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Schrödinger's equation with linear combinations of elementary potentials

Richard L. Hall
Department of Mathematics, Concordia University, Montreal, Quebec, Canada
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Suppose $\epsilon = F(v)$ is the energy of the lowest bound eigenstate of the Hamiltonian $\hat{h} = -\Delta + vf(x)$, where $f(x)$ is an attractive central potential. The Λ transform is defined by $F = \Lambda\{f\}$ and the curve $(v,F(v))$ is called the "energy trajectory" of the problem. In this article it is shown that the energy trajectory of the linear combination $f = \Sigma_{i=1}^{n}\alpha_i f_i$, $\alpha_i \geq 0$, is bounded by curves of the form $v = \{\Sigma_{i=1}^{n}\alpha_i[\theta_i(s)]^{-1}\}^{-1}$, $\epsilon = v\Sigma_{i=1}^{n}\alpha_i F_i(\theta_i(s))\,[\theta_i(s)]^{-1}$, where the curve parameter $s > 0$, and each function $\theta_i(s)$ is defined by an equation $F_i(\theta_i) - \theta_i F_i'(\theta_i) = s$, which is solvable when f_i is "elementary." For the lower bound, $F_i = \Lambda\{f_i\}$, for the upper bound, $F_i(v) = F_i^U(v)$ is the upper trajectory obtained by applying a trial function to the *one*-component problem $-\Delta + vf_i(x)$ and minimizing $\langle\hat{h}\rangle$ with respect to a scale variable. Detailed recipes are given for the trajectory bounds corresponding to potentials which are arbitrary linear combinations of powers, logarithm, Hulthén, and sech^2 in one or three dimensions. For the anharmonic oscillator $f(x) = x^2 + \lambda x^4$ in one dimension, for example, $\epsilon(\lambda)$ is determined by the expression $\lambda = \{1 - 4[\epsilon - (\epsilon^2 - 3/4)^{1/2}]^2\}/A[\epsilon - (\epsilon^2 - 3/4)^{1/2}]^3$, where $A = 22.608$ for the lower bound and $A = 24$ for the upper bound derived from a Gaussian trial function; this formula determines ϵ for a given λ with error less than 1% for all $\lambda \geq 0$. The lower bounds and Gaussian upper bounds at the same time determine the lowest energies of the corresponding N-boson systems for all $N \geq 2$.

I. INTRODUCTION

In this article we continue the study of the Schrödinger eigenvalue problem by geometrical methods which we began in Ref. 1. The new results are applicable to the N-body problem, as we show in Sec. VI, but the main emphasis of the present work is the case $N = 2$. We consider a bound system of two particles with masses m_1 and m_2 interacting by the two-parameter attractive central pair potential

$$V(|\vec{r}_i - \vec{r}_2|) = V_0 f(|\vec{r}_1 - \vec{r}_2|/a), \quad V_0 > 0, \ a > 0 \tag{1.1}$$

and obeying nonrelativistic quantum mechanics. In terms of the dimensionless variables

$$v = 2\mu V_0 a^2/\hbar^2, \qquad \epsilon = 2\mu E a^2/\hbar^2, \qquad \vec{x} = (\vec{r}_1 - \vec{r}_2)/a, \tag{1.2}$$

where $\mu = m_1 m_2/(m_1 + m_2)$ is the reduced mass and E is the energy, Schrödinger's equation may be written

$$[-\Delta_{\vec{x}} + vf(x)]\Psi(\vec{x}) = \hat{h}\Psi(\vec{x}) = \epsilon\Psi(\vec{x}). \tag{1.3}$$

We are using a different sign convention from Ref. 1: In the present paper the potential *shape* f now always has the same sign as the potential, and ϵ has the same sign as the energy E. We define the *energy trajectory* F as the function which tells us how ϵ depends on v, thus

$$\epsilon = F(v), \tag{1.4}$$

and

$$F = \Lambda\{f\},$$

where Λ is the name we give to the nonlinear transform which takes us from the potential to its trajectory. There will be a trajectory for each eigenvalue of $\hat{h}$ but we are currently concerned mainly with the lowest trajectory. Thus for the hydrogen atom we have (using the convenient abuse of notation common in the application of Fourier and Laplace transforms) $\Lambda\{-x^{-1}\} = -v^2/4$ and for the harmonic oscillator $\Lambda\{x^2\} = 3v^{1/2}$.

We shall now state our main result and present two illustrations. Suppose f is a sum of n potentials f_i each of whose trajectories F_i is known exactly; that is

$$f(x) = \sum_{i=1}^{n}\alpha_i f_i(x), \quad \alpha_i > 0. \tag{1.5}$$

Then the parametric equations for a lower bound to the trajectory $F = \Lambda\{f\}$ are as follows:

$$v^{-1} = \sum_{i=1}^{n}\alpha_i[\theta_i(s)]^{-1}, \qquad \epsilon v^{-1} = \sum_{i=1}^{n}\alpha_i F_i(\theta_i(s))[\theta_i(s)]^{-1}, \tag{1.6}$$

where $s > 0$ is a parameter and the n functions $\{\theta_i\}$ are defined by the n equations

$$F_i(\theta_i(s)) - \theta_i(s)F_i'(\theta_i(s)) = s, \quad i = 1, 2, \ldots, n. \tag{1.7}$$

Moreover, suppose a trial function with shape ϕ

is used to estimate F_i and the expectation of the *one*-component Hamiltonian $-\Delta+vf_i(x)$ is minimized with respect to *scale* separately, for each $i=1,2,\ldots,n$, giving the upper bounds $F_i^U(v)$, then the *best* upper bound to F which can be obtained by using ϕ is given by substituting the functions F_i^U and the corresponding θ_i^U in Eq. (1.6). For example, if f is given by

$$f(x)=-\alpha x^{-1}+\beta x^2, \tag{1.8}$$

then the bounds (1.6) to $F=\Lambda\{f\}$ become in this case

$$\begin{aligned} v^{-1}&=\alpha At+\beta Bt^4,\\ \epsilon v^{-1}&=-\alpha At^{-1}+2\beta Bt^2, \end{aligned} \tag{1.9}$$

where the parameter $t=s^{-1/2}>0$ and for the lower bound $(A,B)=(\frac{1}{2},\frac{9}{4})$ and for the upper bound $(A,B)=((2/3\pi)^{1/2},\frac{9}{4})$ with Gaussian ϕ and $(A,B)=(\frac{1}{2},3)$ with exponential ϕ.

The formula (1.6) corresponds to the more general formula Eq. (4.12) of Ref. 1 but the new theory yields far better results because it has been developed specifically for the special case of potential *sums* (1.5). The most novel feature of the present work is the new variational lower bound which depends heavily on the trajectory idea and is derived in Sec. III; the fact that the variational upper bound can also be put in the same *form* is also interesting and very useful in practice. One might expect that solving Eq. (1.7) for the $\theta_i(s)$ could pose difficulties but we shall give explicit recipes for general mixtures of the form

$$\begin{aligned} f(x)=&-\alpha_1x^{-1}-\alpha_2(e^x-1)^{-1}+\alpha_3\ln x+\alpha_4x\\ &+\alpha_5x^2-\alpha_6\operatorname{sech}^2x+\alpha_7x^4+\alpha_8x^6+\alpha_9x^8, \end{aligned} \tag{1.10}$$

which certainly represents a rich variety of problems; potentials for which Eq. (1.7) *can* be solved for $\theta(s)$ we call *elementary potentials*. Whenever there is only one term in f, the lower bound gives the exact answer; otherwise the bound is a kind of optimal mean in the trajectory picture.

For the popular anharmonic-oscillator problem[2-5] $f(x)=x^2+\lambda x^4$ (in one spatial dimension) we are able to show (Sec. VII) that

$$\lambda=\frac{1-4[\epsilon-(\epsilon^2-\frac{3}{4})^{1/2}]^2}{A[\epsilon-(\epsilon^2-\frac{3}{4})^{1/2}]^3}, \tag{1.11}$$

where $A=A^L=22.608$ for the lower bound and $A=A^U=24$ for the upper bound derived from a Gaussian trial function. Consequently we see that λ is determined with error *strictly* less than $100(A^U-A^L)/(A^U+A^L)<3\%$ for all $\lambda\geq 0$; a similar formula for the problem in three spatial dimensions gives λ with error less than 2%. Since $\lambda\,d\epsilon/\epsilon\,d\lambda<\frac{1}{3}$ on the mean trajectory, with $A=(A^L+A^U)/2$, the error in ϵ for a given λ is less than 1% in both cases. Because we have used a *Gaussian* trial function for the upper bound, Eq. (1.11) actually represents a solution to the N-boson problem to the same accuracy for *all* $N\geq 2$ (see Sec. VI).

Equations (1.9) and (1.11) indicate very well the nature of our present contribution to the eigenvalue problem: The bounds exhibit the dependence of the eigenvalue on the potential parameters in a form which allows for further analysis; the separation of the bounds is typically of the order of a few percent. Hill[6] has recently solved the anharmonic-oscillator problem to 21 significant figures, but even so, for many purposes, *explicit* bounds like (1.11) will still be of considerable value.

From the analytical point of view it is of interest to note that although the Λ transform is clearly *not* linear, the general bound formula (1.6) does preserve some aspects of the linear dependence of f on the coefficients $\{\alpha_i\}$. It is also geometrically interesting that if $F_i''(v)<0$ for each $i=1,2,\ldots,n$ [as *is* the case for each of the terms in Eq. (1.10)], then Eq. (1.6) implies the following geometrical properties on each of the trajectory *bounds* of $F=\Lambda\{\sum_i\alpha_if_i\}$:

$$\begin{aligned} &\frac{d(\epsilon v^{-1})}{d(v^{-1})}=s>0,\\ &\text{and}\\ &\frac{d^2(\epsilon v^{-1})}{d(v^{-1})^2}<0. \end{aligned} \tag{1.12}$$

On the upper-bound curve the parameter s is actually equal to the mean kinetic energy.

It may eventually become necessary to study the Λ transform in an abstract and general fashion but the present article is chiefly concerned with presenting concrete results which will be of use in applications where the potential under consideration is a sum of elementary potentials.

II. ELEMENTARY POTENTIALS

Elementary potentials are defined to be those potentials f whose trajectories $F=\Lambda\{f\}$ are known exactly and for which the equation

$$F(\theta(s))-\theta(s)F'(\theta(s))=s \tag{2.1}$$

can be solved explicitly for the function $\theta(s)$. Some potentials like the example[7]

$$\begin{aligned} &f(x)=-2x^{-1}+4\lambda x+4\lambda^2x^2,\quad \lambda\geq 0\\ &F(1)=6\lambda-1 \end{aligned} \tag{2.2}$$

have known exact solutions only for certain isolated values of v so that although these potentials

provide useful tests, they cannot be employed immediately as "building blocks" in our geometrical theory. There *are* many elementary potentials, however, and we now discuss a few of them.

A. Power-law potentials

For potentials of the form

$$f(x)=\mathrm{sgn}(p)x^p,\quad p\geq -1,\ p\neq 0 \tag{2.3}$$

we have[1]

$$F(v)=\mathrm{sgn}(p)F_p v^{2/(p+2)}, \tag{2.4}$$

where the F_p are positive constants. If a trial function ϕ is applied to estimate ϵ and we minimize $\langle\hat{h}\rangle$ with respect to a scale variable (as in Ref. 1 and more generally in Sec. IV below), then the upper trajectory has the same form as Eq. (2.4) but F_p must be replaced by the appropriate F_p^U. These F numbers are shown in Table I for both one and three dimensions. In one dimension we consider symmetric potentials $f(|x|)$ and restrict $p>0$ so that simple Gaussian and exponential trial functions are applicable.

For power-law potentials the $\theta(s)$ functions defined by Eq. (2.1) become

$$\theta_p(s)=[s(p+2)/|p|F_p]^{(p+2)/2}. \tag{2.5}$$

B. The logarithmic potential

For the potential

$$f(x)=\ln x \tag{2.6}$$

in three dimensions we have shown[8] that

$$F(v)=-\tfrac{1}{2}v\ln(v/G_L),\quad v>0 \tag{2.7}$$

where G_L is a positive constant. The "exact" numerical solution of Quigg and Rosner[9] gives $G_L=7.63$ and the corresponding values for variational upper bounds with Gaussian and exponential trial functions are 8.4579 and 8.6057, respectively. Meanwhile the $\theta(s)$ function in this case has the simple form

$$\theta(s)=2s\,. \tag{2.8}$$

C. The Hulthén and sech^2x potentials

The Hulthén potential[10] in three dimensions has the shape

$$f(x)=-(e^x-1)^{-1} \tag{2.9}$$

and

$$F(v)=-(v-1)^2/4,\quad v\geq 1\,. \tag{2.10}$$

Consequently we have from Eq. (2.1)

$$\theta(s)=(1+4s)^{1/2},\quad s\geq 0\,. \tag{2.11}$$

The potential with shape

$$f(x)=-\mathrm{sech}^2x \tag{2.12}$$

has in three dimensions (see Ref. 11)

$$\begin{aligned}&F(v)=-v+3(v+\tfrac{1}{4})^{1/2}-\tfrac{5}{2},\quad v\geq 2\\ &\theta(s)=\tfrac{1}{9}[(s+\tfrac{5}{2})+(s^2+5s+4)^{1/2}]^2-\tfrac{1}{4},\quad s\geq 0\end{aligned} \tag{2.13}$$

and in one dimension

$$\begin{aligned}&F(v)=-v+(v+\tfrac{1}{4})^{1/2}-\tfrac{1}{2},\quad v\geq 0\\ &\theta(s)=[(s+\tfrac{1}{2})+(s^2+s)^{1/2}]^2-\tfrac{1}{4},\quad s\geq 0\,.\end{aligned} \tag{2.14}$$

It is interesting that the θ function is defined for all $s>0$ in all the cases we have studied, so that we do not have to pay special attention to the range of this variable (as we should with v) when we consider arbitrary linear combinations of potentials.

For the Hulthén and sech^2x potentials we are not able to find *explicit* formulas for $F^U(v)$ corresponding to Gaussian and exponential trial functions. However, in Sec. IV we show [Eqs. (4.6)

TABLE I. Trajectory coefficients for pure power-law potentials. The lowest eigenvalue of $\hat{h}=-\Delta+vf(x)$ for $f(x)=\mathrm{sgn}(p)x^p$ is given by $\epsilon=\mathrm{sgn}(p)F_p^{(d)}v^{2/(p+2)}$, where $d=1$ or 3 is the number of spatial dimensions of the problem. For $p=4$, 6, and 8, the F_p numbers are taken from Refs. 4 and 5. The letters G or E indicate upper bounds derived by the use respectively of Gaussian and exponential trial functions.

p	-1	1	2	4	6	8
$F_p^{(1)}$		1.018 793	1	1.060 362	1.144 802	1.225 820
$F_p^{(3)}$	$\frac{1}{4}$	2.338 107	3	3.799 673	4.338 60	4.755 8

$F_p^{(1)G}=(p+2)[\Gamma((p+1)/2)/\Gamma(1/2)]^{2/(p+2)}/2p^{p/(p+2)}$, $p>0$

$F_p^{(1)E}=(p+2)[\Gamma(p+1)]^{2/(p+2)}/2(2p)^{p/(p+2)}$, $p>0$

$F_p^{(3)G}=(p+2)[\Gamma((3+p)/2)/\Gamma(3/2)]^{2/(p+2)}(3/|p|)^{p/(p+2)}/2$, $p\geq -1$

$F_p^{(3)E}=(p+2)[\Gamma(p+3)]^{2/(p+2)}/4|p|^{p/(p+2)}$, $p\geq -1$

and (4.7)] that in the general case of a potential f_i, and an (appropriate) trial function ϕ, expressions can be given for the terms $\theta_i^{-1}F(\theta_i)$ and θ_i^{-1} to be substituted in the general sum (1.6) so that it yields the best upper bound to $\Lambda\{\sum_i \alpha_i f_i\}$ available via ϕ. Thus we see that the general bounds (1.6) only *require* that the component potentials f_i be "elementary" with respect to the lower bound.

III. VARIATIONAL LOWER BOUNDS

We consider a collection of n attractive potentials f_i each of whose energy trajectories $F_i = \Lambda\{f_i\}$ is known exactly. The potential we wish to study is the linear combination

$$f = \sum_{i=1}^{n} \alpha_i f_i \,, \tag{3.1}$$

where the coefficients α_i are positive and fixed. The new variational lower bound is based on the idea that the Hamiltonian

$$\hat{h} = -\Delta + vf \tag{3.2}$$

can be written as a convex sum of n solvable Hamiltonians

$$\hat{h} = \sum_{i=1}^{n} w_i \hat{h}_i \,, \quad w_i > 0 \,, \tag{3.3}$$

where

$$\hat{h}_i = -\Delta + \frac{v\alpha_i}{w_i} f_i$$

and (3.4)

$$\sum_{i=1}^{n} w_i = 1 \,.$$

Suppose Ψ is the normalized exact (unknown) lowest eigenstate of $\hat{h}$ for a fixed value of v, and let us assume that Ψ may be applied as a trial function to each of the $\hat{h}_i$, then we have from Eq. (3.3)

$$(\Psi, \hat{h}\Psi) = F(v) = \sum_{i=1}^{n} w_i (\Psi, \hat{h}_i \Psi) \,. \tag{3.5}$$

But each term $(\Psi, \hat{h}_i \Psi)$ is an upper bound to the lowest eigenvalue of $\hat{h}_i$. We therefore have our fundamental lower-bound inequality

$$F(v) \geq \sum_{i=1}^{n} w_i F_i\left(\frac{v\alpha_i}{w_i}\right) \,, \qquad \sum_{i=1}^{n} w_i = 1 \,, \quad w_i > 0 \,. \tag{3.6}$$

The positive weights w_i may now be chosen to maximize the right-hand side of Eq. (3.6) subject to the constraints that (a) they have sum one, and (b) for the values of α_i and v under consideration the products $(v\alpha_i/w_i)$ do not fall outside the domains of the corresponding trajectory functions F_i. It is certainly possible to use direct methods to find a good lower bound (for example, by letting the w_i be functions of a parameter), or even Monte Carlo methods (the vector $\vec{w}$ of the w_i is a probability vector). However, for *elementary potentials* for which Eq. (1.7) can be solved explicitly, we can actually find a prescription for the best weights. The necessary conditions are simply

$$F_i\left(\frac{v\alpha_i}{w_i}\right) - \left(\frac{v\alpha_i}{w_i}\right) F_i'\left(\frac{v\alpha_i}{w_i}\right) = s \,, \quad i = 1, 2, \ldots, n \,, \tag{3.7}$$

where s is a Lagrange multiplier. Hence, by the definition Eq. (1.7) of the functions $\theta_i(s)$, we have

$$w_i = v\alpha_i [\theta_i(s)]^{-1} \tag{3.8}$$

and consequently our best lower-bound trajectory for linear combinations of elementary potentials becomes in parametric form

$$v^{-1}F(v) \geq \sum_{i=1}^{n} \alpha_i F_i(\theta_i(s))[\theta_i(s)]^{-1} \,, \qquad v^{-1} = \sum_{i=1}^{n} \alpha_i [\theta_i(s)]^{-1} \,. \tag{3.9}$$

In all the cases which we have studied, the question of the various domains of definition of the trajectory functions $F_i(v)$ poses no difficulty because the range of the parameter s is conveniently the same, namely the half line $s > 0$. In the similar formula which we find for upper bounds (Sec. IV) s is equal to the mean kinetic energy. If all but one of the α_i are set equal to zero, the lower bound (3.9) yields the exact answer; in the general case the bound is an optimal mean of the component trajectories, optimized for each choice of $\{\alpha_i\}$ and v.

IV. VARIATIONAL UPPER BOUNDS

We shall show that variational upper bounds obtained by the minimization of the energy expectation with respect to a scale variable σ lead to upper trajectories which have the same *form* as our lower trajectories. Suppose $\phi(x)$ is a trial function and we define the normalization and kinetic energy integrals respectively as

$$\int \phi^2(x) d\tau(x) = I \tag{4.1}$$

and

$$\int \phi(x)\{-\Delta\}\phi(x) d\tau(x) = K \,. \tag{4.2}$$

This notation allows us to treat the one-dimensional and three-dimensional problems at the same time. An upper bound to the lowest eigenvalue of $\hat{h} = -\Delta + vf$ is given by using the trial function

$\phi(x/\sigma)$ and this leads to the expression

$$\epsilon(\sigma)=\frac{K}{\sigma^2 I}+\frac{v}{I}\int \phi^2(\xi)f(\sigma\xi)d\tau(\xi)\,. \tag{4.3}$$

If $\epsilon(\sigma)$ is now minimized with respect to σ we obtain the upper-bound trajectory $F^U(v)$ in parametric form in terms of σ:

$$\begin{aligned} v^{-1}F^U(v)&=\epsilon v^{-1}\\ &=(2I)^{-1}\int \phi^2(\xi)[2f(\sigma\xi)+(\sigma\xi)f'(\sigma\xi)]d\tau(\xi)\,,\\ v^{-1}&=(2K)^{-1}\sigma^2\int \phi^2(\xi)(\sigma\xi)f'(\sigma\xi)d\tau(\xi)\,, \end{aligned} \tag{4.4}$$

where $f(x)=\sum_{i=1}^n \alpha_i f_i(x)$. By differentiating Eq. (4.4) with respect to σ we see that

$$\frac{d}{d\sigma}[v^{-1}F^U(v)]=\left(\frac{K}{I\sigma^2}\right)\frac{d}{d\sigma}(v^{-1}) \tag{4.5}$$

and therefore

$$F^U(v)-vF^{U'}(v)=\frac{K}{I\sigma^2}\,. \tag{4.6}$$

Now the expressions for ϵv^{-1} and v^{-1} are both linear homogeneous in the $\{\alpha_i\}$, and therefore for $i=1,2,\ldots,n$ we have

$$\begin{aligned} \frac{\partial(\epsilon v^{-1})}{\partial\alpha_i}&=(2I)^{-1}\int \phi^2(\xi)[2f_i(\sigma\xi)+(\sigma\xi)f_i'(\sigma\xi)]d\tau(\xi)\,,\\ \frac{\partial(v^{-1})}{\partial\alpha_i}&=(2K)^{-1}\sigma^2\int \phi^2(\xi)(\sigma\xi)f_i'(\sigma\xi)d\tau(\xi)\,. \end{aligned} \tag{4.7}$$

By defining the *single-component* upper trajectories F_i^U to be given by F^U in Eq. (4.4) when $\alpha_i=1$ and $\alpha_{k\neq i}=0$, and by comparing (4.4) with (4.7), we see that (4.7) may be written in the form

$$\begin{aligned} \frac{\partial(\epsilon v^{-1})}{\partial\alpha_i}&=\theta_i{}^{-1}F_i^U(\theta_i)\,,\\ \frac{\partial(v^{-1})}{\partial\alpha_i}&=\theta_i{}^{-1}\,, \end{aligned} \tag{4.8}$$

and consequently, by the same argument which led to Eq. (4.6), we have

$$F_i^U(\theta_i)-\theta_i F_i^{U'}(\theta_i)=\frac{K}{I\sigma^2}\,,\quad i=1,2,\ldots,n\,. \tag{4.9}$$

Thus we conclude that the best upper-bound trajectory for the potential $f(x)=\sum_i \alpha_i f_i(x)$ which can be obtained by using the trial function $\phi(x/\sigma)$ and minimizing $\langle\hat{h}\rangle$ with respect to the scale σ is given in parametric form by

$$\begin{aligned} \epsilon v^{-1}&=\sum_{i=1}^n \alpha_i F_i^U(\theta_i(s))[\theta_i(s)]^{-1}\,,\\ v^{-1}&=\sum_i \alpha_i[\theta_i(s)]^{-1}\,, \end{aligned} \tag{4.10}$$

where the n functions $\theta_i(s)$ are defined by

$$F_i^U(\theta_i(s))-\theta_i(s)F_i^{U'}(\theta_i(s))=s\,,\quad i=1,2,\ldots,n\,, \tag{4.11}$$

and the parameter

$$s=\frac{K}{\sigma^2 I} \tag{4.12}$$

is the mean kinetic energy [see Eq. (4.3)]. We do not *require* the solvability of Eq. (4.11) for the upper bound: In cases where Eq. (4.11) is difficult to solve, the corresponding terms $\theta_i{}^{-1}F_i(\theta_i)$ and $\theta_i{}^{-1}$ of Eq. (4.10) are given as explicit functions by Eqs. (4.7), (4.8), and (4.12).

V. MIXTURES OF POWERS AND THE LOG POTENTIAL

We have established the general formula (1.6) which provides upper and lower bounds to the energy trajectory $\Lambda\{\sum_i \alpha_i f_i\}$ of a sum of potentials. Terms can be added or subtracted from this sum but the variational bounds always remain optimal. This formulation is so very convenient for sums of powers and the log potential that we shall now treat these special components in their own terms. In one dimension we assume f to be a function of $|x|$ and we omit the singular terms x^p for $p<0$, and $\ln x$; otherwise our general arguments and formulas are the same for both cases.

We suppose f to be given by

$$f(x)=\sum_p \alpha_p\,\mathrm{sgn}(p)x^p+\alpha\ln x\,,$$

$$p\geq -1\,,\quad p\neq 0\,,\quad \alpha_p\geq 0\,,\quad \alpha\geq 0\,. \tag{5.1}$$

Then the trajectory bounds are given from Eq. (1.6) by

$$\begin{aligned} \epsilon v^{-1}&=\sum_p \alpha_p\left(\frac{2+p}{p}\right)\left(\frac{|p|F_p}{p+2}\right)^{(p+2)/2}s^{-p/2}-\tfrac{1}{2}\alpha\ln(2s/G_L)\,,\\ v^{-1}&=\sum_p \alpha_p\left(\frac{|p|F_p}{p+2}\right)^{(p+2)/2}s^{-(p+2)/2}+\alpha/(2s)\,, \end{aligned} \tag{5.2}$$

where the F_p numbers and G_L are given in Table I and Sec. II B both for lower bounds, and upper bounds corresponding to Gaussian and exponential trial functions. It is clearly convenient for mixtures of type (5.1) to define the G_p numbers and the parameter t as follows:

$$G_p=\left(\frac{|p|F_p}{p+2}\right)^{(p+2)/2}\,,\quad t=s^{-1/2}>0\,. \tag{5.3}$$

The power-law and log bounds then have the simple form

$$\begin{aligned} \epsilon v^{-1}&=\sum_p \alpha_p\left(\frac{2+p}{p}\right)G_p t^p+\frac{\alpha}{2}\ln(G_L t^2/2)\,,\\ v^{-1}&=\sum_p \alpha_p G_p t^{p+2}+\tfrac{1}{2}\alpha t^2\,,\quad p\geq -1\,,\quad p\neq 0\,, \end{aligned} \tag{5.4}$$

where the G numbers are presented in Table II; for the upper bound we have from Eq. (4.12)

$$t=\sigma(I/K)^{1/2}. \tag{5.5}$$

The rounding of decimals has been chosen in Table II so that the G numbers yield strict bounds via Eq. (5.4).

VI. THE N-BOSON PROBLEM

Consider N identical bosons each of mass m interacting via a central pair potential of the form (1.1). The Hamiltonian for this system may be written[1]

$$H=\sum_{1=i<j}^{N}\left[\frac{(\vec{p}_i-\vec{p}_j)^2}{2mN}+V_{ij}\right]. \tag{6.1}$$

In terms of a set $\{\vec{\rho}_2,\vec{\rho}_3,\ldots,\vec{\rho}_N\}$ of Jacobi orthogonal relative coordinates[1] with $\vec{\rho}_2=(\vec{r}_1-\vec{r}_2)/\sqrt{2}$ we have for expectations of H with respect to boson functions of these variables

$$\langle H\rangle=\langle\mathcal{H}\rangle, \tag{6.2}$$

where

$$\mathcal{H}=(N-1)\left[-\frac{\hbar^2}{2m}\Delta_{\vec{\rho}_2}+\frac{N}{2}V_0 f(\sqrt{2}\rho_2/a)\right]. \tag{6.3}$$

We now define the dimensionless variables

$$\begin{aligned} &v=NV_0a^2m/2\hbar^2,\\ &\epsilon=mE_Na^2/(N-1)\hbar^2,\\ &\hat{h}=-\Delta_{\vec{x}}+vf(x),\\ &\vec{x}=\sqrt{2}\,\vec{\rho}_2/a, \end{aligned} \tag{6.4}$$

where E_N is the lowest eigenvalue of the N-boson problem, and we note that these definitions are consistent with Eq. (1.2) in the case $N=2$ and $m_1=m_2=\mu/2$, and the operators $\hat{h}$ in (1.3) and (6.4) are identical. It then follows (see Ref. 1) that

$$F(v)\leq\epsilon\leq F^G(v), \tag{6.5}$$

where $F(v)$ is the lowest eigenvalue of $\hat{h}$ and $F^G(v)$ is the minimum of $\langle\hat{h}\rangle$ with respect to normalized Gaussian functions of $\vec{x}$; the upper and lower bounds in (6.5) coincide if and only if[12] $f(x)=x^2$, i.e., the harmonic-oscillator potential.

Although the present article is principally concerned with the two-body problem, the search for upper and lower trajectories, F^G and F, in the same *form* has been motivated strongly by the relation (6.5) which immediately extends our results to the N-boson problem for all $N\geq 2$. For the N-boson problem the variable ϵv^{-1}, which appears in our parametric equations for the energy trajectories, becomes

$$\epsilon v^{-1}=(E_N/V_0)\binom{N}{2}^{-1}. \tag{6.6}$$

VII. SOME ILLUSTRATIONS

The following problems are of some interest in themselves and at the same time they give an indication of the quality of the results we should expect when we apply the general formulas for trajectory bounds to specific problems.

A. An exactly soluble test problem

We mentioned in Sec. III the exactly soluble problem[7] in three dimensions:

$$\begin{aligned} &f(x)=-2x^{-1}+4\lambda x+4\lambda^2x^2,\quad \lambda\geq 0\\ &F(1)=(6\lambda-1). \end{aligned} \tag{7.1}$$

This example is covered by our formula (5.4) for general power-law and log mixtures, with $p=-1$,

TABLE II. G numbers for combinations of powers and the log potential. The $G^{(d)}$ numbers are required in Eq. (5.4) which gives upper and lower energy trajectories for arbitrary linear combinations of power-law potentials and the log potential. The number of spatial dimensions is indicated by d, the letters G and E indicate upper bounds derived by the use, respectively, of Gaussian and exponential trial functions, and L indicates the log potential. Decimal approximations have been rounded so as to preserve the validity of the energy bounds.

p	-1	L	1	2	4	6	8
$G_p^{(1)}$			0.197 900	$\frac{1}{4}$	0.353 255	0.543 458	0.906 950
$G_p^{(3)}$	$\frac{1}{2}$	7.63	0.688 041	$\frac{9}{4}$	16.254 17	112.109	797.20

$G_p^{(1)G}=p[\Gamma((p+1)/2)/\Gamma(1/2)]2^{-(p+2)/2}$, $p>0$

$G_p^{(1)E}=p\,\Gamma(p+1)2^{-(p+1)}$, $p>0$

$G_p^{(3)G}=|p|\,3^{p/2}[\Gamma((p+3)/2)/\Gamma(3/2)]2^{-(p+2)/2}$, $p\geq -1$

$G_p^{(3)E}=|p|\,\Gamma(p+3)2^{-(p+2)}$, $p\geq -1$

$G_L^{(3)G}=\frac{3}{4}\exp(3-\gamma)=8.457\,912$ $\qquad$ $G_L^{(3)E}=\frac{1}{2}\exp(4-2\gamma)=8.605\,672$

1, and 2. Thus we have

$$\epsilon v^{-1} = -2G_{-1}t^{-1} + 12\lambda G_1 t + 8\lambda^2 G_2 t^2 ,$$
$$v^{-1} = 2G_{-1}t + 4\lambda G_1 t^3 + 4\lambda^2 G_2 t^4 , \tag{7.2}$$

where $t > 0$ and the G_p for upper and lower bounds are given in Table II. Since it is not possible to find $F(v)$ for $v \neq 1$ from (7.1) by scaling arguments, we take the special case $v = 1$ and exhibit in Table III some values of the positive ratio

$$R(\lambda) = [\epsilon(\lambda) + 1]/6\lambda , \tag{7.3}$$

which has the value 1 if ϵ is exact; the fractional error in ϵ itself is given by $(R-1)6\lambda|6\lambda - 1|^{-1}$. For the lower bound and the exponential upper bound we find from (7.2) that

$$R(0+) \equiv \lim_{\lambda \to 0+} R(\lambda) = 4G_1/3 . \tag{7.4}$$

Consequently $R(0+) = 1$ for the exponential upper bound, and $R(0+) = 0.917$ for the lower bound; this implies that $R^L(\lambda)$ is discontinuous in λ. However, the corresponding errors in ϵ^U and ϵ^L do *both* vanish with λ; for $\lambda = 0.01$ these errors are, respectively, +0.03% and −0.51%.

B. The anharmonic oscillator

For the anharmonic oscillator

$$f(x) = x^2 + \lambda x^4 \tag{7.5}$$

the energy bounds via Eq. (5.4) become

$$\epsilon v^{-1} = 2G_2 t^2 + 3\lambda G_4 t^4/2 ,$$
$$v^{-1} = G_2 t^4 + \lambda G_4 t^6 . \tag{7.6}$$

Since by scaling arguments we find

$$\epsilon(v, \lambda) = v^{1/2}\epsilon(1, \lambda v^{-1/2}) , \tag{7.7}$$

we need only consider the case $v = 1$ for which we use the notation $\epsilon(\lambda)$. If we set $v = 1$ in Eq. (7.6) we can eliminate the parameter t and obtain the formula

$$\lambda = \left(\frac{G_2^2}{G_4}\right)\left\{\frac{G_2 - [\epsilon - (\epsilon^2 - 3G_2)^{1/2}]^2}{[\epsilon - (\epsilon^2 - 3G_2)^{1/2}]^3}\right\} . \tag{7.8}$$

Provided we use a Gaussian trial function for the upper bound, we have $G_2 = G_2^U$ in one or three dimensions. Consequently by taking the mean of the upper and lower λ values we have an error in λ which for *all* ϵ is strictly bounded by the following inequality:

$$(\text{error in } \lambda) \leq 100\left(\frac{G_4^U - G_4}{G_4^U + G_4}\right)\% . \tag{7.9}$$

Hence by using the G_4 numbers in Table II and the mean value $G_4^M = \frac{1}{2}(G_4^U + G_4)$ in formula (7.8) we have the strict inequalities: (error in λ) < 3% in one dimension and (error in λ) < 2% in three dimensions.

TABLE III. Quality of the bounds for a test problem. The lowest eigenvalue of $\hat{h} = -\Delta - 2x^{-1} + 4\lambda x + 4\lambda^2 x^2$ is exactly (Ref. 7) $\epsilon(\lambda) = (6\lambda - 1)$. The table shows values of $R(\lambda) = (\epsilon + 1)/6\lambda$, for $\epsilon = \epsilon^L$, $\epsilon = \epsilon^G$ (Gaussian trial function), and $\epsilon = \epsilon^E$ (exponential trial function). $R(\lambda) = 1$ when ϵ is exact; the fractional error in ϵ for a given λ is $6\lambda(R-1)|6\lambda - 1|^{-1}$.

λ	R (lower)	R (Gaussian)	R (exponential)
0.01	0.919 64	3.519 56	1.004 72
0.1	0.933 16	1.251 96	1.032 15
0.2	0.941 60	1.125 98	1.048 63
0.3	0.947 19	1.083 99	1.059 31
0.5	0.954 46	1.050 39	1.072 98
1.0	0.963 98	1.025 20	1.090 55
2.0	0.972 37	1.012 60	1.105 79
5.0	0.981 20	1.005 04	1.121 61
10.0	0.986 21	1.002 52	1.130 49
100.0	0.995 36	1.000 25	1.146 60

Moreover, on the curves (7.8) we have (independently of G_4)

$$\frac{\lambda\, d\epsilon}{\epsilon\, d\lambda} = \left(\frac{1 - G_2 t^4}{3 + G_2 t^4}\right) < \tfrac{1}{3} . \tag{7.10}$$

Thus by using G_4^M in Eq. (7.8) we determine ϵ for a given λ with error less than 1% (usually much less) for all $\lambda \geq 0$, in one or three dimensions.

With this definite analytical information about the quality of the bounds given by Eq. (7.8) we do not need to exhibit many numerical values of this simple formula which is consistent with earlier data to be found in the extensive literature[2-6] on the problem (the three-dimensional case corresponds to the first *odd* excited state of the one-dimensional system). We have for example with $\lambda = 1$ the following values for one and three dimensions respectively: (lower, exact,[3] upper) = (1.388, 1.392, 1.404) and (4.6398, 4.6590, 4.6783). Since Gaussian trial functions have been used for the upper bounds, we know by Sec. VI and the scaling law (7.7) that the corresponding N-boson problem has also been solved to the same accuracy for all $N \geq 2$.

C. A possible quark-quark potential

For phenomenological quark-quark potentials of the form $f(x) = -\alpha x^{-1} + \beta \ln x + \gamma x$ which we considered in Ref. 1 we may easily apply our new formula (5.4) to obtain expressions for the trajectory bounds. The results are similar in quality to those of the example in Sec. VII A and much better than given by the more general potential-envelope method.[1]

Instead of using the log function to bridge between the Coulombic and linear regions of the potential,[13] we might also consider a combination of Hulthén

and linear potentials given by

$$f(x) = -\alpha(e^x - 1)^{-1} + \beta x \,. \tag{7.11}$$

For small x this potential is like $-\alpha x^{-1}$ and we can control the "rate" at which the linear component βx is approached as x increases by adjusting the range parameter a (which was redundant for the power-law combinations considered earlier). The actual potential has the following form from Eq. (1.1) in which, for analytical convenience, we retain all four parameters:

$$V(r) = V_0[-\alpha(e^{x/a} - 1)^{-1} + \beta x/a] \,. \tag{7.12}$$

By applying the formulas given in Secs. II–V in the general formula (1.6) we find, in terms of $q > 0$, the lower bound

$$\begin{aligned} \epsilon v^{-1} &= E^L/V_0 \\ &= -\alpha[(1+q^2)^{1/2} - 1)]^2/4(1+q^2)^{1/2} + 6\beta G_1 q^{-1} \,, \\ v^{-1} &= (m_1+m_2)\hbar^2/2m_1m_2V_0a^2 = \alpha(1+q^2)^{-1/2} + 8\beta G_1 q^{-3} \end{aligned} \tag{7.13}$$

and the upper bound (exponential trial function)

$$\begin{aligned} \epsilon v^{-1} &= E^U/V_0 = -\alpha q^3[\gamma^2(1+q) + q\gamma^3(1+q)]/4 + 6\beta G_1^U q^{-1} \,, \\ v^{-1} &= (m_1+m_2)\hbar^2/2\,m_1m_2V_0a^2 \\ &= -\alpha q[3\gamma^2(1+q) + q\gamma^3(1+q)] + 8\beta G_1^U q^{-3} \,, \end{aligned} \tag{7.14}$$

where (from Table II) $G_1 = 0.688\,042$ and $G_1^U = \frac{3}{4}$, the polygamma functions[14] are defined by

$$\begin{aligned} (-1)^{n+1}\gamma^n(z) &= \int_0^\infty \frac{x^n e^{-zx}}{(1-e^{-x})}dx \\ &= n! \sum_{k=0}^{\infty} (z+k)^{-(n+1)} \,, \end{aligned} \tag{7.15}$$

and the positive trajectory parameter q is related to earlier parameters by $q = \sigma^{-1} = 2s^{1/2} = 2t^{-1}$ [$I = K^{-1} = 2$ for the exponential trial function $\phi(x) = e^{-x}$; see Eqs. (4.1) and (4.2)]. The upper and lower energy trajectories for the case $\alpha = \beta = 1$ are shown in Fig. Fig. 1. For large values of v *both* bounds approach the pure Coulombic trajectory $\epsilon = -(\alpha v)^2/4$; for small v, a better upper bound is provided by a Gaussian trial function which is known to be excellent for linear potentials (Ref. 1 and Sec. III).

For many purposes the lower trajectory (7.13) gives with adequate accuracy the essential dependence of E on all the potential parameters in a form which is amenable both to further analysis and to computation on a hand calculator. From Eq. (1.12) we know that on *either* trajectory bound we have

$$d(\epsilon v^{-1})/d(v^{-1}) = s = q^2/4 \,; \tag{7.16}$$

on the upper trajectory this quantity is the mean kinetic energy.

VIII. CONCLUSION

We have shown that the nonlinear Λ transform $\Lambda\{f\} = F$ of a sum $f = \sum_i \alpha_i f_i$ of attractive potentials has variational upper and lower bounds that can be specified by writing v^{-1} and ϵv^{-1} as functions of a trajectory parameter $s > 0$; these functions depend *linearly* on the coefficients $\{\alpha_i\}$ of the potential. In the case of elementary potentials the Λ transforms $F_i = \Lambda\{f_i\}$ of the individual components are sufficiently simple that the general formula (1.6) for the trajectory bounds provides a convenient recipe to which terms may be added or subtracted with ease and which determines the eigenvalues, very often to within a few percent. Whenever it is more important to know how the eigenvalue depends on the potential parameters (and particle number for N-boson systems) than it is to have accuracy better than one or two percent, the methods presented in this article will be very useful. In cases where high accuracy is necessary, these methods can be considered as exploratory tools.

The approach we have followed is very general for it deals with operators $\hat{h}$ which can be written as the convex sum

$$\hat{h} = \sum_i w_i \hat{h}^{(i)} \,, \quad \sum_i w_i = 1 \,. \tag{8.1}$$

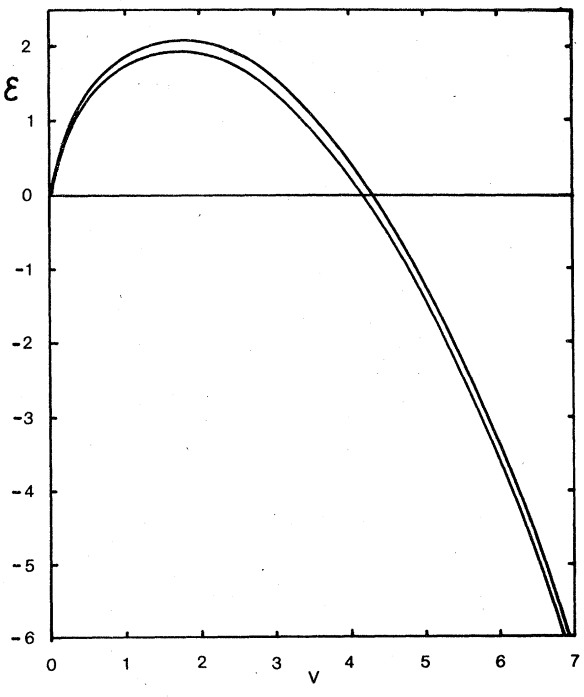

FIG. 1. The trajectories are upper and lower bounds to the lowest eigenvalue $\epsilon = F(v)$ of the Hamiltonian $\hat{h} = -\Delta + v f(x)$, where f is the linear combination $f(x) = -(e^x - 1)^{-1} + x$ of Hulthen and linear potentials.

Such situations may arise, for example, in the classical theory of oscillatory systems and for finite matrices. However, since this paper is concerned with quantum mechanics we shall mention two specific areas in this context where natural generalizations can be made.

A. Projected excited states

In the illustration of Sec. VII B we were able to deal with two eigenvalues of the anharmonic-oscillator problem because the first excited state can be defined by a projector onto the subspace of Hilbert space spanned by odd functions. In a similar fashion in three dimensions we can project the whole problem into the subspace of eigenfunctions of $\vec{L}^2$ with a given eigenvalue $l(l+1)$. The dimensionless operator $\hat{h}$ now becomes

$$\hat{h} = -D^2 + l(l+1)x^{-2} + vf(x) \tag{8.2}$$

and the theory will yield bounds on the lowest ei- eigenvalues of $\hat{h}$ for each value of l.

B. Integral transforms of elementary potentials

In Ref. 1 we discussed potentials which could be written as envelopes of a family of simple potentials. An envelope is a type of *derivative* of the class of curves which generate the envelope. In the present article we are working with *sums* of potentials and it is natural therefore to generalize Eq. (8.1) to *integrals* of the form

$$\hat{h} = \int_0^\infty w(s)\hat{h}^{(s)}ds, \quad \int_0^\infty w(s)ds = 1, \tag{8.3}$$

where

$$f(x) = \int_0^\infty \alpha(s)k^{(s)}(x)\,ds, \tag{8.4}$$

$$\hat{h}^{(s)} = -\Delta + \frac{v\alpha(s)}{w(s)}k^{(s)}(x), \tag{8.5}$$

and $k^{(s)}(x)$ is an elementary potential depending on the parameter s. If $\Lambda\{k^{(s)}\} = K^{(s)}$, and $\Lambda\{f\} = F$, then by a similar argument to that of Sec. III we have

$$F(v) \geq \int_0^\infty w(s)K^{(s)}\left[\frac{v\alpha(s)}{w(s)}\right]ds. \tag{8.6}$$

The best lower bound can now be found by maximizing the right-hand side of Eq. (8.6) with the aid of the calculus of variations. Instead of searching for an optimal probability vector $\vec{w}$ we now look for an optimal probability density $w(s)$. The class of problems reached by the integral transform (8.4) is very interesting. For example, if $k^{(s)}(x) = e^{-sx}$, then $f(x) = \mathcal{L}\{\alpha(s)\}$, the Laplace transform of $\alpha(s)$. However, we shall have to leave the detailed analysis of this idea to a later article.

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