in a sense rather different from conventional perturbation theory. In particular we examine potentials of the form

$$V(r) = vf(-r^{-1} + \omega r) + \omega^2 r^2 \tag{5}$$

where f is a smooth increasing function of $\phi = (-r^{-1} + \omega r)$. The principal idea of our geometrical theory is that a *tangent line* to the curve $(\phi, f(\phi))$ has an equation like $y = \alpha + \beta\phi$ with $\beta > 0$ and therefore generates the 'tangential potential' defined by

$$V^{(t)}(r) = v\alpha + v\beta(-r^{-1} + \omega r) + \omega^2 r^2. \tag{6}$$

Consequently, by equations (3) and (4), we know that the Hamiltonian $H^{(t)} = (-\Delta + V^{(t)}(r))$ has the exact lowest eigenvalue given by

$$E^{(t)} = v\alpha + 3\omega - (v\beta)^2/4. \tag{7}$$

The method of potential envelopes which is outlined in § 2 prescribes sufficient conditions on f which allow us to relate the unknown eigenvalue E to the tangential eigenvalues $E^{(t)}$. In many cases the method yields a simple algebraic formula, in terms of the functions f and f', for bounds on E. In § 3 we return to the potential $V(r)$ of equation (5) and study the illustration $f(\phi) = (e^{\lambda\phi} - 1)/\lambda$ in some detail.

2. The method of potential envelopes

We suppose that the *exact* eigenvalue $\varepsilon(v)$ corresponding to the lowest bound state of the Hamiltonian

$$\hat{h} = -\Delta + v\phi(r) + U(r) \tag{8}$$

is known for each allowed value of the positive coupling constant v. The graph $(v, \varepsilon(v))$ we call the *energy trajectory* of $\hat{h}$ with respect to ϕ. The new Hamiltonian which we wish to analyse in terms of $\hat{h}$ is given by

$$H = -\Delta + vf(\phi(r)) + U(r) \tag{9}$$

and our aim first of all is to approximate the lowest eigenvalue E of H. We assume that the transformation function f is continuously differentiable and that $f'(\phi) > 0$, for all $\phi(r)$ with $r > 0$.

The key additional assumption which leads to energy *bounds* is that f is either convex or concave: we shall take the case that f is convex for all $\phi(r)$, $r > 0$, which leads to lower energy bounds; upper energy bounds are obtained when f is concave, by an exactly similar argument.

Consider the point $r = s$ and $\phi(s) = t$ which, for the present, we keep constant. We have, by the convexity of f,

$$f(\phi(r)) \geqslant f^{(t)}(r) \equiv f(t) + f'(t)\{\phi(r) - t\} \qquad \text{all } r > 0. \tag{10}$$

Equation (10) simply states that f lies above the tangent line $f^{(t)}$ which touches f at $\phi = t$.

We call the collection of functions $\{f^{(t)}(r)\}$ an *envelope representation* for the function $g(r)=f(\phi(r))$ and write this $g=\overset{\text{Envelope}}{t\in R_\phi}\{f^{(t)}\}$, where R_ϕ is the range of the potential function ϕ.

We can rewrite equation (10) (with t still fixed) in the form

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

where the 'constants' $\alpha(t)$ and $\beta(t)$ are given by

$$\alpha(t)=f(t)-tf'(t) \qquad \beta(t)=f'(t)>0 \text{ (by hypothesis).} \tag{12}$$

We now define the *tangential Hamiltonian* $H^{(t)}$ by

$$H^{(t)}=-\Delta+vf^{(t)}(r)+U(r) \tag{13}$$

and observe that, since $f^{(t)}=\alpha+\beta\phi$, where α and β are *constants*, the exact lowest eigenvalue $E^{(t)}$ of $H^{(t)}$ is given in terms of the known energy-trajectory function $\varepsilon(v)$ of $\hat{h}$ by

$$E^{(t)}=\alpha v+\varepsilon(\beta v). \tag{14}$$

Since $f^{(t)}(r)\leqslant f(\phi(r))$, $r>0$, we have, by Weyl's comparison theorem (e.g. Weinstein and Stenger 1972, p 21), that

$$E^{(t)}\leqslant E \qquad \text{for each fixed choice of } t\in R_\phi \tag{15}$$

where R_ϕ is the range of the function ϕ. The lower bound E^{L} is now given by

$$E^{\mathrm{L}}=\overset{\text{Envelope}}{t\in R_\phi}\{E^{(t)}\}\leqslant E. \tag{16}$$

Our smoothness assumption concerning f has been made merely for the convenience of using elementary calculus. In the same spirit, we now assume that $f''(t)$ and $\varepsilon'(v)$ are continuous functions so that the envelope in equation (16) can easily be calculated: our assumption that f is convex now becomes $f''(t)>0$, all $t\in R_\phi$. If we write equation (14) in the form

$$G(v,E,t)=\alpha v+\varepsilon(\beta v)-E=0 \tag{17}$$

and think of this equation as representing a *family* of curves in the (v,E) plane labelled by the parameter t, then we obtain (e.g. Courant 1936, p 172) the *envelope curve* (v,E^{L}) of this family by eliminating the parameter t between the two equations

$$G(v,E,t)=0 \qquad \text{and} \qquad \frac{\partial G}{\partial t}(v,E,t)=0. \tag{18}$$

In our problem these envelope equations become explicitly:

$$\begin{aligned} &E^{\mathrm{L}}=v\{f(t)-tf'(t)\}+\varepsilon(vf'(t)) \\ &t=\varepsilon'(vf'(t)). \end{aligned} \tag{19}$$

If equations (19) were difficult to solve, one might prefer to approach the original problem *directly* by using numerical methods. However, in many cases these equations can be rearranged to give E^{L} and v each as explicit functions of t, that is to say, parametric equations for the graph (v,E^{L}). If, for example, $\phi(r)$ is the pure power law $\phi(r)=\operatorname{sgn}(p)r^p$, where p is a constant greater than or equal to -1, and $U(r)\equiv 0$, then $\varepsilon(v)=\operatorname{sgn}(p)F^{(p)}v^{2/(p+2)}$, where $F^{(p)}$ is a positive constant (Hall 1980), and equations

(19) become in this case (after some algebraic manipulation):

$$E^{\mathrm{L}} = \tfrac{1}{2}v\{2f(t) + ptf'(t)\} \qquad pt > 0$$
$$v = |2F^{(p)}/t(p+2)|^{(p+2)/p}\{f'(t)\}^{-1}. \tag{20}$$

Equations (20) agree, of course, with equation (4.12) of Hall (1980): the actual Hamiltonian for which (v, E^{L}) provides a lower trajectory bound is given in the notation of the present article by

$$H = -\Delta + vf(\mathrm{sgn}(p)r^p) \tag{21}$$

and the equivalence of results is easily verified with the aid of the equations $t = \mathrm{sgn}(p)s^p$ and $ptf'(t) = s\ \mathrm{d}f(\mathrm{sgn}(p)s^p)/\mathrm{d}s$.

Of course, equations (19) and (20) immediately yield *upper* trajectory bounds when f is *concave*. Also, whenever the trajectory function $\varepsilon_k(v)$ is known for the kth excited state of the base problem $\hat{h}$, the corresponding energy bound formula yields a bound on the kth eigenvalue E_k of the transformed problem H: this follows because the comparison theorem of Weyl applies to each eigenvalue separately.

3. An example

In order to illustrate the theory of § 2 we need first to choose $\phi(r)$ and $U(r)$ so that the Hamiltonian $\hat{h}$ corresponds to an exactly soluble problem; then we must choose the convex or concave transformation $f(\phi)$ of ϕ which generates the new Hamiltonian H. The present paper is concerned with the class of Hamiltonians discussed in § 1 above where $U(r) = \omega^2 r^2$. We therefore define $\hat{h}$ as follows

$$\hat{h} = -\Delta + v\phi(r) + \omega^2 r^2$$
$$\phi(r) = (-r^{-1} + \omega r) \tag{22}$$
$$\varepsilon(v) = 3\omega - v^2/4$$

where $(v, \varepsilon(v))$ is the exact energy trajectory of $\hat{h}$ with respect to ϕ. The Hamiltonian H which we study then becomes

$$H = -\Delta + vf(-r^{-1} + \omega r) + \omega^2 r^2 \tag{23}$$

where f is increasing and either convex or concave, and will be chosen explicitly later. By applying the theory of § 2 we find the following approximation E^{A} to the exact energy trajectory $E(v)$ of H (equations (22) have been substituted directly in equations (19) and the resulting equations have been rearranged to give v and E in terms of the parameter t):

$$v = -2t\{f'(t)\}^{-1} \qquad E^{\mathrm{A}} = vf(t) + t^2 + 3\omega. \tag{24}$$

The parameter t must be in the range of ϕ which, in this example with $\omega \neq 0$, is the entire real line; moreover, since f is assumed to be increasing and v is positive, we see that $t \leqslant 0$. This means that, in this example, we only make use of that subset of the enveloping family of curves $\{\alpha + \beta\phi(r)\}$ corresponding to points of contact $r = s \leqslant \omega^{-1/2}$: the rest of the enveloping family gives suboptimal energy estimates.

We now choose the transformation f of ϕ. For the identity $f(\phi) = \phi$, we see from equation (24) that $E^{\mathrm{A}} = \varepsilon(v)$, as we expect. If we choose for f a function which is

convex, then equation (24) will yield a lower trajectory bound which we can compare with an independent variational upper bound. The example we present is

$$f(\phi) = \lambda^{-1}\{e^{\lambda\phi} - 1\} \qquad \lambda > 0 \tag{25}$$

which approaches the identity $f(\phi) = \phi$ as $\lambda \downarrow 0$. The actual potential generated in this way (with $\lambda > 0$) has the form

$$V(r) = v\lambda^{-1}\{\exp[\lambda(-r^{-1} + \omega r)] - 1\} + \omega^2 r^2. \tag{26}$$

A sketch of $V(r)$ for the case $v = 2$ and $\omega = 20\lambda = 1$ is shown in figure 1: for $\lambda > 0$, the Coulomb singularity of $\phi(r)$ is removed by the transformation $f(\phi)$ for we have $V(r) \geqslant \lim_{r\downarrow 0} V(r) = -v\lambda^{-1}$; for large values of r, $V(r) \sim v\lambda^{-1}\exp(\lambda\omega r)$. The (lower) trajectory bound equation (24) becomes (in parametric form)

$$v = 2q\, e^{\lambda q} \qquad q \geqslant 0 \tag{27a}$$

$$E^{L} = v\lambda^{-1}\{e^{-\lambda q} - 1\} + q^2 + 3\omega \tag{27b}$$

where we have used the positive parameter $q = -t$. Thus we have in equation (27) a formula for a lower bound to the lowest eigenvalue of the Hamiltonian $H = \{-\Delta + V(r)\}$ which depends on $v \geqslant 0$, $\omega \geqslant 0$ and $\lambda > 0$; in the limiting case $\lambda \downarrow 0$, this formula yields of course the exact result $E = 3\omega - v^2/4$. For $\omega = 1$, the graph of $E^{L}(v)$ for $\lambda = 0.05$ is shown in figure 2 together with a variational upper trajectory bound $E^{U}(v)$ found by

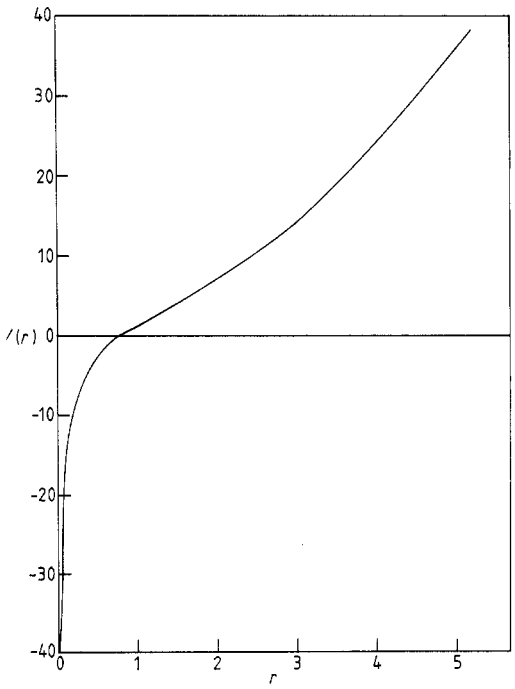

Figure 1. The potential in the example is the smooth transformation $vf(\phi) + \omega^2 r^2$ of the potential $\phi(r) = (-r^{-1} + \omega r)$, in which $f(\phi) = \lambda^{-1}\{\exp(\lambda\phi) - 1\}$. Explicitly we have $V(r) = \omega\lambda^{-1}[\exp\{\lambda(-r^{-1} + \omega r)\} - 1] + \omega^2 r^2$, and the figure illustrates the case $\omega = 20\lambda = 1$, and $v = 2$.

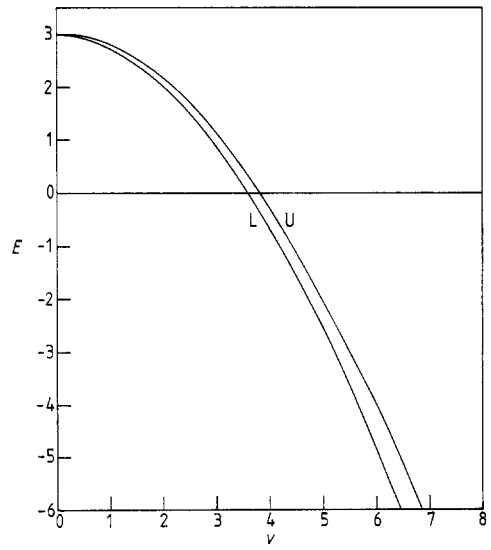

Figure 2. Upper and lower bounds to the lowest eigenvalues $E(v)$ of the Hamiltonian $H = -\Delta + v\lambda^{-1}[\exp\{\lambda(-r^{+1} + \omega r)\} - 1] + \omega^2 r^2$, with $\omega = 1$ and $\lambda = 0.05$: in the limit as $\lambda \downarrow 0$, we have $H = -\Delta + v(-r^{-1} + \omega r) + \omega^2 r^2$ and $E(v) = 3\omega - v^2/4$ exactly.

using the trial function $\psi(r) = \exp\{-ar - br^2\}$ and minimising the expectation of H with respect to the scale variables a and b.

In order to find E^{L} for a given v *numerically*, one first solves equation (27*a*) for q and then substitutes this value of q into (27*b*). For the case $\omega = 1$, $v = 5$, and $\lambda = 0.01$, 0.05 and 0.1 Killingbeck (1981) has found a numerical approximation E^{K} to E by the method described in his (1977a) article: these results together with ours are respectively $(E^{\mathrm{L}}, E^{\mathrm{K}}, E^{\mathrm{U}}) = (-3.099, -2.917, -2.908)$, $(-2.578, -1.971, -1.950)$, and $(-2.066, -1.230, -1.160)$.

Of course, our lower bound equation (27) gives the general *form* of the dependence of E on the triple (v, λ, ω) and this analytical information, which is always interesting, is particularly important for the N-body problem, $N \geq 2$, as we have shown in Hall (1980, 1981). Even for the rather general class of potentials (23), we have a simple recipe (24) which yields lower bounds when $f'' > 0$ and upper bounds when $f'' < 0$.

4. Conclusion

The minimal properties of the eigenvalues of the semi-bounded self-adjoint operators of wave mechanics allow us to use the geometrical ideas of convexity and envelope representations in their study. In this article we submit a *component* $\phi(r)$ of the potential in the Hamiltonian $\hat{h}$ to a smooth convex or concave transformation $f(\phi)$. This generates a new Hamiltonian H whose kth eigenvalue can be easily approximated provided we know how the kth eigenvalue of $\hat{h}$ depends on the coupling constant v of the component $\phi(r)$, that is to say, the kth energy trajectory of $\hat{h}$ with respect to ϕ. In terms of perturbation theory one can also write

$$H = \hat{h} + v\{f(\phi(r)) - \phi(r)\}. \tag{28}$$

We do not, however, require v to be small: provided f is convex or concave the method always yields a strict energy *bound*; whenever the *curvature* of f is small in the region over which the square of wavefunction $|\psi(r)|^2$ is significantly large, the approximation will be good. The purpose of this geometrical theory is to provide a new tool with which to analyse potentials that are near to one of the few potentials we have whose corresponding energy trajectories are known exactly.

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