Spectral Bounds and Comparison Theorems

for Schrödinger Operators

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ABSTRACT

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One of the most important problems in quantum physics is to find the energy eigenvalues for Schrödinger's equation. This equation is exactly solvable only for a small class of potentials. For one-particle problems numerical solutions can always be obtained, but in the absence of exact solutions, the next best thing is an analytical formula for an approximation, such as energy bound. In this thesis we use geometrical techniques such as the envelope method to obtain analytical spectral bounds for Schrödinger's equation for wide classes of potential. Our geometrical approach leans heavily on the comparison theorem, to the effect that $V_1 < V_2 \Rightarrow E_1 < E_2$. For the bottom of an angular-momentum subspace it is possible to generalize the comparison theorem by allowing the comparison potentials V_1 and V_2 to cross over in a controlled way and still imply spectral ordering $E_1 < E_2$. We prove and use these theorems to sharper some earlier upper and lower bounds obtained using the 'envelope method'. In chapter two we introduce the envelope method that is used in the subsequent chapters. In chapter three we study the Hellmann potential in quantum physics: we prove that discrete eigenvalues exist and we obtain formulae for upper and lower bounds to them. In chapter four, we prove the existence of a discrete spectrum for the cutoff-Coulomb potential, and we obtain upper and lower-bound formulae. In chapter five we prove the monotonicity of the wave function $\psi(r)$ for the ground state in the case of attractive central potentials in N

N spatial dimensions. By using this result we establish some generalized comparison theorems in which the comparison potentials intersect. We use these theorems, together with the sum approximation, to improve the upper and the lower bounds obtained earlier with the aid of the envelope method. In chapter six, we study the representation $P(q)$ for the eigenvalues $E(q)$ of the operator $H = -\Delta + \mathrm{sgn(q)r^q}$ defined by $E(q) = \min_{r>0}\{\frac{P(q)^2}{r^2} + \mathrm{sgn(q)r^q}\}$. It had earlier been proved that $P(q)$ is monotone increasing. We strengthen this result for the ground state (and the bottom of each angular-momentum subspace) by using the generalized comparison theorems to prove that a new function $Q(q) = Z(q)P(q)$ is monotone increasing, where the factor $Z(q)$ is monotone decreasing. Thus we know that $P(q)$ cannot increase too slowly: this in turn allows us to obtain same improved bounds for the eigenvalues $E(q)$ in N dimensions. In the last chapter we analyse bounds for the Coulomb plus power-law potentials obtained by variational methods and the sum approximation.

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Preliminaries

I.1 Introduction

We study the Schrödinger differential equation $H\psi = E\psi$ and regard the Schrödinger operator $H = -\Delta + V$ as an operator in the Hilbert space $L^2(R^N)$. We now give a short synopsis of Hermitian, symmetric, and self-adjoint operators in general Hilbert spaces. To this end we let $\mathcal{H}$ denote a Hilbert space with inner product $(\cdot,\cdot)$, where $(\cdot,\cdot) : \mathcal{H} \times \mathcal{H} \to C$ satisfies the properties of linearity and sesquilinearity with respect to the first and second variables. This is indeed the case for $\mathcal{H} = L^2(R^N)$, where the inner product is given by $(f,g) = \int_{R^N} \overline{f(r)} g(r) d^N r$.

When dealing with bounded linear operators in Hilbert spaces, the boundedness of these operators permits the extension of these operators to all of $\mathcal{H}$. All we need to do is to define these operators by continuity in the closure of their respective domains of definition, and zero on the complement of these closures, in case the domain of definition fails to be dense in $\mathcal{H}$. Many of the linear operators of particular interest in quantum mechanics are unbounded. It follows that the domains of definition of these unbounded operators cannot be the entire Hilbert space, as is clearly indicated by theorem of "Hellinger-Toeplitz" [2] to the effect that if the operator H is defined on all of $\mathcal{H}$, then H is bounded.

Let $< \mathcal{H}_1, (\cdot,\cdot)_1 >$ and $< \mathcal{H}_2, (\cdot,\cdot)_2 >$ be two Hilbert spaces, where it is understood that $(\cdot,\cdot)_1$ and $(\cdot,\cdot)_2$ are the inner products of $\mathcal{H}_1$ and $\mathcal{H}_2$ respectively.

Let the operator T from Hilbert space $\mathcal{H}_1$ into Hilbert space $\mathcal{H}_2$ be defined as follows. The domain of definition of the operator T, denoted by $D(T)$, is a linear manifold in $\mathcal{H}_1$ and the transformation $T : D(T) \rightarrow \mathcal{H}_2$ is linear. In case $D(T) = \mathcal{H}_1$, we say the operator is a linear operator from $\mathcal{H}_1$ into $\mathcal{H}_2$, however, $D(T) \subset \mathcal{H}_1$ is the general situation.

Without loss of generality, we assume that $\mathcal{H}_1 = \mathcal{H}_2 = \mathcal{H}$, and we will define some of the basic concepts for unbounded operators:

Definition: The graph of the linear operator T in the Hilbert space $\mathcal{H}$ is the set of all pairs

$$\Gamma(T) = \{\{\psi, T\psi\} \mid \psi \in D(T)\}$$

and is a submanifold of $\mathcal{H} \times \mathcal{H}$.

An operator T is closed if its graph $\Gamma(T)$ is closed in the product topology of the Hilbert space $\mathcal{H}_1 \times \mathcal{H}_2$. This means that if f_n is a sequence in $D(T)$, such that $f_n \rightarrow f$ and $T(f_n) \rightarrow g$, then this implies that (f, g) is an element of the graph $\Gamma(T)$ and f is an element of $D(T)$ and $T(f) = g$ (i.e. $\overline{\Gamma}(T) = \Gamma(\overline{T}) = \Gamma(T)$).

Definition: An operator T is formally-adjoint to S if $(Tf, g) = (f, Sg)$ $\forall f \in D(T)$, $g \in D(S)$.

Due to the fact that there could be many operators S formally adjoint to T, we are interested under what conditions does the operator have only one adjoint. This is iff $D(T)$ is dense in $\mathcal{H}_1$.

Definition: The adjoint T^* of the linear operator T in the Hilbert space $\mathcal{H}$ is

defined as

$$D(T^*) = \{\psi \in \mathcal{H} : \exists\, \psi^* \in \mathcal{H} \text{ satisfying } (T\phi, \psi) = (\phi, \psi^*)\ \forall\, \phi \in D(T)\} \text{ and } T^*\psi = \psi^*.$$

Definition: An operator T in $\mathcal{H}$ is called Hermitian if $D(T) \subset D(T^*)$ and $T\psi = T^*\psi \quad \forall \psi \in D(T)$.

Definition: An Hermitian operator T of $\mathcal{H}$ is positive if $(\psi, T\psi) \geq 0\ \forall \psi \in D(T)$.

Definition: An operator T is symmetric if it is densely defined and $(Tf, g) = (g, Tf)\ \forall\ f,\ g \in D(T)$.

Definition: An operator T in $\mathcal{H}$ is called self-adjoint if $D(T) = D(T^*)$ and $T\psi = T^*\psi \quad \forall \psi \in D$.

Now, let us combine a concept of self-adjointness with that of the closure $\overline{T}$ of an operator T, namely we say that T is essentially self-adjoint if $\overline{T}$ is self-adjoint, i.e. $\overline{T}^* = \overline{T}$. Since we are dealing in this thesis with the symmetric operator $H = -\Delta + V$, we are interested in the spectrum $\sigma(H)$ of our operator H, in particular the discrete $\sigma_d(H)$ and continuous spectrum $\sigma_c(H)$, where $\sigma(H) = \sigma_d(H) \cup \sigma_c(H)$. Nevertheless, in this thesis we shall be dealing with the discrete spectrum only, which has significant advantages. Namely, we can easily write the spectral decomposition of the operator provided a self-adjoint extention of it can be found. Moreover, the arduous construction of the spectral projectors ranging over the continuous spectrum is avoided.

Now, we define the discrete, continuous, and essential spectrum as follows:

Definition: A number E is called an eigenvalue of the operator T, if there exists

a non-zero $\psi \in D(T)$, such that, $T\psi = E\psi$.

Definition: The resolvent operator $R(E,T)$ of T in $\mathcal{H}$ at E is $R(E,T) = (EI - T)^{-1}$, and $\rho(T) = \{E \in C \mid R(E,T) \in B(\mathcal{H})\}$ is called the resolvent set of the operator T, where $B(\mathcal{H})$ denotes the Banach-algebra of bounded linear operators.

Definition: The spectrum of the operator T is $C \setminus \rho(T)$.

Definition: The essential spectrum $\sigma_e(T)$, of a self-adjoint operator T is the set of points in $\sigma(T)$, that are either accumulation points of $\sigma(T)$ or isolated eigenvalues of infinite multiplicity.

Definition: The complement of the essential spectrum in the spectrum space is called the discrete spectrum, in other word $\sigma_d(T) = \sigma(T) \setminus \sigma_e(T)$.

Definition: The ratio $\frac{(\psi,T\psi)}{(\psi,\psi)}$, where $\psi \in D(T)$ is called the Rayleigh quotient.

Throughout this thesis we shall assume that the operator T is semi-bounded below, that is to say that, there exists $k \in R$ such that $\frac{(\psi,T\psi)}{(\psi,\psi)} \geq k$, $\forall \psi \in D(T)$. In another words, the Rayleigh quotient is bounded below.

Definition: The function f is of bounded variation iff $\sup\{\sum_{i=1}^{n} |f(\lambda_i) - f(\lambda_{i-1})|$, $P = \{\lambda_0, \lambda_1, \ldots, \lambda_n\}$ is any partition of any finite interval of R $\} < \infty$.

In most cases in quantum mechanics the operators considered are at best symmetric on the appropriate Hilbert space $\mathcal{H}$, in our case $L^2(R^N)$. For spectral decomposition to hold for such a symmetric operator T, we must have that T posses a self-adjoint extention, which extention we also denote by T again. Such a spec-

tral decomposition of a self-adjoint T means the following: There exists a unique λ parameter family of projections operators P_λ, increasing in λ $(\mu \leq \lambda \rightarrow P_\mu \leq P_\lambda)$ on the Hilbert space $\mathcal{H}$ satisfying $\lim_{\lambda \rightarrow -\infty} P_\lambda = 0$, $\lim_{\lambda \rightarrow +\infty} P_\lambda = I$ and $P_{\lambda+0} = P_\lambda$, in the strong sense $\forall \lambda \in R$, i.e. $\lim_{s \rightarrow 0} P_{\lambda+s} f = P_\lambda f$, $\forall f \in \mathcal{H}$ and $\forall \lambda \in R$. Now the Stieltjes integral representation of T is $T = \int_{-\infty}^{+\infty} \lambda dP_\lambda$. This representation is understood to mean $(Tf, g) = \int_{-\infty}^{+\infty} \lambda d_\lambda (P_\lambda f, g)$, $\forall f \in D(T)$, $\forall g \in \mathcal{H}$, where the function (in variable λ) of bounded variation acting as the integrator is $(P_\lambda f, g)$. All this spectral decomposition presupposes, that the operator T posses a self-adjoint extension . Because we are dealing with semi-bounded operators on $L^2(R^N)$, we are guaranteed the existence of a self-adjoint extension of T by means of Theorem I.1. For a semi-bounded operator S with lower bound γ we define $s[f, g] = (Sf, g)$ for f, $g \in D(S)$, and H_s is the completion of the domain $D(S)$ under the norm $||.||_s$ defined by $(f, g)_s = (1-\gamma)(f, g) + s[f, g]$ $(||f||_s \geq ||f||)$ $||.||_s$ is compatible with the $||.||$ in the sense of: if $\{f_m\}_{m=1}^{\infty}$ is a $||.||-$ Cauchy sequence in $D(S)$ with $\lim_{n \rightarrow \infty} ||f_n|| = 0$, then $\lim_{n \rightarrow \infty} ||f_n||_s = 0$. This compatability condition always exists for a semi-bounded operator, as guaranteed by Friedrichs' extension theorem:

Theorem I.1.: [1]

Let S be a semi-bounded symmetric operator with lower-bound γ. Then there exists a semi-bounded self-adjoint extension of S with lower-bound γ. If we define $s[f, g] = (Sf, g)$ for f, $g \in D(S)$, and H_s as above, then we have: The operator

T defined by

$$D(T) = D(S^*) \cap H_s \text{ and } Tf = S^* f \text{ for } f \in D(T)$$

is a self-adjoint extension of S with lower bound γ. The operator T is the only self-adjoint extension of S having the property $D(T) \subset H_s$.

Now we are ready to introduce the min-max principle for the discrete spectrum.

I.2 Min-max principle and spectral characterization

The Rayleigh-Ritz theorem is the most notable method used to characterize and approximate the discrete eigenvalues of a self-adjoint operator. It restricts the operator of interest to a finite dimensional subspace, then the eigenvalues of the original operator are approximated by eigenvalues of the constrained operator. Let T be a self adjoint operator 'semi-bounded below' with eigenvalues $\{E_1, E_2, \ldots\}$ such that $E_1 \leq E_2 \leq \ldots$. We will explain how to use Rayleigh-Ritz method to find upper bounds:

Theorem I.2.: (Rayleigh-Ritz) [3]

For an arbitrary function ψ in $D(T)$ the expectation value (mean value) of T in the state ψ is such that

$$E = \frac{(\psi, T\psi)}{(\psi, \psi)} \geq E_1, \tag{I.2.1}$$

where the equality holds if and only if ψ is the eigenstate of T with the eigenvalue E_1.

In the more general case the trial function is chosen as a linear combination of a finite number of linearly independent functions ϕ_i:

$$\psi = \sum_{i=1}^{n} c_i \phi_i.$$

The restriction of the eigenvalue problem of T to the n-dimensional subspace D_n can yield interesting approximate solutions. If $D_n = Span\{\phi_1, \phi_2, ..., \phi_n\} \subset D(T)$, then in a sense, we reduce the problem to a matrix problem $TC = \mathcal{E}C$ where T is the $n \times n$ matrix $T_{ij} = (\phi_i, T\phi_j)$ with eigenvalues $\{\mathcal{E}_1, \mathcal{E}_2, \ldots\}$ such that $\mathcal{E}_1 \leq \mathcal{E}_2 \ldots \leq \mathcal{E}_n$. We obtain upper bounds using the following:

Theorem I.3.: (Generalized Ritz Theorem) [3]

(1) $E_i \leq \mathcal{E}_i^{(n)}$, $i = 1, ..., n$ provided the E_i exist.

(2) $\lim_{n\to\infty} \mathcal{E}_i^{(n)} = E_i$, provided $\text{span}\{\phi_n : n \in N\}$ is dense in $D(H)$.

The min-max principle for the self-adjoint operators is a useful characterization of the eigenvalues of the operator. In fact it is the foundation of the Rayleigh-Ritz method for eigenvalue approximation. We state the min-max principle in the following theorem:

Theorem I.4.: [3]

Given a complex, separable Hilbert space $\mathcal{H}$ with norm $(.,.)^{\frac{1}{2}}$, we consider a self-adjoint operator T in $\mathcal{H}$ bounded below with spectrum $E_{n+1} \geq E_n$ (allowing for multiplicities). If $\mathcal{D}_n$ denotes the family of all n-dimensional subspaces D_n of $D(T)$, let $D_n^{\perp}$ be the orthogonal complement of D_n in $D(T)$. Then the eigenvalues of $\{E_n\}_{n\in N}$ can be characterized in the following ways:

$$E_n = \min_{\mathcal{D}_n} \max_{\psi \in (D_n \cap D(T)) \setminus \{0\}} \frac{(\psi, T\psi)}{(\psi, \psi)} \tag{I.2.2}$$

$$E_n = \sup_{\mathcal{D}_{n-1}} \inf_{\psi \in (D_{n-1}^{\perp} \cap D(T)) \setminus \{0\}} \frac{(\psi, T\psi)}{(\psi, \psi)} \tag{I.2.3}$$

We are interested in the discrete spectrum of the Hamiltonian $H = -\Delta + V$, which is known as a Schrödinger operator. The following example is an application of the Rayleigh-Ritz method for Schrödinger operator in one dimension.

Example: (Harmonic Oscillator) Consider a one dimensional harmonic oscillator, given by

$$H = -\frac{d^2}{dx^2} + \omega^2 x^2,$$

we apply the Rayleigh-Ritz method to obtain a bound for its ground state eigenvalue E_1. Let $\psi_\alpha = e^{-\alpha x^2} \in D(H)$, where $\alpha > 0$, then for each α we have

$$E_1 \leq \mathcal{E}(\alpha) = \min_{\alpha > 0} \frac{(\psi_\alpha, H\psi_\alpha)}{(\psi_\alpha, \psi_\alpha)}$$

thereafter we optimize over α the expression

$$H\psi_\alpha = 2\alpha e^{-\alpha x^2} + (w^2 x - 4\alpha^2) x^2 e^{-\alpha x^2}$$

now computing $(\psi_\alpha, H\psi_\alpha)$ we find that,

$$(\psi_\alpha, H\psi_\alpha) = \int_{-\infty}^{+\infty} (e^{-\alpha x^2}(2\alpha e^{-\alpha x^2} + (\omega^2 x - 4\alpha^2) x^2 e^{-\alpha x^2}) dx$$

$$= (2\alpha + \frac{\omega^2 - 4\alpha^2}{4\alpha})(\psi_\alpha, \psi_\alpha)$$

and finally substituting into the Rayleigh-Ritz quotient we find that for $\alpha = \hat{\alpha} = \frac{\omega}{2}$,

$$E_1 \leq \mathcal{E}(\hat{\alpha}) = \mathcal{E}(\omega/2) = \omega$$

We know that the eigenfunction for the ground state is $\psi = e^{-\frac{\omega}{2}x^2} \in D(H)$ with the eigenvalue ω. Since in this case $\psi = \psi_{\omega/2}$, the trial set includes the 'lowest' eigenfunction, which is recovered by the minimization.

We shall make extensive use of the set $C_0^\infty(R^N)$ of infinitely differentiable functions having compact support .A further utilized notion is that of local integrability of a function, in particular $L^2_{loc}(R^N) = \{f(r)$ measurable on $R^N : \int_A |f|^2 d^N r < \infty$, $\forall$ compact subsets A of $R^N\}$. Their use is in the following useful theorems:

Theorem I.5.: [3]

For non-zero $V \in C_0^\infty(R)$, $-\frac{d^2}{dx^2} + \lambda V$ has a negative eigenvalue for all positive λ if and only if

$$\int_{-\infty}^{+\infty} V(x)dx \leq 0. \tag{I.2.4}$$

Theorem I.6.: [4]

If $V \in L^2_{loc}(R)$ and satisfies

$$\int_a^{a+1} |V(x)|^2 dx \to 0, \text{ as } |a| \to \infty, \tag{I.2.5}$$

then the essential spectrum $\sigma_e(-\frac{d^2}{dx^2} + \lambda V) = [0, \infty)$.

The spectrum of a self-adjoint operator is always a subset of R. However, because the spectrum $\sigma(H)$ is a union of discrete spectrum and the essential spectrum (as already stated), we would like to consider how the essential spectrum brings about conditions on discrete spectrum as, for instance, the following:

Theorem I.7.: [4]

If T is self-adjoint, $\sigma_e(T) \subset [0, \infty)$ and there is a $\psi \in D(T)$ such that $(T\psi, \psi) < 0$, then T has a negative eigenvalue.

For example if $V(r) = -1/r^{0.2}$, then $\sigma_e(T) = [0, \infty)$ and if we choose $\psi = e^{-0.3r}$, then $(\psi, (-\Delta + V)\psi)/(\psi, \psi) = -0.3621 < 0$ this implies (using the previous theorem) that the Hamiltonian $H\psi = -\Delta\psi - r^{-0.2}\psi$ has a negative discrete eigenvalue. Moreover, we know by the Rayleigh-Ritz theorem that this number is an upper bound for the ground-state eigenvalue $EX \approx -0.6297$. In chapters VI and VII we discuss in detail how to compute upper and lower bounds for discrete eigenvalues for the power-law potentials $V(r) = \mathrm{sgn(q)r^q}$ in N dimensions.

Theorem I.8.: [4]

For V_1, $V_2 \in L^2_{loc}(R)$ such that

$$\sup_a \int_a^{a+1} |V_1(x)|^2 dx < \infty \tag{I.2.6}$$

and

$$\int_a^{a+1} |V_2(x)|^2 dx \to 0, \text{ as } |a| \to \infty, \tag{I.2.7}$$

we have

$$\sigma_e(-\frac{d^2}{dx^2} + V_1 + V_2) = \sigma_e(-\Delta + V_1).$$

We note that if we add $V_2(r) = c|x|^{-\alpha}$, $0 < \alpha < \frac{1}{2}$, to any Hamiltonian $H = -\Delta + V_1$ the essential spectrum is unchanged because $V_2(x)$ satisfies $(I.2.7)$.

Theorem I.9.: [4]

If $\sigma_e(H) \subset [0, \infty)$ and $V(x) \leq 0$ for $x \geq a$, for some $a \geq 0$ with

$$\int_a^{\infty} V(x) dx = -\infty, \tag{I.2.8}$$

then $H = -\frac{d^2}{dx^2} + V$ has an infinite number of negative eigenvalues.

The quadratic form associated with Schrödinger operator $H = -\Delta + V$ is $q(f) = (-\Delta f, f) + (Vf, f)$, $\forall f \in D(q)$. We look at the quadratic form as an entity which yields a lower or upper bound of the operator if such bounds exists. This finds its application in the following theorems:

Theorem I.10.: [3] Let V be a locally bounded positive function with $V(x) \to \infty$ as $x \to \infty$. Define $-\Delta + V$ as a sum of quadratic forms, then $-\Delta + V$ has purely discrete spectrum (e.g harmonic oscillator).

Theorem I.11.: [3]

Let V be a non-zero negative function in $C_0^\infty(R^N)$ ($N = 1$ or 2). Then the Schrödinger operator $-\Delta + \lambda V$ acting on $L^2(R^N)$ has at least one negative eigenvalue for all $\lambda > 0$.

Theorem I.12.: [3]

Let $V \in L^1_{loc}(R^N)$, be bounded from below and suppose that $V \to \infty$ at infinity. Then $H = -\Delta + V$ defined as a sum of quadratic forms has purely discrete spectrum and a complete set of eigenfunctions.

Theorem I.13.: [3]

If $V \in L^1_{loc}(R^N)$ is positive and

$$\lim_{|x| \to 0} V(x) = \infty, \tag{I.2.9}$$

then $H = -\Delta + V$ has nondegenerate strictly positive ground state.

Theorem I.14.: (The Comparison Theorem [5,6,7,8,9])

If S, T are self-adjoint operators such that $S \leq T$, in the sense that $D(S) \subset D(T)$ and $(\psi, S\psi) \leq (\psi, T\psi)$ for all $\psi \in D(S)$, then the eigenvalues of S are not larger than the corresponding eigenvalues of T, i.e

$$E_n(S) \leq E_n(T), \ n = 1, 2, 3, ..., \tag{I.2.10}$$

where $E_n(S)$ denotes the n-th eigenvalues of S in ascending order.

As a special case we have the following comparison corollary for our operator $H = -\Delta + V$:

Corollary I.1.: [5]

If $S = -\Delta + V_1$, $T = -\Delta + V_2$ and $V_1 \leq V_2$ (as in Figure I.1), then $E_n(S) \leq E_n(T)$.

Theorem I.15.: (Weyl's Theorem for a Sum of Operators) [3,10,11]

If for the sum $S + T$ of two self-adjoint operators S and T, defined on $D(S) \cap D(T)$, we denote by $\{E_k[S]\}_{k=1}^{\infty}$ and $\{E_l[T]\}_{l=1}^{\infty}$ the discrete eigenvalues of S and T respectively, then

$$E_{k+l-1}[S+T] \geq E_k[S] + E_l[T]. \tag{I.2.11}$$

This result is weak [12] for $k, l > 1$.

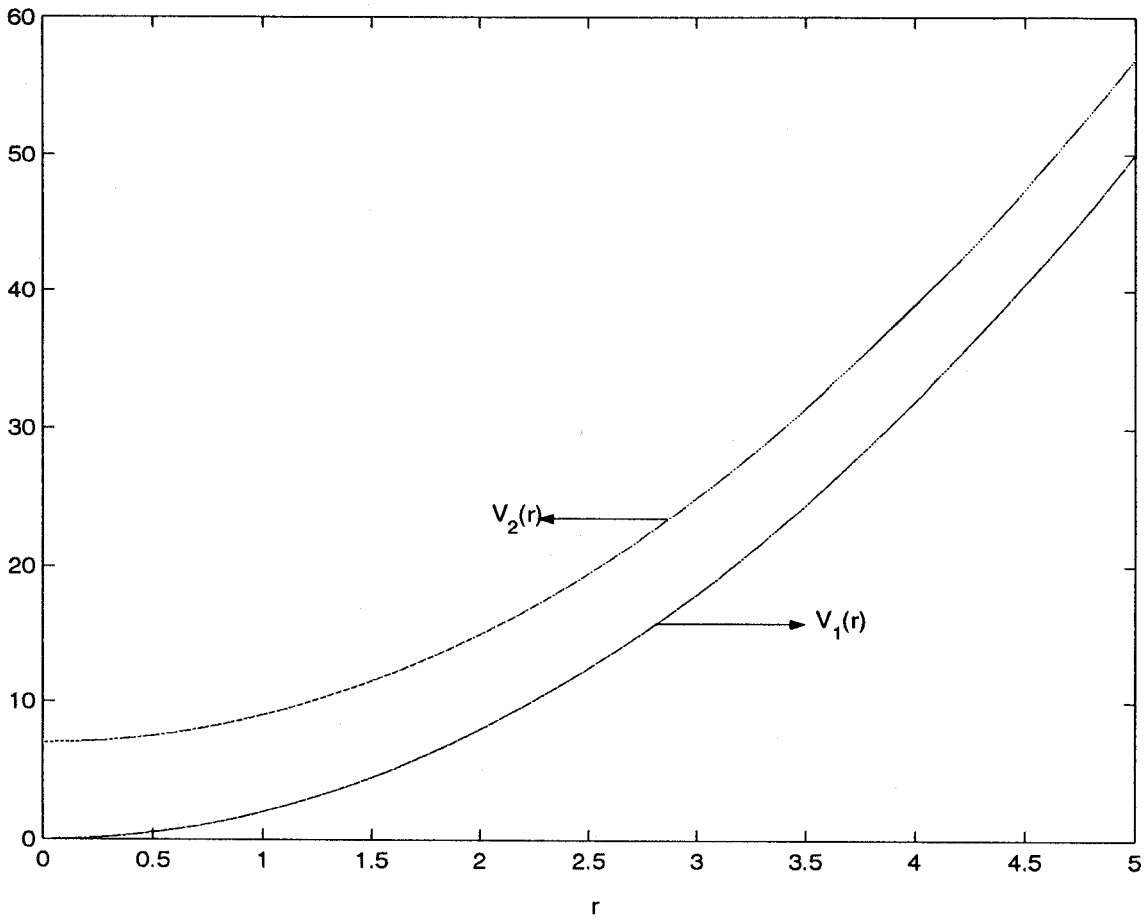

Figure I.1 Consider $H_1 = -\Delta + V_1$ and $H_2 = -\Delta + V_2$. The comparison theorem implies that $E_n(H_1) \leq E_n(H_2)$, $n = 1, 2, 3, \ldots$.

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Chapter II

Geometrical methods

Many different approaches have been proposed to solve Schrödinger's equation approximately, such as the large-N approximation, and JWKB approximation and the method of potential envelopes. The envelope method has advantages over other methods because it provides simple and accurate formulas for upper and lower bounds to the eigenvalues. The method of potential envelopes was first introduced in 1980 by Hall [1]. This method provides us with analytical bounds for the spectrum of Schrödinger's equation for wide classes of potential.

II.1 Schrödinger's equation in N dimensions:

We consider a particle which moves in R^N subject to a central potential $V(r)$, $r = ||r||$ and is governed by Schrödinger's equation

$$H\psi = -\Delta\psi(r) + V(r)\psi(r) = E\psi(r), \; r = ||r|| \text{ and } r \in R^N. \tag{II.1.1}$$

We can separate the Laplacian operator into a radial and an angular part:

$$\Delta = \hat{R} - \frac{1}{r^2}\hat{L}(\theta_2, \ldots, \theta_N) \tag{II.1.2}$$

where

$$\hat{R} = \frac{\partial^2}{\partial r^2} + \frac{(N-1)}{r}\frac{\partial}{\partial r}$$

and $\hat{L}(\theta_2, \ldots, \theta_N)$ is the angular momentum operator in N dimensions. We separate the radial and angular parts by substituting $\psi(r) = R(r)Y(\theta_2, \ldots, \theta_N)$ to

obtain,

$$\frac{r^2}{R}\hat{R}R + r^2(E - V(r)) = \frac{\hat{L}Y}{Y} = \ell(\ell + N - 2) \qquad \text{(II.1.3)}$$

where $\hat{Y}(\theta_2, \ldots, \theta_N)$ represents the spherical harmonics in N dimensions. Now we separate the radial part $R(r)$ (where $R \in L^2(R^+, r^{N-1}dr)$) and the angular momentum part $\hat{Y}$ to get

$$\{-(\frac{\partial^2}{\partial r^2} + \frac{(N-1)}{r}\frac{\partial}{\partial r}) + \frac{\ell(\ell + N - 2)}{r^2} + V(r)\}R(r) = ER(r) \qquad \text{(II.1.4)}$$

and

$$\hat{L}\hat{Y}(\theta_2, \ldots, \theta_N) = \ell(\ell + N - 2)\hat{Y}(\theta_2, \ldots, \theta_N). \qquad \text{(II.1.5)}$$

We note from equation (II.1.5) that the spherical harmonics in N dimensions are eigenstates of the angular momentum operator $\hat{L}$ with eigenvalues $\ell(\ell + N - 2)$. We can reduce the radial part to simpler form by writing $R(r) = \frac{\phi(r)}{r^{(N-1)/2}}$, $r > 0$ and $\phi(0) = 0$, to obtain

$$-\phi''(r) + (\frac{(\ell + N/2 - 3/2)(\ell + N/2 - 1/2)}{r^2} + V(r))\phi(r) = E\phi(r). \qquad \text{(II.1.6)}$$

The radial function $\phi \in L^2(R^+, dr)$ is normalized according to $\int_0^\infty \phi(r)^2 dr = 1$. The eigenvlaue $E = E_{n\ell}^N$ in $N \geq 2$ spatial dimensions has degeneracy 1 for $\ell = 0$ and, for $\ell > 0$, the degeneracy is given [2] by the function $\Lambda(N, \ell)$, where

$$\Lambda(N, \ell) = (2\ell + N - 2)(\ell + N - 3)!/\{\ell!(N-2)!\}, \quad N \geq 2, \ \ell > 0. \qquad \text{(II.1.7)}$$

II.2 Kinetic potentials:

We shall need some established results concerning 'kinetic potentials' [3] and 'envelope theory' [4, 5]; which rely strongly on the comparison theorem discussed in chapter I. In order to fix ideas and simplify the presentation, let us suppose that E is a discrete eigenvalue at the bottom of the spectrum of $H = -\Delta + V$ in N dimensions. It follows that $E = \inf(\psi, H\psi)$ where $\psi \in \mathcal{D}(H)$, and $\|\psi\| = 1$. We perform the total minimization in two stages: first we constrain the process by fixing the mean kinetic energy $(\psi, -\Delta\psi) = s$, and then we minimize over $s > 0$. The mean potential-energy function under the constraint is called the 'kinetic potential' $\overline{V}(s)$ associated with the potential $V(r)$. Thus we have

$$\overline{V}(s) = \inf_{\substack{\psi\in\mathcal{D}(H) \\ (\psi,\psi)=1 \\ (\psi,-\Delta\psi)=s}} (\psi, V\psi) \quad \Rightarrow \quad E = \min_{s>0}\left\{s + \overline{V}(s)\right\}. \tag{II.2.1}$$

The variational definition of the kinetic potentials implies that (i) $\overline{cV}(s) = c\overline{V}(s)$, and (ii) $\overline{V}^{(1)}(s) \leq \overline{V}^{(2)}(s) \Rightarrow E^{(1)} \leq E^{(2)}$. Kinetic potentials can be defined [3] for higher eigenvalues and they can then be reconstructed from 'energy trajectories', the functions which describe how the eigenvalues vary with the coupling parameter $v > 0$. We have in general for coupling $v > 0$

$$H = -\Delta + vf(r) \rightarrow E_{n\ell} = F_{n\ell}(v) \tag{II.2.2a}$$

and

$$s = F_{n\ell}(v) - vF'_{n\ell}(v), \quad \overline{f}_{n\ell}(s) = F'_{n\ell}(v). \tag{II.2.2b}$$

The relationship $F(v) \leftrightarrow \overline{f}(s)$ is essentially a Legendre transformation [6] $\{v, F(v)\} \rightarrow \{s, \overline{f}(s)\}$ since $F(v)$ is concave and $\overline{f}(s)$ is convex, in fact we

have [3] $F''(v)\overline{f}(s) = -1/v^3$. The main purpose for this two-step reformulation of 'min-max' is that certain spectral approximations are very effectively developed in terms of kinetic potentials. We shall consider next the 'envelope approximation'.

II.3 Envelope method

We consider Schrödinger Hamiltonian of the form

$$H = -\Delta + vf(r),\ v > 0, \tag{II.3.1}$$

where f is an attractive central potential and v a coupling constant. These eigenenergies are ordered according to $E_{n\ell} \geq E_{n'\ell},\ n > n'$. The method of potential envelopes is a technique for approximating the energy trajectories of Schrödinger equation (II.2.2a). Envelope theory relies on the envelope representation and variational characterization of the eigenvalues. Consider a smooth function $f(r)$, any tangent line to f can be expressed in terms of the linear potential r by the following: we define

$$f^{(t)}(r) = A + Br, \tag{II.3.2}$$

where A, B are constants depending on the point of contact $r = t$. In fact,

$$A(t) = f(t) - tf'(t), \text{ and } B(t) = f'(t). \tag{II.3.3}$$

As shown in Figure II.1. We thus have an envelope representation for our potential, namely,

$$f(r) = \text{Envelope}_t\{f^{(t)}(r)\}. \tag{II.3.4}$$

Now, if f has definite convexity, say f is convex (as in Figure II.2), then each tangential linear potential $f^{(t)}(r)$ will lie beneath $f(r)$ and, by using the comparison theorem, we see that $-\Delta + vf^{(t)}(r)$ has eigenvalues which are lower bounds to those of the required eigenvalue problem $-\Delta + vf(r)$.

Now, we can generalize this idea by using a change of variables as follows,

$$f(r) = g(h(r)) \tag{II.3.5}$$

where g is a smooth increasing transformation, and we shall assume that g is concave ($g'' < 0$). In fact, we will have

$$f(r) = g(h) = \text{Envelope}_t\{g^{(t)}(h)\} \tag{II.3.6}$$

as in Figure II.3, and

$$g^{(t)}(h(r)) = A(t) + B(t)h(r) \tag{II.3.7}$$

with

$$A(t) = g(h(t)) - h(t)g'(h(t)),\ B(t) = g'(h(t)). \tag{II.3.8}$$

The min-max theorem implies

$$-\Delta + vf(r) \leq -\Delta + v(A + Bh(r)). \tag{II.3.9}$$

Let $H_{n\ell}(v)$ be the exact eigenvalues of $vh(r)$, then using the min-max principle we will have

$$E_{n\ell} \leq vA(t) + H_{n\ell}(vB(t)). \tag{II.3.10}$$

The best upper bound is given by

$$EU = \min_{t>0}\{vg(h(t)) - vh(t)g'(h(t)) + H_{n\ell}(vg'(h(t)))\} \qquad \text{(II.3.11)}$$

Now, we can state the following theorems which formulate spectral bounds based on the approximation $\bar{f}(s) \approx g(\bar{h}(s))$:

Theorem II.1.: [7]

Suppose that $f(r) = g(h(r))$ and $g(h)$ is monotone increasing, then

(a) $g(h)$ is convex $\Rightarrow \bar{f}(s) \geq g(\bar{h}(s))$

(b) $g(h)$ is concave $\Rightarrow \bar{f}(s) \leq g(\bar{h}(s))$.

Theorem II.2.: [7]

If $g(h)$ convex $\Rightarrow E_{n\ell} \geq \min_{s>0}\{s + vg(\bar{h}_{n\ell}(s))\}$.

If $g(h)$ concave $\Rightarrow E_{n\ell} \leq \min_{s>0}\{s + vg(\bar{h}_{n\ell}(s))\}$.

Now we discuss well-known class of potentials; the power-law potentials in N dimensions and see the connection between the kinetic potentials and a certain function P which we shall study in this thesis.

II.4 Power-law potentials in quantum mechanics: $P(q)$

In this section we simplify the spectral representation by including the potential $f(r)$ itself in the formulae: we effect this by a change of variables $\bar{f}(s) = f(r)$.

$$E_{n\ell} = \min_{s>0}\{s + v\bar{f}_{n\ell}(s)\} \qquad \text{(II.4.1)}$$

we will obtain new formulation for the energy in terms of the potential $f(r)$,

$$E_{n\ell} = \min_{r>0}\{K^{(f)}_{n\ell}(r) + vf(r)\}, \qquad \text{(II.4.2)}$$

where

$$K_{n\ell}^{(f)}(r) = (\bar{f}_{n\ell}^{-1} o f)(r). \tag{II.4.3}$$

This function is known exactly for certain potentials. For example, we consider $f(r) = \mathrm{sgn(q)r^q}$ pure powers in N dimensions, we find that [5]

$$K^{(q)}(r) = (P(q)/r)^2, \tag{II.4.4}$$

where

$$P_{n\ell}(q) = |E_{n\ell}(q)|^{(2+q)/2q} \left[\frac{2}{2+q}\right]^{1/q} \left[\frac{|q|}{2+q}\right]^{1/2}, \ q \neq 0. \tag{II.4.5}$$

Specifically, we have

$$P_{n\ell}(-1) = (n + \ell + N/2 - 3/2), \quad N \geq 2, \tag{II.4.6}$$

and

$$P_{n\ell}(2) = (2n + \ell + N/2 - 2), \quad N \geq 2, \tag{II.4.7}$$

and in one dimension (keeping $n = 1, 2, 3, \ldots$)

$$P_n(2) = (n - \frac{1}{2}), \quad N = 1. \tag{II.4.8}$$

Therefore, we may represent the discrete spectrum of these Schrödinger operators by means of the P function. In [4] it was proved, by writing one power-law potential as a convex or concave transformation of an other and using envelope theory, that $P(q)$ is monotone increasing . Such results derived by envelope theory thus lean on

the fundamental comparison theorem of quantum mechanics. Further analysis and new results concerning the power law-potentials and the corresponding P function in higher dimensions, one obtained in chapter VI: the new results are found by use of a 'refined' comparison theorem in which the comparison potentials are allowed to intersect in a controlled fashion; this leads to sharper estimates for the power spectral function $P(q)$.

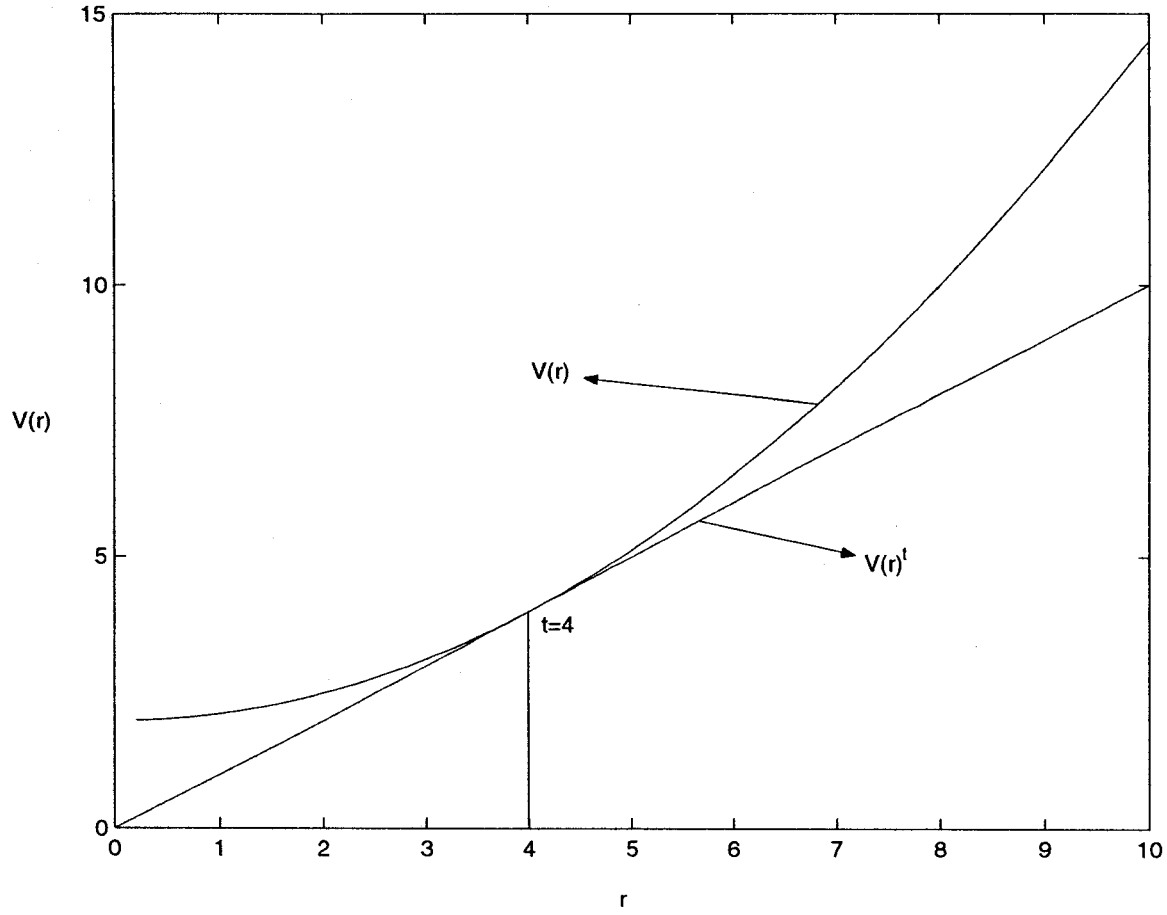

Figure II.1 The tangential potential $V^t(r) = a(t) + b(t)h(r)$ to the potential $V(r)$ using the base potential $h(r) = r$, where $a(t)$ and $b(t)$ are given in (II.3.3).

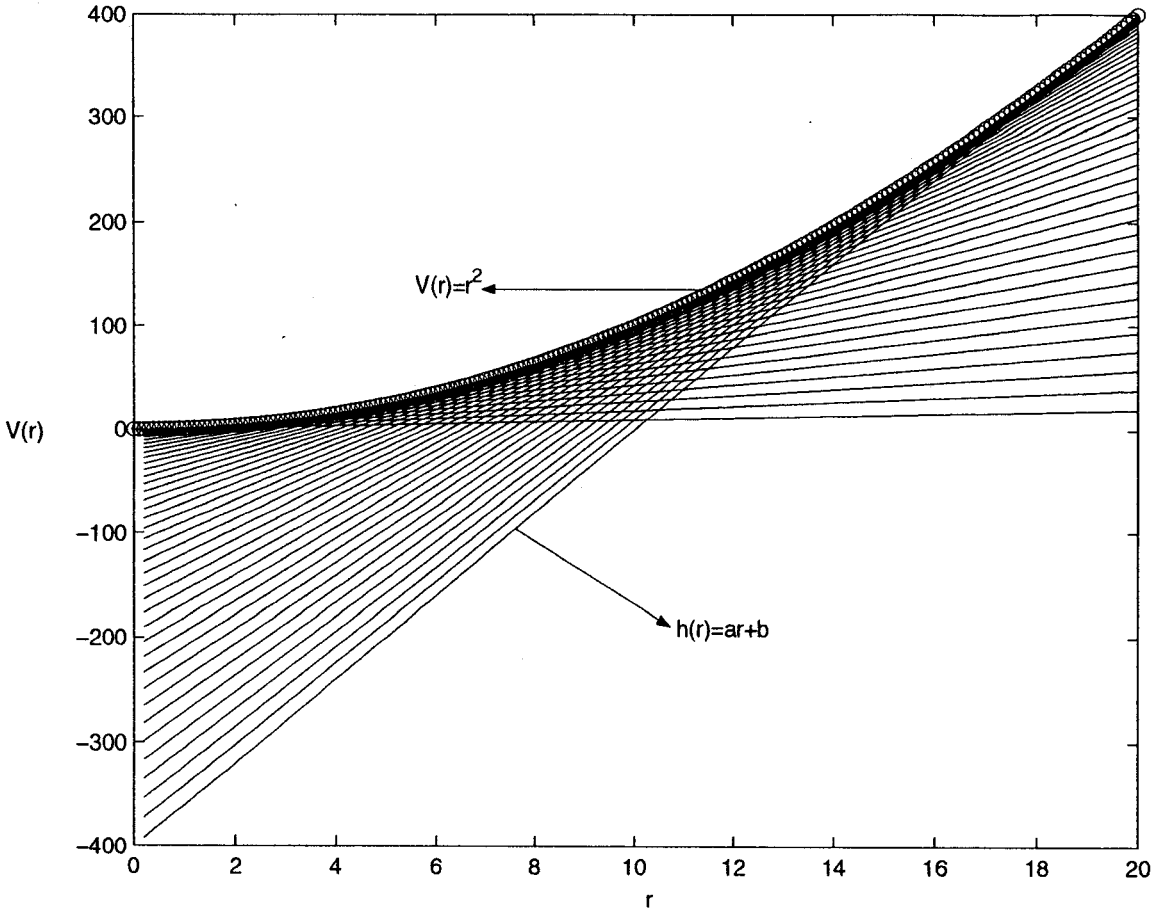

Figure II.2 The family of the tangential potentials used in (II.3.6) to obtain lower bound to the exact eigenvalues.

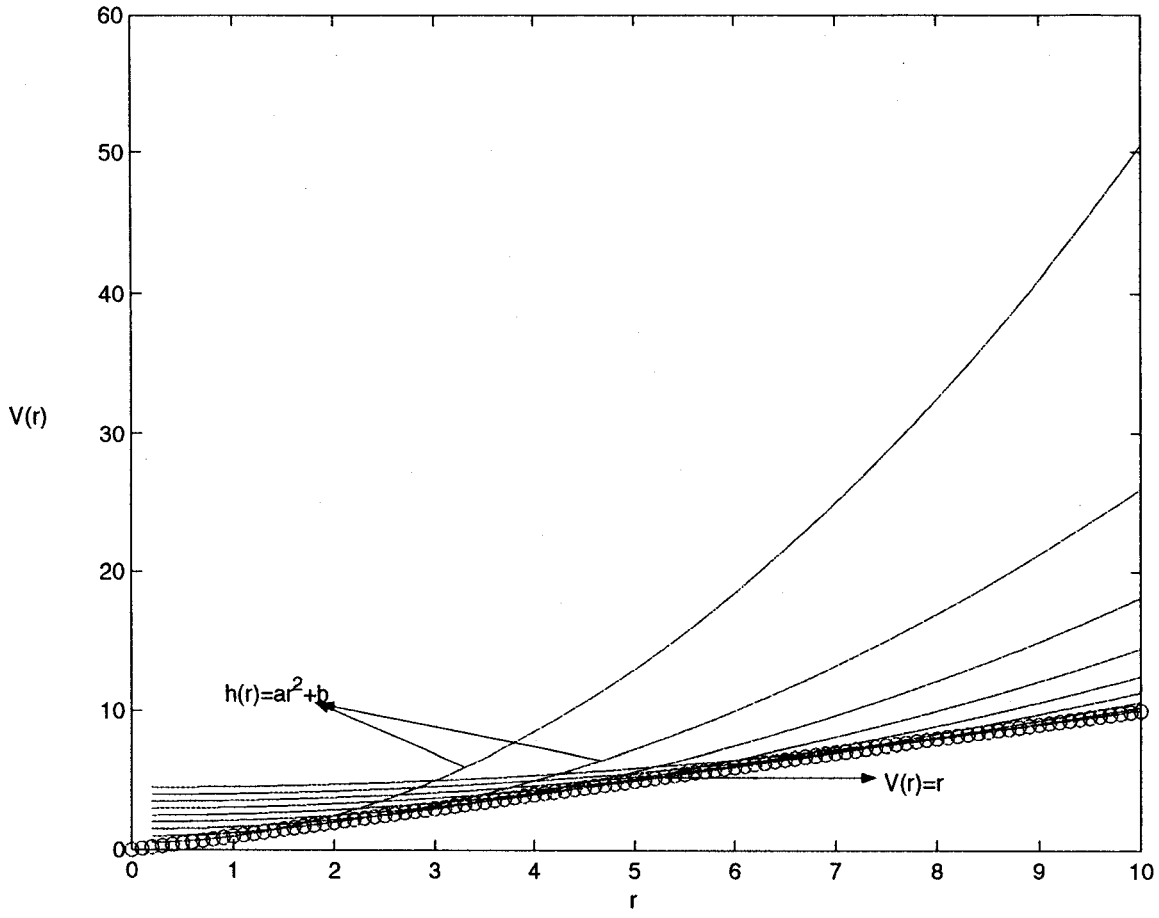

Figure II.3 The family of the tangential potentials used in (II.3.6) to obtain upper bound to the exact eigenvalues.

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Chapter III

Spectral bounds for the Hellmann potential

In this chapter the method of potential envelopes is used to analyse the bound state spectrum of the Schrödinger Hamiltonian $H = -\Delta + V(r)$, where $V(r)$ is the Hellmann potential given by $V(r) = -A/r + Be^{-Cr}/r$, A and C are positive constants, and B can be positive or negative. We established simple formulae yielding upper and lower energy bounds for the energy eigenvalues.

III.1 Introduction

The Hellmann potential $V(r)$ given by

$$V(r) = -A/r + Be^{-Cr}/r \tag{III.1.1}$$

has many applications in atomic physics and condensed-matter physics [1-11]. The Hellmann potential, with B positive, was suggested originally by Hellmann [1-2] and henceforth called the Hellmann potential if B is positive or negative. The Hellmann potential was used as a model for alkali hydride molecules [4]. It was used also to represent the electron-ion [5-6] and electron core interaction [7-8]. It has also been shown that the main properties of the effective two-particle interaction for charged particles in polar crystals may be described by this potential [9-11].

III.2 The discrete spectrum : Scaling

Many authors have studied the eigenvalues generated by the Hellmann potential and have tried to estimate them [1-14]. For example Adamoski [3] used a variational

framework to obtain accurate eigenvalues. Dutt, Mukherji and Varshni [12] and Kwato Njock *et al* [14] applied the method of large-N expansion to approximate the bound states energies. In this chapter we present simple upper- and lower-bound formulae obtained by the use of the comparison theorem and the envelope method [15-18].

We first show that discrete eigenvalues exist for the Hellmann potential for all values of $A > 0$, B, and $C > 0$. This result allows us to transcend the limit $B < A$ assumed to be necessary in an earlier attempt at this problem by geometrical methods [13]. Suppose that $B \leq 0$, then we immediately have that $-(A+B)/r < V(r) < -A/r$. Since both upper and lower bounds are Hydrogenic potentials with discrete eigenvalues, the same follows for $V(r)$.

Now we suppose that $B > 0$. In this case the concern is that, for sufficiently large B, the positive term might dominate the Coulomb term. We see that this does not happen by the following argument. The function re^{-Cr} has maximum value $1/(eC)$. Hence, for $B > 0$, we have $Be^{-Cr}/r < (B/eC)/r^2$, and we conclude that $-A/r < V(r) < -A/r+(B/eC)/r^2$. But the 'effective potential' for the Hydrogenic Atom in a state of orbital angular momentum ℓ is given by

$$V_{\text{eff}}(r) = -A/r + \ell(\ell+1)/r^2. \qquad \text{(III.2.1)}$$

Hence, again, we see that $V(r)$ is bounded above and below by Hydrogenic potentials whose corresponding Hamiltonians have discrete eigenvalues. This establishes our claim.

If we denote the eigenvalues of $H = -\omega\Delta + A/r + Be^{-Cr}$ by $\mathcal{E}(\omega, A, B, C)$, and consider a scale change of the form $s = r/\sigma$, and choose the scale $\sigma = 1/C$, then it is easy to show that,

$$\mathcal{E}(\omega, A, B, C) = C^2\omega\mathcal{E}(1, \frac{A}{\omega C}, \frac{B}{\omega C}, 1). \tag{III.2.2}$$

Hence, the full problem is now reduced to the simpler two-parameter problem

$$H = -\Delta - \alpha/r + \beta e^{-r}/r, \quad \mathcal{E} = \mathcal{E}(\alpha, \beta), \alpha > 0. \tag{III.2.3}$$

III.3 Energy bounds by the Envelope Method

The Comparison Theorem of quantum mechanics, discussed in the first chapter, tells us that an ordering between potentials implies a corresponding ordering of the eigenvalues. The 'envelope method' discussed in chapter II is based on this result and provides us with simple formulae for lower and upper bounds [16-18]. We need a solvable model which we can use as an envelope basis as shown in Figures III.1 and III.2. The natural basis to use in the present context is the hydrogenic potential

$$h(r) = -1/r. \tag{III.3.1}$$

The spectrum generated by the potential $h(r)$ may be represented exactly by the semi-classical expression $(II.4.1)$,

$$\mathcal{E}_{n\ell}(v) = \min_{s>0}\{s + v\bar{h}_{n\ell}(s)\}, \tag{III.3.2}$$

where the 'kinetic potential' $\bar{h}_{n\ell}(s)$ associated with the potential $h(r) = -1/r$ is given, in this case, exactly by $\bar{h}_{n\ell}(s) = -s^{\frac{1}{2}}/(n + \ell)$.

If we now consider a potential, such as $V(r)$, which is a smooth transformation $V(r) = g(h(r))$ of $h(r)$, then it follows that a useful approximation for the corresponding kinetic potential $\bar{f}_{n\ell}(s)$ is given by

$$\bar{f}_{n\ell}(s) \approx g(\bar{h}_{n\ell}(s)). \tag{III.3.3}$$

If g is convex in (III.3.3), we get lower bounds ($\simeq = \geq$) for all n and ℓ, and if g is concave we get upper bounds ($\simeq = \leq$) for all n and ℓ by Theorem II.2. For the Hellmann potential, if we use the potential $h = -1/r$ as the envelope basis, then the sign of g'' depends only on the sign of B. An elementary calculation shows that

$$g''(h) = -BC^2 e^{(C/h)}/h^3 = BC^2 r^3 e^{-Cr}. \tag{III.3.4}$$

Hence, g is convex if $B > 0$ or concave if $B < 0$. Thus in this application of the envelope method explained in chapter II, we obtain upper energy bounds for $B < 0$ and lower bounds for $B > 0$ and by substituting (III.3.3) in (III.3.2) and using Theorems II.1 and II.2, we find that

$$\mathcal{E}_{n\ell} \approx \min_{r>0}\{s + g(s^{1/2}/(n+\ell))\}, \tag{III.3.5}$$

which yields an upper bound if $B < 0$ and a lower bound if $B > 0$. This can be further simplified by changing the minimization variable s to r by the relation,

$$g(\bar{h}_{n\ell}(s)) = g(-s^{1/2}/(n+\ell)) = V(r), \tag{III.3.6}$$

which, in turn, implies $s = (n+\ell)^2/r^2$. Hence we obtain finally the following semi-classical eigenvalue formula involving the potential $V(r)$ itself

$$\mathcal{E}_{n\ell} \approx \min_{r>0}\{(n+\ell)^2/r^2 + V(r)\}. \tag{III.3.7}$$

III.4 Results

We now have a simple formula (III.3.7) for lower and upper bounds to the eigenvalues for the Hellmann potential. In Fig.(III.3) we plot the ground-state eigenvalue bound (full line) as a function of B for the case $A = 2,\ C = 1,$ along with the corresponding point results of Adamowski [3] as hexagons, and some accurate numerical values (dashed line). It is clear from this figure that the simple approximation formula gives an accurate estimate of the eigenvlues which is an upper bound if $B < 0,$ and a lower bound when $B > 0,$ as predicted by the theory.

If we fix $A, B,$ and C and consider the Hamiltonian $H = -\Delta + vV(r),$ with eigenvalues $\mathcal{E}(v)$, then from (III.3.7) we immediately obtain the following explicit parametric equations for the corresponding energy curve $\{v, \mathcal{E}(v)\},$ namely

$$\begin{aligned} v &= \frac{2(n+\ell)^2}{r^3 V'(r)} \\ \mathcal{E}(v) &= \frac{(n+\ell)^2}{r^2} + \frac{2(n+\ell)^2 V(r)}{r^3 V'(r)}. \end{aligned} \tag{III.4.1}$$

In Fig.(III.4) we exhibit the corresponding graphs of the function $\mathcal{E}(v)/v^2$ for $B = +1$ and $B = -1,$ again with $A = 2,$ and $C = 1,$ along with accurate numerical data shown as a dashed curve. The main point of this work is to show that by elementary geometric reasoning one can obtain simple semi-classical approximations for the eigenvalues. These results are complementary to purely numerical solutions and have the advantage that they are expressed analytically and allow one to explore the parameter space without having to attend to the arbitrary additional parameters and considerations which necessarily accompany numerical approaches with the aid of a computer.

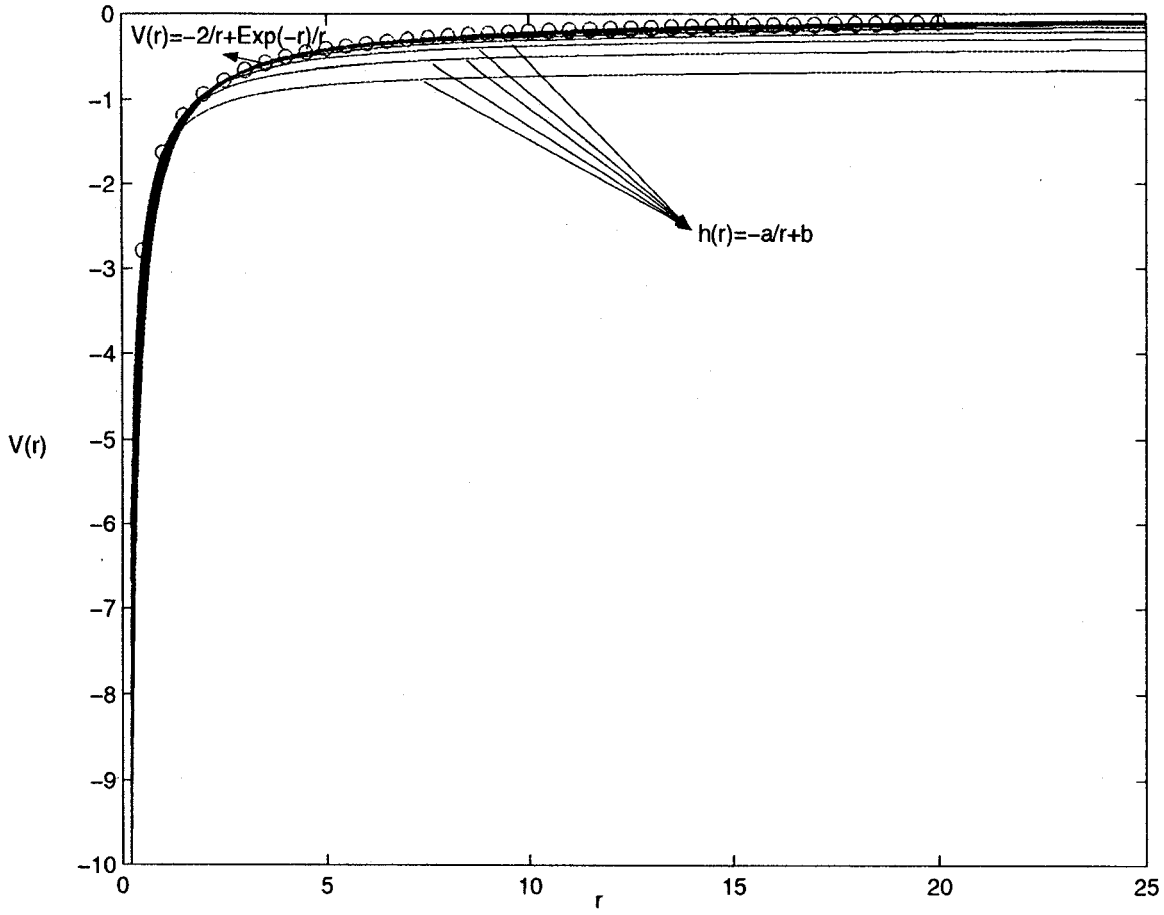

Figure III.1 The Hellmann potential $V(r) = -2/r + \exp(-r)/r$ represented as a lower envelope curve of a family of potentials of the form $-a/r + b$.

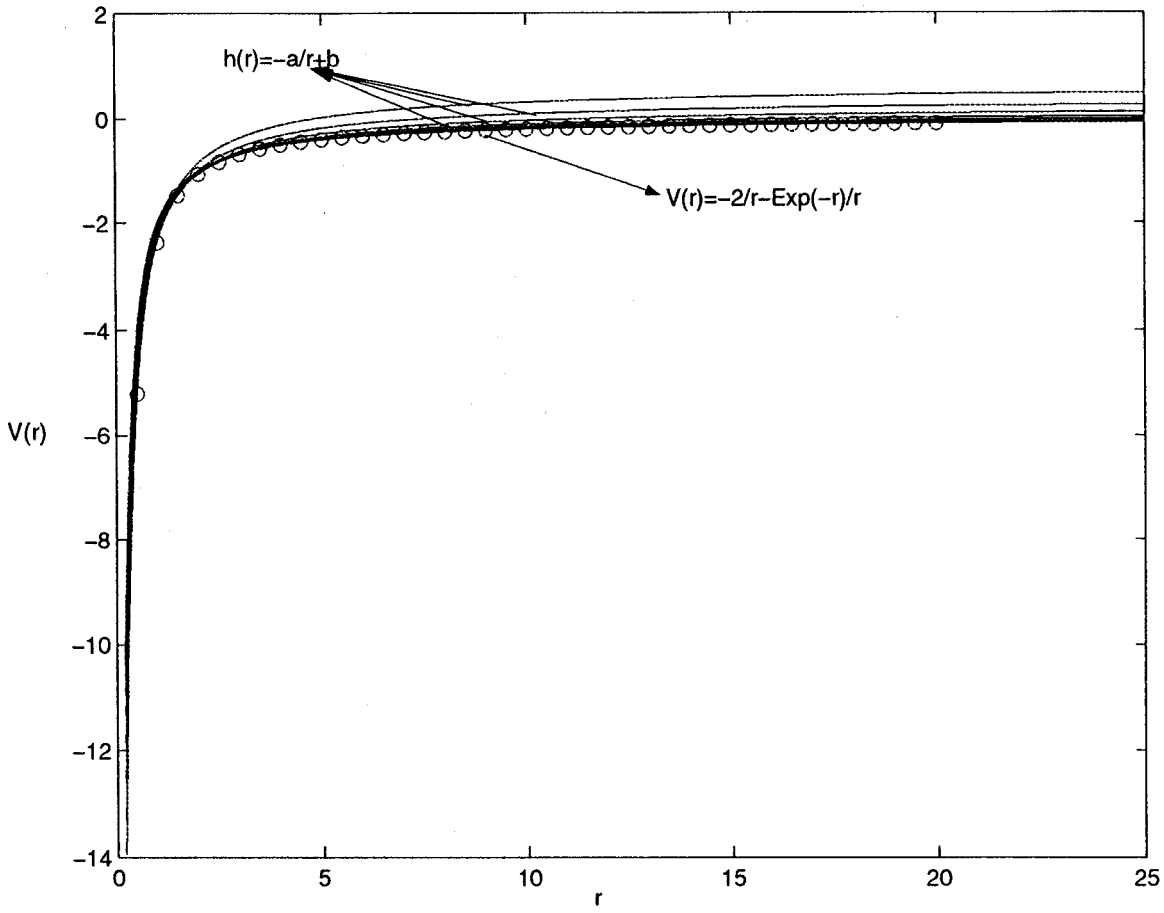

Figure III.2 The Hellmann potential $V(r) = -2/r - \exp(-r)/r$ represented as an upper envelope curve of a family of potentials of the form $-a/r + b$.

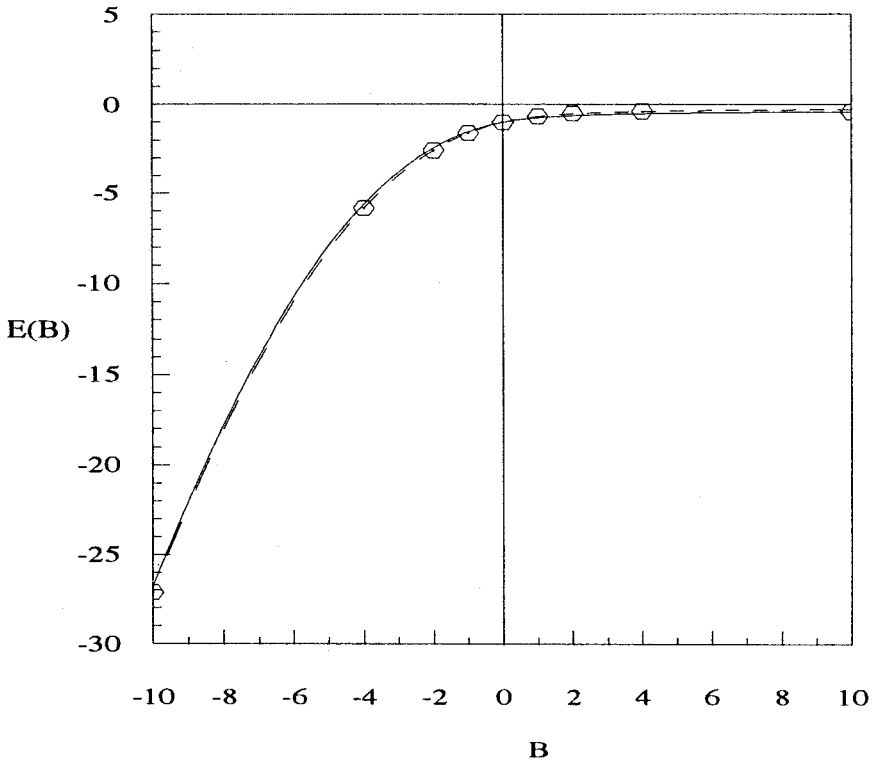

Figure III.3 The eigenvalues $\mathcal{E}(B)$ of the Hamiltonian $H = -\Delta - 2/r + Be^{-r}/r$ for $n = 1$ and $\ell = 0$. The continuous curve shows the bounds given by the formula (III.3.7), the dashed curve represents accurate numerical data, and the hexagons are the results of Adamowski [3]. It is clear that the formula provides us with upper bounds when $B < 0$ and lower bounds when $B > 0$.

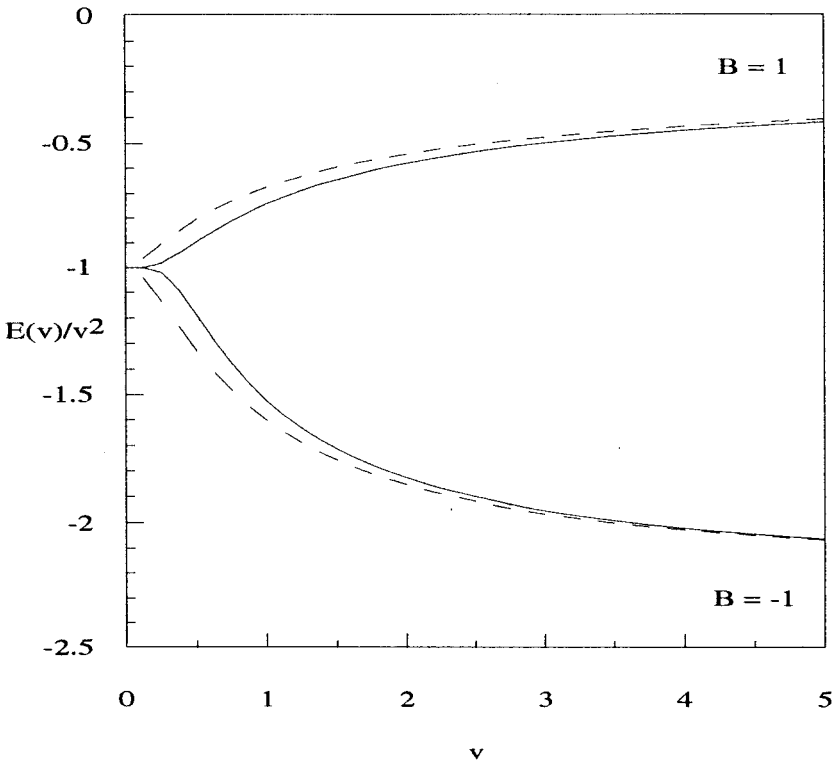

Figure III.4 The eigenvalue bounds (full-line) for $\mathcal{E}(v)/v^2$, where $\mathcal{E}(v)$ is the ground-state eigenvalue of the Hamiltonian $H = -\Delta + vV(r)$, for $A = 2$, $C = 1$, and $B = +1, -1$, together with accurate numerical data (dashed-line). The parametric equations (III.4.1) yield upper bounds when $B < 0$, and lower bounds when $B > 0$.

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Chapter IV

Spectral bounds for the cutoff Coulomb potential

The method of potential envelopes is used to analyse the bound-state spectrum of the Schrödinger Hamiltonian $H = -\Delta - v/(r+b)$, where v and b are positive constant. We establish simple formulae yielding upper and lower energy bounds for all the energy eigenvalues.

IV.1. Introduction

The cutoff Coulomb potential $f(r)$ given by

$$f(r) = -v/(r+b) \tag{IV.1.1}$$

is an approximation to the potential due to a smeared charge distribution, rather than a point charge, and is appropriate for describing mesonic atoms [1]. Many authors have studied the eigenvalues $E_{n\ell}, n = 1,2,3,...,\ell = 0,1,2,...$ generated by the cutoff Coulomb potential and have tried to estimate them. For example Ray and Mahata [2] applied the method of large-N expansion to approximate the bound states energies from $n = 1$ to $n = 4$. Mehta and Patil [1] rigorously analysed the S-wave bound-state eigenvalues of this potential as a function of b.

In this chapter we offer an elementary proof that the cutoff Coulomb potential has infinitely many discrete negative eigenvalues $E_{n\ell}, n = 1,2,3,...,\ell = 0,1,2,...$ by using the comparison methods. We then use the comparison theorem I.13 and

the envelope method discussed in chapter II and in [3-8] to obtain simple upper- and lower-bound formulae for all the eigenvalues.

IV.2. The discrete spectrum : Scaling

The Hamiltonian for the problem is given by,

$$H = -\Delta - v/(r+b),\ v,\ b > 0. \tag{IV.2.1}$$

A concern might be that, for sufficiently small coupling v, the potential, like a square well, might not have any discrete spectrum. However, the Coulomb tail averts this problem. It has been proved [4] by general methods that for any potential, like $-v/(r+b)$, which is negative and decays at infinity slower than $1/r^{2-\epsilon}$, the corresponding Hamiltonian operator has infinitly many negative eigenvalues. The specific result for our problem may also be obtained by an elementary application of the comparison theorem, as we now show by the following argument. We note that the potential can be written

$$f(r) = \frac{-v}{r} + \frac{vb}{r^2} - \frac{vb^2}{r^2(r+b)}. \tag{IV.2.2}$$

It therefore follows that

$$-\frac{v}{r} < f(r) < \frac{-v}{r} + \frac{vb}{r^2},$$

and consequently

$$V_l = -\frac{v}{r} + \frac{\ell(\ell+1)}{r^2} < f(r) + \frac{\ell(\ell+1)}{r^2} < \frac{-v}{r} + \frac{\lambda(\lambda+1)}{r^2} = V_u, \tag{IV.2.3}$$

where

$$\lambda = ((\ell + \frac{1}{2})^2 + vb)^{\frac{1}{2}} - \frac{1}{2}. \tag{IV.2.4}$$

Hence, we see that the effective potential associated with $f(r)$ is bounded above and below by Hydrogenic effective potentials with discrete negative eigenvalues. This implies that the potential V has infinitely many negative discrete eigenvalues $E_{n\ell}$ bounded by

$$\frac{-v^2}{4(n+\ell)^2} \leq E_{n\ell} \leq \frac{-v^2}{4(n+\lambda)^2}. \tag{IV.2.5}$$

These bounds are asymptotically close for large n. Another upper bound is provided by the linear potential since $f(r) < -\frac{v}{b} + \frac{v}{b^2}r$. Hence,

$$E_{n\ell} < -\frac{v}{b} + (\frac{v}{b^2})^{\frac{2}{3}}\mathcal{E}_{n\ell}(1), \tag{IV.2.6}$$

where $\mathcal{E}_{n\ell}(1)$ are the eigenvalues of the Hamiltonian $-\Delta + r$ for linear potential.

For the S-states the radial equation may be transformed into Whittaker's equation which has known exact solutions [9]. The general solution is written [9] in terms of the confluent hypergeometric functions $M[x,y,z]$ and $U[x,y,z]$ where,

$$U(x,y,z) = \frac{1}{\Gamma(x)}\int_0^\infty e^{-zt}t^{x-1}(1+t)^{y-x-1}dt = z^{-x}{}_2F_0[x, 1+x-y;;-1/z] \tag{IV.2.7}$$

and $M[x,y,z] = {}_1F_1[x;y;z]$. Mehta and Patil [1] used the bounded property of the radial wave function and the boundary conditions to demonstrate that the eigenvalues are determined by the equation

$$U[1 - v/(2\sqrt{-E}), 2, 2b\sqrt{-E}] = 0. \tag{IV.2.8}$$

As an alternative, we shall apply the envelope method to approximate all the eigenvalues. We first reduce the complexity of the problem by the use of scaling arguments. If we denote the eigenvalues of $H = -\omega\Delta - v/(r+b)$ by $\mathcal{E}(\omega, v, b)$, and consider a scale change of the form $s = r/\sigma$, and choose the scale $\sigma = \omega/v$, then it is easy to show that,

$$\mathcal{E}(\omega, v, b) = \frac{v^2}{\omega}\mathcal{E}(1, 1, \frac{vb}{\omega}). \tag{IV.2.9}$$

Hence, the full problem is now reduced essentially to the simpler 1-parameter problem

$$H = -\Delta - 1/(r+b), \quad \mathcal{E} = \mathcal{E}(b), b > 0. \tag{IV.2.10}$$

IV.3. Energy bounds by the Envelope Method

As another application of the Comparison Theorem of quantum mechanics I.14 and the 'envelope method' we obtain simple formulae for lower and upper bounds [5-8] as explained above (in chapter II) for the cutoff Coulomb potential. We need a solvable model which we can use as an envelope basis as shown in Figures IV.1 and IV.2. The natural bases to use in the present context are the hydrogenic and linear potentials

$$h(r) = \mathrm{sgn(q)r^q}, \quad \text{where} \quad \mathrm{q} = -1, 1. \tag{IV.3.1}$$

The spectrum generated by the potential $h(r)$ may be represented exactly by the semi-classical expression

$$\mathcal{E}_{n\ell}(v) = \min_{s>0}\{s + v\bar{h}_{n\ell}(s)\}, \tag{IV.3.2}$$

where the 'kinetic potential' $\bar{h}_{n\ell}(s)$ associated with the power-law potentials (IV.3.1) are given by (II.4.5) [8]

$$\bar{h}(s) = (2/q)|q\mathcal{E}_{n\ell}^{(q)}/(2+q)|^{(q+2)/2}s^{-q/2}, \tag{IV.3.3}$$

and $\mathcal{E}_{n\ell}^{(q)}$ is the exact eigenvalue of $-\Delta + \mathrm{sgn(q)r^q}$, that is to say, corresponding to the pure-power potential with unit coupling. If we now consider a potential, such as $f(r)$, which is a smooth transformation $f(r) = g(h(r))$ of $h(r)$, then it follows that a useful approximation for the corresponding kinetic potential $\bar{f}_{n\ell}(s)$ is given by

$$\bar{f}_{n\ell}(s) \approx g(\bar{h}_{n\ell}(s)). \tag{IV.3.4}$$

If g in (IV.3.4) is convex, we get [5-8] lower bounds ($\simeq=\geq$) for all n and ℓ, and if g is concave we get upper bounds ($\simeq=\leq$) for all n and ℓ, by Theorem II.2.

For the cutoff Coulomb potential, if we use the potential $h = -1/r$ as an envelope basis, then g is convex. An elementary calculation shows in this case that

$$g''(h) = \frac{2vb}{(\frac{b}{r}+1)^3} > 0. \tag{IV.3.5}$$

And if we use the potential $h = r$ as an envelope basis, then g is concave, in fact

$$g''(h) = \frac{-2v}{(b+r)^3} < 0. \tag{IV.3.6}$$

Thus in this application of the method we obtain upper energy bounds if we use $h = -1/r$ and lower energy bounds if we use $h = r$. Theorem II.1 and Theorem II.2 imply the following spectral inequality

$$E_{n\ell}(v) \geq va(t) + \mathcal{E}_{n\ell}(vb(t)). \tag{IV.3.7}$$

The optimal lower bound thus obtained may then eventually [8] be re-written as

$$E_{n\ell} \geq \min_{s>0} \left\{ s + g(\bar{h}_{n\ell}(s)) \right\}. \tag{IV.3.8}$$

In the complementary case where g is concave, the inequalities are reversed and one obtains upper bounds.

For the power-law potentials $h(r) = \mathrm{sgn(q)r^q}$ we can simplify (IV.3.8) by changing the minimization variable s to r defined in each case by the equation $\bar{h}_{n\ell}(s) = h(r)$ so that $g(h(r)) = f(r) = \frac{-v}{(r+b)}$ and the minimization (IV.3.2), which yields eigenvalue approximations for the Hamiltonian $H = -\omega\Delta + f(r)$, where $\omega > 0$, can be expressed in the form

$$E_{n\ell} \approx \min_{r>0} \left\{ \omega \frac{P^2_{n\ell}(q)}{r^2} - \frac{v}{(r+b)} \right\}. \tag{IV.3.9}$$

We obtain a lower bound for $P_{n\ell} = P_{n\ell}(-1) = (n+\ell)$, an upper bound for $P_{n\ell} = P_{n\ell}(1)$, and a good approximation with the mean value $P_{n\ell} = P^M_{n\ell} = \frac{1}{2}(P_{n\ell}(-1) + P_{n\ell}(1))$. These P-numbers are provided in Table IV.1.

A natural question to ask is whether there exists a set of numbers $\{P_{n\ell}\}$ such that $E_{n\ell} = \min_{r>0}\left\{\frac{P^2_{n\ell}}{r^2} + f(r)\right\}$ *exactly.* We can see that the answer is "no" by an argument based on the 'concentration lemma' [10], which provides us with the relation between the concentration of the ground-state wave function and the size of the coupling constant v. More precisely, the wave function becomes

more concentrated near the origin as v increases. Since for large values of the coupling v the "linear" upper bound (IV.3.9) is very accurate (concentration near $r = 0$), if there were one "exact" P_{10}, it would have to be the linear potential value $P_{10} = P_{10}(1)$. But our upper bound is clearly above $E_{n\ell}$ for small values of v. Hence there are no such "exact" $P_{n\ell}$.

IV.4. Conclusion

We have derived a simple formula (IV.3.12) for lower and upper bounds to the eigenvalues for the cutoff Coulomb potential. In Figure IV.3 we plot the eigenvalue when $(n, \ell) = (1, 1)$ as a function of b for the case $v = 1$, accurate numerical values (dashed line), and our approximation with the average value $P_{n\ell} = \frac{1}{2}(P_{n\ell}(-1) + P_{n\ell}(1))$ as stars.

If we fix b and consider the Hamiltonian $H = -\Delta + vf(r)$, with eigenvalues $\mathcal{E}(v)$, then from (3.12) we obtain the following explicit parametric equations for the corresponding approximate energy curve $\{v, \mathcal{E}(v)\}$, namely

$$\begin{aligned} v &= \frac{2(P_{n\ell})^2}{r^3 f'(r)} \\ \mathcal{E}(v) &= \frac{(P_{n\ell})^2}{r^2} + \frac{2(P_{n\ell})^2 f(r)}{r^3 f'(r)}. \end{aligned} \tag{IV.4.1}$$

These parametric equations yield upper bounds when $P_{n\ell} = P_{n\ell}(1)$ lower bounds when $P_{n\ell} = (n+\ell)$, and a good approximation when we use the arithmetic average of $P_{n\ell}(-1)$ and $P_{n\ell}(1)$. It is interesting, perhaps, that all these curves are scaled versions of any one of them; it is unknown if such a symmetry is true for the

corresponding exact curves. In Figure IV.4 we exhibit the graphs of the function $\mathcal{E}(v)$ for $b = 1$ along with accurate numerical data shown as a dashed curve. The main point of this work is to show that by elementary geometric reasoning one can obtain simple semi-classical approximations for the eigenvalues. These results are complementary to purely numerical solutions and have the advantage that they are expressed simply and analytically and therefore allow one to explore the parameter space of the problem.

Table IV.1 The 'input' P-values $P^L_{n\ell}$, $P^U_{n\ell}$, and the mean $P^M_{n\ell} = \frac{1}{2}(P_{n\ell}(-1) + P_{n\ell}(1))$ used in the general formula (IV.3.9).

n	ℓ	$P^L_{n\ell} = n + \ell$	$P^M_{n\ell}$	$P^U_{n\ell}$
1	0	1	1.18804	1.37608
2	0	2	2.59065	3.18131
3	0	3	3.99627	4.99255
4	0	4	5.40257	6.80514
5	0	5	6.80911	8.61823
1	1	2	2.18596	2.37192
2	1	3	3.57750	4.15501
3	1	4	4.97650	5.95300
4	1	5	6.37850	7.75701
5	1	6	7.78204	9.56408
1	2	3	3.18509	3.37018
2	2	4	4.57067	5.14135
3	2	5	5.96455	6.92911
4	2	6	7.36257	8.72515
5	2	7	8.76298	10.52596
1	3	4	4.18461	4.36923
2	3	5	5.56649	6.13298
3	3	6	6.95652	7.91304
4	3	7	8.35118	9.70236
5	3	8	9.74874	11.49748
1	4	5	5.18431	5.36863
2	4	6	6.56366	7.12732
3	4	7	7.95074	8.90148
4	4	8	9.34260	10.68521
5	4	9	10.73766	12.47532

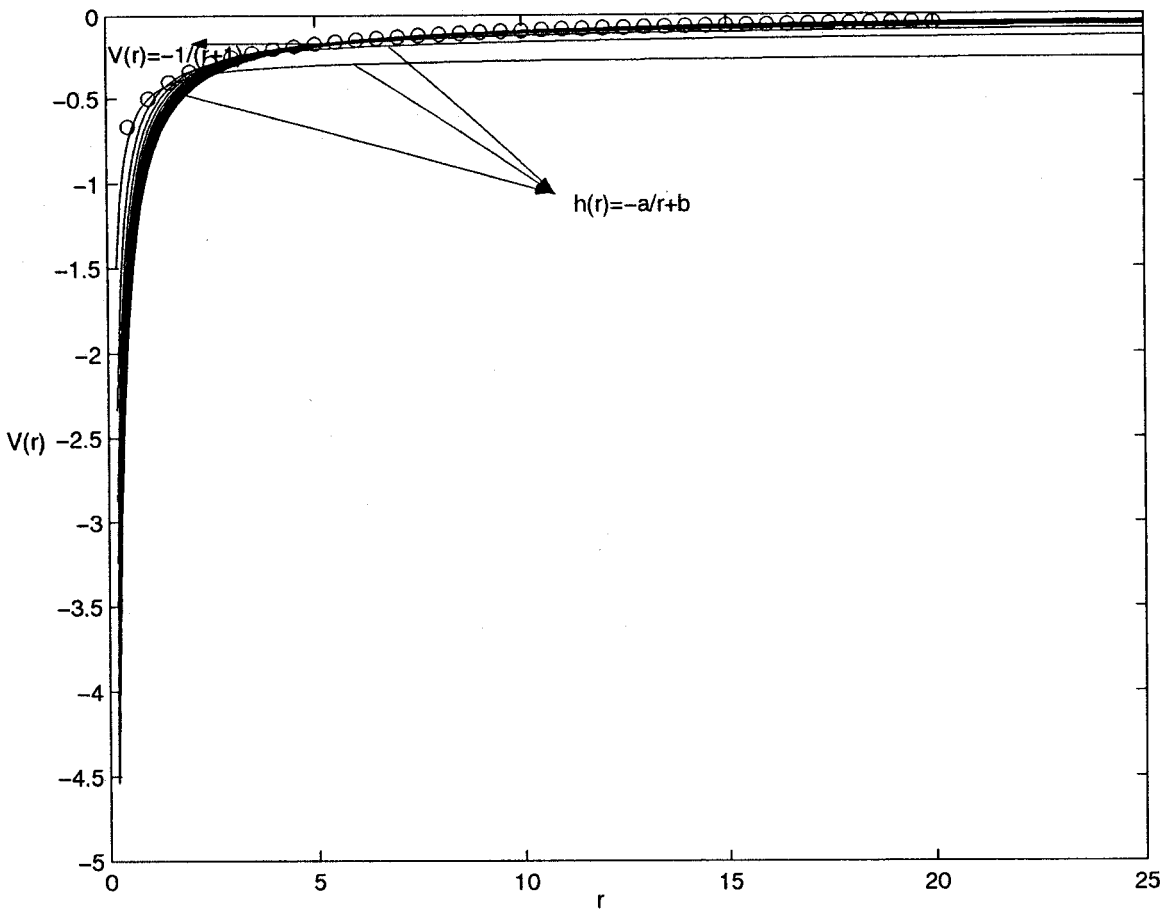

Figure IV.1 The cutoff Coulomb potential $V(r) = -1/(r+1)$ represented as a lower envelope curve of a family of potentials of the form $-a/r + b$.

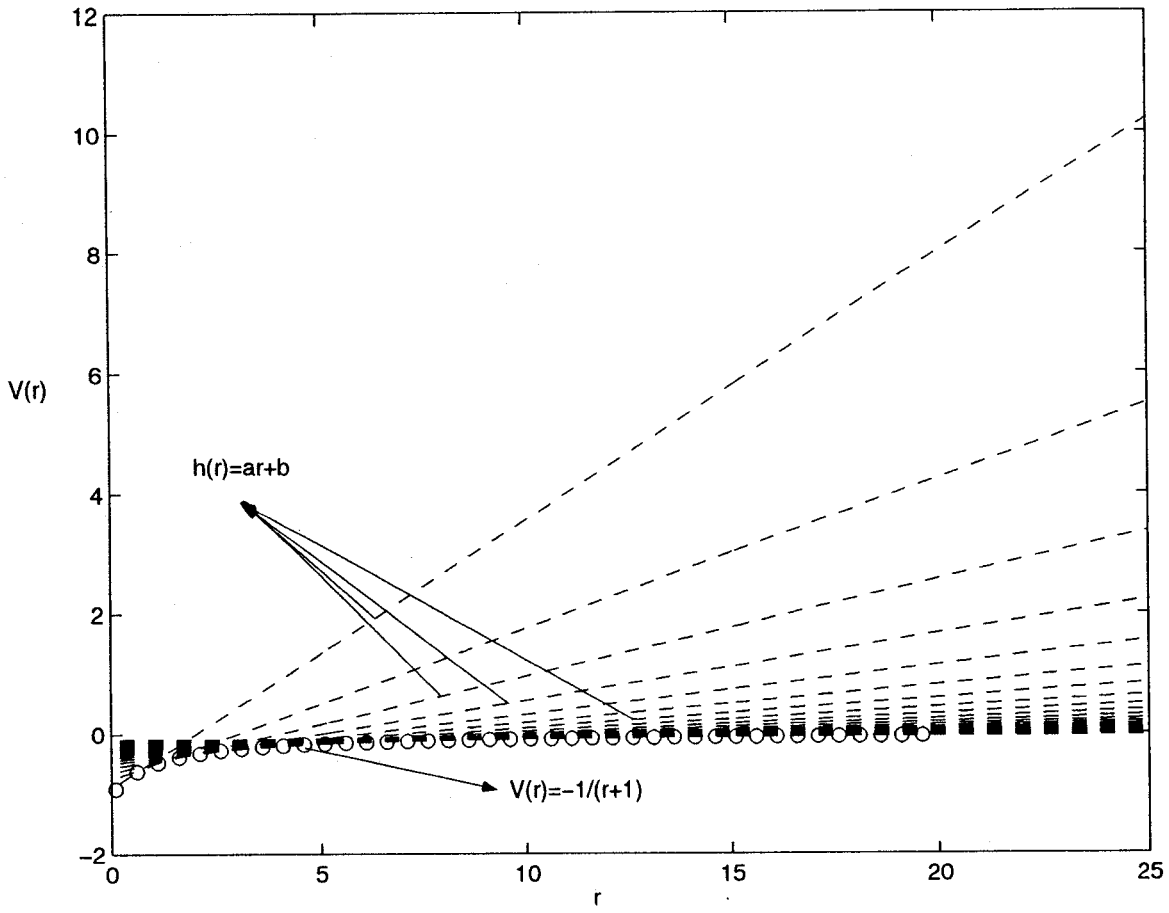

Figure IV.2 The cutoff Coulomb potential $V(r) = -1/(r+1)$ represented as an upper envelope curve of a family of potentials of the form $-a/r + b$.

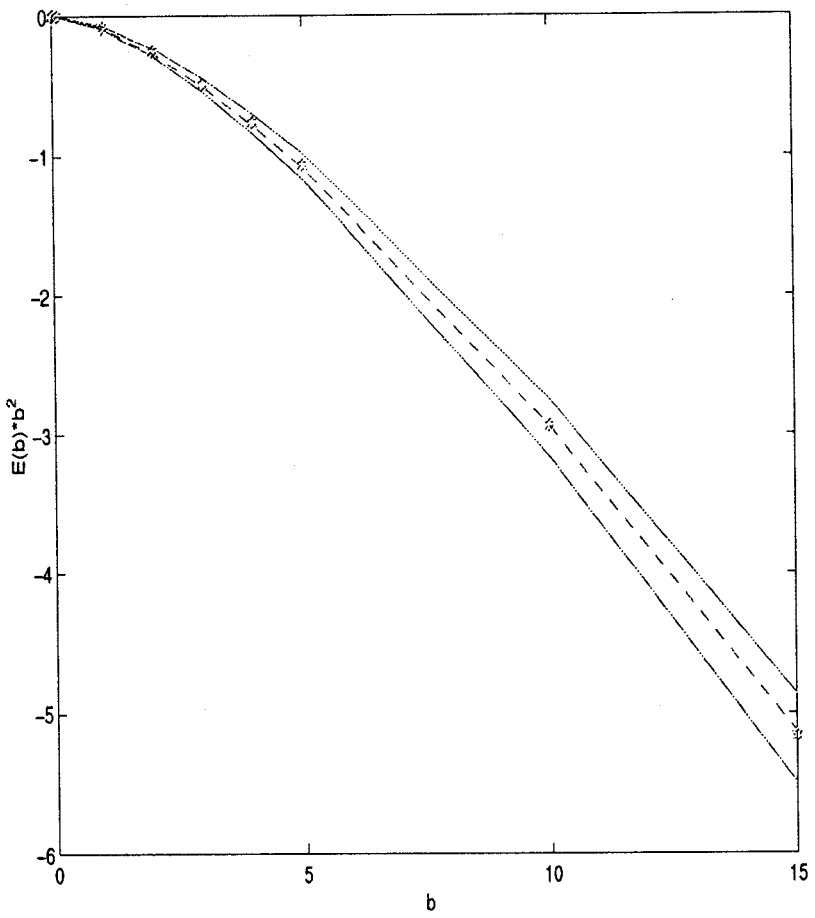

Figure IV.3 The eigenvalues $\mathcal{E}(b)$ of the Hamiltonian $H = -\frac{1}{2}\Delta - 1/(r+b)$ for $n = \ell = 1$ (in atomic units $\hbar = m = 1$). The continuous curves show the bounds given by formula (IV.3.9), the dashed curve represents accurate numerical data, and the stars are the 'mean approximation' $P_{n\ell} = \frac{1}{2}(P_{n\ell}(-1) + P_{n\ell}(1))$.

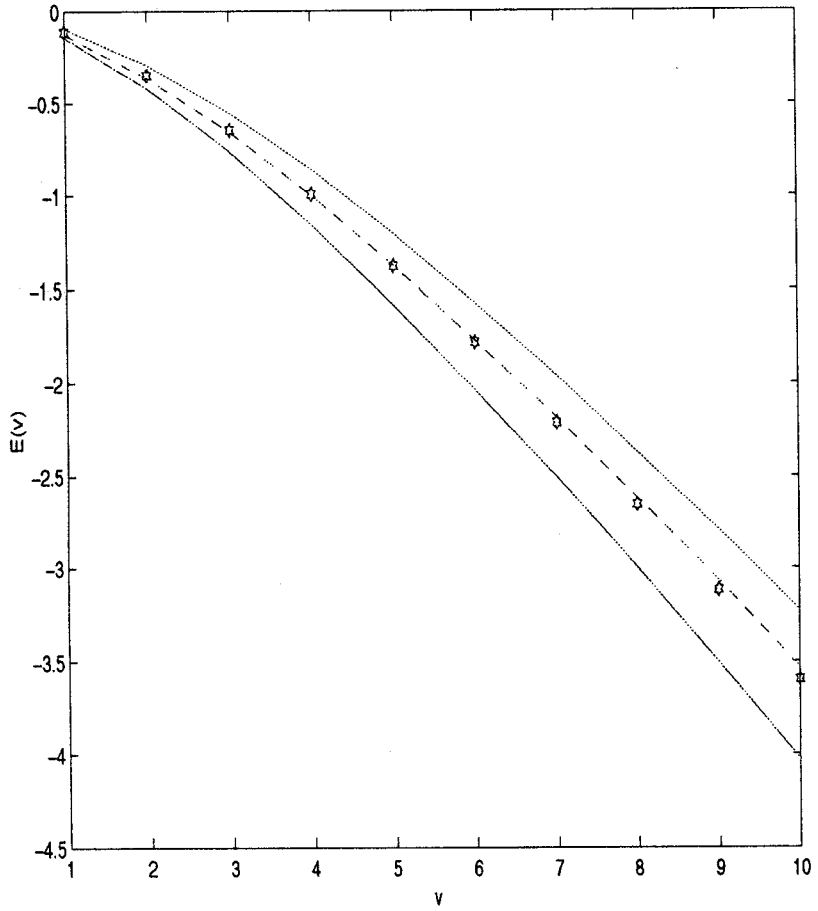

Figure IV.4 Eigenvalue bounds(full-line)for the ground-state eigenvalue $\mathcal{E}(v)$ $(n = 1, \ell = 0)$of the Hamiltonian $H = -\Delta + vf(r)$ (in units $\hbar = 2m = 1$) for $b = 1$, together with accurate numerical data (dashed curve). The parametric equations (IV.4.1) yield upper bounds when $P_{n\ell} = P_{n\ell}(1)$, lower bounds when $P_{n\ell} = P_{n\ell}(-1)$ and good approximation when $P_{n\ell} = \frac{1}{2}(P_{n\ell}(-1) + P_{n\ell}(1))$, shown as stars.

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Chapter V

Generalized comparison theorems in quantum mechanics

This chapter is concerned with the discrete spectra of Schrödinger operators $H = -\Delta + V$, where $V(r)$ is an attractive potential in N spatial dimensions. Two principal results are reported for the bottom of the spectrum of H in each angular-momentum subspace: (i) an optimized lower bound when the potential is a sum of terms $V(r) = V^{(1)}(r) + V^{(2)}(r)$, and (ii) a generalized comparison theorem which predicts spectral ordering when the graphs of the comparison potentials $V^{(1)}(r)$ and $V^{(2)}(r)$ intersect in a controlled way. Pure power-law potentials are studied and an application of the results to the Coulomb-plus-linear potential $V(r) = -a/r + br$ is presented in detail: for this problem an earlier formula for energy bounds is sharpened and generalized to N dimensions.

V.1 Introduction

This chapter has two principal aspects: the potential-sum approximation, and the generalization of the comparison theorem of quantum mechanics to cases where the comparison potentials intersect. We study spherically-symmetric problems in N spatial dimensions. There is much interest in problems posed in arbitrary dimension [1–9] and the geometrical methods we use are insensitive to the dimension N, which can usually be carried as a free parameter. We consider examples with Hamiltonians of the form $H = -\Delta + v\ \mathrm{sgn(q)r^q}$ or with sums of such potential terms. We

suppose that the Hamiltonian operators $H = -\Delta + V(r)$, $r = \|\mathbf{r}\|$, have domains $\mathcal{D}(H) \subset L^2(R^N)$, they are bounded below, essentially self adjoint, and have at least one discrete eigenvalue at the bottom of the spectrum. Because the potentials are spherically symmetric, the discrete eigenvalues $E_{n\ell}$ can be labelled by two quantum numbers, the total angular momentum $\ell = 0, 1, 2, \ldots$, and a 'radial' quantum number, $n = 1, 2, 3, \ldots$, which counts the eigenvalues in each angular-momentum subspace. Since the discrete spectrum may be characterized variationally [10], the elementary **comparison theorem I.14** $V^{(1)} < V^{(2)} \Rightarrow E^{(1)}_{n\ell} < E^{(2)}_{n\ell}$ immediately follows. The generalization we shall study (in Section V.3) involves comparison potentials whose graphs 'cross over' in such a way that spectral ordering is still guaranteed.

In Section V.2 we shall use the envelope method (explained in chapter II) along with the kinetic potential and the P-function representation for single power spectra to study the Coulomb-plus-linear potential $V(r) = -1/r + \lambda r$. This potential is clearly at once a convex transformation of the Hydrogenic potential $h(r) = -1/r$ and a concave transformation of the linear potential $h(r) = r$. We shall show that we are also able to express both the upper and lower bounds for the entire discrete spectrum in the form of an explicit rational function $\lambda = \lambda(E_{n\ell})$.

The base potentials used for the Coulomb-plus-linear potential are both pure powers. Thus we shall need to use the corresponding base kinetic potentials. In fact is has been shown in general [12] that

$$-\Delta + \mathrm{sgn(q)r^q} \quad \Rightarrow \quad \mathrm{E} = \min_{\mathrm{r>0}} \left\{ \left(\frac{\mathrm{P^N_{n\ell}(q)}}{\mathrm{r}} \right)^2 + \mathrm{sgn(q)r^q} \right\}, \qquad \text{(V.1.1)}$$

where, for example, we find in N dimensions that $P^N_{n\ell}(-1) = (n + \ell + N/2 - 3/2)$ and $P^N_{n\ell}(2) = (2n + \ell + N/2 - 2)$. These P-numbers and the underlying eigenvalues $E^N_{n\ell}$ satisfy the relation $E^N_{n\ell} = E^{N+2\ell}_{n0}$: this is generally true for central potentials and is the content of Theorem V.2, which we prove in Section V.4. Numerical values for $P^N_{n0}(1)$ are given in Table V.1 for $N = 2, ..., 12$. It is interesting that the case $q = 0$ corresponds *exactly* to the $\ln(r)$ potential [13]. The expression in (V.1.1) is derived by a change of variable $s \to (P^N/r)^2$ in the kinetic-potential formalism. The application to the Coulomb-plus-linear potential is not our only interest in these P^N-numbers. They provide through (V.1.1) a nice representation for the pure-power eigenvalues since the P^N-numbers vary smoothly with q through $q = 0$ whereas the eigenvalues themselves do not [12]. We have proved [12] that $P^N_{n\ell}(q)$ are monotone increasing in q. This result was obtained by using envelope theory: we considered one power q as a smooth transformation of another p, and then took the limit $p \to q$.

In Section V.3 we prove Theorem V.1 which provides a lower bound for the bottom of the spectrum in each angular momentum subspace using the sum approximation. In Section V.4 we prove Theorem V.2, which establishes the invariance of the eigenvalues with respect to changes in ℓ and N that leave the sum $N + 2\ell$ invariant. This allows us to restrict our considerations to the ground state in suf-

ficiently high dimension N. We reformulate the **refined comparison theorem** (Theorem 3 of Ref. [15]) which becomes Theorem V.3 here. We first prove the monotonicity of the ground-state wave function in N dimensions; then we prove Theorem V.4, which extends Theorem V.3 to $N \geq 2$ dimensions. Finally we prove Theorems V.5, V.6, and V.7 which provide simple explicit sufficient conditions for the application of Theorem V.4 under a variety of crossing schemes. In Section V.4 we apply Theorem V.5 to sharpen the envelope bounds already found in Section V.2 for the bottom of the spectrum E of H when V is the Coulomb-plus-linear potential $V(r) = -a/r + br$.

V.2 Coulomb-plus-linear potential: an eigenvalue formula

The Coulomb-plus-linear potential $V(r) = -a/r + br$ is of interest in physics because it serves as a nonrelativistic model for the principal part of the quark-quark interaction. First, we will use the envelope method to derive a simple formula for upper and lower bounds for all the eigenvalues $E_{n\ell}$, $n = 1, 2, 3, ...$, $\ell = 0, 1, 2, ...$ Because the linear potential, rather than the harmonic oscillator, is used as a basis for the upper bound, the new bounds are shaper than those of the earlier chapter [16].

If we denote the eigenvalues of $H = -\omega\Delta - \alpha/r + \beta r$ by $E(\omega, \alpha, \beta)$ and consider a scale of change of the form $r' = r/\sigma$, and if we further choose $\sigma = \alpha/\omega$, then it is easy to show that

$$E(\omega, \alpha, \beta) = \alpha^2 \omega^{-1} E(1, 1, \lambda), \ \lambda = \frac{\beta\omega^2}{\alpha^3}. \tag{V.2.1}$$

Thus it is sufficient to study the special case $H = -\Delta - 1/r + \lambda r$.

We need a solvable model which we can use as an envelope basis. The natural bases to use in the present context are the hydrogenic and linear potentials

$$h(r) = \mathrm{sgn(q)r^q}, \quad \text{where} \quad \mathrm{q} = -1, 1. \tag{V.2.2}$$

The spectrum generated by the potential $h(r)$ is represented precisely by means of the semi-classical expression $(II.2.1)$ as follows:

$$\mathcal{E}_{n\ell}(v) = \min_{s>0}\{s + v\bar{h}_{n\ell}(s)\}, \tag{V.2.3}$$

where the 'kinetic potentials' $\bar{h}_{n\ell}(s)$ associated with the power-law potentials (II.2.1) are given [13] by

$$\bar{h}(s) = \frac{2}{q}\left|\frac{q\mathcal{E}^{(q)}_{n\ell}}{2+q}\right|^{\frac{q+2}{2}} s^{-q/2} \tag{V.2.4}$$

and $\mathcal{E}^{(q)}_{n\ell}$ is the eigenvalue of $-\Delta + \mathrm{sgn(q)r^q}$ in N dimensions, that is to say, corresponding to the pure-power potential with coupling 1. If we use the potential $h(r) = -\frac{1}{r}$ as an envelope basis, then $V(r) = -\frac{1}{r} + \lambda r = g(-\frac{1}{r})$ implies g is convex. And if we use the linear potential $h(r) = r$ as an envelope basis, then g is concave. A weaker upper bound is provided by the harmonic oscillator $h(r) = r^2$, for which, again $g(h)$ is convex.

For the power-law potentials $h(r) = \mathrm{sgn(q)r^q}$ we can simplify (V.2.3) by changing the minimization variable s to r defined in each case by the equation $\bar{h}_{n\ell}(s) = h(r)$ so that $g(h(r)) = f(r) = -\frac{1}{r} + \lambda r$. The minimization on

the other hand, which yields eigenvalue approximations for the Hamiltonian $H = -\omega\Delta + f(r)$ $(\omega > 0)$, can be expressed in the form

$$E^N_{n\ell} \approx \min_{r>0}\left\{\omega\left(\frac{P^N_{n\ell}(q)}{r}\right)^2 - \frac{1}{r} + \lambda r\right\}, \tag{V.2.5}$$

where

$$P^N_{n\ell}(q) = \left|E^{(q)}_{n\ell}\right|^{\frac{2+q}{2q}}\left[\frac{2}{2+q}\right]^{\frac{1}{q}}\left|\frac{q}{2+q}\right|^{\frac{1}{2}}, \quad q \neq 0. \tag{V.2.6}$$

We obtain a lower bound with $P^N_{n\ell}(-1) = (n + \ell + N/2 - 3/2)$ and the harmonic-oscillator upper bound (of Ref.[16]) with $P^N_{n\ell}(2) = 2n + \ell + N/2 - 2$, and a sharper upper bound with $P^N_{n\ell}(1)$; the $P^N_{n0}(1)$-numbers are provided in Table V.1 for $N = 2, ..., 12$. This table allows $\ell > 0$ since $P^N_{n\ell} = P^{N+2\ell}_{n0}$: it is clear that $E^N_{n\ell}(-1)$ and $E^N_{n\ell}(2)$, and the corresponding P-numbers, are invariant with respect to changes in ℓ and N, which preserve the sum $2\ell + N$; this symmetry is also true for $E^N_{n\ell}(1)$, indeed for *all* eigenvalues generated by a central potential. This property is the content of Theorem V.2, which we state and prove is Section V.4. We thus obtain the following energy bounds

$$\min_{r>0}\left\{\left(\frac{P^N_{n\ell}(-1)}{r}\right)^2 - \frac{1}{r} + \lambda r)\right\} \leq E_{n\ell} \leq \min_{r>0}\left\{\left(\frac{P^N_{n\ell}(1)}{r}\right)^2 - \frac{1}{r} + \lambda r\right\} \tag{V.2.7}$$

for $n = 1, 2, 3, ...,$ $\ell = 0, 1, 2, ...$ Consequently, the energy bounds are given by the parametric equations

$$E_{n\ell} = -\frac{1}{2\nu t} + \frac{3\lambda\mu t}{2} \tag{V.2.8a}$$

$$1 = \frac{t}{2\nu} + \frac{\lambda\mu t^3}{2}, \quad t = rP^N_{n\ell}(q) \quad q = -1, 1, \tag{V.2.8b}$$

wherein the lower and upper bounds take the values $\nu = \mu = P_{n\ell}^N(-1)$ and $\nu = \mu = P_{n\ell}^N(1)$ respectively. It is interesting that we can actually solve Eqs. (V.2.8a) and (V.2.8b) to obtain λ as an explicit function of $E = E_{n\ell}^N$; the result namely is

$$\lambda = \frac{\left\{2(\nu E)^3 - \nu E^2\left[(1+3\nu^2 E)^{\frac{1}{2}} - 1\right]\right\}}{\mu\left[(1+3\nu^2 E)^{\frac{1}{2}} - 1\right]^3} \tag{V.2.9}$$

with $E \geq -\frac{1}{4\nu^2}$ (corresponding to $\lambda = 0$ for the pure hydrogenic spectrum). We emphasis that these bounds are valid for all the discrete eigenvalues in arbitrary dimension $N \geq 2$. The bounds are weak for $n > 1$, but at the bottom of each angular momentum subspace $n = 1$ they are sharp and improve with increasing $\ell, N,$ and λ. The lower bound for the bottom of each angular-momentum subspace $(n = 1)$ can be improved by use of the 'sum approximation' ([17] and Section V.3 below) in which $\nu = P_{n\ell}^N(1)$ (Table V.1) and $\mu = P_{n\ell}^N(-1) = (n + \ell + N/2 - 3/2)$. In Figure V.1 we exhibit these bounds for $n = 1$, $N = 3,$ and $\ell = 0, 1, 2, 3$.

V.3 The sum approximation: lower bounds

We now consider potentials which are sums of terms. Since further generalizations easily follow, we first look at the problem of the sum of only two potential terms. We assume that each potential $vh^{(i)}(r)$ alone, when added to the kinetic-energy operator $-\Delta$, has a discrete eigenvalue E at the bottom of the spectrum for sufficiently large coupling v. We note that the proof is unchanged if we restrict the problem to a given angular-momentum subspace labelled by ℓ; our claim then concerns the bottom of the spectrum of H in such a subspace; in the more general

case, all the kinetic potentials would be labelled by ℓ. We express our result in terms of kinetic potentials and prove (for the case $\ell = 0$) the following:

Theorem V.1 If E is the bottom of the spectrum of the Hamiltonian $H = -\Delta + V$, and the potential V is the sum $V(r) = h^{(1)}(r) + h^{(2)}(r)$, then it follows that the sum of the component kinetic potentials yields a lower bound to $\overline{V}$, that is to say

$$\overline{V}(s) \geq \overline{h}^{(1)}(s) + \overline{h}^{(2)}(s). \tag{V.3.1}$$

We shall now prove this theorem, which is in effect an optimized Weyl lower bound [18–20]. From the definition (II.2.1) of kinetic potentials we have

$$\overline{V}(s) = \inf_{\substack{\psi\in\mathcal{D}(H)\\(\psi,\psi)=1\\(\psi,K\psi)=s}} (\psi, V\psi) = \inf_{\substack{\psi\in\mathcal{D}(H)\\(\psi,\psi)=1\\(\psi,K\psi)=s}} \left(\psi, \left(h^{(1)} + h^{(2)}\right)\psi\right).$$

But the latter minimum mean-value is clearly bounded below by the sum of the *separate* minima. Thus we have

$$\overline{V}(s) \geq \inf_{\substack{\psi\in\mathcal{D}(H)\\(\psi,\psi)=1\\(\psi,-\Delta\psi)=s}} \left(\psi, h^{(1)}\psi\right) + \inf_{\substack{\psi\in\mathcal{D}(H)\\(\psi,\psi)=1\\(\psi,-\Delta\psi)=s}} \left(\psi, h^{(2)}\psi\right) = \overline{h}^{(1)}(s) + \overline{h}^{(2)}(s),$$

which inequality establishes the theorem. □

Another approach, which would eventually yield an alternative proof of the theorem, exhibits the relationship between Theorem V.1 and the classical Weyl lower bound [20–22] for the eigenvalues of the sum of two operators. Let us suppose that Ψ is the exact normalized lowest eigenfunction of $H = -\Delta + V$, so that

$H\Psi = E\Psi$. If the positive real parameter w satisfies $0 < w < 1$, then $E = (\Psi, (-\Delta + V)\Psi)$ may be written as follows:

$$\begin{aligned} E = \; & w\left(\Psi, \left(-\Delta + \frac{1}{w}\, h^{(1)}(r)\right)\Psi\right) + (1-w)\left(\Psi, \left(-\Delta + \frac{1}{1-w}\, h^{(2)}(r)\right)\Psi\right) \\ \geq \; & w \inf_{\substack{\psi\in\mathcal{D}(H) \\ (\psi,\psi)=1}} \left(\psi, \left(-\Delta + \frac{1}{w}\, h^{(1)}(r)\right)\psi\right) \\ + \; & (1-w) \inf_{\substack{\psi\in\mathcal{D}(H) \\ (\psi,\psi)=1}} \left(\psi, \left(-\Delta + \frac{1}{1-w}\, h^{(2)}(r)\right)\psi\right). \end{aligned}$$

That is to say, in terms of component kinetic potentials, we arrive at Weyl's inequality for the lowest eigenvalue E of the operator sum H, where

$$H = -w\Delta + h^{(1)} \quad + \quad -(1-w)\Delta + h^{(2)},$$

and we conclude

$$E \geq w \min_{s>0}\left\{s + \frac{1}{w}\,\overline{h}^{(1)}(s)\right\} + (1-w)\min_{s>0}\left\{s + \frac{1}{1-w}\,\overline{h}^{(2)}(s)\right\}.$$

Since w is an essentially free parameter in the last expression, we may optimize the Weyl lower bound with respect to the choice of w: this forces the individual values of s at the minima, $\{s_1(w), s_2(w)\}$, to be related. More specifically we find from the individual minimizations over s,

$$E \geq \mathcal{E}(w) = ws_1(w) + (1-w)s_2(w) + \overline{h}^{(1)}(s_1(w)) + \overline{h}^{(2)}(s_2(w)),$$

where

$$w = -\frac{\partial \overline{h}^{(1)}}{\partial s}\,(s_1(w)), \quad \text{and} \quad 1-w = -\frac{\partial \overline{h}^{(2)}}{\partial s}\,(s_2(w)).$$

The critical condition $\mathcal{E}'(w) = 0$ for the subsequent maximization over w then yields $s_1(w) = s_2(w)$. Thus the best lower energy bound is given by

$$E \geq \min_{s>0} \left\{ s + \overline{h}^{(1)}(s) + \overline{h}^{(2)}(s) \right\}.$$

The kinetic-potential inequality of Theorem V.1 leads, of course, to the same energy lower bound: the optimization just performed above is therefore seen to be automatically 'built in' by the kinetic-potential formalism.

It follows immediately from the above kinetic-potential comparison theorem and coupling-parameter absorption that a lower bound to the lowest energy E of the Hamiltonian $H = -\Delta + \sum_i c_i h^{(i)}(r)$, $\{c_i > 0\}$, is provided by the formula

$$E \geq \min_{s>0} \left\{ s + \sum_i c_i \overline{h}^{(i)}(s) \right\}. \tag{V.3.2}$$

Similarly we can extend this result to 'continuous sums' such as $V(r) = \int_{t_1}^{t_2} c(t) h^{(t)}(r) dt$.

Meanwhile, since the proof is identical, the bound is valid for the bottom of each angular-momentum subspace. Thus, more generally, the fundamental inequality becomes

$$\overline{V}_{1\ell}(s) \geq \overline{h}^{(1)}_{1\ell}(s) + \overline{h}^{(2)}_{1\ell}(s), \ \ell = 0, 1, 2, \ldots. \tag{V.3.3}$$

V.4 Generalized Comparison Theorems

The proof of our generalized comparison theorem (Theorem V.4) depends on monotone behaviour of the wave function induced by the assumed monotonicity of

the potential. We are able to establish this monotonicity for the lowest eigenfunction in arbitrary many spatial dimensions $N \geq 1$. We shall then be able to apply our eigenvlaue results to the case $\ell > 0$ and $n = 1$ because of Theorem V.2 which claims that $E^N_{n\ell} = E^{N+2\ell}_{n0}$; this general result is then employed in the special case $n = 1$.

Theorem V.2

Suppose that $H = -\Delta + V(r)$, where $V(r)$ is a central potential in $N \geq 2$ dimensions, has a discrete eigenvlaue $E^N_{n\ell}$ with n radial nodes in the angular-momentum subspace labelled by ℓ, then $E^N_{n\ell} = E^{N+2\ell}_{n0}$.

Proof: We suppose that ψ is the eigenfunction corresponding to $E^N_{n\ell}$. We express $-\Delta$ in spherical coordinates [1-9] and write the radial eigenequation explicitly as

$$-\psi''(r) - \frac{(N-1)}{r}\psi'(r) + \frac{\ell(\ell+N-2)}{r^2}\psi(r) + V(r)\psi(r) = E^N_{n\ell}\psi(r).$$

If we now define the reduced radial function $u(r) \in L^2(R^+)$ by $\psi(r) = u(r)r^{-(N-1)/2}$, $r > 0$, and $u(0) = 0$, we obtain

$$-u''(r) + \left[\frac{\frac{(N-1)}{2}\frac{(N-3)}{2} + \ell(\ell+N-2)}{r^2} + V(r)\right] u(r) = E^N_{n\ell}u(r). \qquad \text{(V.4.1)}$$

If we consider the spherically-symmetric potential $V(r)$ in M dimensions such that $(M-1)(M-3)/4 = \ell(\ell+N-2) + (N-1)(N-3)/4$, we find that $M = 2\ell + N$. The eigenequation (V.4.1) then may be written equivalently

$$-u''(r) + \left[\frac{\frac{(M-1)}{2}\frac{(M-3)}{2}}{r^2} + V(r)\right] u(r) = E^N_{n\ell}u(r). \qquad \text{(V.4.2)}$$

It therefore follows immediately that $E^N_{n\ell} = E^M_{n0} = E^{2\ell+N}_{n0}$. □

For the purpose of our comparison theory we may now consider the special case $n = 1$, $\ell = 0$ in arbitrary $N \geq 1$ spatial dimensions: the energy results which we derive will then be applicable to the family of equivalent problems in N' spatial dimension with $n = 1$, $\ell > 0$, and $N = N' + 2\ell$. In order to prove an appropriate extension of the comparison theorem in N dimensions, we shall first need to establish an elementary monotonicity property for the ground-state ψ. We prove the following:

Lemma

Suppose $\psi = \psi(r)$, $r = \|\mathbf{r}\|$, $\mathbf{r} \in R^N$, satisfies Schrödinger's equation:

$$H\psi(r) = (-\Delta + V(r))\psi(r) = E\psi(r), \tag{V.4.3}$$

where $V(r)$ is a central potential which is monotone increasing, $r > 0$, and $\lim_{r\to 0} rV(r) = \gamma < \infty$. Suppose that E is a discrete eigenvalue at the bottom of the spectrum of the operator $H = -\Delta + V$, defined on some suitable domain $\mathcal{D}(H)$ in $L^2(R^N)$. Suppose that $\psi(r)$ has no nodes, so that, without loss of generality, we can assume $\psi(r) > 0$, $r > 0$, then $\psi'(r) \leq 0$, $r > 0$.

Proof: The proof for the case $N = 1$ is given in Ref. [15], Eq.(V.2.2). Henceforth we shall now assume $N \geq 2$. If we express $-\Delta$ in spherical coordinates in N spatial dimensions, then we have

$$-\Delta\psi + V\psi = E\psi$$

$$-\frac{1}{t^{N-1}}\frac{\partial}{\partial t}(t^{N-1}\frac{\partial}{\partial t})\psi(t) + V(t)\psi(t) = E\psi(t).$$

We now multiply by t^{N-1} both sides and integrate with respect to t, to obtain

$$\psi'(r) = (1/r^{N-1}) \int_0^r [V(t) - E]\psi(t)t^{N-1}dt.$$

Since V is monotone increasing, it follows that there is one point $\hat{r} > 0$ satisfying $V(\hat{r}) = E$. First, we prove that $s(r) = \int_{\hat{r}}^r [V(t) - E]\psi(t)t^{N-1}dt$ is monotone increasing and bounded. For $t > \hat{r}$, $[V(t) - E]\psi(t)t^{N-1} > 0$, because $V(t) > E$ and hence $s(r)$ is increasing as $r \to \infty$. If there exists $r_1 < \infty$ such that $s(r_1) = -\int_0^{\hat{r}} [V(t) - E]\psi(t)t^{N-1}dt$, then $\int_0^r [V(t) - E]\psi(t)t^{N-1}dt > 0$, $r > r_1$, and $\psi'(r) > 0$, $r > r_1$; this contradicts the fact that the wave function $\psi(r)$ is positive and belongs to $L^2(R^N)$. This means that $\int_0^r [V(t) - E]\psi(t)t^{n-1}dt \leq 0$, $\forall r > 0$. Consequently $\psi'(r) \leq 0$, $\forall r > 0$. □

We now consider two potentials $V_1(r)$ and $V_2(r)$ both of the type described above. We have two Schrödinger equations for the respective ground-states ψ_1 and ψ_2 and the corresponding discrete eigenvalues E_1 and E_2 at the bottoms of the spectra. Thus we have the following pair of eigenequations

$$(-\Delta + V_1(r))\psi_1(r) = E_1\psi_1(r) \tag{V.4.4}$$

$$(-\Delta + V_2(r))\psi_2(r) = E_1\psi_2(r) \tag{V.4.5}$$

The radial wave functions in the present chapter satisfy the normalization condition $\int_0^\infty \psi_i^2(r)r^{N-1}dr < \infty$, $i = 1, 2$. With this notation, and $N = 3$, Theorem V.3 of Ref. [15] becomes

Theorem V.3

$$k(r) = \int_0^r (V_1(t) - V_2(t))\psi_i(t)t^2dt \leq 0, \ \forall r > 0, \ i = 1 \text{ or } 2 \Rightarrow E_1 \leq E_2. \tag{V.4.6}$$

We shall now generalize this theorem to general dimension $N \geq 1$. We first establish a fundamental comparison formula (Eq.(V.4.7)) below.

By multiplying $(V.4.4)$ by ψ_2 and $(V.4.5)$ by ψ_1, and subtracting, we find

$$\psi_1 \Delta \psi_2 - \psi_2 \Delta \psi_1 + [V1 - V2]\psi_1 \psi_2 = [E1 - E2]\psi_1 \psi 2.$$

Integrating over R^N and using the following identity,

$$\nabla.(\psi_1 \nabla \psi_2) = \nabla \psi_1 . \nabla \psi_2 + \psi_1 \nabla^2 \psi_2,$$

we find that

$$\int_{R^N} \nabla.[\psi_1 \nabla \psi_2 - \psi_2 \nabla \psi_1] d^N r + \int_{R^N} [V1 - V2]\psi_1 \psi_2 d^N r = [E1 - E2] \int_{R^N} \psi_1 \psi_2 d^N r.$$

Now by Gauss's theorem [23] we find that the first term becomes a surface integral which vanishes because $\psi_i \in L^2(R^N)$. In the remaining integrals the angular factors yield $2\pi^{N/2}/\Gamma(N/2)$. Hence we find

$$\frac{2\sqrt{\pi^N}}{\Gamma(N/2)} \int_0^\infty [V_1(r) - V_2(r)]\psi_1(r)\psi_2(r) r^{N-1} dr = \frac{2\sqrt{\pi^N}}{\Gamma(N/2)} [E_1 - E_2] \int_0^\infty \psi_1(r)\psi_2(r) r^{N-1} dr,$$

which implies

$$s = \int_0^\infty [V_1 - V_2]\psi_1\psi_2 r^{N-1}dr = [E_1 - E_2]\int_0^\infty \psi_1\psi_2 r^{N-1}dr. \qquad \text{(V.4.7)}$$

Now we may state our generalization of Theorem V.3 to N dimensions:

Theorem V.4

$$k(r) = \int_0^r (V_1(t) - V_2(t))\psi_i(t)t^{N-1}dt \leq 0,\ \forall r > 0,\ i = 1 \text{ or } 2 \Rightarrow E_1 \leq E_2. \quad \text{(V.4.8)}$$

Proof: For definiteness we assume that $i = 1$; the proof is just the same with the other choice. We study the integral s on the left side of $(V.4.7)$. Integrating by parts we find that

$$s = [k(r)\psi_2(r)]_0^\infty - \int_0^\infty k(r)\psi_2'(r)r^{N-1}dr \qquad \text{(V.4.9)}$$

Since $k(0) = \psi_2(\infty) = 0$, the first term vanishes, and s is therefore equal to the negative of the integral of the right side of $(V.4.9)$. But the integrand of this integral is positive because $k(r) \leq 0$, by hypothesis, and we know that $\psi_2'(r) \leq 0$ by the above lemma. This proves that $s \leq 0$. Consequently, by $(V.4.7)$, we obtain $E_1 \leq E_2$. □

It may be difficult to apply Theorem V.4 in practice. Thus it would be helpful to establish some simpler sufficient conditions, depending on the number and nature of the crossings over of the two comparison potentials. We treat three useful cases: Theorem V.5, one potential crossing, with use of the wave function; Theorem V.6, two crossings and the use of the wave function; Theorem V.7, two crossings

and no wave function used. In these Theorems we shall assume that the integrals $\int_0^\infty (V_1(r) - V_2(r))\psi_i(r) r^{N-1} dr,\ i = 1, 2,$ exists for the given problem, even though we use at most one wave function factor.

Theorem V.5. If the potentials $V_1(r)$ and $V_2(r)$ cross exactly once for $r > 0$ at $r = r_1$, with

(i) $V_1(r) < V_2(r)\ \ (0 < r < r_1)$ and

(ii) $\int_0^\infty [V_1(t) - V_2(t)]\psi_i(t) t^{N-1} dt = 0,\ i = 1$ or 2,

then

$$k(r) = \int_0^r [V_1(t) - V_2(t)] t^{N-1} \psi_i(r) dt \leq 0,\ \forall\ r > 0,\ i = 1 \text{ or } 2, \qquad \text{(V.4.10)}$$

from which $E_1 \leq E_2$ follows, by Theorem V.4.

Proof: We choose $i = 1$: the proof is identical for $i = 1$ or 2 . First, we show that $s(r) = \int_{r_1}^r [V_1(t) - V_2(t)]\psi_1(t) t^{N-1} dt$ is monotone increasing. For $t > r_1$, $s'(r) = [V_1(r) - V_2(r)]\psi_1(r) r^{N-1} > 0$, because $V_1(r) > V_2(r)$; hence $s(r)$ is increasing on (r_1, ∞). Moreover, (ii) implies that the maximum value of $s(r)$ is reached at $r = \infty$; i.e $s(r) \leq s(\infty)$ we have therefore

$$\int_0^\infty [V_1(t) - V_2(t)]\psi_1(t) t^{N-1} dt =$$

$$\int_0^{r_1} [V_1(t) - V_2(t)]\psi_1(t) t^{N-1} dt + \int_{r_1}^\infty [V_1(t) - V_2(t)]\psi_1(t) t^{N-1} dt = 0$$

and therefore

$$\lim_{r\to\infty} s(r) = -\int_0^{r_1} [V_1(t) - V_2(t)]\psi_1(t)t^{N-1}dt.$$

Now, we have the following two cases to consider

Case 1: for $r < r_1$, $k(r) = \int_0^r [V_1(t) - V_2(t)]\psi_1(t)t^{N-1}dt < 0$, since $V_1(t) < V_2(t)$ for $0 < t < r$.

Case 2: if $r > r_1$, then

$$k(r) = \int_0^{r_1} [V_1(t)-V_2(t)]\psi_1(t)t^{N-1}dt+\int_{r_1}^{r} [V_1(t)-V_2(t)]\psi_1(t)t^{N-1}dt = s(r)-s(\infty) < 0.$$

Therefore, $k(r) \leq 0, \forall r > 0$. □

Theorem V.6. If the potentials $V_1(r)$ and $V_2(r)$ cross twice for $r > 0$ at $r = r_1, r = r_2$ $(r_1 < r_2)$ with,

(i) $V_1(r) < V_2(r)$ for $0 < r < r_1$ and

(ii) $\int_0^{r_2} (V_1(t) - V_2(t))\psi_i(t)t^{N-1}dt = 0$, $i = 1$ or 2,

then,

$$k(r) = \int_0^r (V_1(t) - V_2(t))\psi_i(t)t^{N-1}dt \leq 0, \ \forall r > 0, \ i = 1 \text{ or } 2, \qquad \text{(V.4.11)}$$

from which $E_1 \leq E_2$ follows, by Theorem V.4.

Proof: $k'(r) = (V_1(r) - V_2(r))r^{N-1}\psi_1(r)$, now $k(0) = 0$, $k'(r) < 0$, $0 < r < r_1$, implies $k(r) < 0$, $0 < r < r_1$. Next, $k(r_2) = 0$, $k'(r) > 0$, $r_1 < r < r_2$, implies $k(r) < 0$, $r_1 < r < r_2$. Lastly, $k(r_2) = 0$, $k'(r) < 0$, $r > r_2$, implies $k(r) < 0$, $r > r_2$. □

Theorem V.7. If the potentials $V_1(r)$ and $V_2(r)$ cross twice for $r > 0$ at $r = r_1,\ r_2\ \ (r_1 < r_2)$ with

(i) $V_1(r) < V_2(r)$ for $0 < r < r_1$ and

(ii) $\int_0^{r_2}(V_1(t) - V_2(t))t^{N-1}dt = 0$

then,

$$k(r) = \int_0^r [V_1(t) - V_2(t)]\psi_i(t)t^{N-1}dt \leq 0,\ \forall r > 0\ ,\ i = 1 \text{ or } 2, \qquad \text{(V.4.12)}$$

from which $E_1 < E_2$ follows, by Theorem V.4.

Proof: We choose $i = 1$: the proof is identical if $i = 2$. Define $h(r) = \int_0^r (V_1(t) - V_2(t))t^{N-1}dt$, the proof of Theorem V.3 shows that $h(r) \leq 0,\ 0 \leq r \leq r_2$. But

$$\begin{aligned} k(r) &= \int_0^r (V_1(t) - V_2(t))\psi_1(t)t^{N-1}dt \\ &= [h(t)\psi_1(t)]_0^r - \int_0^r h(t)\psi_1'(t)dt \\ &= h(r)\psi_1(r) - \int_0^r h(t)\psi_1'(t)dt < 0, \end{aligned}$$

meanwhile, $k'(r) < 0,\ r > r_2$. Therefore, $k(r) < 0,\ \forall r > 0$. □

V.5 Application to the Coulomb-plus-linear potential

As an example, we employ the comparison theorems to improve the bounds obtained in Section V.2 for the eigenvalues corresponding to the Coulomb-plus-linear potential $V(r) = -a/r + br$, where a and b are positive coupling parameters. For the upper bound we use as a comparison potential the shifted linear potential $h(r) = -\alpha + \beta r$, where α and $\beta > 0$. We allow the potentials $V(r)$ and $h(r)$ to

cross over exactly twice, as illustrated in Figure V.2. Let A and B represent the absolute values of the areas (or of the ψ-weighted areas) between the potentials. We vary α and β so that $A = B$, and thereafter Theorems V.5 and V.6 imply $E^V \leq E^h$. For simplicity of derivation of the upper-bound formula, we will use Theorem V.7 (with no use of the wave function ψ). Thus we have two equations to solve in this case,

$$-\frac{a}{r} + br = -\alpha + \beta r,$$

$$\int_0^r [-\frac{a}{t} + bt + \alpha - \beta t] t^{N-1} dt = 0,$$

where $r = r_2$ is the second crossing point. These reduce to the quadratic equations

$$(\beta - b)r^2 - \alpha r + a = 0,$$

$$N(N-1)(b-\beta)r^2 + \alpha(N-1)(N+1)r - aN(N+1) = 0,$$

with simultaneous solution $r = \frac{2aN}{\alpha(N-1)}$. Now the best upper bound is obtained after minimizing with respect to r, giving

$$E^U = \min_{r>0} \left\{ -\left(\frac{2aN}{(N-1)r}\right) + \left(\frac{(N+1)a}{(N-1)r^2} + b\right)^{\frac{2}{3}} \mathcal{E}^N(1) \right\}. \qquad \text{(V.5.1)}$$

At the expense of further complication, the use of $\psi_1(r)$ (the Airy function) would lower this upper bound.

Similarly, to improve our lower bound, we allow the Coulomb-plus-linear potential to intersect twice with the Hydrogenic potential $h(r) = -\frac{\alpha}{r} + \beta$, with the exact wave function solution $\psi = e^{-\alpha r/(N-1)}$ and the exact energy $E^h = \beta - \alpha^2/(N-1)^2$,

where α and β are positive parameters. Again, let A and B represent the absolute values of the areas (or of the ψ-weighted areas) between the potentials. We vary α and β so that $A = B$, as illustrated in Figure V.3, and thereafter Theorems V.5 and V.6 imply $E^h \leq E^V$. Subsequently, we obtain the lower bound (without ψ) by solving the following three equations:

$$\frac{-a}{t} + bt = -\frac{\alpha}{t} + \beta$$

$$\int_0^t [\frac{-a}{r} + br + \frac{\alpha}{r} - \beta] r^{N-1} dr = 0$$

$$E^L = \min_{t>0} \{\beta - (\alpha/(N-1))^2\}. \qquad \text{(V.5.2)}$$

For the case $a = 1$ and $b = 1$, we compare in Figure V.4 the upper and lower bounds obtained by means of the classical envelope method and by the comparison theorems introduced in Section V.3.

V.6 Conclusion

Our proof of the lower-bound for the bottom of the spectrum of the operator $H = -\Delta + V^{(1)}(r) + V^{(2)}(r)$, based on kinetic potentials, is more compact and direct than the original proof, and is valid in N dimensions; the principal steps of the earlier proof are repeated because they show that the final result is equivalent to an optimization of the classical theorem of Weyl. The generalized comparison theorem is proved in the present chapter for all dimensions N, whereas, in its original form, it required two distinct theorems, for $N = 1$, and $N = 3$. Moreover, we are now able to apply the results to the bottom of each angular-momentum

subspace since we have proved that this energy is identical to the lowest eigenvalue of a higher-dimensional problem, in $R^{N+2\ell}$. Meanwhile, in order to be practical, weaker sufficient conditions were sought which would guarantee in a simple way that the comparison potentials cross over so as to imply definite spectral ordering. These results greatly clarify the application of the generalized comparison theorem to specific problems.

The Coulomb-plus-linear problem provides a convenient example on which to test the effectiveness of the energy bounds. At the same time it offers an opportunity to sharpen an earlier energy-bound formula for this problem, and to extend its validity to all $N \geq 2$ dimensions. The energy bounds provided by this formula are remarkably accurate for the bottom of each angular-momentum subspace ($n = 1$), and, as we have shown, they become sharper with increasing N or ℓ. If the sum approximation is capriciously applied also to the higher discrete eigenvalues $n > 1$, the resulting *ad hoc* approximation formula continues to give very accurate estimates, which, however, are no longer bounds. What additional conditions might guarantee bounds from such a formula is an interesting open question.

Table V.1 The 'input' P-values $P_{n0}^{N}(1)$ used in the general formula (V.1.1), for $N = 2, 3, \ldots, 12$. The same data applies to $\ell > 0$ since, by Theorem V.2, we have $P_{n\ell}^{N} = P_{n0}^{N+2\ell}$.

N	$n=1$	$n=2$	$n=3$	$n=4$
2	0.9348	2.8063	4.6249	6.4416
3	1.3761	3.1813	4.9926	6.8051
4	1.8735	3.6657	5.4700	7.2783
5	2.3719	4.1550	5.9530	7.7570
6	2.8709	4.6472	6.4398	8.2396
7	3.3702	5.1413	6.9291	8.7251
8	3.8696	5.6367	7.4204	9.2129
9	4.3692	6.1330	7.9130	9.7024
10	4.8689	6.6299	8.4068	10.1932
11	5.3686	7.1274	8.9053	10.7453
12	5.8684	7.6253	9.4045	11.2744

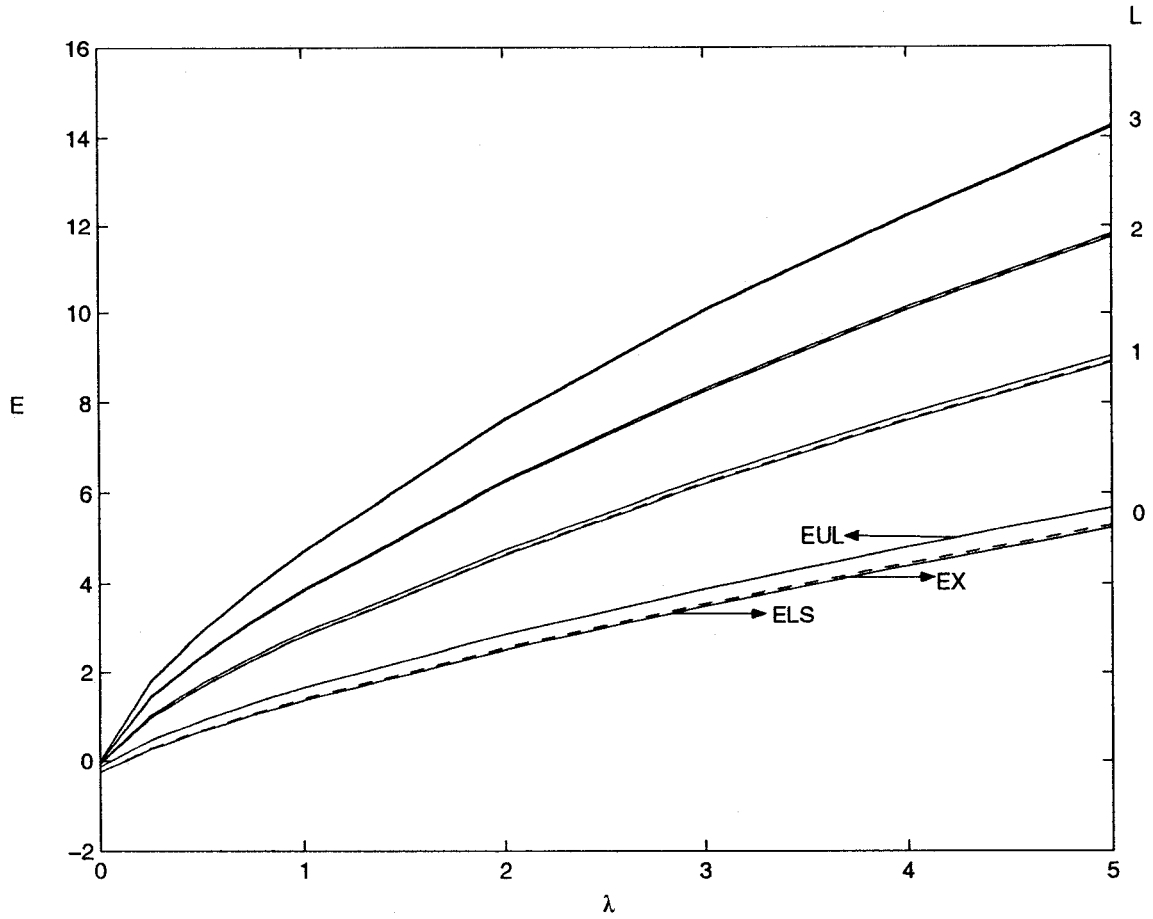

Figure V.1 The eigenvalues $E(\lambda)$ of the Hamiltonian $H = -\Delta - 1/r + \lambda r$ for $N = 3$, $n = 1$, and $\ell = L = 0, 1, 2, 3$. The continuous curves show the upper bound EUL given by the envelope formula (V.2.9) with $\nu = \mu = P^3_{1\ell}(1)$, and the lower bound ELS by the sum approximation given by the same formula but with $\nu = P^3_{1\ell}(1)$ and $\mu = P^3_{1\ell}(-1)$. The dashed curve EX represents accurate numerical data.

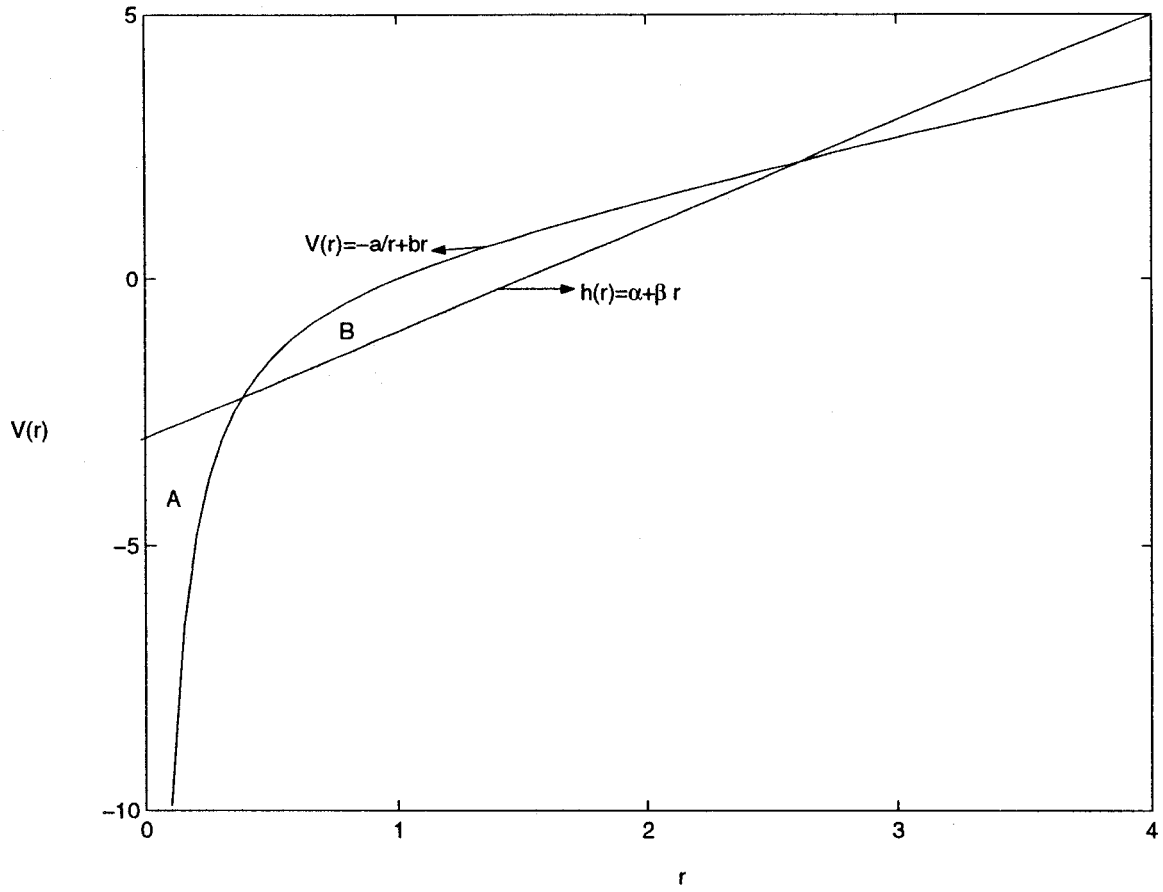

Figure V.2 The linear potential $h(r) = \alpha r + \beta$ used to estimate an upper bound for the eigenvalues of the Coulomb-plus-linear potential $V(r) = -a/r + br$. A and B are the absolute values of the inter-potential areas (or ψ-weighted areas). We vary α and β so that $A = B$, and thereafter Theorems V.5 and V.6 imply $E^V \leq E^h$.

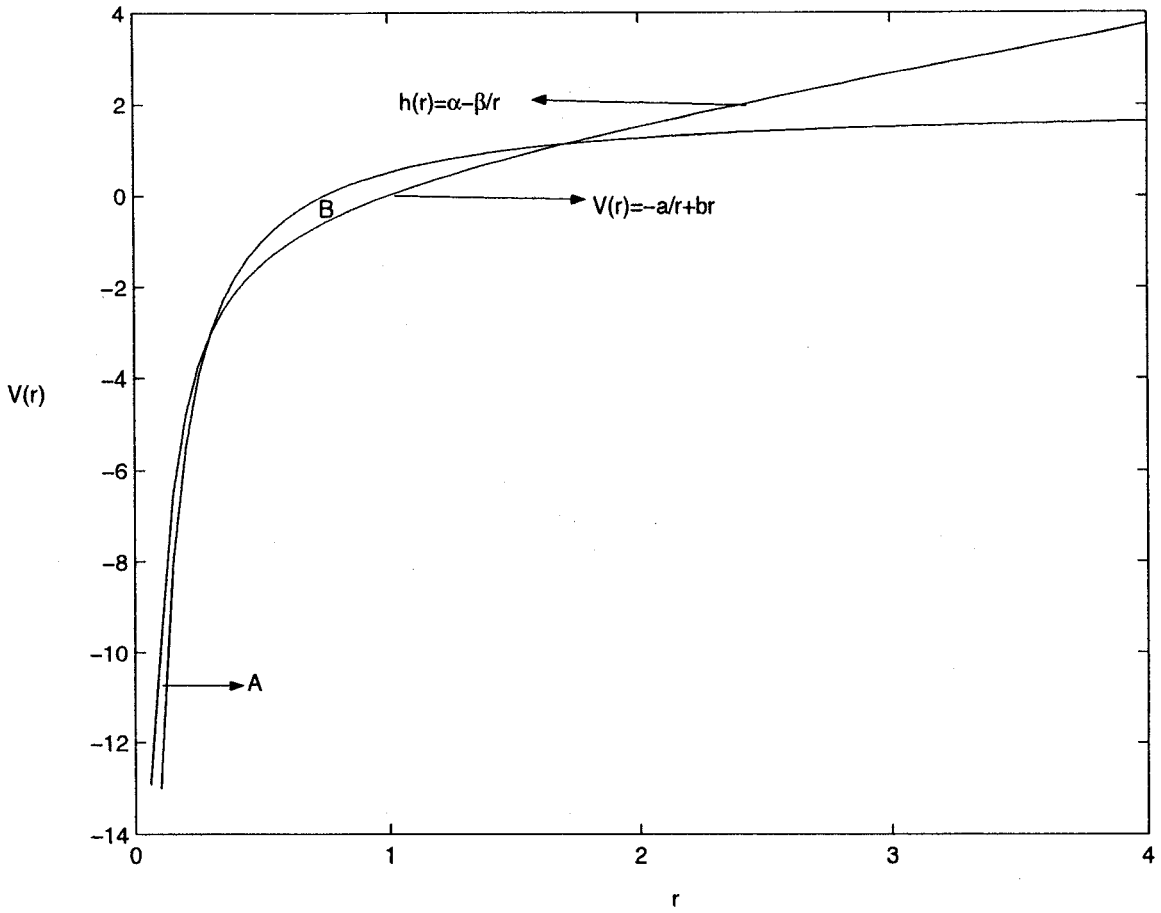

Figure V.3 The hydrogenic potential $h(r) = -\alpha/r + \beta$ used to estimate a lower bound for the eigenvalues of the Coulomb-plus-linear potential $V(r) = -a/r + br$. A and B are the absolute values of the inter-potential areas (or ψ-weighted areas). We vary α and β so that $A = B$, and thereafter Theorems V.5 and V.6 imply $E^h \leq E^V$.

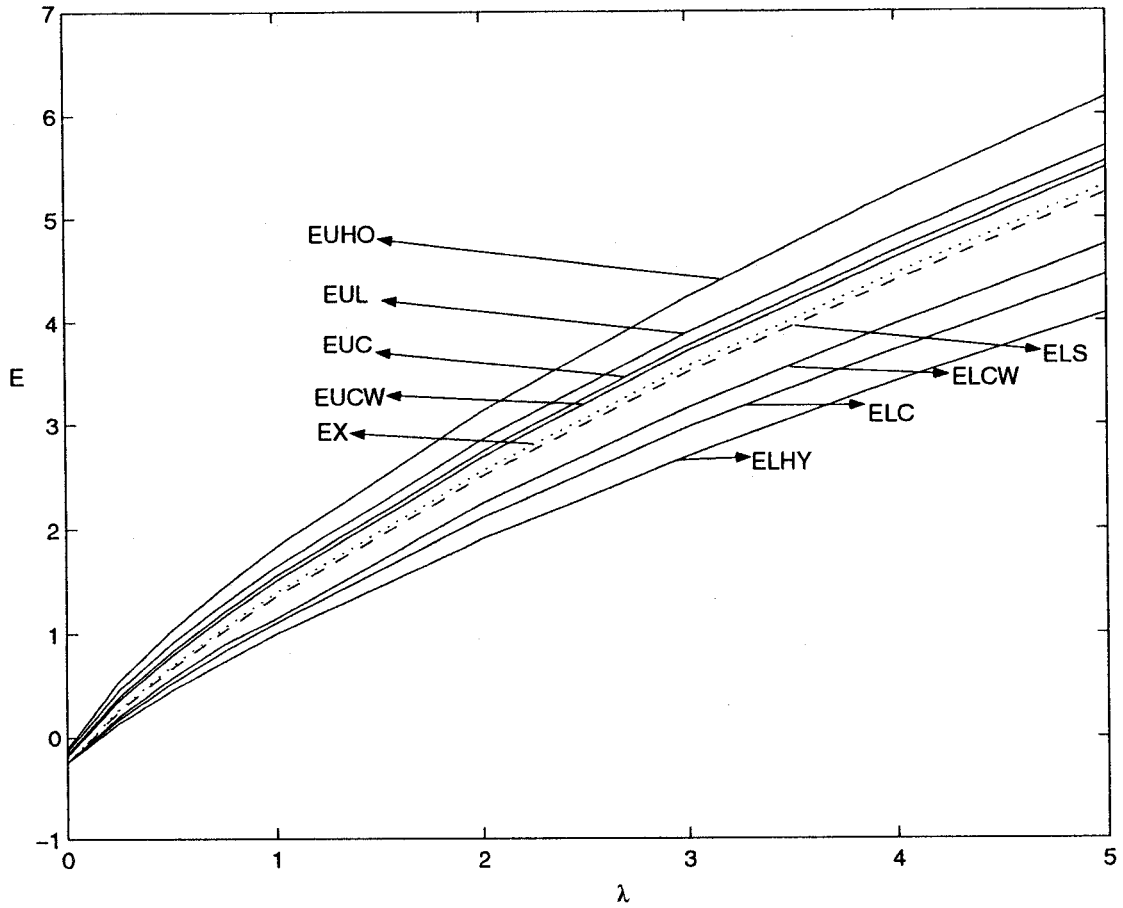

Figure V.4 We compare the bounds for $E(\lambda)$, where $E(\lambda)$ is the ground-state eigenvalue $(n = 1,\ \ell = 0)$ of the Hamiltonian $H = -\Delta - 1/r + \lambda r$. The upper bounds (full-line) are by harmonic-oscillator tangents EUHO, linear tangents EUL, linear chords EUC, and linear chords with the wave function EUCW. The lower bounds (lower full-lines) are by hydrogenic tangents ELHY, Hydrogenic chords ELC, and Hydrogenic chords with the wave function ELCW. The dashed curve ELS represent the lower bound given by the sum approximation. Accurate numerical data (dotted-curve) EX is shown for comparison.

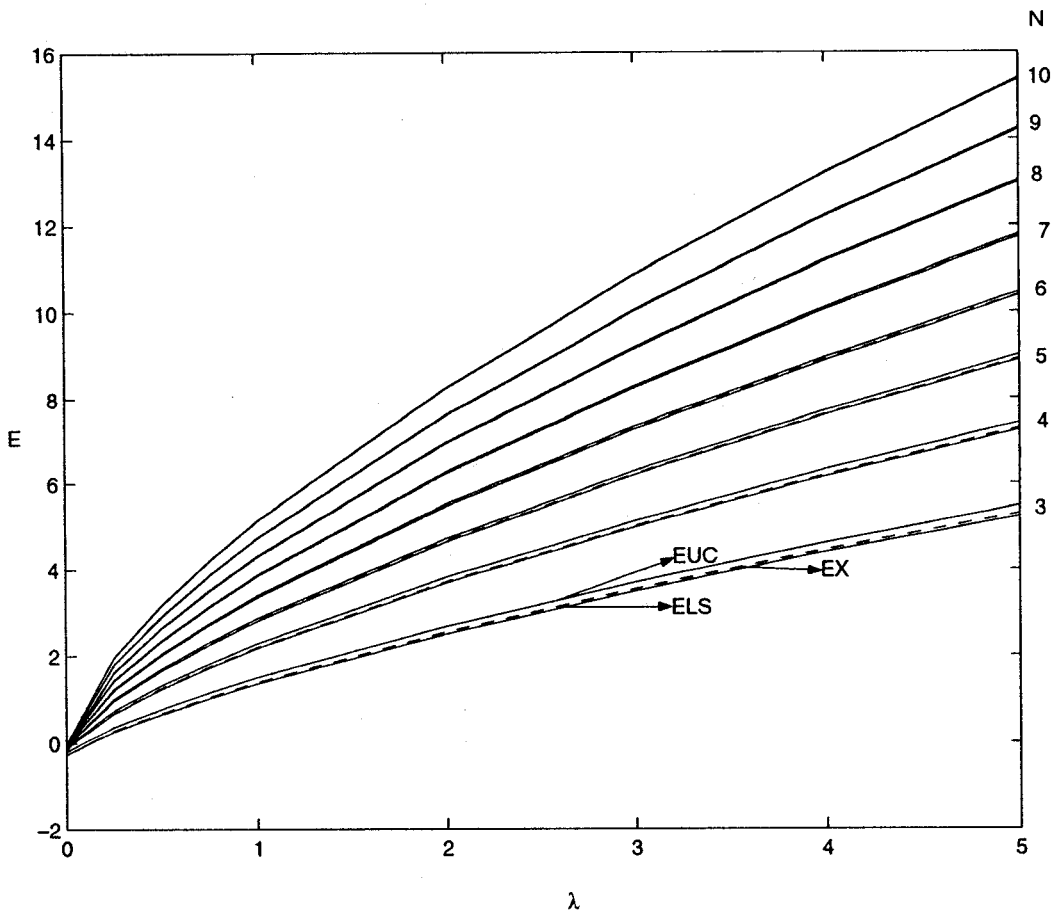

Figure V.5 Bounds on the eigenvalues $E_{10}^{N}(\lambda)$ corresponding to the Coulomb-plus-linear potential $V(r) = -1/r + \lambda r$ in N dimensions. Upper bounds EUC by the generalized comparison theorem, lower bounds ELS by the sum approximation, and accurate numerical data (dashed-line), for $n = 1$, $\ell = 0$, and $N = 3, 4, \ldots 7$. By Theorem V.2 we know that the same curves apply also to $\ell > 0$ since $E_{1\ell}^{N} = E_{10}^{N+2\ell}$.

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Chapter VI

Semiclassical energy formulas for power-law and log potentials in quantum mechanics

We study a single particle which obeys non-relativistic quantum mechanics in R^N with Hamiltonian $H = -\Delta + V(r)$, where $V(r) = \mathrm{sgn(q)r^q}$. If $N \geq 2$, then $q > -2$, and if $N = 1$, then $q > -1$. The discrete eigenvalues $E_{n\ell}$ may be represented exactly by the semiclassical expression $E_{n\ell}(q) = \min_{r>0}\{P_{n\ell}(q)^2/r^2 + V(r)\}$. The case $q = 0$ corresponds to $V(r) = \ln(r)$. By writing one power as a smooth transformation of another, and using envelope theory, it has earlier been proved that the $P_{n\ell}(q)$ functions are monotone increasing. Recent refinements to the comparison theorem of QM, in which comparison potentials can cross over, allow us to prove for $n = 1$ that $Q(q) = Z(q)P(q)$ is monotone increasing, even though the factor $Z(q) = (1+q/N)^{1/q}$ is monotone decreasing. Thus $P(q)$ cannot increase too slowly. This result yields some sharper estimates for power-potential eigenvlaues at the bottom of each angular-momentum subspace.

VI.1. Introduction

In this chapter we study a certain representation, the P-representation, for the Schrödinger spectra generated by the power-law potentials $f(r) = \mathrm{sgn(q)r^q}$ in N spatial dimensions. Considerable interest has been shown in the Schrödinger spectra generated by this elementary class of potentials [1-15]. The Hamiltonian H is given

explicitly by

$$H = -\Delta + v\ \mathrm{sgn(q)r^q},\ \text{where r} = \|\mathrm{r}\| \text{ and v} > 0,\ \text{and q} \neq 0, \qquad \text{(VI.1.1a)}$$

where $q > -1$ for $N = 1$, and $q > -2$ for $N \geq 2$. Corresponding to the case $q = 0$ we have

$$H = -\Delta + v \ln(r),\ v > 0. \qquad \text{(VI.1.1b)}$$

It is certainly possible to include the log potential as a limiting case of the power potentials if in place of the potential family $f(r) = \mathrm{sgn(q)r^q}$, we use $V(r,q) = (r^q - 1)/q$ whose limit as $q \to 0$ is $V(r,0) = \ln(r)$. However, we have chosen instead to leave the power-potentials themselves in their simplest form and incorporate the $q \to 0$ limit smoothly in the spectral domain by means of the P-representation. This limit will be discussed again in this section, after the P-representation has been introduced. As with Eq.(VI.1), our policy of favouring simple powers will again lead to two equations instead of one at various points in the development.

The operators H have domains $\mathcal{D}(H) \subset L^2(R^N)$, they are bounded below, and essentially self adjoint. For the most part we shall be concerned with the cases $N \geq 2$, but we may also include $N = 1$ provided $q > -1$. The one-dimensional hydrogen atom ($N = 1$, $q = -1$) has been extensively studied [16-22] but requires special side conditions not consistent with the class of problems we consider in this chapter. For the operators we consider, the essential spectrum is in $[0, \infty)$ and, by using a normalized Gaussian trial function ϕ, it is easy to select a scale so that $(\phi, H\phi) < 0$, thus estalishing the existence of a discrete eigenvalue; for $q > 0$, the

entire spectrum is discrete by Theorem I.12 in chapter I. The eigenvalues $E^N_{n\ell}$ for the power-law potential can be labelled by two quantum numbers, the total angular momentum $\ell = 0, 1, 2, \ldots$, and a 'radial' quantum number, $n = 1, 2, 3, \ldots$, which represents 1 plus the number of nodes in the radial part of the wave function. These eigenvalues satisfy the relation $E^N_{n\ell} \leq E^N_{m\ell}$, $n < m$. With our labelling convention, the eigenvlaue $E^N_{n\ell}(q)$ in $N \geq 2$ spatial dimensions has degeneracy 1 for $\ell = 0$ and, for $\ell > 0$, the degeneracy is given [24] by the function $\Lambda(N, \ell)$, where

$$\Lambda(N, \ell) = (2\ell + N - 2)(\ell + N - 3)!/\{\ell!(N-2)!\}, \quad N \geq 2, \ \ell > 0. \qquad \text{(VI.1.2)}$$

We first review some general elementary results for the power-law eigenvalues [2]. Nieto and Simons [6] have proved that the eigenvalues $E_n = E^1_{n0}$ for the power-law potentials in one dimension increase with the quantum number n at a higher rate when q is greater. However, for any q, this increase never attains n^2, i.e., $\lim_{n\to\infty} E_n/n^2 = 0$, $q < \infty$. In general, the dependence of the eigenvalues $E^N_{n\ell}$ on the coupling parameter v may be established with the aid of elementary scaling arguments in which r is replaced by σr, where $\sigma > 0$. We find that

$$E^N_{n\ell}(v) = v^{2/(q+2)} E^N_{n\ell}(1). \qquad \text{(VI.1.3)}$$

Thus, without loss of generality, we may limit further discussion to the case of unit coupling, $v = 1$. We shall henceforth let expression such as $E(q)$ represent the dependence of an eigenvalue of unit coupling on the power q.

We do have *some* exactly solvable potentials in N dimensions. For example, for the well-known hydrogenic atom and the harmonic oscillator potentials we have for $n = 1, 2, 3, ...$

$$E^N_{n\ell}(-1) = -[2(n + \ell + N/2 - 3/2)]^{-2}, \quad N \geq 2, \tag{VI.1.4}$$

and

$$E^N_{n\ell}(2) = 4n + 2\ell + N - 4, \quad N \geq 2, \tag{VI.1.5a}$$

and in one dimension (keeping $n = 1, 2, 3, \ldots$)

$$E_n(2) = 2n - 1, \quad N = 1. \tag{VI.1.5b}$$

Analytical solutions are also possible for the linear potential in one dimension, and for the S states in three dimensions. For $N = 1$ and $N = 3$ the repulsive $1/r^2$ term in the 'effective potential' $V_{\text{eff}}(r) = (N-1)(N-3)/4r^2$, obtained using the transformation $\psi(r) = \phi(r)/r^{(N-1)/2}$, is zero. The exact solution in these cases is in terms of the zeros of Airy's function $\text{Ai}(r)$ in three dimensions and the zeros of the first derivative $\text{Ai}'(r)$ of Airy's function in one dimension. We have

$$E^1_n(v) = v^{\frac{2}{3}} r_{n+1}, \quad \text{Ai}'(-r_{n+1}) = 0, \; n = 0, 1, 2, \ldots. \tag{VI.1.6}$$

and

$$E^3_{n0}(v) = v^{\frac{2}{3}} r_n, \quad \text{Ai}(-r_n) = 0, \; n = 1, 2, 3, \ldots. \tag{VI.1.7}$$

Unfortunately, for $N = 2$ or $N > 3$, and for higher angular momenta $\ell > 0$ generally, exact solutions are unavailable at this time. However, by using Theorem V.1 [25,

Theorem 2] we have for $N \geq 2$ the general correspondence $E^N_{n\ell} = E^{N+2\ell}_{n0}$. In Figure VI.1 we exhibit the graphs of the eigenvalues $E^3_{n0}(q)$ for $n = 1 \ldots 5$. In the limit $q \to \infty$ the problem is equivalent to an infinite square well with width 1 in N dimensions. Thus we have $\lim_{q\to\infty} |E^3_{n0}(q)| = (n\pi)^2$. For small values of q, the $|E(q)|$ curves are asymptotically like $|E(q)| \sim C|q/2|^{q/2}$ and have infinite slopes in the limit $q \to 0$ [2,26,27].

The approach in the present chapter is to study a representation for $E_{n\ell}(q)$ which is smoother and easier to approximate than the 'raw' eigenvalues themselves. We shall write many of our equations for the case $N \geq 2$: they are also valid for $N = 1$ provided $q > -1$. In both cases we keep the convention $n = 1, 2, 3, \ldots)$. We have:

$$E^N_{n\ell} = \min_{r>0} \left\{ \left(\frac{P^N_{n\ell}(q)}{r} \right)^2 + \mathrm{sgn(q)r^q} \right\}, \quad q > -2,\ q \neq 0, \tag{VI.1.8a}$$

and

$$E^N_{n\ell} = \min_{r>0} \left\{ \left(\frac{P^N_{n\ell}(0)}{r} \right)^2 + \ln(r) \right\}. \tag{VI.1.8b}$$

The form of this representation, in which the kinetic energy is represented by P^2/r^2 and the power-potential is represented by itself, is what leads us to use the term 'semiclassical' in the title of the paper: the two parts of the quantum-mechanical problem are replaced by simple real functions of r, scaling as the classical terms would scale, and their sum is exactly equal to the quantum-mechanical energy. This is a quite different use of the term 'semiclassical' from that describing a reformulation of the quantum-mechanical problem itself. Such a method is the JWKB

approximation which has been applied to estimate the pure-power spectra [12,13] and could in principle therefore be employed to approximate $P_{n\ell}^N(q)$: however, this approach would not yield exact analytical information about the P-functions, such as bounds or convexity. The existence of this representation $P(q)$ for $E(q)$ is guaranteed because the functions

$$g(P,q) = \min_{r>0}\left\{\left(\frac{P}{r}\right)^2 + \mathrm{sgn(q)r^q}\right\} = \mathrm{sgn(q)}\left(1+\frac{\mathrm{q}}{2}\right)\left(\frac{2\mathrm{P}^2}{|\mathrm{q}|}\right)^{\frac{\mathrm{q}}{2+\mathrm{q}}} \qquad \mathrm{q} > -2,\ \mathrm{q} \neq 0, \tag{VI.1.9a}$$

and

$$g(P,0) = \min_{r>0}\left\{\left(\frac{P}{r}\right)^2 + \ln(r)\right\} = \frac{1}{2}(1+\ln(2)) + \ln(P). \tag{VI.1.9b}$$

are monotone increasing in P. Indeed we find

$$\frac{\partial g}{\partial P}(P,q) = P^{\frac{q}{2+q}}\left(\frac{|q|}{2P}\right)^{\frac{2}{q+2}} > 0, \quad q > -2,\ q \neq 0 \tag{VI.1.10a}$$

and

$$\frac{\partial g}{\partial P}(P,0) = \frac{1}{P} > 0. \tag{VI.1.10b}$$

From $(VI.1.4)$ and $(VI.1.5)$ we find:

$$P_{n\ell}^N(-1) = (n+\ell+N/2-3/2), \quad N \geq 2, \tag{VI.1.11}$$

and

$$P_{n\ell}^N(2) = (2n+\ell+N/2-2), \quad N \geq 2, \tag{VI.1.12a}$$

and in one dimension (keeping $n = 1,2,3,\ldots$)

$$P_n(2) = (n-\frac{1}{2}), \quad N = 1. \tag{VI.1.12b}$$

In Table V.1 we exhibit some numerical values for $P^N_{n\ell}(1)$. The case $q = 0$ corresponds *exactly* to the $\ln(r)$ potential [26]. In this chapter we shall usually denote by $E(q)$ and $P(q)$ the ground-state eigenvalues and P-functions in N dimensions.

We now return briefly to the question of considering the log potential as the limit of the family $V(r,q) = (r^q - 1)/q$, as $q \to 0$, where we define $V(r,0) = \ln(r)$. A useful feature of the P-representation is that, for a given eigenvalue, only one P-number is required to determine the eigenvalue $\mathcal{E}$ corresponding to the 'scaled' power potential $A + B\mathrm{sgn(q)r^q}$, B > 0. Thus, we may write (exactly)

$$\mathcal{E}^N_{n\ell}(A,B,q) = \min_{r>0}\left\{\left(\frac{P^N_{n\ell}(q)}{r}\right)^2 + A + B\mathrm{sgn(q)r^q}\right\}, \quad q > -2,\ q \neq 0,\ B > 0. \tag{VI.1.13}$$

In particular, with $A = -1/q$, $B = 1/|q|$ we have

$$V(r,q) = (r^q - 1)/q \quad \Rightarrow \quad \mathcal{E}^N_{n\ell}(q) = \min_{r>0}\left\{\left(\frac{P^N_{n\ell}(q)}{r}\right)^2 + \frac{r^q - 1}{q}\right\}, \quad q > -2,\ q \neq 0. \tag{VI.1.14}$$

Provided $P(q)$ is continuous, it follows immediately from (VI.1.14) that

$$V(r) = \ln(r) \quad \Rightarrow \quad \mathcal{E}^N_{n\ell} = \min_{r>0}\left\{\left(\frac{P^N_{n\ell}(0)}{r}\right)^2 + \ln(r)\right\}. \tag{VI.1.15}$$

As we mentioned above, the continuity (in fact, monotonicity) of $P^N_{n\ell}(q)$ was proved in Ref. [2]. It is our opinion that the advantage of accommodating this limit easily does not justify the concomitant complication of having to work, for example, with a harmonic oscillator having the form $V(r,2) = (r^2 - 1)/2$.

For $N \geq 2$, the P-numbers and the underlying eigenvalues $E^N_{n\ell}$ satisfy the relation $P^N_{n\ell} = P^{N+2\ell}_{n0}$. This result is obtained using the following theorem

Theorem VI.1. [25, Theorem 2] Suppose that $H = -\Delta + V(r)$, where $V(r)$ is a central potential in $N \geq 2$ dimensions, has a discrete eigenvalue $E^N_{n\ell}$, then $E^N_{n\ell} = E^{N+2\ell}_{n0}$. This theorem expresses the invariance of the eigenvalues with respect to changes in ℓ and N that leave the sum $N + 2\ell$ invariant.

The advantage of the P-representation is illustrated by comparing Figure VI. 1 with Figure VI.2 which show, respectively, the eigenvalues $E_{n\ell}(q)$ and the corresponding P-representations $P_{n\ell}(q)$ for the case $N = 3$. The P-functions of Figure VI.2 are evidently monotone increasing. This property has been proved mathematically by means of envelope theory [2]: one power q was written as a smooth transformation of another p, and then the limit $p \to q$ was taken in the P-picture. The infinite slopes of $E(q)$ at $q = 0$, mentioned above, are not visible in Figure VI.1 because the approach of the slopes to infinity is very slow for such functions: if , for example, we consider [27] the function $f(q) = |q|^q$, then, although $f'(0) = -\infty$, we have $f'(10^{-5}) \approx -10.51$.

The principal result of the present chapter is Theorem VI.4, to the effect that for $N \geq 1$, $Q(q) = Z(q)P(q)$ is monotone increasing, where $Z(q) = (1 + q/N)^{\frac{1}{q}}$: this result is stronger than the monotonicity of $P(q)$ because the factor $Z(p)$ is decreasing; thus we know more about $P(q)$ than we did. This theorem is proved in Section 2 and principally concerns the power-law potentials, but also treats the log case by the use of the limit $q \to 0$ and continuity. As consequences of Theorem VI.4 we shall be able to derive some specific formulas for upper and lower bounds for the power-law energy eigenvalues, by using nearby comparisons. However, it should be

clearly emphasized at this point that the main purpose of the present chapter is to strengthen our knowledge of the monotone function $P(q)$.

Theorem VI.4 has been made possible by the emergence of generalized comparison theorems that allow comparison potentials to cross over and still predict spectral ordering. In Section 2 we restate the generalized comparison theorem (Theorem V.4, of Ref. [25]) which becomes Theorem V.2 here, and we state Theorem VI.3 (Theorem VI.7, of Ref. [25]), which provides explicit sufficient conditions for the application of Theorem VI.3 under a variety of potential crossing schemes. Theorem VI.3 allows us to prove our main result, Theorem VI.4. In Section 3, we use Theorem VI.4 to prove Theorem VI.5 which sharpens the envelope bounds found earlier in Ref. [2]. The earlier result used 'envelope theory' based on the 'standard' comparison theorem, which may be written $V_1 < V_2 \Rightarrow E[V_1] < E[V_2]$. As an illustration of Theorem VI.5 we apply it to generate spectral bounds for the bottom of the spectrum of $-\Delta + r^{\frac{3}{2}}$ in dimensions $N = 3 \ldots 10$.

VI.2. Power-law potentials and generalized comparison theorems

We discussed the generalized comparison theorems which we shall apply to obtain our main result in the previous chapter. We consider the two eigenproblems $(-\Delta + V_1(r))\psi_1(r) = E[V_1]\psi_1(r)$ and $(-\Delta + V_2(r))\psi_2(r) = E[V_2]\psi_2(r)$ in $N \geq 1$ dimensions, where $\psi_i(r)$, $i = 1, 2$, are the respective ground states (or the bottoms of angular-momentum subspaces labelled by a fixed $\ell \geq 0$).

Theorem VI.2. [25, Theorem 4]

$$k(r) = \int_0^r [V_1(t) - V_2(t)]\psi_i(t)t^{N-1}dt < 0, \ \forall r > 0, \ i = 1 \text{ or } 2 \Rightarrow E[V_1] < E[V_2]. \tag{VI.2.1}$$

We stated this theorem (and the following theorem) with strict inequalites: the proofs are essentially the same as given in chapter V and in Ref. [25]. It may be difficult to apply Theorem VI.2 in practice since the positivity of the function $k(r)$ depends on the detailed properties of the comparison potentials. Thus it is helpful to have simpler sufficient conditions, depending on the number and nature of the crossings over of the two comparison potentials. In particular we shall employ the case of two crossings, and sufficient conditions not involving the wave function. Thus we have:

8@Ââ8p@p[illegible]

Theorem VI.3. [23, Theorem 7] If the potentials $V_1(r)$ and $V_2(r)$ cross twice for $r > 0$ at $r = r_1,\ r_2\ \ (r_1 < r_2)$ with

(i) $V_1(r) < V_2(r)$ for $0 < r < r_1$ and

(ii) $\int_0^{r_2} [V_1(t) - V_2(t)] t^{N-1} dt = 0$

then,

$$k(r) = \int_0^r [V_1(t) - V_2(t)] \psi_i(t) t^{N-1} dt < 0,\ \forall r > 0\ ,\ i = 1 \text{ or } 2, \qquad \text{(VI.2.2)}$$

from which $E[V_1] < E[V_2]$ follows, by Theorem VI.2.

Now we shall use the generalized comparison theorems to prove the monotonicity of a new function $Q(q)$, which does not 'vary' so much as the function $P(q)$.

As a consequence we shall be able to derive specific formulas for upper and lower bounds for the power-law energy eigenvalues. We are able to prove the following:

Theorem VI.4. $P(q)$ represents via (VI.1.8) the bottom $E(q)$ of the spectrum of $H = -\Delta + \mathrm{sgn(q)r^q}$, where $q \neq 0$, and $q > -2$, in $N \geq 2$ dimensions (or $q > -1$ for $N = 1$). Define $Q(q) = (1 + q/N)^{1/q} P(q)$, and $Q(0) = \lim_{q \to 0} Q(q) = e^{1/N} P(0)$, then $Q(q)$ is monotone increasing for $N \geq 2$, $q > -2$ (or $N = 1$, $q > -1$).

Proof: Let $p > q$, $p, q > -2$ for $N \geq 2$ and $p, q > -1$ for $N = 1$. We shall first suppose $p \neq 0$ and $q \neq 0$. Our goal is to prove that $Q(p) > Q(q)$. Assume that $V_1(r) = A + B\ \mathrm{sgn(p)r^p}$ and $V_2(r) = \mathrm{sgn(q)r^q}$. Now, we choose A and B so that the potentials $V_1(r)$ and $V_2(r)$ cross over exactly twice, as illustrated in Figure VI.3. Let A_1 and B_1 represent the absolute values of the areas between the potentials. We vary A and B so that $A_1 = B_1$. Then Theorem VI.3 implies $E[V_1] \leq (\geq) E[V_2]$ depending, as r increases from zero, on which potential lies beneath the other when they first differ. Without loss of generality, we will assume, in this sense, that V_1 starts above V_2; this leads to an upper bound. Since $V_1(r)$ is designed to intersect $V_2(r)$ exactly twice, we shall have two equations to solve to provide sufficient conditions for a bound.

$$V_1(R) = V_2(R) \Rightarrow A + B\ \mathrm{sgn(p)R^p} = \mathrm{sgn(q)R^q} \text{ and} \tag{VI.2.3a}$$

$$\int_0^R [V_1(r) - V_2(r)] r^{N-1} dr = 0 \Rightarrow A\frac{R^N}{N} + B\ \mathrm{sgn(p)}\frac{\mathrm{R^{p+N}}}{\mathrm{p+N}} - \mathrm{sgn(q)}\frac{\mathrm{R^{q+N}}}{\mathrm{q+N}} = 0, \tag{VI.2.3b}$$

where R is the second potential intersection point. We let $t = R^{p/q}$ and, solve (2.3a) and (2.3b) for $A(t)$ and $B(t)$, to find

$$A(t) = \frac{\mathrm{sgn(q)Nt^{q^2/p}(p-q)}}{\mathrm{p(q+N)}} \tag{VI.2.4}$$

$$B(t) = \frac{|q|(p+N)}{|p|(N+q)t^{q/p(p-q)}}. \tag{VI.2.5}$$

Without loss of generality, we may consider only the case when p and $q > 0$, since the proof of the other cases is exactly similar. Theorem IV.3 thus implies that

$$\min_t\{A(t) + B(t)^{\frac{2}{(p+2)}} E(p)\} > E(q) \tag{VI.2.6}$$

Optimizing the left side over t, we find the critical point as follows. We define

$$F(t) = A(t) + (B(t))^{\frac{2}{p+2}} E(p) = \frac{Nt^{q^2/p}(p-q)}{p(q+N)} + \left(\frac{q(p+N)}{p(N+q)t^{q/p(p-q)}}\right)^{\frac{2}{p+2}} E(p) \tag{VI.2.7}$$

We now simplify the equation to find the critical point in terms of p and q. We define the following:

$$n = q^2/p,$$

$$m = \frac{q}{p}(p-q)\left(\frac{2}{2+p}\right),$$

$$a_1 = \left(\frac{N(p-q)}{p(q+N)}\right),$$

and

$$b_1 = \left(\frac{q(p+N)}{p(N+q)}\right)^{\frac{2}{2+p}} E(p).$$

Thus we have

$$F(t) = a_1 t^n + b_1 t^{-m}$$

$$F'(t) = a_1 n t^{n-1} - b_1 m t^{-m-1}$$

for which the minimum occurs at $\hat{t} = \left[\frac{b_1 m}{a_1 n}\right]^{\frac{1}{n+m}}$. Meanwhile, the minimum value $F(\hat{t})$ is given by

$$F(\hat{t}) = a_1 \left[\frac{b_1 m}{a_1 n}\right]^{\frac{n}{n+m}} + b_1 \left[\frac{b_1 m}{a_1 n}\right]^{-\frac{m}{n+m}}$$

$$= a_1^{\frac{m}{n+m}} b_1^{\frac{n}{n+m}} \left[\frac{m}{n}\right]^{-\frac{m}{n+m}} \left[\frac{m}{n} + 1\right] \quad \geq E(q).$$

By substituting $F(\hat{t})$ and $E(p)$ given by (VI.1.9) in (VI.2.6), we find that

$$\left(\frac{N(p-q)}{p(q+N)}\right)^{\frac{2(p-q)}{p(q+2)}} \left[\left(\frac{q(N+p)}{p(q+N)}\right)^{\frac{2}{2+p}} \left(\frac{p+2}{2}\right) \left(\frac{2P(p)^2}{p}\right)^{\frac{p}{p+2}}\right]^{\frac{q(2+p)}{p(q+2)}} \times$$

$$\left[\frac{q(p+2)}{2(p-q)}\right]^{\frac{2(p-q)}{p(q+2)}} \left[\frac{p(q+2)}{q(p+2)}\right] > \left(\frac{q+2}{2}\right) \left(\frac{2P(q)^2}{q}\right)^{\frac{q}{2+q}}. \qquad \text{(VI.2.8)}$$

By simplifying this expression, we find eventually that $Q(q) = (1+q/N)^{1/q} P(q)$ is monotone increasing, that is to say

$$Q(p) > Q(q). \qquad \text{(VI.2.9)}$$

Now for $N \geq 2$, $P(q)$ is continuous, $q > -2$, (or for $N = 1$, $q > -1$), and, if we define $Z(0) = \lim_{q \to 0} Z(q) = e^{1/N}$, then $Q(0) = Z(0)P(0)$. It follows immediately that $Q(q) = Z(q)P(q)$ is continuous and monotone increasing $q > -2$ (or for $N = 1$, $q > -1$). □

The three functions $P(q)$, $Z(q)$, and $Q(q)$ are illustrated for $N = 3$ in Figure VI.4: Theorem VI.4 states that in all dimensions $N \geq 1$, $Q(q)$ is a monotone increasing function of q.

VI.3. Application

By using the monotonicity of the function $Q(q)$, we now prove a special comparison theorem (a corollary to Theorem VI.4) for the comparison of eigenvalues generated by power-law potentials.

Theorem IV.5. Consider the power-law potentials $V_i(r) = \mathrm{sgn}(q_i) r^{q_i}$, $q_i > -2$, ($q_i > -1$, for $N = 1$), $i = 1, 2$, where $q_1 < q_2$. Let $Z(q) = (1 + q/N)^{1/q}$, $Z(0) = \lim_{q \to} Z(q) = e^{1/N}$, $Q(q) = Z(q)P(q)$, and $g(P, q)$ be given by (VI.1.9a) and (VI.1.9b), then

(i) $E[V_1] < E_1^U = g(P(q_2), q_1)$,

(ii) $E[V_2] > E_1^L = g(P(q_1), q_2)$,

(iii) $E[V_1] < E_2^U = g\left(\frac{Q(q_2)}{Z(q_1)}, q_1\right) < E_1^U$,

(iv) $E[V_2] > E_2^L = g\left(\frac{Q(q_1)}{Z(q_2)}, q_2\right) > E_1^L$.

Proof: We first establish the upper bound (iii). We note that the function $Z(q) = (1 + q/N)^{1/q}$ is decreasing. Thus $q_1 < q_2$, implies $Z(q_2) < Z(q_1)$, and by using the monotonicity of the functions $P(q)$ [2] and $g(P, q)$, we may conclude that $P(q_1) < Z(q_2)P(q_2)/Z(q_1) = Q(q_2)/Z(q_1) < P(q_2)$, which, in turn, implies $E[V_1] < E_2^U < E_1^U$. This proves (i) and (iii). After a reversal of the inequalities, the proofs for the lower bounds (ii) and (iv) follow similarly. □

We note that Theorem IV.5 includes applications to the log potential. For example, if $q_1 = 0$ and $q_2 = q > 0$, then we have from Theorem IV.5 (iv)

$$E(q) > \min_{r>0} \left\{ \left(\frac{Q(0)}{Z(q)r} \right)^2 + \mathrm{sgn(q)r^q} \right\}, \quad q > 0. \tag{VI.3.1}$$

Example: $V(r) = r^{\frac{3}{2}}$

We illustrate Theorem IV.5 by applying it to the potential $V(r) = r^{\frac{3}{2}}$ in $N \geq 3$ dimensions. We first use the linear and the harmonic oscillator problems to obtain upper and lower bounds by envelope theory. That is to say, we first use Eq.(VI.1.9a) to give the envelope lower bound ELP given by $g(P(1), 3/2)$, and the envelope upper bound EUP given by $g(P(2), 3/2)$. Then we use Theorem IV.5 (iv) to generate the improved lower bound ELQ given by $g(Q(1)/Z(3/2), 3/2)$, and Theorem IV.5 (iii) to generate the improved upper bound EUQ given by $g(Q(2)/Z(3/2), 3/2)$. These results are shown in Figure VI.5, along with accurate numerical data EX, for $N = 3 \ldots 10$: they illustrate the improvement obtained in the approximation when Q is used rather then P in the semiclassical energy formulas.

VI.4. Conclusion

The eigenvalues $E(q)$ of $H = -\Delta + \mathrm{sgn(q)r^q}$, $q > -2$, $q \neq 0$, may be conveniently represented by the functions $P(q)$, which are known [2] to be positive, continuous, and monotone increasing. In the proof of the earlier result, each q-potential was written as a smooth transformation of a p-potential with definite

convexity, and then 'envelope theory' was applied. The envelope method, in turn, depends on the 'standard' comparison theorem of quantum mechanics. In the present chapter we use a stronger comparison theorem, valid for node-free states in N dimensions, and we are able thereby to learn more about $P(q)$ for the bottom of each angular-momentum subspace ($n = 1$). If $N > 1$ and $\ell > 0$, we use the equivalence $E^N_{1\ell} = E^{2\ell+N}_{10}$. We have shown for all these problems that $Q(q) = P(q)Z(q)$ is monotone increasing, where the factor $Z(q) = (1 + q/N)^{1/q}$ is decreasing. This immediately leads to some sharpened spectral inequalites concerning pairs of power-law Hamiltonians.

The $P(q)$ functions are important for an established general lower bound for potentials which are sums of powers. Thus if $V(r) = \sum_q a(q)\mathrm{sgn(q)r^q} + \mathrm{a(0)\,ln(r)}$, then we have [1, 31] for the bottom of each angular-momentum subspace in $N \geq 2$ dimensions:

$$E^N_{1\ell} \geq \min_{r>0}\left\{\frac{1}{r^2} + \sum_q a(q)\ \mathrm{sgn(q)}\left(\mathrm{P^N_{1\ell}(q)r}\right)^{\mathrm{q}}\ + \mathrm{a(0)\ln}\left(\mathrm{P^N_{1\ell}(0)r}\right)\right\}.$$

This formula, which is easily extended to smooth mixtures defined by an integral, is exact whenever the non-negative 'weight' $a(q)$ is concentrated on a single term. The lower bound is preserved if the P-numbers are replaced by lower bounds to them. Thus any information concerning these fundamental numbers for the power-law potentials immediately has application to this general lower bound. These numbers have yielded useful energy bounds also for the many-body problem [32], and for relativistic problems [33, 34].

In spite of the simplicity of the power-law potentials and the attractive scaling

properties of the corresponding Schrödinger eigenvalues, general results concerning the unit-coupling eigenvalues $E(q)$ seem to be difficult to obtain. One might expect that the results of the present chapter would extend to all the excited states, but we know of no way at present to prove such general results. Even more ellusive seems to be a proof of the apparent concavity of all the $P(q)$ functions, some of which are illustrated for $N = 3$ in Figure VI.2. The establishment of concavity of $P(q)$ (or better, $Q(q)$) would immediately yield a large number of new spectral inequalities arising from the use of tangents and chords to the corresponding graphs.

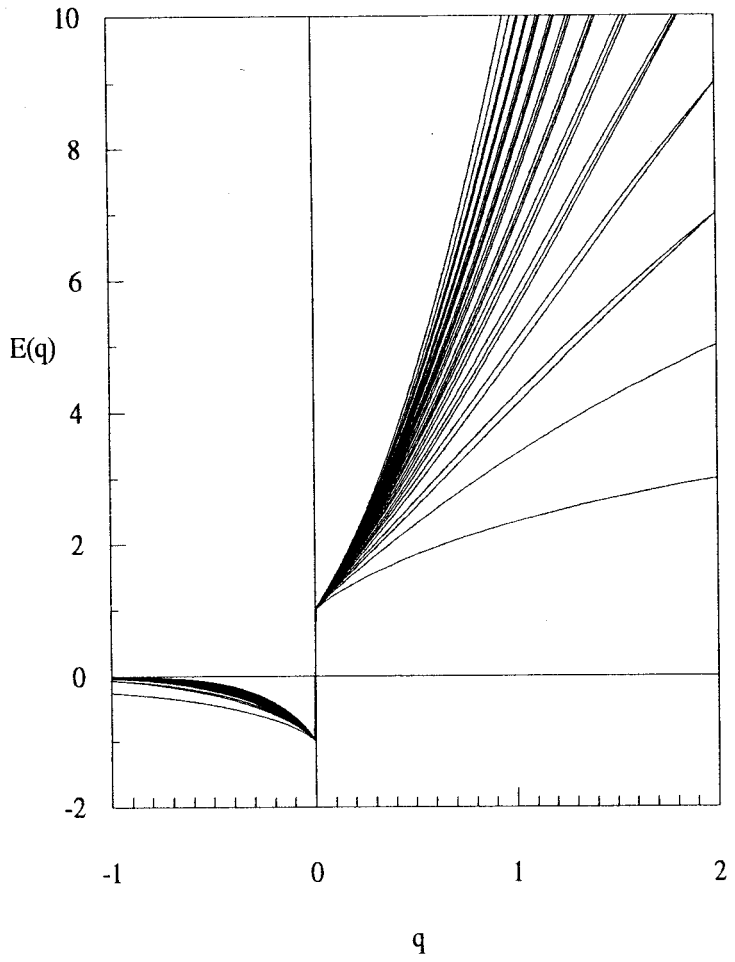

Figure VI.1. The first 30 eigenvalues $E_{n\ell}(q)$, $1 \leq n \leq 5$, $0 \leq \ell \leq 5$, corresponding to the power potential $V(r) = \mathrm{sgn(q)r^q}$ in $N = 3$ dimensions. For $q > 0$, the eigenvalues increase with q from 1 to $E_{n\ell}(2) = 4n + 2\ell - 1$; for $q < 0$, they decrease (as q increases) from $E_{n\ell}(-1) = -[2(n + \ell)]^{-2}$. to -1. Both sets of curves increase with n and ℓ.

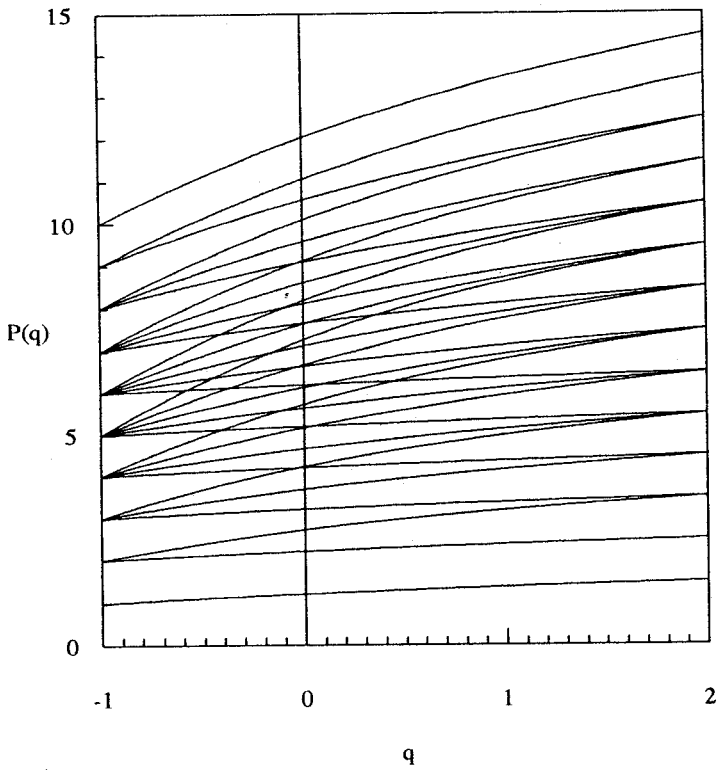

Figure VI.2. In the P-representation, the same set of 30 eigenvalues shown in Fig.(1) now lie on monotone smooth curves. The log-power theorem states that the P values for the log potential are precisely $P_{n\ell}(0)$. As q increases from -1 to 2, the degeneracy of the Coulomb problem $P_{n\ell}(-1) = n + \ell$ evolves into the degeneracy of the harmonic oscillator $P_{n\ell}(2) = 2n + \ell - \frac{1}{2}$.

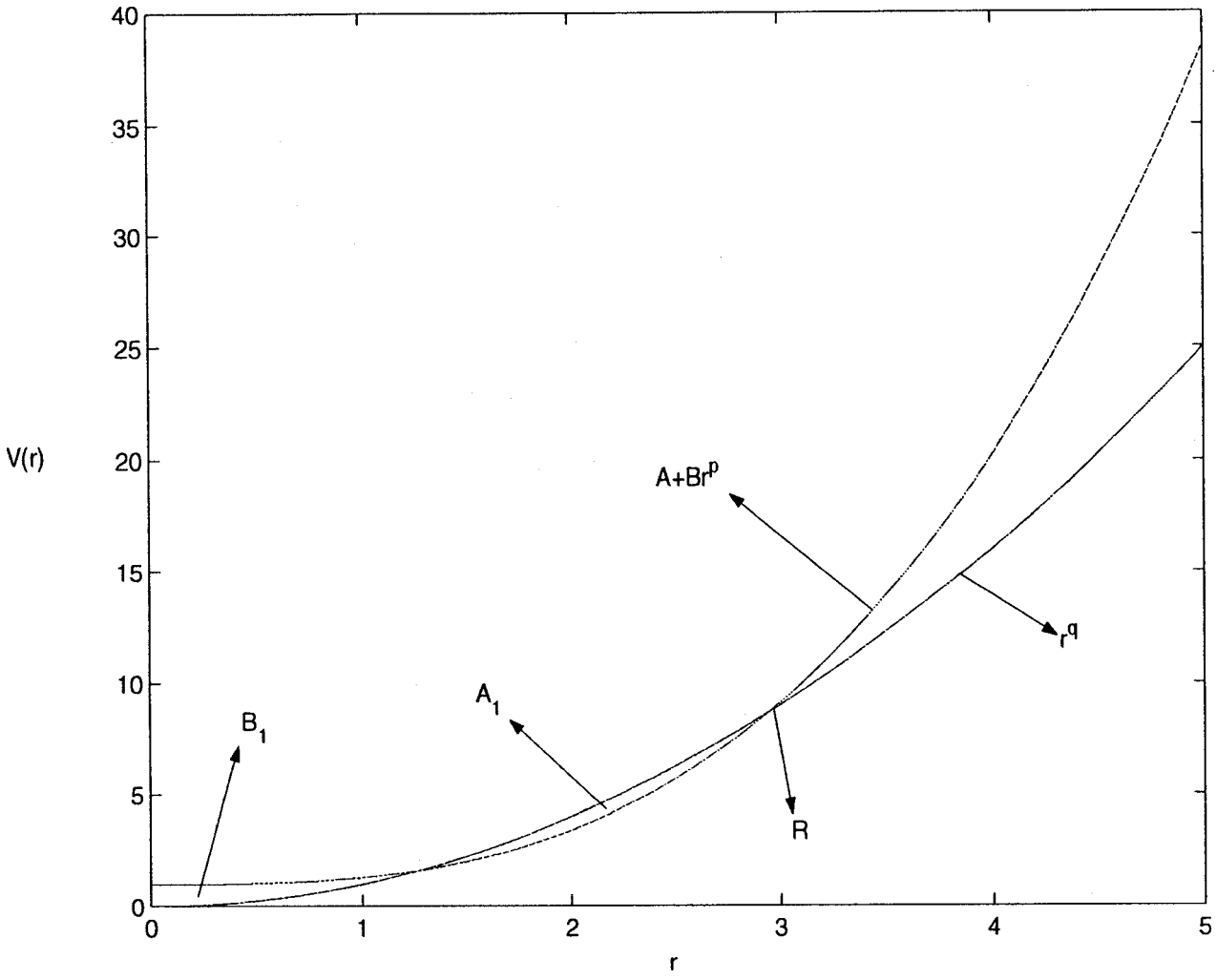

Figure VI.3. The shifted linear potential $V_1(r) = A + Br^p$ used to estimate an upper bound for the eigenvalues corresponding to the potential $V_2(r) = r^q$. A_1 and B_1 are the absolute values of the inter-potential areas. We vary A and B so that $A_1 = B_1$, where R is the second intersection point. Thereafter, Theorem VI.3 implies that $E[V_2] \leq E[V_1]$. This result is used to prove the monotonicity of $Q(q)$.

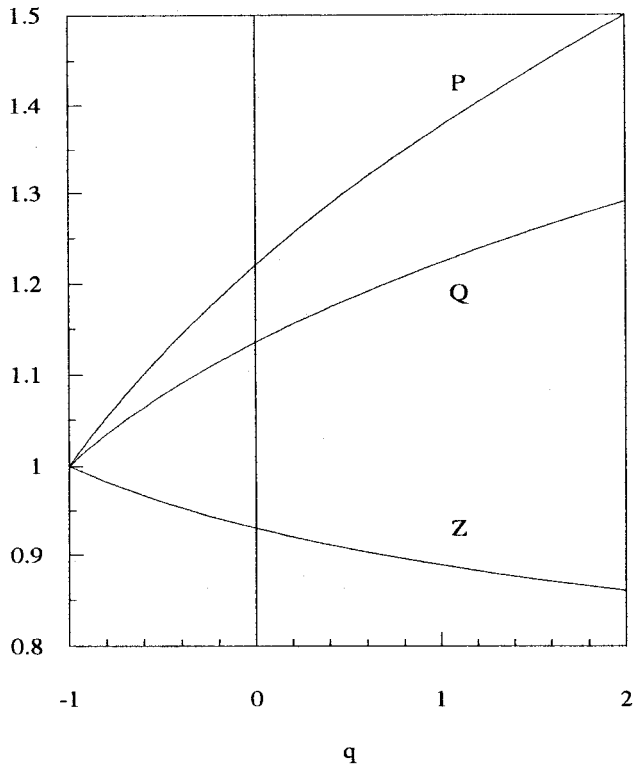

Figure VI.4. The functions $P(q)$, $Z(q)$, and $Q(q) = P(q)Z(q)$ for the ground state in dimension $N = 3$. Theorem VI.4 states that for the ground state in all dimensions $N \geq 1$, $Q(q)$ is monotone increasing with q.

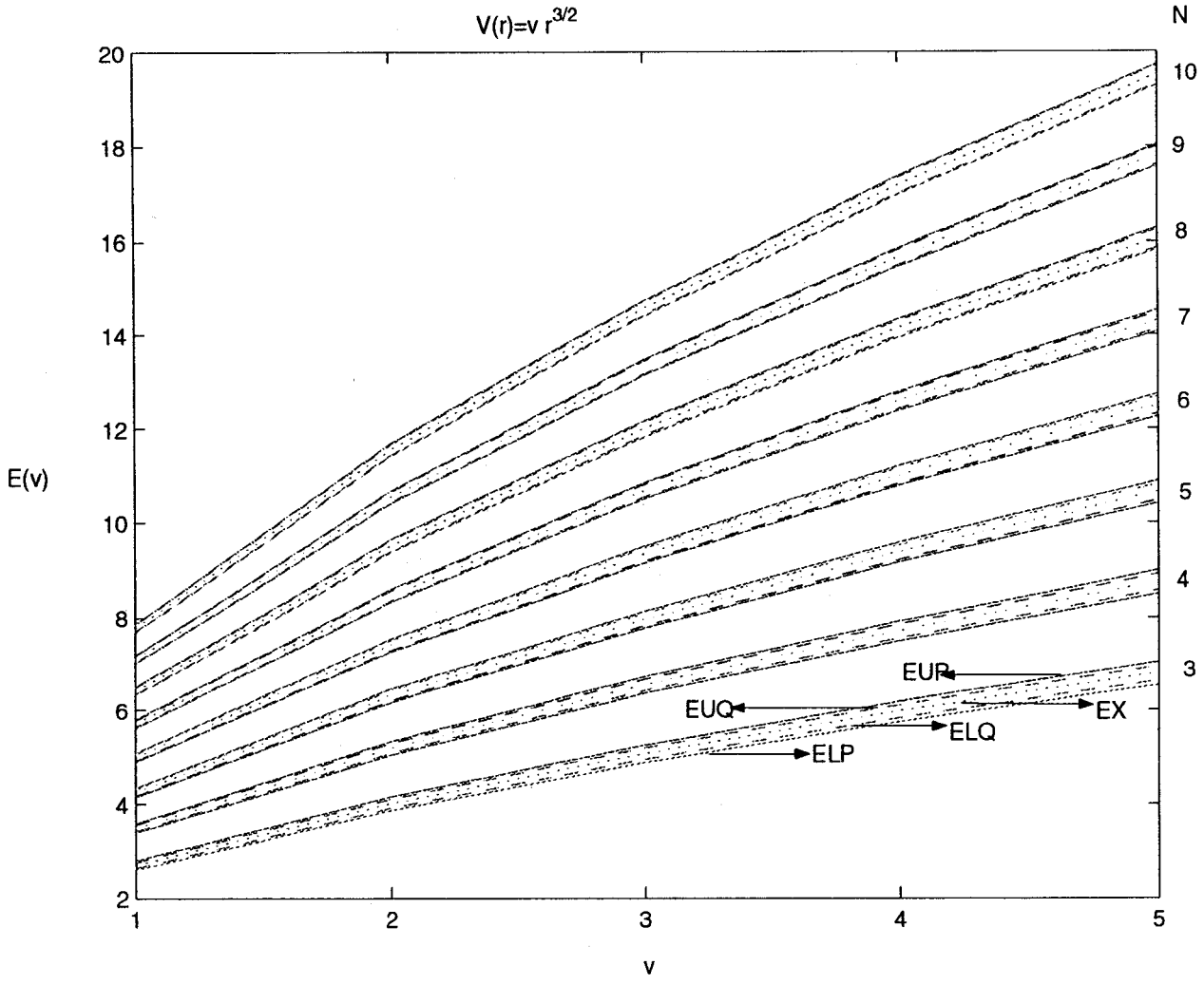

Figure VI.5. Bounds on the eigenvalues $E_{10}^{N}(v)$ corresponding to the power potential $V(r) = vr^{\frac{3}{2}}$ in N dimensions. The upper and lower bounds (full lines) are obtained by harmonic-oscillator tangents EUP, and linear tangents ELP (Theorem VI.5 (i),(ii)). The dashed curves EUQ and ELQ represent respectively the improved upper and lower bounds (Theorem VI.5 (iii),(iv)). Accurate numerical data (dotted curves) EX are shown for comparison.

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Chapter VII

Coulomb plus power-law potentials in quantum mechanics

We study the discrete spectrum of the Hamiltonian $H = -\Delta + V(r)$ for the Coulomb plus power-law potential $V(r) = -1/r + \beta\ \mathrm{sgn(q)r^q}$, where $\beta > 0$, $q > -2$ and $q \neq 0$. We show by envelope theory that the discrete eigenvalues $E_{n\ell}$ of H may be approximated by the semiclassical expression $E_{n\ell}(q) \approx \min_{r>0}\{1/r^2 - 1/(\mu r) + \mathrm{sgn(q)}\beta(\nu \mathrm{r})^{\mathrm{q}}\}$. Values of μ and ν are prescribed which yield upper and lower bounds. Accurate upper bounds are also obtained by use of a trial function of the form, $\psi(r) = r^{\ell+1}e^{-(\alpha r)^d}$. We give detailed results for $V(r) = -1/r + \beta r^q$, $q = 0.5, 1, 2$ for $n = 1$, $\ell = 0, 1, 2$, along with comparison eigenvalues found by direct numerical methods.

[Note: Section VII.3 of this chapter is joint work with Dr. Hakan Ciftci of Ankara, Turkey].

VII.1. Introduction

In this chapter we derive upper and lower bound formulas for the spectrum of a single particle in three dimensions that obeys non-relativistic quantum mechanics and has Hamiltonian

$$H = -\omega\Delta - A/r + B\mathrm{sgn(q)r^q}, \quad \omega,\ \mathrm{A},\ \mathrm{B} > 0,\ \text{and}\ \mathrm{q} \neq 0,\ \mathrm{q} > -2. \qquad \text{(VII.1.1)}$$

The Coulomb plus power-law potential is of interest in particle physics where it serves as a non-relativistic model for principle part of the quark-quark interac-

tion. This class of potentials has been well studied and much work has been done to approximate the eigenvalues, with or without the Coulomb term necessitated by QCD [1-14]. Our goal in this chapter is to provide simple formulas for upper and lower energy bounds for this class of potentials. Firstly, we use the 'envelope method' [15,16] to obtain upper and lower bound formulas for all the discrete eigenvalues. We also use a Gaussian trial function and the 'sum approximation' [17,18] to improve the bounds for the bottom of each angular-momentum subspace. The energy bounds so far discussed may all be expressed in terms of the following semi-classical energy formula:

$$\mathcal{E} \approx \min_{r>0}\left\{\omega\frac{1}{r^2} - \frac{A}{\mu r} + B\mathrm{sgn(q)}(\nu \mathrm{r})^{\mathrm{q}}\right\} \qquad \text{(VII.1.2)}$$

for suitable choices of the parameters $\mu > 0$ and $\nu > 0$. We also apply a variational method used earlier [19] which is based on the exact Coulomb wave function and yields accurate upper bounds for the bottom of each angular momentum subspace. We compare all these results with 'exact' eigenvalues computed by direct numerical integration.

For the class of potentials studied some exactly solvable cases exist for suitable values of the couplings ω, A, B, and the power q. For example, for the well-known hydrogenic atom and the harmonic oscillator potentials we have explicitly for $n = 1, 2, 3, ...$

$$q = -1 \quad \Rightarrow \quad E_{n\ell} = -\frac{A^2}{4\omega(n+\ell)^2} \qquad \text{(VII.1.3)}$$

and

$$q = 2 \quad \Rightarrow \quad E_{n\ell} = (\omega B)^{\frac{1}{2}}(4n + 2\ell - 1). \tag{VII.1.4}$$

For $\ell = 0$, exact solutions are also available for the linear potential $q = 1$. We can simplify the coupling problem in general by the use of scaling arguments. If, for each fixed q, we denote the eigenvalues of $H = -\omega\Delta - A/r + Br^q$ by $\mathcal{E}(\omega, A, B)$, and consider a scale change of the form $s = r/\sigma$, and choose the scale $\sigma = \omega/A$, then it is straightforward to show that,

$$\mathcal{E}(\omega, A, B) = \left(\frac{A^2}{\omega}\right)\mathcal{E}(1, 1, \beta), \quad \beta = \left(\frac{B}{\omega}\right)\left(\frac{\omega}{A}\right)^{q+2}. \tag{VII.1.5}$$

Hence, the full problem is now reduced to the simpler one-parameter problem

$$H = -\Delta - 1/r + \beta\ \mathrm{sgn(q)r^q}, \quad \mathrm{E} = \mathrm{E}(\beta) = \mathcal{E}(1, 1, \beta),\ \beta > 0. \tag{VII.1.6}$$

VII.2. Energy bounds by the envelope method and the sum approximation

We use again the 'envelope method' [15, 16] explained in the previous chapters to analyse the spectrum for the Coulomb plus power-law potentials. In Table VII.1 we exhibit some numerical values for $P_{n\ell}(\frac{1}{2})$ and $P_{n\ell}(1)$. We have found the exact eigenvalues for the linear potential in terms of the zeros of the Airy function, but those for $q = \frac{1}{2}$ have to be computed numerically: this use of some isolated numerical input is justified since, for each $\{n, \ell\}$ pair, the resulting approximation formulas include all the potential parameters but depend only on a single 'numerical input'. Envelope theory [12, 17] shows that the eigenvalues of the Coulomb plus

power-law potential may be approximated by the following semiclassical expression,

$$\mathcal{E} \approx \min_{r>0}\left\{\frac{1}{r^2} - \frac{1}{\mu r} + \beta\ \mathrm{sgn(q)}(\nu \mathrm{r})^{\mathrm{q}}\right\},\ \text{where } \mu,\ \nu > 0. \qquad \text{(VII.2.1)}$$

Since $V(r) = g(h(r))$ is at once a convex function of $h(r) = -1/r$ and a concave function of $h(r) = \mathrm{sgn(q)r^q}$, the spectral representation $P_{n\ell}(q)$ allows us to specify upper and lower bounds formulas as follows. If $\mu = \nu = P_{n\ell}(-1)$, then $\mathcal{E}$ is a lower bound for $E_{n\ell}$, and if $\mu = \nu = P_{n\ell}(q)$, then $\mathcal{E}$ is an upper bound. We may improve the lower bound for the bottom of each angular momentum subspace by using the sum approximation [17,18], which is equivalent to the choice $\mu = P_{1\ell}(-1) = (\ell + 1)$ and $\nu = P_{1\ell}(q)$. For the bottom of the spectrum we can also improve the upper bound by using a Gaussian trial function and minimizing over scale: this is equivalent [12] to using the parameter values

$$\mu = \nu = P_{10}^{U} = \left(\frac{3}{2}\right)^{\frac{1}{2}}\left[\frac{2\Gamma((3+q)/2)}{\sqrt{\pi}}\right]^{\frac{1}{q}}. \qquad \text{(VII.2.2)}$$

We note that the *same* parameters μ and ν which guarantee that (VII.2.1) yields various energy bounds may also be used in the 'full' semiclassical formula (VII.1.2), including all the original Hamiltonian parameters $\{\omega, A, B\}$. In Section VII.3 we apply (VII.2.1) to the explicit cases $V(r) = -1/r + \beta\ r^q$ for $\ell = 0, 1, 2$, where $q = 1, 2$, and 0.5.

VII.3. Variational method

The second approach in this chapter is to use a trial function explored in previous work [19] to obtain accurate upper bounds for the bottom of each angular momentom subspace. We start with Schrödinger's equation

$$H\psi(r) = \left(-\Delta - \frac{1}{r} + \beta\ \mathrm{sgn(q)r^q}\right)\psi(r) = E_{n\ell}(\beta)\psi(r), \quad q \neq 0,\ q > -2. \quad \text{(VII.3.1)}$$

This problem is solvable if $\beta = 0$, and the corresponding wave function $\psi(r)$ is given by

$$\psi(r) = r^{\ell+1}e^{-xr}L_n^{2\ell+1}(2xr). \quad \text{(VII.3.2)}$$

In order to obtain an upper bound for the bottom of each angular momentum subspace $E_{1\ell}$ for fixed power q we choose $\psi(r)$ to be of the following form

$$\psi(r) = r^{\ell+1}e^{-(xr)^d} \quad \text{(VII.3.3)}$$

and define $\mathcal{E}$ by $\mathcal{E}(\beta, x, d) = \frac{(\psi, H\psi)}{(\psi,\psi)}$, where x and d are variational parameters. Now, we minimize $\mathcal{E}$ with respect to x and d. The necessary conditions for a critical point are $\frac{\partial \mathcal{E}}{\partial x} = 0$ and $\frac{\partial \mathcal{E}}{\partial d} = 0$. Consequently, using (VII.3.1) and (VII.3.3), we obtain the following upper bound formula for the eigenvalues $E_{1\ell}$

$$\mathcal{E}_{1\ell}(\beta, d, x) = a_1x^2 - a_2x + a_3x^{-q}, \quad \text{(VII.3.4)}$$

where a_1, a_2 and a_3 are as given below

$$a_1 = 2^{\frac{2-2d}{d}}\frac{(2\ell+1)(2\ell+d+1)\Gamma(\frac{2\ell+1}{d})}{\Gamma(\frac{2\ell+3}{d})}$$

$$a_2 = 2^{\frac{1}{d}} \frac{\Gamma(\frac{2\ell+2}{d})}{\Gamma(\frac{2\ell+3}{d})},$$

$$a_3 = \mathrm{sgn(q)}\beta 2^{\frac{-q}{d}} \frac{\Gamma(\frac{2\ell+q+3}{d})}{\Gamma(\frac{2\ell+3}{d})}.$$

By using (VII.3.4) we derive the following equation for x

$$x^{q+2} - \frac{a_2}{2a_1}x^{q+1} - \frac{qa_3}{2a_1} = 0. \qquad \text{(VII.3.5)}$$

After solving Eq.(VII.3.5) to obtain x, from the numerical solution of $\frac{\partial \varepsilon}{\partial d} = 0$ we find d for $n = 1$ and $\ell = 0$, and then we use the same d value for all ℓ.

VII.4. Conclusion

We have found general semiclassical energy formulas (VII.1.2) and (VII.2.1) for the eigenvalues generated by the Coulomb plus power-law potentials. Specific values for the parameters μ and ν are given which guarantee that the formulas yield bounds for all the discrete energies. By using a more finely tuned wavefunction, we have also derived an improved upper bound (VII.3.4) valid for the bottom of each angular momentum subspace. We may rewrite (VII.2.1) in the form of a pair of parametric equations for the curve $\{\beta,\ E(\beta)\}$. For fixed $q > -1$ we obtain:

$$\beta = \frac{1}{|q|(\nu r)^q}\left(\frac{2}{r^2} - \frac{1}{\mu r}\right),$$

$$E(\beta) = \frac{1+2/q}{r^2} - \frac{1+1/q}{\mu r}. \qquad \text{(VII.4.1)}$$

By envelope theory, we know that these parametric equations yield a lower bound if $\mu = \nu = P_{n\ell}(-1) = (n+\ell)$, and an upper bound when $\mu = \nu = P_{n\ell}(q)$. For the

bottom of each angular momentum subspace the prescription $\mu = P_{1\ell}(-1) = (\ell+1)$, $\nu = P_{1\ell}(q)$ yields an improved lower bound. An improved upper bound for the bottom of the spectrum is given by using the 'Gaussian' P-numbers (VII.2.2). In Figures 1, 2, and 3, we plot the function $E(\beta)$ for $n = 1\,, \ell = 0, 1, 2$ for the Coulomb plus harmonic oscillator $(q = 2)$, Coulomb plus linear $(q = 1)$, and Coulomb plus $r^{0.5}$ potentials, along with the corresponding accurate variational bounds using (VII.3.4) (dashed line), and some comparison numerical values represented as stars. The advantage of the semiclassical formulas is that they describe in approximate analytical form how the eigenvalues depend on all the parameters of the problem.

Table VII.1 The 'input' values $P_{n\ell}(\frac{1}{2})$ and $P_{n\ell}(1)$ to be used in the general formula (VII.2.1) for the energies corresponding to the potential $V(r) = -1/r + \beta\ \mathrm{sgn(q)r^q}$. These P-values yield upper bounds when $q \leq \frac{1}{2}$, or $q \leq 1$, respectively.

n	ℓ	$P_{n\ell}(\frac{1}{2})$	$P_{n\ell}(1)$
1	0	1.30266	1.37608
2	0	2.97387	3.18131
3	0	4.65440	4.99255
4	0	6.33742	6.80514
5	0	8.02149	8.61823
1	1	2.29747	2.37192
2	1	3.93966	4.15501
3	1	5.60154	5.95300
4	1	7.27194	7.75701
5	1	8.94679	9.56408
1	2	3.29535	3.37018
2	2	4.92261	5.14135
3	2	6.57089	6.92911
4	2	8.23022	8.72515
5	2	9.89619	10.52596
1	3	4.29424	4.36923
2	3	5.91240	6.13298
3	3	7.55077	7.91304
4	3	9.20118	9.70236
5	3	10.85929	11.49748
1	4	5.29352	5.36863
2	4	6.90560	7.12732
3	4	8.53658	8.90148
4	4	10.17964	10.68521
5	4	11.83110	12.47532

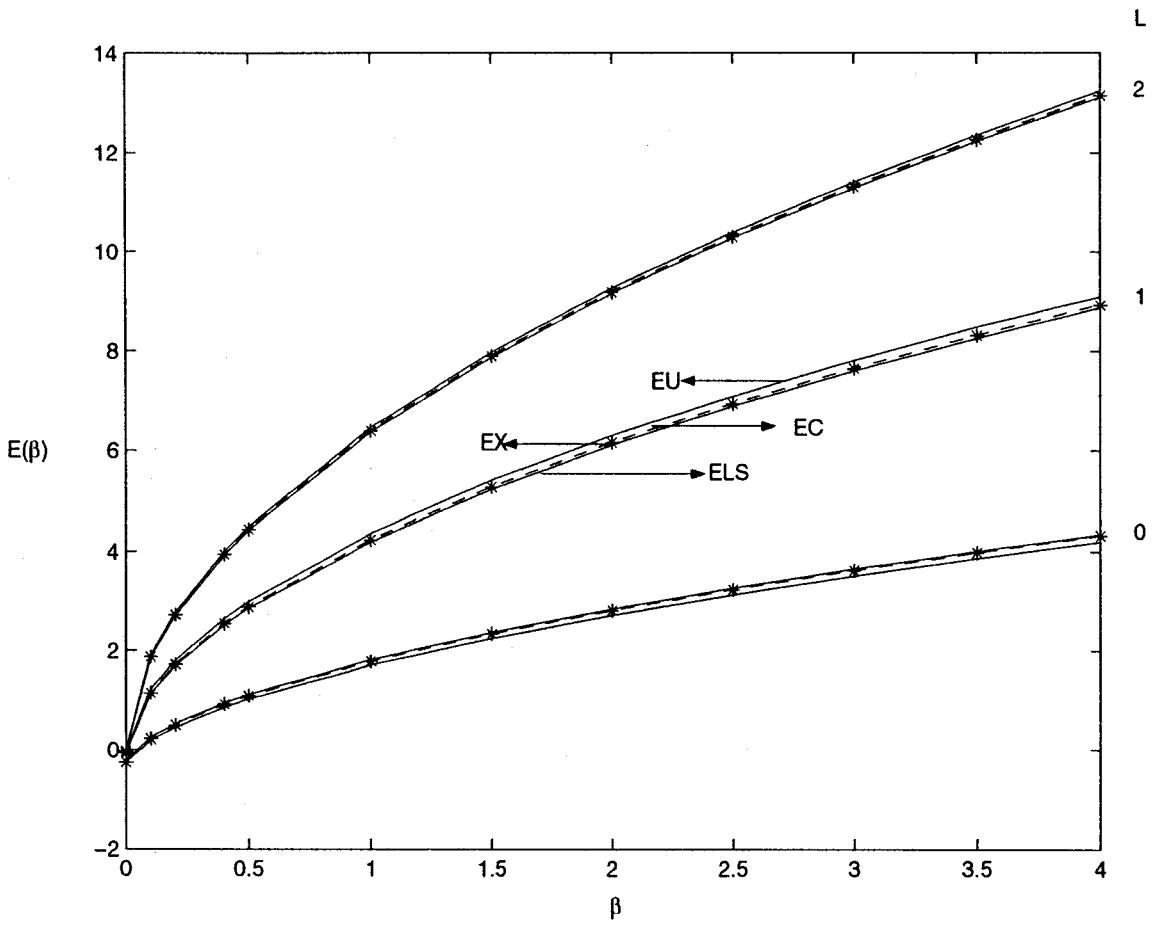

Figure VII.1 the eigenvalues $E(\beta)$ of the Hamiltonian $H = -\Delta - 1/r + \beta r^2$ for $N = 3$, $n = 1$, and $\ell = 0, 1, 2$. The continuous curves show the upper bound EU given by the envelope formula (VII.2.1) with $\nu = \mu = P_{1\ell}(2)$, for $\ell = 1, 2$ and the lower bound ELS by the sum approximation given by the same formula but with $\nu = P_{1\ell}(2)$ and $\mu = P_{1\ell}(-1)$. The upper bound for $\ell = 0$ is calculated using $\nu = P^U_{1\ell}(2)$ and $\mu = P^U_{1\ell}(-1)$ in formula (VII.2.1). The dashed curve EC represents the upper bound by formula (VII.3.4). The stars EX represent accurate numerical data.

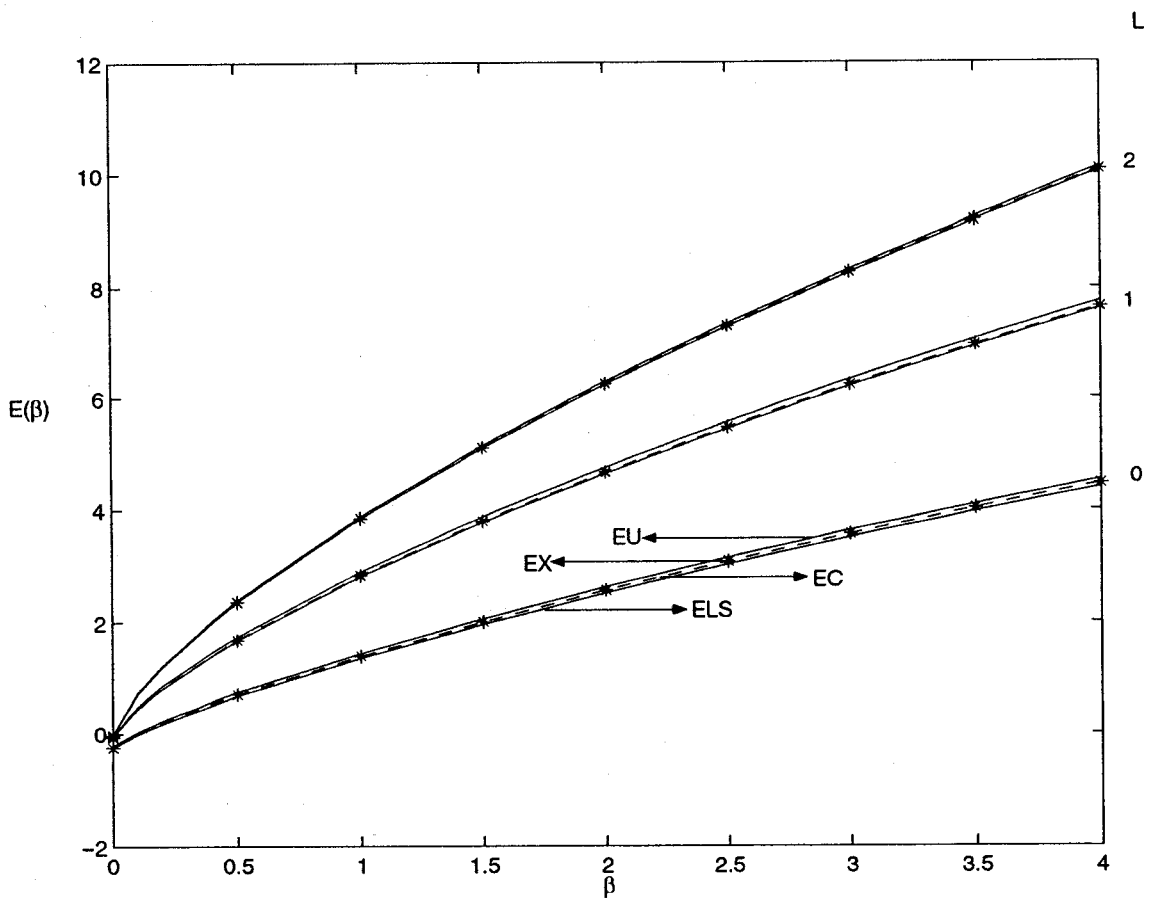

Figure VII.2 the eigenvalues $E(\beta)$ of the Hamiltonian $H = -\Delta - 1/r + \beta r$ for $N = 3$, $n = 1$, and $\ell = 0, 1, 2$. The continuous curves show the upper bound EU given by the envelope formula (2.5) with $\nu = \mu = P_{1\ell}(2)$, and the lower bound ELS by the sum approximation given by the same formula but with $\nu = P_{1\ell}(1)$ and $\mu = P_{1\ell}(-1)$. The upper bound for $\ell = 0$ is calculated using $\nu = P^U_{1\ell}(1)$ and $\mu = P^U_{1\ell}(-1)$ in formula (VII.2.1). The dashed curve EC represents the upper bound by formula (VII.3.4). The stars EX represent accurate numerical data.

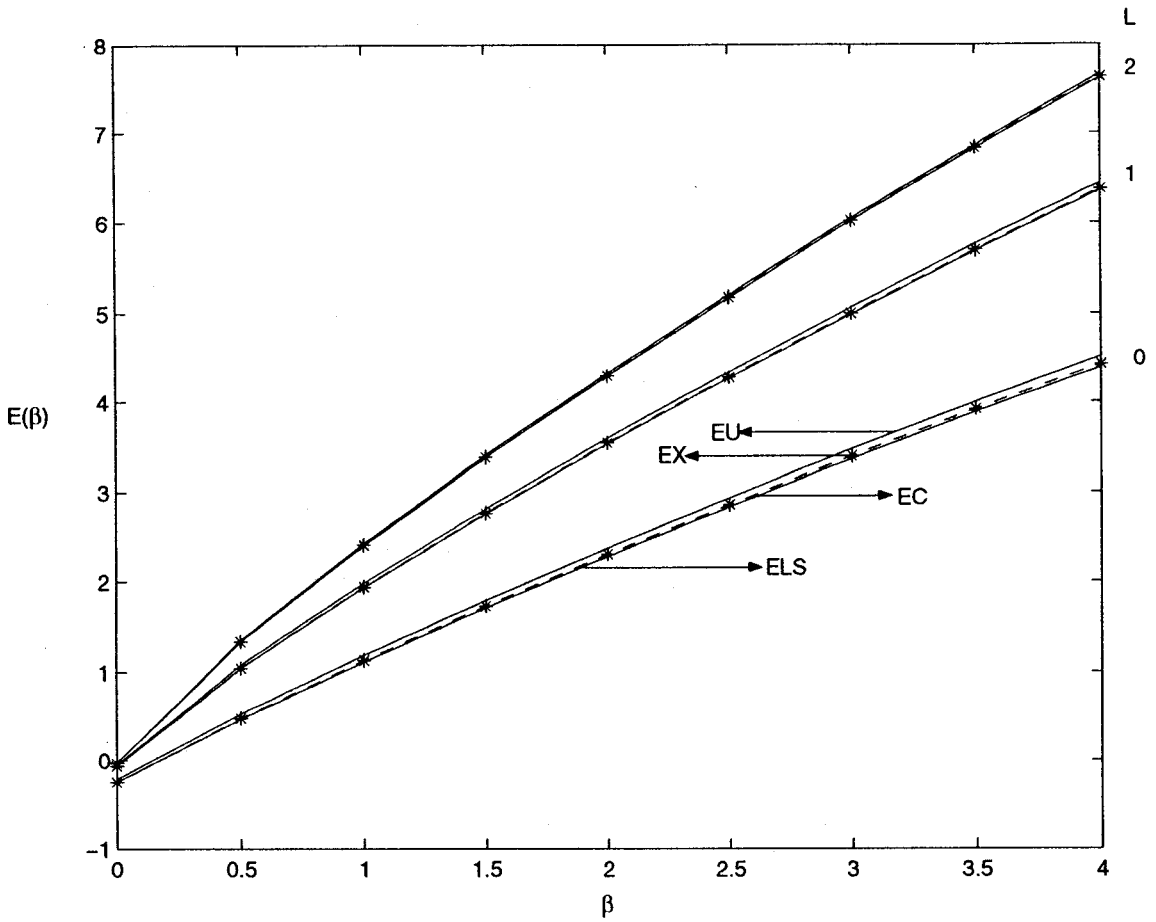

Figure VII.3 the eigenvalues $E(\beta)$ of the Hamiltonian $H = -\Delta - 1/r + \beta r^{0.5}$ for $N = 3$, $n = 1$, and $\ell = 0, 1, 2$. The continuous curves show the upper bound EU given by the envelope formula (VII.2.1) with $\nu = \mu = P_{1\ell}(0.5)$, and the lower bound ELS by the sum approximation given by the same formula but with $\nu = P_{1\ell}(0.5)$ and $\mu = P_{1\ell}(-1)$. The upper bound for $\ell = 0$ is calculated using $\nu = P^U_{1\ell}(0.5)$ and $\mu = P^U_{1\ell}(-1)$ in formula (VII.2.1). The dashed curve EC represents the upper bound by formula (VII.3.4). The stars EX represent accurate numerical data.

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Conclusion

In this thesis we have studied a collection of interesting spectral problems in quantum mechanics. We have obtained a spectral bounds for wide classes of potential V in Schrödinger operators of the form $H = \Delta + V$. We have used the comparison theorem to prove that discrete eigenvalues exist for the Hellman and cutoff-Coulomb potentials . We then employed the envelope method to obtain simple formulae for upper and lower bounds for these eigenvalues. We have generalized the comparison theorem in N dimensions to allow for intersecting comparison potentials and angular momenta $\ell > 0$. Moreover, we are able to obtain bounds for the bottom of each angular-momentum subspace since we have proved that this energy is identical (Theorem V.2) to the lowest eigenvalue of a higher-dimensional problem in $R^{N+2\ell}$. We study the representation $P(q)$ for the eigenvalues $E(q)$ of the operator $H = -\Delta + \mathrm{sgn(q)r^q}$ defined by $E(q) = \min_{r>0}\{\frac{P(q)^2}{r^2} + \mathrm{sgn(q)r^q}\}$. It had previously been proved that $P(q)$ is monotone increasing. We strengthen this result for the ground state by utilizing the generalized comparison theorem to demonstrate the monotonicity of a new function $Q(q) = Z(q)P(q)$, where $Z(q)$ is specified and is monotone decreasing. Thus we know that $P(q)$ cannot increase too slowly: this in turn allows us to obtain improved bounds for the eigenvalues $E(q)$ in N dimensions. Finally we find energy bounds for the Coulomb plus power-law potential be means of the envelope method, a variational method, and the sum approximation. In future it is hoped to improve these analytical results, for example by proving the concavity of the function $P(q)$ (so far known only numerically) and

by more narrowly bounding its rate of increase. An interesting class of unsolved problems is to extend some of our results to the excited states. The 'refined' comparison theorem and the sum approximation in their present forms are both limited to states at the bottom of an angular-momentum subspace.

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Spectral bounds for the Hellmann potential

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Abstract

The method of potential envelopes is used to analyse the bound state spectrum of the Schrödinger Hamiltonian $H = -\Delta + V(r)$, where the Hellmann potential is given by $V(r) = -A/r + Be^{-Cr}/r$, A and C are positive, and B can be positive or negative. We established simple formulas yielding upper and lower bounds for all the energy eigenvalues. © 2001 Elsevier Science B.V. All rights reserved.

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1. Introduction

The Hellmann potential $V(r)$ given by

$$V(r) = -A/r + Be^{-Cr}/r \tag{1.1}$$

has many applications in atomic physics and condensed matter physics [1–11]. The Hellmann potential, with B positive, was suggested originally by Hellmann [1,2] and henceforth called the Hellmann potential if B is positive or negative. The Hellmann potential was used as a model for alkali hydride molecules [4]. It was used also to represent the electron–ion [5,6] and electron core interaction [7,8]. It has also been shown that the main properties of the effective two-particle interaction for charged particles in polar crystals may be described by this potential [9–11].

2. The discrete spectrum: scaling

Many authors have studied the eigenvalues generated by the Hellmann potential and have tried to estimate them [1–14]. For example, Adamowski [3] used a variational framework to obtain accurate eigenvalues. Dutt, Mukherji and Varshni [12] and Kwato Njock et al. [14] applied the method of large-N expansion to approximate the bound states energies. In this paper we present simple upper- and lower-bound formulas obtained by the use of the comparison theorem and the envelope method [15–18].

We first show that discrete eigenvalues exist for the Hellmann potential for all values of $A > 0$, B, and $C > 0$. This result allows us to transcend the limit $B < A$ assumed to be necessary in an earlier attempt at this problem by geometrical methods [13]. Suppose that $B \leqslant 0$, then we immediately have that $-(A - B)/r < V(r) < -A/r$. Since both upper and lower bounds are hydrogenic potentials with discrete eigenvalues, the same follows for $V(r)$. Now we suppose that $B > 0$. In this case the concern is that, for sufficiently large B, the positive term might

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dominate the Coulomb term. We see that this does not happen by the following argument. The function re^{-Cr} has maximum value $1/(eC)$. Hence, for $B > 0$, we have $Be^{-Cr}/r < (B/eC)/r^2$, and we conclude that $-A/r < V(r) < -A/r + (B/eC)/r^2$. But the 'effective potential' for the hydrogenic atom in a state of orbital angular momentum ℓ is given by

$$V_{\text{eff}}(r) = -A/r + \ell(\ell+1)/r^2. \tag{2.1}$$

Hence, again, we see that $V(r)$ is bounded above and below by hydrogenic potentials whose corresponding Hamiltonians have discrete eigenvalues. This establishes our claim.

If we denote the eigenvalues of $H = -\omega\Delta + A/r + Be^{-Cr}$ by $\mathcal{E}(\omega, A, B, C)$, and consider a scale change of the form $s = r/\sigma$, and choose the scale $\sigma = \omega/A$, then it is easy to show that,

$$\mathcal{E}(\omega, A, B, C) = C^2\omega\mathcal{E}\left(1, \frac{A}{\omega C}, \frac{B}{\omega C}, 1\right). \tag{2.2}$$

Hence, the full problem is now reduced to the simpler two-parameter problem

$$H = -\Delta - \alpha/r + \beta e^{-r}/r, \qquad \mathcal{E} = \mathcal{E}(\alpha, \beta), \quad \alpha > 0. \tag{2.3}$$

3. Energy bounds by the envelope method

The comparison theorem of quantum mechanics tells us that an ordering between potentials implies a corresponding ordering of the eigenvalues. The 'envelope method' is based on this result and provides us with simple formulas for lower and upper bounds [16–18]. We need a solvable model which we can use as an envelope basis. The natural basis to use in the present context is the hydrogenic potential

$$h(r) = -1/r. \tag{3.1}$$

The spectrum generated by the potential $h(r)$ may be represented exactly by the semi-classical expression

$$\mathcal{E}_{n\ell}(v) = \min_{s>0}\{s + v\bar{h}_{n\ell}(s)\}, \tag{3.2}$$

where the 'kinetic potential' $\bar{h}_{n\ell}(s)$ associated with the potential $h(r) = -1/r$ is given, in this case, exactly by $\bar{h}_{n\ell}(s) = -s^{1/2}/(n+\ell)$. If we now consider a potential, such as $V(r)$, which is a smooth transformation $V(r) = g(h(r))$ of $h(r)$, then it follows that a useful approximation for the corresponding kinetic potential $\bar{f}_{n\ell}(s)$ is given by

$$\bar{f}_{n\ell}(s) \approx g\big(\bar{h}_{n\ell}(s)\big). \tag{3.3}$$

If g is convex in (3.3), we get lower bounds ($\simeq = \geqslant$) for all n and ℓ, and if g is concave we get upper bounds ($\simeq = \leqslant$) for all n and ℓ.

For the Hellmann potential, if we use the potential $h = -1/r$ as the envelope basis, then the sign of g'' depends only on the sign of B. An elementary calculation shows that

$$g''(h) = -BC^2e^{(C/h)}/h^3 = BC^2r^3e^{-Cr}. \tag{3.4}$$

Hence, g is convex if $B > 0$ or concave if $B < 0$. Thus in this application of the method we obtain upper energy bounds for $B < 0$ and lower bounds for $B > 0$. The following remarks explain briefly how these results are obtained.

We suppose for definiteness that the transformation $g(h)$ is smooth and convex, i.e., $g'' > 0$, then each tangent to g is an affine transformation of h of the form

$$V^{(t)}(r) = a(t) + b(t)h(r), \tag{3.5}$$

where the variables $a(t)$ and $b(t)$ are chosen such that the graph of the potential $V(r)$ lies above the graph of the potential $h(r)$, but it is tangential to it at a point, say $r = t$. That is to say

$$V(t) = a(t) + b(t)h(t) \quad \text{and} \tag{3.6}$$

$$V'(t) = b(t)h'(t). \tag{3.7}$$

This means that the 'tangential potential', $V^{(t)}(r)$, and its derivative agree with $V(r)$ at the point of contact, $r = t$.

Thus, by substituting (3.3) in (3.2), we find

$$\mathcal{E}_{n\ell} \approx \min_{r>0}\{s + g\big(s^{1/2}/(n+\ell)\big)\}, \tag{3.8}$$

which yields an upper bound if $B < 0$ and a lower bound if $B > 0$. This can be further simplified by changing the minimization variable s to r by the relation,

$$g\big(\bar{h}_{nl}(s)\big) = g\big(-s^{1/2}/(n+\ell)\big) = V(r), \tag{3.9}$$

which, in turn, implies $s = (n+\ell)^2/r^2$. Hence we obtain finally the following semi-classical eigenvalue

formula involving the potential $V(r)$ itself

$$\mathcal{E}_{n\ell} \approx \min_{r>0}\{(n+\ell)^2/r^2 + V(r)\}. \tag{3.10}$$

4. Results and conclusion

We now have a simple formula (3.10) for lower and upper bounds to the eigenvalues for the Hellmann potential. In Fig. 1 we plot the ground-state eigenvalue bound (full line) as a function of B for the case $A = 2$, $C = 1$, along with the corresponding point results of Adamowski [3] as hexagons, and some accurate numerical values (dashed line). It is clear from this figure that the simple approximation formula gives an accurate estimate of the eigenvalues which is an upper bound if $B < 0$, and a lower bound when $B > 0$, as predicted by the theory.

If we fix A, B, and C and consider the Hamiltonian $H = -\Delta + vV(r)$, with eigenvalues $\mathcal{E}(v)$, then from (3.10) we immediately obtain the following explicit parametric equations for the corresponding energy curve $\{v, \mathcal{E}(v)\}$, namely

$$v = \frac{2(n+\ell)^2}{r^3 V'(r)},$$

$$\mathcal{E}(v) = \frac{(n+\ell)^2}{r^2} + \frac{2(n+\ell)^2 V(r)}{r^3 V'(r)}. \tag{4.1}$$

In Fig. 2 we exhibit the corresponding graphs of the function $\mathcal{E}(v)/v^2$ for $B = +1$ and $B = -1$, again with $A = 2$, and $C = 1$, along with accurate numerical data shown as a dashed curve. The main point of this work is to show that by elementary geometric reasoning one

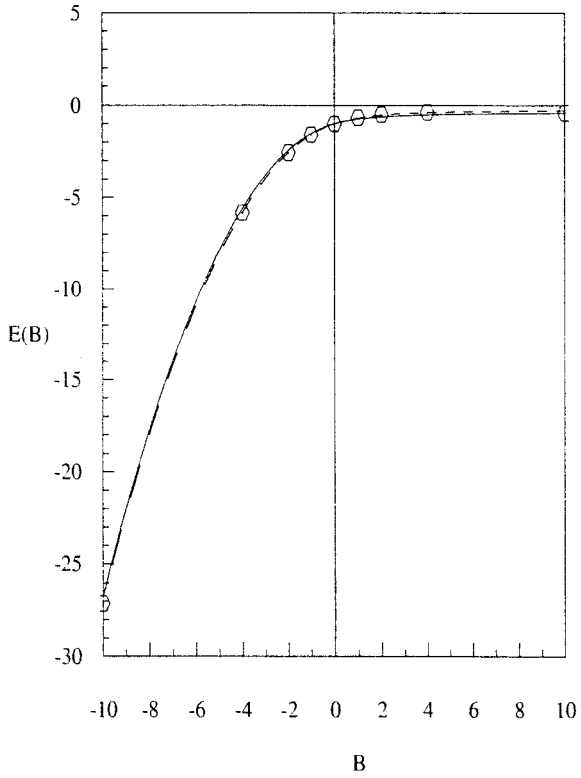

Fig. 1. The eigenvalues $\mathcal{E}(B)$ of the Hamiltonian $H = -\Delta - 2/r + Be^{-r}/r$ for $n = 1$ and $\ell = 0$. The continuous curve shows the bounds given by the formula (3.10), the dashed curve represents accurate numerical data, and the hexagons are the results of Adamowski [3]. It is clear that the formula provides us with upper bounds when $B < 0$ and lower bounds when $B > 0$.

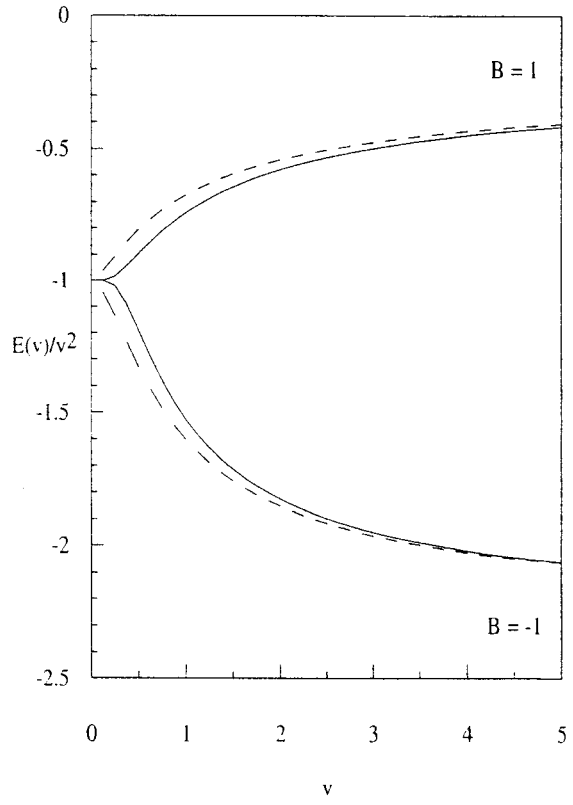

Fig. 2. The eigenvalue bounds (full-line) for $\mathcal{E}(v)/v^2$, where $\mathcal{E}(v)$ is the ground-state eigenvalue of the Hamiltonian $H = -\Delta + vV(r)$, for $A = 2$, $C = 1$, and $B = +1, -1$, together with accurate numerical data (dashed-line). The parametric equations (4.1) yield upper bounds when $B < 0$, and lower bounds when $B > 0$.

can obtain simple semi-classical approximations for the eigenvalues. These results are complementary to purely numerical solutions and have the advantage that they are expressed analytically and allow one to explore the parameter space without having to attend to the arbitrary additional parameters and considerations which necessarily accompany numerical approaches with the aid of a computer.

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Spectral bounds for the cutoff Coulomb potential

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Abstract

The method of potential envelopes is used to analyse the bound-state spectrum of the Schrödinger Hamiltonian $H = -\Delta - v/(r+b)$, where v and b are positive. We established simple formulas yielding upper and lower energy bounds for all the energy eigenvalues. © 2002 Elsevier Science B.V. All rights reserved.

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1. Introduction

The cutoff Coulomb potential $f(r)$ given by

$$f(r) = -v/(r+b) \tag{1.1}$$

is an approximation to the potential due to a smeared charge distribution, rather than a point charge, and is appropriate for describing mesonic atoms [1]. Many authors have studied the eigenvalues $E_{n\ell}$, $n = 1, 2, 3, \ldots$, $\ell = 0, 1, 2, \ldots$, generated by the cutoff Coulomb potential and have tried to estimate them. For example, Ray and Mahata [2] applied the method of large-N expansion to approximate the bound states energies from $n = 1$ to $n = 4$. Mehta and Patil [1] rigorously analysed the S-wave bound-state eigenvalues of this potential as a function of b.

In this Letter we offer an elementary proof that the cutoff Coulomb potential has infinitely many discrete negative eigenvalues $E_{n\ell}$, $n = 1, 2, 3, \ldots$, $\ell = 0, 1, 2, \ldots$, by using comparison methods. We then use the comparison theorem and the envelope method [4–8] to obtain simple upper- and lower-bound formulas for all the eigenvalues.

2. The discrete spectrum: scaling

The Hamiltonian for the problem is given by

$$H = -\Delta - v/(r+b), \quad v, b > 0. \tag{2.1}$$

A concern might be that, for sufficiently small coupling v, the potential, like a square well, might not have any discrete spectrum. However, the Coulomb tail averts this problem. It has been proved [5] by general methods that for any potential, like $-v/(r+b)$, which is negative and decays at infinity slower than $1/r^{2-\epsilon}$, the corresponding Hamiltonian operator has infinitely many negative eigenvalues. The specific result for our problem may also be obtained by an elementary application of the comparison theorem, as we now show by the following argument. We note that the

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potential can be written

$$f(r) = \frac{-v}{r} + \frac{vb}{r^2} - \frac{vb^2}{r^2(r+b)}. \tag{2.2}$$

It therefore follows that

$$-\frac{v}{r} < f(r) < \frac{-v}{r} + \frac{vb}{r^2},$$

and, consequently,

$$V_l = -\frac{v}{r} + \frac{\ell(\ell+1)}{r^2} < f(r) + \frac{\ell(\ell+1)}{r^2} < \frac{-v}{r} + \frac{\lambda(\lambda+1)}{r^2} = V_u, \tag{2.3}$$

where

$$\lambda = \left(\left(\ell + \frac{1}{2}\right)^2 + vb\right)^{1/2} - \frac{1}{2}. \tag{2.4}$$

Hence, we see that the effective potential associated with $f(r)$ is bounded above and below by hydrogenic effective potentials with discrete negative eigenvalues. This implies that the potential V has infinitely many negative discrete eigenvalues $E_{n\ell}$ bounded by

$$\frac{-v^2}{4(n+\ell)^2} \leqslant E_{n\ell} \leqslant \frac{-v^2}{4(n+\lambda)^2}. \tag{2.5}$$

These bounds are asymptotically close for large n. Another upper bound is provided by the linear potential since $f(r) < -v/b + (v/b^2)r$. Hence,

$$E_{n\ell} < -\frac{v}{b} + \left(\frac{v}{b^2}\right)^{2/3} \mathcal{E}_{n\ell}(1), \tag{2.6}$$

where $\mathcal{E}_{n\ell}(1)$ are the eigenvalues of the Hamiltonian $-\Delta + r$ for linear potential.

For the S-states the radial equation may be transformed into Whittaker's equation which has known exact solutions [3]. Some closed-form results have also been obtained for $\ell > 0$ [9,10]. The general solution is written [3] in terms of the confluent hypergeometric functions $M[x, y, z]$ and $U[x, y, z]$, where

$$U(x, y, z) = \frac{1}{\Gamma(x)} \int_0^\infty e^{-zt} t^{x-1} (1+t)^{y-x-1}\, dt = z^{-x}\, {}_2F_0[x, 1+x-y;\ ;-1/z] \tag{2.7}$$

and $M[x, y, z] = {}_1F_1[x; y; z]$. Mehta and Patil [1] used the bounded property of the radial wave function and the boundary conditions to demonstrate that the eigenvalues are determined by the equation

$$U\left[1 - v/\left(2\sqrt{-E}\right), 2, 2b\sqrt{-E}\right] = 0. \tag{2.8}$$

As an alternative, we shall apply the envelope method to approximate all the eigenvalues. We first reduce the complexity of the problem by the use of scaling arguments. If we denote the eigenvalues of $H = -\omega\Delta - v/(r+b)$ by $\mathcal{E}(\omega, v, b)$ and consider a scale change of the form $s = r/\sigma$, and choose the scale $\sigma = \omega/v$, then it is easy to show that

$$\mathcal{E}(\omega, v, b) = \frac{v^2}{\omega} \mathcal{E}\left(1, 1, \frac{vb}{\omega}\right). \tag{2.9}$$

Hence, the full problem is now reduced essentially to the simpler 1-parameter problem

$$H = -\Delta - 1/(r+b), \quad \mathcal{E} = \mathcal{E}(b), \quad b > 0. \tag{2.10}$$

3. Energy bounds by the envelope method

The comparison theorem of quantum mechanics tells us that an ordering between potentials implies a corresponding ordering of the eigenvalues. The 'envelope method' is based on this result and provides us with simple formulas for lower and upper bounds [6–8]. We need a solvable model which we can use as an envelope basis. The natural bases to use in the present context are the hydrogenic and linear potentials

$$h(r) = \operatorname{sgn}(q) r^q, \quad \text{where } q = -1, 1. \tag{3.1}$$

The spectrum generated by the potential $h(r)$ may be represented exactly by the semi-classical expression

$$\mathcal{E}_{n\ell}(v) = \min_{s>0}\left\{s + v\bar{h}_{n\ell}(s)\right\}, \tag{3.2}$$

where the 'kinetic potential' $\bar{h}_{n\ell}(s)$ associated with the power-law potentials (3.1) are given by [8]

$$\bar{h}(s) = (2/q)\left|q\mathcal{E}_{n\ell}^{(q)}/(2+q)\right|^{(q+2)/2} s^{-q/2}, \tag{3.3}$$

and $\mathcal{E}_{n\ell}^{(q)}$ is the exact eigenvalue of $-\Delta + \operatorname{sgn}(q) r^q$, that is to say, corresponding to the pure-power potential with coupling 1. If we now consider a potential, such as $f(r)$, which is a smooth transformation $f(r) = g(h(r))$ of $h(r)$, then it follows that a useful approximation for the corresponding kinetic potential

$\bar{f}_{n\ell}(s)$ is given by

$$\bar{f}_{n\ell}(s) \approx g\big(\bar{h}_{n\ell}(s)\big). \tag{3.4}$$

If g is convex in (3.4), we get [6–8] lower bounds ($\simeq = \geqslant$) for all n and ℓ, and if g is concave we get upper bounds ($\simeq = \leqslant$) for all n and ℓ.

For the cutoff Coulomb potential, if we use the potential $h = -1/r$ as an envelope basis, then g is convex. An elementary calculation shows in this case that

$$g''(h) = \frac{2vb}{(b/r+1)^3} > 0. \tag{3.5}$$

And if we use the potential $h = r$ as an envelope basis, then g is concave, in fact

$$g''(h) = \frac{-2v}{(b+r)^3} < 0. \tag{3.6}$$

Thus in this application of the method we obtain upper energy bounds if we use $h = -1/r$ and lower energy bounds if we use $h = r$. The following remarks explain briefly how these results are obtained.

We suppose for definiteness that the transformation $g(h)$ is smooth and *convex*, i.e., $g'' > 0$, then each tangent $f^{(t)}(r)$ to g is an affine transformation of h satisfying

$$f^{(t)}(r) = a(t) + b(t)h(r) < f(r), \tag{3.7}$$

where the variables $a(t)$ and $b(t)$ are given by solving the contact equations

$$f(t) = a(t) + b(t)h(t) \tag{3.8}$$

and

$$f'(t) = b(t)h'(t), \tag{3.9}$$

which mean that the 'tangential potential', $f^{(t)}(r)$, and its derivative agree with $f(r)$ at the point of contact, $r = t$. The potential inequality (3.7) implies the spectral inequality

$$E_{n\ell}(v) \geqslant va(t) + \mathcal{E}_{n\ell}\big(vb(t)\big). \tag{3.10}$$

The optimal lower bound thus obtained may then eventually [8] be rewritten

$$E_{n\ell} \geqslant \min_{s>0}\big\{s + g\big(\bar{h}_{n\ell}(s)\big)\big\}. \tag{3.11}$$

In the complementary case where g is concave, the inequalities are reversed, and one obtains upper bounds.

Table 1
The 'input' P-values $P^L_{n\ell}$, $P^U_{n\ell}$, and the mean $P^M_{n\ell} = (1/2) \times (P_{n\ell}(-1) + P_{n\ell}(1))$ used in the general formula (3.12)

n	ℓ	$P^L_{n\ell} = n+\ell$	$P^M_{n\ell}$	$P^U_{n\ell}$
1	0	1	1.18804	1.37608
2	0	2	2.59065	3.18131
3	0	3	3.99627	4.99255
4	0	4	5.40257	6.80514
5	0	5	6.80911	8.61823
1	1	2	2.18596	2.37192
2	1	3	3.57750	4.15501
3	1	4	4.97650	5.95300
4	1	5	6.37850	7.75701
5	1	6	7.78204	9.56408
1	2	3	3.18509	3.37018
2	2	4	4.57067	5.14135
3	2	5	5.96455	6.92911
4	2	6	7.36257	8.72515
5	2	7	8.76298	10.52596
1	3	4	4.18461	4.36923
2	3	5	5.56649	6.13298
3	3	6	6.95652	7.91304
4	3	7	8.35118	9.70236
5	3	8	9.74874	11.49748
1	4	5	5.18431	5.36863
2	4	6	6.56366	7.12732
3	4	7	7.95074	8.90148
4	4	8	9.34260	10.68521
5	4	9	10.73766	12.47532

For the power-law potentials $h(r) = \mathrm{sgn}(q)r^q$ we can simplify (3.11) by changing the minimization variable s to r defined in each case by the equation $\bar{h}_{n\ell}(s) = h(r)$ so that $g(h(r)) = f(r) = -v/(r+b)$, and minimization (3.2), which yields eigenvalue approximations for the Hamiltonian $H = -\omega\Delta + f(r)$, where $\omega > 0$, can be expressed in the form

$$E_{n\ell} \approx \min_{r>0}\left\{\omega\frac{P^2_{n\ell}(q)}{r^2} - \frac{v}{(r+b)}\right\}. \tag{3.12}$$

We obtain a lower bound for $P_{n\ell} = P_{n\ell}(-1) = n+\ell$, an upper bound for $P_{n\ell} = P_{n\ell}(1)$, and a good approximation with the mean value $P_{n\ell} = P^M_{n\ell} = (1/2) \times (P_{n\ell}(-1) + P_{n\ell}(1))$. These P-numbers are provided in Table 1.

A natural question to ask is whether there exists a set of numbers $\{P_{n\ell}\}$ such that $E_{n\ell} = \min_{r>0}\{P^2_{n\ell}/r^2 + f(r)\}$ *exactly*. We can see that the answer is 'no' by an argument based on the 'concentration lemma' [11], which provides us with the relation between the concentration of the ground-state wave function and the

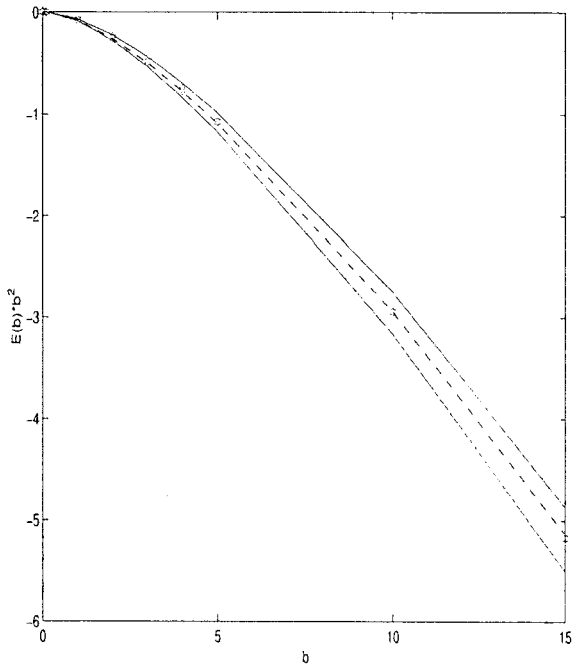

Fig. 1. The eigenvalues $\mathcal{E}(b)$ of the Hamiltonian $H = -(1/2)\Delta - 1/(r+b)$ for $n = \ell = 1$ (in atomic units $\hbar = m = 1$). The continuous curves show the bounds given by formula (3.12), the dashed curve represents accurate numerical data, and the stars are the 'mean approximation' $P_{n\ell} = (1/2)(P_{n\ell}(-1) + P_{n\ell}(1))$.

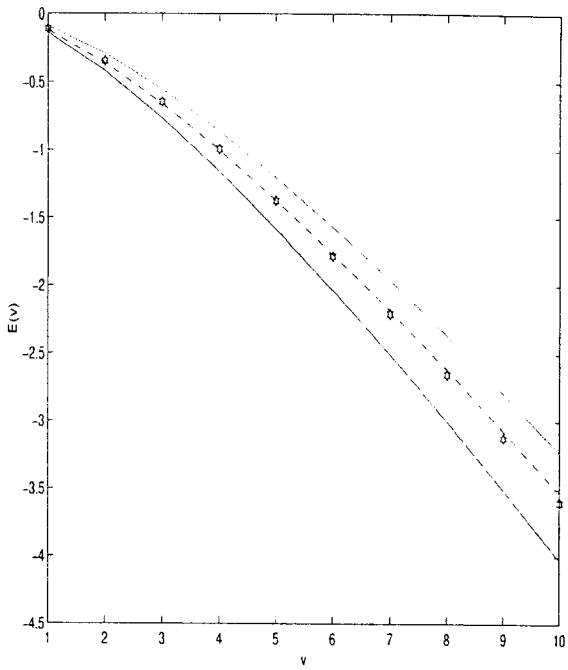

Fig. 2. Eigenvalue bounds (full line) for the ground-state eigenvalue $\mathcal{E}(v)$ $(n = 1,\ \ell = 0)$ of the Hamiltonian $H = -\Delta + vf(r)$ (in units $\hbar = 2m = 1$) for $b = 1$, together with accurate numerical data (dashed curve). The parametric equations (4.1) yield upper bounds when $P_{n\ell} = P_{n\ell}(1)$, lower bounds when $P_{n\ell} = P_{n\ell}(-1)$, and good approximation when $P_{n\ell} = (1/2)(P_{n\ell}(-1) + P_{n\ell}(1))$, shown as stars.

size of the coupling constant v. More precisely, the wave function becomes more concentrated near the origin as v increases. Since for large values of the coupling v the 'linear' upper bound (3.12) is very accurate (concentration near $r = 0$), if there were one 'exact' P_{10}, it would have to be the linear potential value $P_{10} = P_{10}(1)$. But our upper bound is clearly above $E_{n\ell}$ for small values of v. Hence there are no such 'exact' $P_{n\ell}$.

4. Results and conclusion

We have derived a simple formula (3.12) for lower and upper bounds to the eigenvalues for the cutoff Coulomb potential. In Fig. 1 we plot the eigenvalue when $(n, \ell) = (1, 1)$ as a function of b for the case $v = 1$, accurate numerical values (dashed line), and our approximation with the average value $P_{n\ell} = (1/2)(P_{n\ell}(-1) + P_{n\ell}(1))$ as stars.

If we fix b and consider the Hamiltonian $H = -\Delta + vf(r)$, with eigenvalues $\mathcal{E}(v)$, then from (3.12) we obtain the following explicit parametric equations for the corresponding approximate energy curve $\{v, \mathcal{E}(v)\}$, namely

$$v = \frac{2(P_{n\ell})^2}{r^3 f'(r)},$$

$$\mathcal{E}(v) = \frac{(P_{n\ell})^2}{r^2} + \frac{2(P_{n\ell})^2 f(r)}{r^3 f'(r)}. \tag{4.1}$$

These parametric equations yield upper bounds when $P_{n\ell} = P_{n\ell}(1)$, lower bounds when $P_{n\ell} = n + \ell$, and a good approximation when we use the arithmetic average of $P_{n\ell}(-1)$ and $P_{n\ell}(1)$. It is interesting, perhaps, that all these curves are scaled versions of any one of them; it is unknown if such a symmetry is true for the corresponding exact curves. In Fig. 2 we exhibit the graphs of the function $\mathcal{E}(v)$ for $b = 1$ along with accurate numerical data shown as a dashed curve. The

main point of this work is to show that by elementary geometric reasoning one can obtain simple semiclassical approximations for the eigenvalues. These results are complementary to purely numerical solutions and have the advantage that they are expressed simply and analytically and therefore allow one to explore the parameter space of the problem.

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Generalized comparison theorems in quantum mechanics

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Abstract

This paper is concerned with the discrete spectra of Schrödinger operators $H = -\Delta + V$, where $V(r)$ is an attractive potential in N spatial dimensions. Two principal results are reported for the bottom of the spectrum of H in each angular-momentum subspace $\mathcal{H}_\ell$: (i) an optimized lower bound when the potential is a sum of terms $V(r) = V^{(1)}(r) + V^{(2)}(r)$, and the bottoms of the spectra of $-\Delta + V^{(1)}(r)$ and $-\Delta + V^{(2)}(r)$ in $\mathcal{H}_\ell$ are known, and (ii) a generalized comparison theorem which predicts spectral ordering when the graphs of the comparison potentials $V^{(1)}(r)$ and $V^{(2)}(r)$ intersect in a controlled way. Pure power-law potentials are studied and an application of the results to the Coulomb-plus-linear potential $V(r) = -a/r + br$ is presented in detail: for this problem an earlier formula for energy bounds is sharpened and generalized to N dimensions.

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1. Introduction

This paper has two principal aspects: the potential-sum approximation, and the generalization of the comparison theorem of quantum mechanics to cases where the comparison potentials intersect. We study spherically-symmetric problems in N spatial dimensions. There is much interest in problems posed in arbitrary dimension N [1–9], rather than specifically, say, for $N = 1$, or $N = 3$. References [1, 4] are useful for technical results such as the form of the Laplacian in N-dimensional spherical coordinates; the other papers are concerned with solving problems such as the hydrogen atom [3, 7] and the linear, harmonic-oscillator, hydrogen atom, and Morse potentials [8] in higher dimensions than $N = 3$. The geometrical methods we use in this paper are independent of dimension, which can usually be carried as a free parameter N. We consider examples with Hamiltonians of the form $H = -\Delta + v\,\mathrm{sgn}(q)r^q$ or with sums of such potential terms. We suppose that the Hamiltonian operators $H = -\Delta + V(r)$, $r = \|\boldsymbol{r}\|$,

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have domains $\mathcal{D}(H) \subset L^2(R^N)$, they are bounded below, essentially self-adjoint, and have at least one discrete eigenvalue at the bottom of the spectrum. Because the potentials are spherically symmetric, the discrete eigenvalues $E_{n\ell}$ can be labelled by two quantum numbers, the total angular momentum $\ell = 0, 1, 2, \ldots$, and a 'radial' quantum number, $n = 1, 2, 3, \ldots$, which counts the eigenvalues in each angular-momentum subspace. Since the discrete spectrum may be characterized variationally [10, 12], the elementary *comparison theorem* $V^{(1)} < V^{(2)} \Rightarrow E^{(1)}_{n\ell} < E^{(2)}_{n\ell}$ immediately follows. The generalization we shall study (in section 3) involves comparison potentials whose graphs 'cross over' in such a way that spectral ordering is still guaranteed.

Before we study the generalized comparison theorem, we shall need some established results concerning 'kinetic potentials' [13] and 'envelope theory' [14, 15]. In order to fix ideas and simplify the presentation, let us suppose that E is a discrete eigenvalue at the bottom of the spectrum of $H = -\Delta + V$ in N dimensions. It follows that $E = \inf(\psi, H\psi)$ where $\psi \in \mathcal{D}(H)$ and $\|\psi\| = 1$. We perform the total minimization in two stages: first we constrain the process by fixing the mean kinetic energy $(\psi, -\Delta\psi) = s$, and then we minimize over $s > 0$. The mean potential-energy function under the constraint is called the 'kinetic potential' $\overline{V}(s)$ associated with the potential $V(r)$. Thus we define

$$\overline{V}(s) = \inf_{\substack{\psi \in \mathcal{D}(H) \\ (\psi,\psi)=1 \\ (\psi,-\Delta\psi)=s}} (\psi, V\psi) \quad \Rightarrow \quad E = \min_{s>0}\{s + \overline{V}(s)\}. \tag{1.1}$$

The variational definition of the kinetic potentials implies that (i) $\overline{cV}(s) = c\overline{V}(s)$ and (ii) $\overline{V}^{(1)}(s) \leqslant \overline{V}^{(2)}(s) \Rightarrow E^{(1)} \leqslant E^{(2)}$. Kinetic potentials can be defined [13] for higher eigenvalues and they can then be reconstructed from 'energy trajectories', the functions which describe how the eigenvalues vary with the coupling parameter $v > 0$. We have, in general, for coupling

$$H = -\Delta + vf(r) \quad \rightarrow \quad E_{n\ell} = F_{n\ell}(v) \tag{1.2a}$$

and

$$s = F_{n\ell}(v) - vF'_{n\ell}(v) \qquad \overline{f}_{n\ell}(s) = F'_{n\ell}(v) \tag{1.2b}$$

where $E_{n\ell}$ is the nth eigenvalue in the angular-momentum space labelled by ℓ and $F_{n\ell}(v)$ describes how this eigenvalue depends on the coupling $v > 0$; the corresponding kinetic potentials may then be defined by (1.2*b*). The relationship $F(v) \leftrightarrow \overline{f}(s)$ is essentially a Legendre transformation [16]: for the ground state (or the bottom $E_{1\ell}$ of each angular-momentum subspace) $F(v)$ is concave [11–13] and consequently $\overline{f}(s)$ is convex; it follows [17] immediately from (1.2*b*) that $F''(v)\overline{f}''(s) = -v^{-3} < 0$ whenever $F''(v) \neq 0$; thus in general $F(v)$ and $\overline{f}(s)$ have opposite convexities almost everywhere. For the important class of examples $H = -\Delta + v\,\mathrm{sgn}(q)r^q$, corresponding to pure powers $q > -2$, we know that $F(v)$ is *concave* for every (discrete) eigenvalue since, by scaling arguments, we have $F_{n\ell}(v) = F_{n\ell}(1)v^{\frac{2}{2+q}}$, and $\mathrm{sgn}(F_{n\ell}(1)) = \mathrm{sgn}(q)$.

The main purpose for this two-step reformulation of 'min-max' is that certain spectral approximations are very effectively developed in terms of kinetic potentials. We shall consider first the 'envelope approximation', which in its most succinct form can be summarized as follows:

$$f(r) = g(h(r)) \quad \Rightarrow \quad \overline{f_{n\ell}}(s) \approx g(\overline{h_{n\ell}}(s)). \tag{1.3}$$

Here $f(r)$ is a smooth transformation of a 'base' potential $h(r)$. We suppose that the transformation g is monotone increasing and, if it also has definite convexity, the following important conclusions may be drawn: if g is concave, we get an upper bound $\approx = \leqslant$; and,

Table 1. The 'input' P-values $P^N_{n0}(1)$ used in the general formula (1.4), for $N = 2, 3, \ldots, 12$. The same data apply to $\ell > 0$ since by theorem 2 we have $P^N_{n\ell} = P^{N+2\ell}_{n0}$.

N	$n=1$	$n=2$	$n=3$	$n=4$
2	0.9348	2.8063	4.6249	6.4416
3	1.3761	3.1813	4.9926	6.8051
4	1.8735	3.6657	5.4700	7.2783
5	2.3719	4.1550	5.9530	7.7570
6	2.8709	4.6472	6.4398	8.2396
7	3.3702	5.1413	6.9291	8.7251
8	3.8696	5.6367	7.4204	9.2129
9	4.3692	6.1330	7.9130	9.7024
10	4.8689	6.6299	8.4068	10.1932
11	5.3686	7.1274	8.9053	10.7453
12	5.8684	7.6253	9.4045	11.2744

if g is convex, we obtain a lower bound $\approx = \geqslant$. These results may also be derived by the use of families of upper and lower 'tangential' potentials [18]. In section 2, we shall apply this result to study the Coulomb-plus-linear potential $V(r) = -1/r + \lambda r$ which is clearly at once a convex transformation of the hydrogenic potential $h(r) = -1/r$ and a concave transformation of the linear potential $h(r) = r$. We shall show that we are also able to express both the upper and lower bounds for the entire discrete spectrum in the form of explicit rational functions $\lambda = \lambda(E_{n\ell})$.

The base potentials used for the Coulomb-plus-linear potential are both pure powers. Thus we shall need to use the corresponding base kinetic potentials. In fact, we have shown in general [14] that

$$-\Delta + \mathrm{sgn}(q)r^q \quad \Rightarrow \quad E^N_{n\ell} = \min_{r>0}\left\{\left(\frac{P^N_{n\ell}(q)}{r}\right)^2 + \mathrm{sgn}(q)r^q\right\} \tag{1.4}$$

where, for example, $P^N_{n\ell}(-1) = (n + \ell + N/2 - 3/2)$ and $P^N_{n\ell}(2) = (2n + \ell + N/2 - 2)$. These P-numbers and the underlying eigenvalues $E^N_{n\ell}$ satisfy the relation $E^N_{n\ell} = E^{N+2\ell}_{n0}$: this is generally true for central potentials and is the content of theorem 2, which we prove in section 4. Numerical values for $P^N_{n0}(1)$ are given in table 1 for $N = 2, \ldots, 12$. It is interesting that the case $q = 0$ corresponds *exactly* to the $\ln(r)$ potential [15]. The expression in (1.4) is derived by a change of variable $s \to (P^N/r)^2$ in the kinetic-potential formalism. The application to the Coulomb-plus-linear potential is not our only interest in these P^N-numbers. They provide through (1.4) a nice representation for the pure-power eigenvalues since the P^N-numbers vary smoothly with q through $q = 0$ whereas the eigenvalues themselves do not [14]. We have proved [14] that $P^N_{n\ell}(q)$ are monotone increasing in q. This result was obtained by using envelope theory: we considered one power q as a smooth transformation of another p and then took the limit $p \to q$.

In section 3 we prove theorem 1 which provides a lower bound for the bottom of the spectrum in each angular-momentum subspace using the sum approximation. In section 4 we prove theorem 2, which establishes the invariance of the eigenvalues with respect to changes in ℓ and N that leave the sum $N + 2\ell$ invariant. This allows us to restrict our considerations to the ground state in sufficiently high dimension N. We reformulate the *refined comparison theorem* (theorem 3 of [19]) which becomes theorem 3 here. We first prove the monotonicity of the ground-state wavefunction in N dimensions; then we prove theorem 4, which extends theorem 3 to $N \geqslant 2$ dimensions. Finally, we prove theorems 5–7 which provide simple

explicit sufficient conditions for the application of theorem 4 under a variety of crossing schemes. In section 4, we apply theorem 5 to sharpen the envelope bounds already found in section 2 for the bottom of the spectrum E of H when V is the Coulomb-plus-linear potential $V(r) = -a/r + br$.

2. Coulomb-plus-linear potential: an eigenvalue formula

The Coulomb-plus-linear potential $V(r) = -a/r + br$ is of interest in physics because it serves as a nonrelativistic model for the principal part of the quark–quark interaction. First, we will use the envelope method to derive a simple formula for upper and lower bounds for all the eigenvalues $E_{n\ell}$, $n = 1, 2, 3, \ldots$, $\ell = 0, 1, 2, \ldots$. Because the linear potential, rather than the harmonic oscillator, is used as a basis for the upper bound, the new bounds are sharper than those of the earlier paper [20].

If we denote the eigenvalues of $H = -\omega\Delta - \alpha/r + \beta r$ by $E(\omega, \alpha, \beta)$ and consider a scale of change of the form $r' = r/\sigma$, and if we further choose $\sigma = \alpha/\omega$, then it is easy to show that

$$E(\omega, \alpha, \beta) = \alpha^2\omega^{-1}E(1, 1, \lambda) \qquad \lambda = \frac{\beta\omega^2}{\alpha^3}. \tag{2.1}$$

Thus it is sufficient to study the special case $H = -\Delta - 1/r + \lambda r$.

We need a solvable model which we can use as an envelope basis. The natural bases to use in the present context are the hydrogenic and linear potentials

$$h(r) = \mathrm{sgn}(q)r^q \qquad \text{where} \quad q = -1, 1. \tag{2.2}$$

The spectrum generated by the potential $h(r)$ is represented precisely by means of the semi-classical expression (1.1) as follows:

$$\mathcal{E}_{n\ell}(v) = \min_{s>0}\{s + v\bar{h}_{n\ell}(s)\} \tag{2.3}$$

where the 'kinetic potentials' $\bar{h}_{n\ell}(s)$ associated with the power-law potentials (1.1) are given [15] by

$$\bar{h}_{n\ell}(s) = \frac{2}{q}\left|\frac{q\mathcal{E}_{n\ell}^{(q)}}{2+q}\right|^{\frac{q+2}{2}} s^{-q/2} \tag{2.4}$$

and $\mathcal{E}_{n\ell}^{(q)}$ is the eigenvalue of $-\Delta + \mathrm{sgn}(q)r^q$ in N dimensions, that is to say, corresponding to the pure-power potential with coupling 1. If we use the potential $h(r) = -\frac{1}{r}$ as an envelope basis, then $V(r) = -\frac{1}{r} + \lambda r = g\left(-\frac{1}{r}\right)$ implies g is convex. And if we use the linear potential $h(r) = r$ as an envelope basis, then g is concave. A weaker upper bound is provided by the harmonic oscillator $h(r) = r^2$, for which again $g(h)$ is convex.

For the power-law potentials $h(r) = \mathrm{sgn}(q)r^q$ we can simplify (2.3) by changing the minimization variable s to r defined in each case by the equation $\bar{h}_{n\ell}(s) = h(r)$ so that $g(h(r)) = f(r) = -\frac{1}{r} + \lambda r$. The minimization on the other hand, which yields eigenvalue approximations for the Hamiltonian $H = -\omega\Delta + f(r)$ ($\omega > 0$), can be expressed in the form

$$E_{n\ell}^N \approx \min_{r>0}\left\{\omega\left(\frac{P_{n\ell}^N(q)}{r}\right)^2 - \frac{1}{r} + \lambda r\right\} \tag{2.5}$$

where

$$P_{n\ell}^N(q) = \left|E_{n\ell}^{(q)}\right|^{\frac{2+q}{2q}}\left[\frac{2}{2+q}\right]^{\frac{1}{q}}\left|\frac{q}{2+q}\right|^{\frac{1}{2}} \qquad q \neq 0. \tag{2.6}$$

We obtain a lower bound with $P^N_{n\ell}(-1) = (n+\ell+N/2-3/2)$ and the harmonic-oscillator upper bound (of [20]) with $P^N_{n\ell}(2) = 2n+\ell+N/2-2$, and a sharper upper bound with $P^N_{n\ell}(1)$; the $P^N_{n0}(1)$-numbers are provided in table 1 for $N = 2, \ldots, 12$. This table allows $\ell > 0$ since $P^N_{n\ell} = P^{N+2\ell}_{n0}$: it is clear that $E^N_{n\ell}(-1)$ and $E^N_{n\ell}(2)$, and the corresponding P-numbers, are invariant with respect to changes in ℓ and N which preserve the sum $2\ell + N$; this symmetry is also true for $E^N_{n\ell}(1)$, indeed for *all* eigenvalues generated by a central potential. This property is the content of theorem 2, which we state and prove in section 4. We thus obtain the following energy bounds:

$$\min_{r>0}\left\{\left(\frac{P^N_{n\ell}(-1)}{r}\right)^2 - \frac{1}{r} + \lambda r\right\} \leqslant E_{n\ell} \leqslant \min_{r>0}\left\{\left(\frac{P^N_{n\ell}(1)}{r}\right)^2 - \frac{1}{r} + \lambda r\right\} \tag{2.7}$$

for $n = 1, 2, 3, \ldots, \ell = 0, 1, 2, \ldots$. Consequently, the energy bounds are given by the parametric equations

$$E_{n\ell} = -\frac{1}{2vt} + \frac{3\lambda\mu t}{2} \tag{2.8a}$$

$$1 = \frac{t}{2v} + \frac{\lambda\mu t^3}{2} \qquad t = rP^N_{n\ell}(q) \qquad q = -1, 1 \tag{2.8b}$$

wherein the lower and upper bounds take the values $v = \mu = P^N_{n\ell}(-1)$ and $v = \mu = P^N_{n\ell}(1)$, respectively. It is interesting that we can actually solve equations (2.8*a*) and (2.8*b*) to obtain λ as an explicit function of $E = E^N_{n\ell}$; the result namely is

$$\lambda = \frac{\left\{2(vE)^3 - vE^2\left[(1+3v^2E)^{\frac{1}{2}} - 1\right]\right\}}{\mu\left[(1+3v^2E)^{\frac{1}{2}} - 1\right]^3} \tag{2.9}$$

with $E \geqslant -\frac{1}{4v^2}$ (corresponding to $\lambda = 0$ for the pure hydrogenic spectrum). We emphasis that these bounds are valid for all the discrete eigenvalues in arbitrary dimension $N \geqslant 2$. The bounds are weak for $n > 1$, but at the bottom of each angular-momentum subspace $n = 1$ they are sharp and improve with increasing ℓ, N and λ. The lower bound for the bottom of each angular-momentum subspace ($n = 1$) can be improved by the use of the 'sum approximation' ([21] and section 3 below) in which $v = P^N_{n\ell}(1)$ (table 1) and $\mu = P^N_{n\ell}(-1) = (n+\ell+N/2-3/2)$. In figure 1 we exhibit these bounds for $n = 1$, $N = 3$ and $\ell = 0, 1, 2, 3$.

3. The sum approximation: lower bounds

We now consider potentials which are sums of terms. Since further generalizations easily follow, we first look at the problem of the sum of only two potential terms. We assume that each potential $vh^{(i)}(r)$ alone, when added to the kinetic-energy operator $-\Delta$, has a discrete eigenvalue E at the bottom of the spectrum for sufficiently large coupling v. We note that the proof is unchanged if we restrict the problem to a given angular-momentum subspace labelled by ℓ; our claim then concerns the bottom of the spectrum of H in such a subspace; in the more general case, all the kinetic potentials would be labelled by ℓ. We express our result in terms of kinetic potentials and prove (for the case $\ell = 0$) the following:

Theorem 1. *If E is the bottom of the spectrum of the Hamiltonian $H = -\Delta + V$, and the potential V is the sum $V(r) = h^{(1)}(r) + h^{(2)}(r)$, then it follows that the sum of the component kinetic potentials yields a lower bound to $\overline{V}$, that is to say*

$$\overline{V}(s) \geqslant \overline{h}^{(1)}(s) + \overline{h}^{(2)}(s). \tag{3.1}$$

We shall now prove this theorem, which is in effect an optimized Weyl lower bound [22–24].

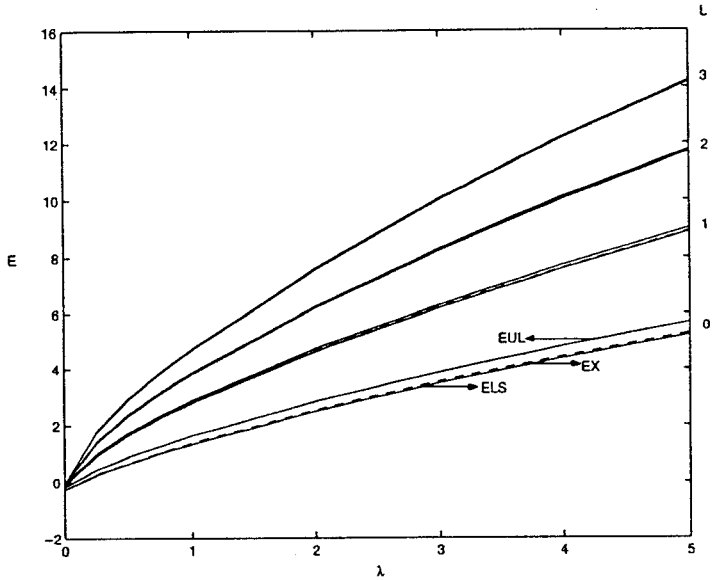

Figure 1. The eigenvalues $E(\lambda)$ of the Hamiltonian $H = -\Delta - 1/r + \lambda r$ for $N = 3$, $n = 1$ and $\ell = L = 0, 1, 2, 3$. The continuous curves show the upper bound EUL given by the envelope formula (2.9) with $\nu = \mu = P^3_{1\ell}(1)$, and the lower bound ELS by the sum approximation given by the same formula but with $\nu = P^3_{1\ell}(1)$ and $\mu = P^3_{1\ell}(-1)$. The dashed curve EX represents accurate numerical data.

Proof. From the definition (1.1) of kinetic potentials we have

$$\overline{V}(s) = \inf_{\substack{\psi\in\mathcal{D}(H)\\(\psi,\psi)=1\\(\psi,K\psi)=s}} (\psi, V\psi) = \inf_{\substack{\psi\in\mathcal{D}(H)\\(\psi,\psi)=1\\(\psi,K\psi)=s}} (\psi, (h^{(1)} + h^{(2)})\psi).$$

But the latter minimum mean value is clearly bounded below by the sum of the *separate* minima. Thus we have

$$\overline{V}(s) \geqslant \inf_{\substack{\psi\in\mathcal{D}(H)\\(\psi,\psi)=1\\(\psi,-\Delta\psi)=s}} (\psi, h^{(1)}\psi) + \inf_{\substack{\psi\in\mathcal{D}(H)\\(\psi,\psi)=1\\(\psi,-\Delta\psi)=s}} (\psi, h^{(2)}\psi) = \overline{h}^{(1)}(s) + \overline{h}^{(2)}(s)$$

which inequality establishes the theorem. □

Another approach, which would eventually yield an alternative proof of the theorem, exhibits the relationship between theorem 1 and the classical Weyl lower bound [24–26] for the eigenvalues of the sum of two operators. Let us suppose that Ψ is the exact normalized lowest eigenfunction of $H = -\Delta + V$, so that $H\Psi = E\Psi$. If the positive real parameter w satisfies $0 < w < 1$, then $E = (\Psi, (-\Delta + V)\Psi)$ may be written as follows:

$$E = w\left(\Psi, \left(-\Delta + \frac{1}{w}h^{(1)}(r)\right)\Psi\right) + (1-w)\left(\Psi, \left(-\Delta + \frac{1}{1-w}h^{(2)}(r)\right)\Psi\right)$$

$$\geqslant w \inf_{\substack{\psi\in\mathcal{D}(H)\\(\psi,\psi)=1}} \left(\psi, \left(-\Delta + \frac{1}{w}h^{(1)}(r)\right)\psi\right)$$

$$+ (1-w) \inf_{\substack{\psi\in\mathcal{D}(H)\\(\psi,\psi)=1}} \left(\psi, \left(-\Delta + \frac{1}{1-w}h^{(2)}(r)\right)\psi\right).$$

That is to say, in terms of component kinetic potentials, we arrive at Weyl's inequality for the lowest eigenvalue E of the operator sum H, where

$$H = -w\Delta + h^{(1)} + (-(1-w)\Delta + h^{(2)})$$

and we conclude

$$E \geqslant w \min_{s>0}\left\{s + \frac{1}{w}\overline{h}^{(1)}(s)\right\} + (1-w)\min_{s>0}\left\{s + \frac{1}{1-w}\overline{h}^{(2)}(s)\right\}.$$

Since w is an essentially free parameter in the last expression, we may optimize the Weyl lower bound with respect to the choice of w: this forces the individual values of s at the minima, $\{s_1(w), s_2(w)\}$, to be related. More specifically, we find from the individual minimizations over s,

$$E \geqslant \mathcal{E}(w) = ws_1(w) + (1-w)s_2(w) + \overline{h}^{(1)}(s_1(w)) + \overline{h}^{(2)}(s_2(w))$$

where

$$w = -\frac{\partial \overline{h}^{(1)}}{\partial s}\ (s_1(w)) \qquad \text{and} \qquad 1-w = -\frac{\partial \overline{h}^{(2)}}{\partial s}\ (s_2(w)).$$

The critical condition $\mathcal{E}'(w) = 0$ for the subsequent maximization over w then yields $s_1(w) = s_2(w)$. Thus the best lower energy bound is given by

$$E \geqslant \min_{s>0}\{s + \overline{h}^{(1)}(s) + \overline{h}^{(2)}(s)\}.$$

The kinetic-potential inequality of theorem 1 leads, of course, to the same energy lower bound: the optimization just performed above is therefore seen to be automatically 'built in' by the kinetic-potential formalism.

It follows immediately from the above kinetic-potential comparison theorem and coupling-parameter absorption that a lower bound to the lowest energy E of the Hamiltonian $H = -\Delta + \sum_i c_i h^{(i)}(r)$, $\{c_i > 0\}$ is provided by the formula

$$E \geqslant \min_{s>0}\left\{s + \sum_i c_i \overline{h}^{(i)}(s)\right\}. \tag{3.2}$$

Similarly, we can extend this result to 'continuous sums' such as $V(r) = \int_{t_1}^{t_2} c(t)h^{(t)}(r)\,dt$.

Meanwhile, since the proof is identical, the bound is valid for the bottom of each angular-momentum subspace. Thus, more generally, the fundamental inequality becomes

$$\overline{V}_{1\ell}(s) \geqslant \overline{h}^{(1)}_{1\ell}(s) + \overline{h}^{(2)}_{1\ell}(s) \qquad \ell = 0, 1, 2, \ldots. \tag{3.3}$$

4. Generalized comparison theorems

The proof of our generalized comparison theorem (theorem 4) depends on monotone behaviour of the wavefunction induced by the assumed monotonicity of the potential. We are able to establish this monotonicity for the lowest eigenfunction in arbitrary many spatial dimensions $N \geqslant 1$. We shall then be able to apply our eigenvalue results to the case $\ell > 0$ and $n = 1$ because of theorem 2 which claims that $E^N_{n\ell} = E^{N+2\ell}_{n0}$; this general result is then employed in the special case $n = 1$.

Theorem 2. *Suppose that $H = -\Delta + V(r)$, where $V(r)$ is a central potential in $N \geqslant 2$ dimensions, has a discrete eigenvalue $E^N_{n\ell}$ with $n - 1$ radial nodes in the angular-momentum subspace labelled by ℓ, then $E^N_{n\ell} = E^{N+2\ell}_{n0}$.*

Proof. We suppose that ψ is the eigenfunction corresponding to $E^N_{n\ell}$. We express $-\Delta$ in spherical coordinates [1–9] and write the radial eigenequation explicitly as

$$-\psi''(r) - \frac{(N-1)}{r}\psi'(r) + \frac{\ell(\ell+N-2)}{r^2}\psi(r) + V(r)\psi(r) = E^N_{n\ell}\psi(r).$$

If we now define the reduced radial function $u(r) \in L^2(R^+)$ by $\psi(r) = u(r)r^{-(N-1)/2}$, $r > 0$, and $u(0) = 0$, we obtain

$$-u''(r) + \left[\frac{\frac{(N-1)}{2}\frac{(N-3)}{2} + \ell(\ell+N-2)}{r^2} + V(r)\right]u(r) = E^N_{n\ell}u(r). \tag{4.1}$$

If we consider the spherically-symmetric potential $V(r)$ in M dimensions such that $(M-1)(M-3)/4 = \ell(\ell+N-2) + (N-1)(N-3)/4$, we find that $M = 2\ell + N$. The eigenequation (4.1) then may be written equivalently as

$$-u''(r) + \left[\frac{\frac{(M-1)}{2}\frac{(M-3)}{2}}{r^2} + V(r)\right]u(r) = E^N_{n\ell}u(r). \tag{4.2}$$

It therefore follows immediately that $E^N_{n\ell} = E^M_{n0} = E^{2\ell+N}_{n0}$. □

For the purpose of our comparison theory we may now consider the special case $n = 1, \ell = 0$ in arbitrary $N \geqslant 1$ spatial dimensions: the energy results which we derive will then be applicable to the family of equivalent problems in N' spatial dimensions with $n = 1$, $\ell > 0$ and $N = N' + 2\ell$. In order to prove an appropriate extension of the comparison theorem in N dimensions, we shall first need to establish an elementary monotonicity property for the ground state ψ. We prove the following:

Lemma. *Suppose $\psi = \psi(r)$, $r = \|\mathbf{r}\|$, $\mathbf{r} \in R^N$, satisfies Schrödinger's equation*

$$H\psi(r) = (-\Delta + V(r))\psi(r) = E\psi(r) \tag{4.3}$$

where $V(r)$ is a central potential which is monotone increasing for $r > 0$. Suppose that E is a discrete eigenvalue at the bottom of the spectrum of the operator $H = -\Delta + V$, defined on some suitable domain $\mathcal{D}(H)$ in $L^2(R^N)$. Suppose that $\psi(r)$ has no nodes, so that, without loss of generality, we can assume $\psi(r) > 0, r > 0$. Then $\psi'(r) \leqslant 0, r > 0$.

Proof. The proof for the case $N = 1$ is given in [19], equation (2.2). Henceforth, we shall now assume $N \geqslant 2$. If we express $-\Delta$ in spherical coordinates in N spatial dimensions, then we have

$$-\Delta\psi + V\psi = E\psi \qquad -\frac{1}{t^{N-1}}\frac{\partial}{\partial t}\left(t^{N-1}\frac{\partial}{\partial t}\right)\psi(t) + V(t)\psi(t) = E\psi(t).$$

We now multiply both sides by t^{N-1} and integrate with respect to t to obtain

$$\psi'(r) = (1/r^{N-1})\int_0^r [V(t) - E]\psi(t)t^{N-1}\,dt.$$

Since V is monotone increasing, it follows that there is one point $\hat{r} > 0$ satisfying $V(\hat{r}) = E$. First, we prove that $s(r) = \int_{\hat{r}}^r [V(t) - E]\psi(t)t^{N-1}\,dt$ is monotone increasing and bounded. For $t > \hat{r}$, $[V(t) - E]\psi(t)t^{N-1} > 0$, because $V(t) > E$ and hence $s(r)$ is increasing as $r \to \infty$. If there exists $r_1 < \infty$ such that $s(r_1) = -\int_0^{\hat{r}} [V(t) - E]\psi(t)t^{N-1}\,dt$, then $\int_0^r [V(t) - E]\psi(t)t^{N-1}\,dt > 0, r > r_1$ and $\psi'(r) > 0, r > r_1$; this contradicts the fact that the wavefunction $\psi(r)$ is positive and belongs to $L^2(R^N)$. This means that $\int_0^r [V(t) - E]\psi(t)t^{n-1}\,dt \leqslant 0, \forall r > 0$. Consequently $\psi'(r) \leqslant 0, \forall r > 0$. □

We now consider two potentials $V_1(r)$ and $V_2(r)$, both of the type described above. We have two Schödinger equations for the respective ground states ψ_1 and ψ_2 and the corresponding discrete eigenvalues E_1 and E_2 at the bottoms of the spectra. Thus we have the following pair of eigenequations:

$$(-\Delta + V_1(r))\psi_1(r) = E_1\psi_1(r) \tag{4.4}$$

$$(-\Delta + V_2(r))\psi_2(r) = E_1\psi_2(r). \tag{4.5}$$

The radial wavefunctions in the present paper satisfy the normalization condition $\int_0^\infty \psi_i^2(r)r^{N-1}\,dr < \infty$, $i = 1, 2$. With this notation and $N = 3$, theorem 3 of [19] becomes

Theorem 3.

$$k(r) = \int_0^r (V_1(t) - V_2(t))\psi_i(t)t^2\,dt \leqslant 0 \qquad \forall r > 0 \quad i = 1 \text{ or } 2 \quad \Rightarrow \quad E_1 \leqslant E_2. \tag{4.6}$$

We shall now generalize this theorem to general dimension $N \geqslant 1$. We first establish a fundamental comparison formula (equation (4.7)) below.

By multiplying (4.4) by ψ_2 and (4.5) by ψ_1, and subtracting, we find

$$\psi_1\Delta\psi_2 - \psi_2\Delta\psi_1 + [V_1 - V_2]\psi_1\psi_2 = [E_1 - E_2]\psi_1\psi_2.$$

Integrating over R^N and using the following identity:

$$\nabla \cdot (\psi_1\nabla\psi_2) = \nabla\psi_1 \cdot \nabla\psi_2 + \psi_1\nabla^2\psi_2$$

we find that

$$\int_{R^N} \nabla \cdot [\psi_1\nabla\psi_2 - \psi_2\nabla\psi_1]\,d^Nr + \int_{R^N} [V_1 - V_2]\psi_1\psi_2\,d^Nr = [E_1 - E_2]\int_{R^N} \psi_1\psi_2\,d^Nr.$$

Now by Gauss's theorem [27] we find that the first term becomes a surface integral which vanishes because $\psi_i \in L^2(R^N)$. In the remaining integrals the angular factors yield $2\pi^{N/2}/\Gamma(N/2)$. Hence we find

$$\frac{2\sqrt{\pi^N}}{\Gamma(N/2)}\int_0^\infty [V_1(r) - V_2(r)]\psi_1(r)\psi_2(r)r^{N-1}\,dr = \frac{2\sqrt{\pi^N}}{\Gamma(N/2)}[E_1 - E_2]\int_0^\infty \psi_1(r)\psi_2(r)r^{N-1}\,dr$$

which implies

$$s = \int_0^\infty [V_1 - V_2]\psi_1\psi_2 r^{N-1}\,dr = [E_1 - E_2]\int_0^\infty \psi_1\psi_2 r^{N-1}\,dr. \tag{4.7}$$

Now we may state our generalization of theorem 3 to N dimensions:

Theorem 4.

$$k(r) = \int_0^r (V_1(t) - V_2(t))\psi_i(t)t^{N-1}\,dt \leqslant 0 \qquad \forall r > 0 \quad i = 1 \text{ or } 2 \quad \Rightarrow \quad E_1 \leqslant E_2. \tag{4.8}$$

Proof. For definiteness we assume that $i = 1$; the proof is just the same with the other choice. We study the integral s on the left side of (4.7). Integrating by parts we find that

$$s = [k(r)\psi_2(r)]_0^\infty - \int_0^\infty k(r)\psi_2'(r)r^{N-1}\,dr. \tag{4.9}$$

Since $k(0) = \psi_2(\infty) = 0$, the first term vanishes, and s is therefore equal to the negative of the integral of the right side of (4.9). But the integrand of this integral is positive because $k(r) \leqslant 0$, by hypothesis, and we know that $\psi_2'(r) \leqslant 0$ by the above lemma. This proves that $s \leqslant 0$. Consequently, by (4.7), we obtain $E_1 \leqslant E_2$. □

It may be difficult to apply theorem 4 in practice. Thus it would be helpful to establish some simpler sufficient conditions, depending on the number and nature of the crossings of the two comparison potentials. We treat three useful cases: theorem 5, one potential crossing, with the use of the wavefunction; theorem 6, two crossings and the use of the wavefunction; theorem 7, two crossings and no wavefunction used. In these theorems we shall assume that the integrals $\int_0^\infty (V_1(r) - V_2(r))\psi_i(r)r^{N-1}\,dr$, $i = 1, 2$, exist for the given problem, even though we use at most one wavefunction factor.

Theorem 5. *If the potentials $V_1(r)$ and $V_2(r)$ cross exactly once for $r > 0$ at $r = r_1$, with,*

(i) $V_1(r) < V_2(r)$ $(0 < r < r_1)$ and
(ii) $\int_0^\infty [V_1(t) - V_2(t)]\psi_i(t)t^{N-1}\,dt \leqslant 0$, $i = 1$ or 2,

then

$$k(r) = \int_0^r [V_1(t) - V_2(t)]t^{N-1}\psi_i(r)\,dt \leqslant 0 \qquad \forall r > 0 \quad i = 1 \text{ or } 2 \tag{4.10}$$

from which $E_1 \leqslant E_2$ follows, by theorem 4.

Remark. The best bound is obtained with the equality in hypothesis (ii).

Proof of theorem 5. We choose $i = 1$: the proof is identical for $i = 1$ or 2. First, we show that $s(r) = \int_{r_1}^r [V_1(t) - V_2(t)]\psi_1(t)t^{N-1}\,dt$ is monotone increasing. For $t > r_1$, $s'(r) = [V_1(r) - V_2(r)]\psi_1(r)r^{N-1} > 0$, because $V_1(r) > V_2(r)$; hence $s(r)$ is increasing on (r_1, ∞). Moreover, (ii) implies that the maximum value of $s(r)$ is reached at $r = \infty$, i.e. $s(r) \leqslant s(\infty)$; we have therefore

$$\int_0^\infty [V_1(t) - V_2(t)]\psi_1(t)t^{N-1}\,dt$$
$$= \int_0^{r_1} [V_1(t) - V_2(t)]\psi_1(t)t^{N-1}\,dt + \int_{r_1}^\infty [V_1(t) - V_2(t)]\psi_1(t)t^{N-1}\,dt \leqslant 0$$

and therefore

$$\lim_{r\to\infty} s(r) \leqslant -\int_0^{r_1} [V_1(t) - V_2(t)]\psi_1(t)t^{N-1}\,dt.$$

Now, we have the following two cases to consider:

Case 1. For $r < r_1$, $k(r) = \int_0^r [V_1(t) - V_2(t)]\psi_1(t)t^{N-1}\,dt \leqslant 0$, since $V_1(t) < V_2(t)$ for $0 < t < r$.

Case 2. If $r > r_1$, then

$$k(r) = \int_0^{r_1} [V_1(t) - V_2(t)]\psi_1(t)t^{N-1}\,dt + \int_{r_1}^r [V_1(t) - V_2(t)]\psi_1(t)t^{N-1}\,dt$$
$$= s(r) - s(\infty) < 0.$$

Therefore, $k(r) \leqslant 0$, $\forall r > 0$. □

Theorem 6. *If the potentials $V_1(r)$ and $V_2(r)$ cross twice for $r > 0$ at $r = r_1$, $r = r_2$ $(r_1 < r_2)$ with*

(i) $V_1(r) < V_2(r)$ for $0 < r < r_1$ and

(ii) $\int_0^{r_2}(V_1(t)-V_2(t))\psi_i(t)t^{N-1}\,dt \leqslant 0, i = 1 \text{ or } 2,$

then

$$k(r) = \int_0^r (V_1(t)-V_2(t))\psi_i(t)t^{N-1}\,dt \leqslant 0 \qquad \forall r > 0 \quad i = 1 \text{ or } 2 \tag{4.11}$$

from which $E_1 \leqslant E_2$ *follows, by theorem 4.*

Remark. The best bound is obtained with the equality in hypothesis (ii).

Proof of theorem 6. We choose $i = 1$; the proof is the same if $i = 2$. $k'(r) = (V_1(r)-V_2(r))r^{N-1}\psi_1(r)$, now $k(0) = 0$, $k'(r) < 0, 0 < r < r_1$ implies $k(r) < 0$, $0 < r < r_1$. Next, $k(r_2) = 0$, $k'(r) > 0, r_1 < r < r_2$ implies $k(r) < 0, r_1 < r < r_2$. Lastly, $k(r_2) = 0, k'(r) < 0, r > r_2$ implies $k(r) \leqslant 0, r > r_2$. □

Theorem 7. *If the potentials* $V_1(r)$ *and* $V_2(r)$ *cross twice for* $r > 0$ *at* $r = r_1, r_2$ $(r_1 < r_2)$ *with*

(i) $V_1(r) < V_2(r)$ *for* $0 < r < r_1$ *and*
(ii) $\int_0^{r_2}(V_1(t)-V_2(t))t^{N-1}\,dt \leqslant 0$

then

$$k(r) = \int_0^r [V_1(t)-V_2(t)]\psi_i(t)t^{N-1}\,dt \leqslant 0 \qquad \forall r > 0 \quad i = 1 \text{ or } 2 \tag{4.12}$$

from which $E_1 < E_2$ *follows, by theorem 4.*

Remark. The best bound is obtained with the equality in hypothesis (ii).

Proof of theorem 7. We choose $i = 1$: the proof is identical if $i = 2$. Define $h(r) = \int_0^r (V_1(t)-V_2(t))t^{N-1}\,dt$, the proof of theorem 3 shows that $h(r) \leqslant 0, 0 \leqslant r \leqslant r_2$. But

$$\begin{aligned} k(r) &= \int_0^r (V_1(t)-V_2(t))\psi_1(t)t^{N-1}\,dt \\ &= [h(t)\psi_1(t)]_0^r - \int_0^r h(t)\psi_1'(t)\,dt \\ &= h(r)\psi_1(r) - \int_0^r h(t)\psi_1'(t)\,dt < 0 \end{aligned}$$

meanwhile, $k'(r) < 0, r > r_2$. Therefore, $k(r) \leqslant 0, \forall r > 0$. □

5. Application to the Coulomb-plus-linear potential

As an example, we employ the comparison theorems to improve the bounds obtained in section 2 for the eigenvalues corresponding to the Coulomb-plus-linear potential $V(r) = -a/r + br$, where a and b are positive coupling parameters. For the upper bound we use as a comparison potential the shifted linear potential $h(r) = -\alpha + \beta r$, where α and $\beta > 0$. We allow the potentials $V(r)$ and $h(r)$ to cross over exactly twice, as illustrated in figure 2. Let A and B represent the absolute values of the areas (or of the ψ-weighted areas) between the potentials. We vary α and β so that $A = B$, and thereafter theorems 5 and 6 imply $E^V \leqslant E^h$. For simplicity of derivation of the upper-bound formula, we will use theorem 7 (with no use of the wavefunction ψ). Thus we have two equations to solve in this case,

$$-\frac{a}{r} + br = -\alpha + \beta r \qquad \int_0^r \left[-\frac{a}{t} + bt + \alpha - \beta t\right] t^{N-1}\,dt = 0$$

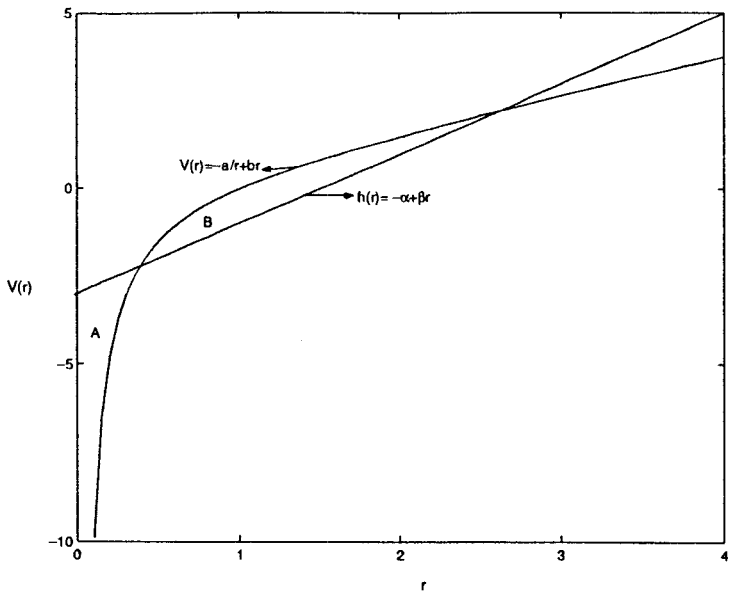

Figure 2. The linear potential $h(r) = \alpha r + \beta$ used to estimate an upper bound for the eigenvalues of the Coulomb-plus-linear potential $V(r) = -a/r + br$. A and B are the absolute values of the inter-potential areas (or ψ-weighted areas). We vary α and β so that $A = B$, and thereafter theorems 5 and 6 imply $E^V \leqslant E^h$.

where $r = r_2$ is the second crossing point. These reduce to the quadratic equations

$$(\beta - b)r^2 - \alpha r + a = 0 \qquad N(N-1)(b-\beta)r^2 + \alpha(N-1)(N+1)r - aN(N+1) = 0$$

with the simultaneous solution $r = \frac{2aN}{\alpha(N-1)}$. Now the best upper bound is obtained after minimizing with respect to r, giving

$$E^U = \min_{r>0}\left\{-\left(\frac{2aN}{(N-1)r}\right) + \left(\frac{(N+1)a}{(N-1)r^2} + b\right)^{\frac{1}{3}} \mathcal{E}^N(1)\right\}. \tag{5.1}$$

At the expense of further complication, the use of $\psi_1(r)$ (the Airy function) would lower this upper bound.

Similarly, to improve our lower bound, we allow the Coulomb-plus-linear potential to intersect twice with the hydrogenic potential $h(r) = -\frac{\alpha}{r} + \beta$, with the exact wavefunction solution $\psi = \mathrm{e}^{-\alpha r/(N-1)}$ and the exact energy $E^h = \beta - \alpha^2/(N-1)^2$, where α and β are positive parameters. Again, let A and B represent the absolute values of the areas (or of the ψ-weighted areas) between the potentials. We vary α and β so that $A = B$, as illustrated in figure 3, and thereafter theorems 5 and 6 imply $E^h \leqslant E^V$. Subsequently, we obtain the lower bound (without ψ) by solving the following three equations:

$$\frac{-a}{t} + bt = -\frac{\alpha}{t} + \beta \qquad \int_0^t \left[\frac{-a}{r} + br + \frac{\alpha}{r} - \beta\right] r^{N-1}\,\mathrm{d}r = 0$$

$$E^L = \min_{t>0}\{\beta - (\alpha/(N-1))^2\}. \tag{5.2}$$

For the case $a = 1$ and $b = 1$, we compare in figure 4 the upper and lower bounds obtained by means of the classical envelope method and by the comparison theorems introduced in

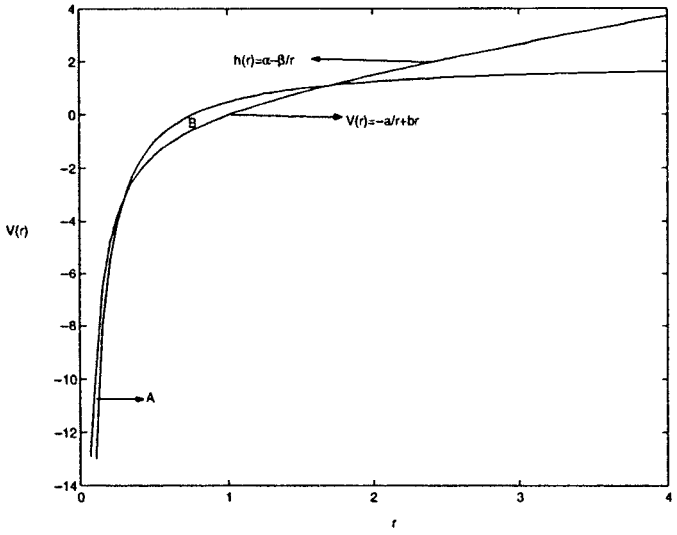

Figure 3. The hydrogenic potential $h(r) = -\alpha/r + \beta$ used to estimate a lower bound for the eigenvalues of the Coulomb-plus-linear potential $V(r) = -a/r + br$. A and B are the absolute values of the inter-potential areas (or ψ-weighted areas). We vary α and β so that $A = B$, and thereafter theorems 5 and 6 imply $E^h \leqslant E^V$.

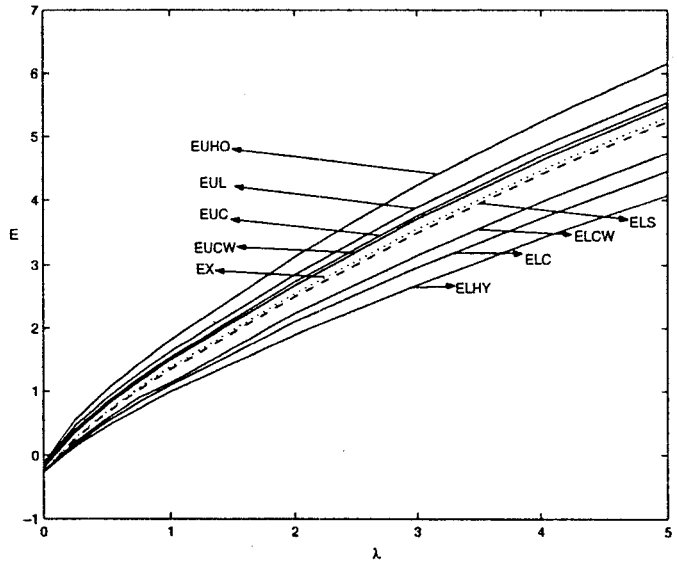

Figure 4. We compare the bounds for $E(\lambda)$, where $E(\lambda)$ is the ground-state eigenvalue ($n = 1, \ell = 0$) of the Hamiltonian $H = -\Delta - 1/r + \lambda r$. The upper bounds (full lines) are by harmonic-oscillator tangents EUHO, linear tangents EUL, linear chords EUC and linear chords with the wavefunction EUCW. The lower bounds (lower full lines) are by hydrogenic tangents ELHY, hydrogenic chords ELC and hydrogenic chords with the wavefunction ELCW. The dashed curve ELS represents the lower bound given by the sum approximation. Accurate numerical data (dotted curve) EX are shown for comparison.

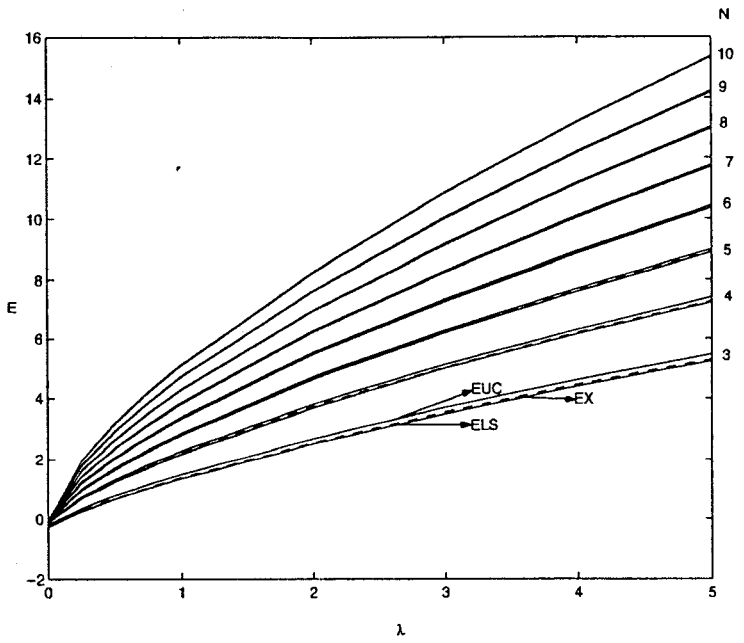

Figure 5. Bounds on the eigenvalues $E_{10}^{N}(\lambda)$ corresponding to the Coulomb-plus-linear potential $V(r) = -1/r + \lambda r$ in N dimensions. Upper bounds EUC by the generalized comparison theorem, lower bounds ELS by the sum approximation and accurate numerical data (dashed line) for $n = 1$, $\ell = 0$ and $N = 3, 4, \ldots, 7$. By theorem 2 we know that the same curves also apply to $\ell > 0$ since $E_{1\ell}^{N} = E_{10}^{N+2\ell}$.

section 3. Generalizations to cases where there are large numbers of potential crossings are discussed in [37].

6. Conclusion

Our proof of the lower bound for the bottom of the spectrum of the operator $H = -\Delta + V^{(1)}(r) + V^{(2)}(r)$, based on kinetic potentials, is more compact and direct than the original proof, and is valid in N dimensions; the principal steps of the earlier proof are repeated because they show that the final result is equivalent to an optimization of the classical theorem of Weyl. The generalized comparison theorem is proved in the present paper for all dimensions N, whereas, in its original form, it required two distinct theorems, for $N = 1$ and $N = 3$. Moreover, we are now able to apply the results to the bottom of each angular-momentum subspace since we have proved that this energy is identical to the lowest eigenvalue of a higher-dimensional problem, in $R^{N+2\ell}$. Meanwhile, in order to be practical, weaker sufficient conditions were sought which would guarantee in a simple way that the comparison potentials cross over so as to imply definite spectral ordering. These results greatly clarify the application of the generalized comparison theorem to specific problems.

The Coulomb-plus-linear problem provides a convenient example on which to test the effectiveness of the energy bounds. At the same time it offers an opportunity to sharpen

an earlier energy-bound formula for this problem, and to extend its validity to all $N \geqslant 2$ dimensions. For most of the parameter space of the problem, the energy bounds provided by this formula for the bottom of each angular-momentum subspace ($n = 1$) are accurate to a few per cent and, as we have shown, they become sharper with increasing N or ℓ. If the sum approximation is capriciously applied also to the higher discrete eigenvalues $n > 1$, the resulting *ad hoc* approximation formula continues to give very accurate estimates, which, however, are no longer bounds. What additional conditions might guarantee bounds from such a formula is an interesting open question.

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Semiclassical energy formulae for power law and log potentials in quantum mechanics

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Abstract

We study a single particle which obeys non-relativistic quantum mechanics in $\Re^N$ and has Hamiltonian $H = -\Delta + V(r)$, where $V(r) = \mathrm{sgn}(q)r^q$. If $N \geqslant 2$, then $q > -2$, and if $N = 1$, then $q > -1$. The discrete eigenvalues $E_{n\ell}$ may be represented exactly by the semiclassical expression $E_{n\ell}(q) = \min_{r>0}\{P_{n\ell}(q)^2/r^2 + V(r)\}$. The case $q = 0$ corresponds to $V(r) = \ln(r)$. By writing one power as a smooth transformation of another, and using envelope theory, it has earlier been proved that the $P_{n\ell}(q)$ functions are monotone increasing. Recent refinements to the comparison theorem of QM in which comparison potentials can cross over, allow us to prove for $n = 1$ that $Q(q) = Z(q)P(q)$ is monotone increasing, even though the factor $Z(q) = (1 + q/N)^{1/q}$ is monotone decreasing. Thus, $P(q)$ cannot increase too slowly. This result yields some sharper estimates for power-potential eigenvalues at the bottom of each angular momentum subspace.

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1. Introduction

In this paper we study a certain representation, the P-representation, for the Schrödinger spectra generated by the power-law potentials $f(r) = \mathrm{sgn}(q)r^q$ in N spatial dimensions. Considerable interest has been shown in the Schrödinger spectra generated by this elementary class of potentials [1–15]. The Hamiltonian H is given explicitly by

$$H = -\Delta + v\,\mathrm{sgn}(q)r^q \qquad \text{where} \quad r = \|r\| \quad \text{and} \quad v > 0 \quad \text{and} \quad q \neq 0 \tag{1.1a}$$

where $q > -1$ for $N = 1$, and $q > -2$ for $N \geqslant 2$. Corresponding to the case $q = 0$ we have

$$H = -\Delta + v\ln(r) \qquad v > 0. \tag{1.1b}$$

It is certainly possible to include the log potential as a limiting case of the power potentials if in place of the potential family $f(r) = \mathrm{sgn}(q)r^q$, we use $V(r, q) = (r^q - 1)/q$ whose

limit as $q \to 0$ is $V(r, 0) = \ln(r)$. However, we have chosen instead to leave the power potentials themselves in their simplest form and incorporate the $q \to 0$ limit smoothly in the spectral domain by means of the P-representation. This limit will be discussed again in this section, after the P-representation has been introduced. As with equation (1), our policy of favouring simple powers will again lead to two equations instead of one at various points in the development.

The operators H have domains $\mathcal{D}(H) \subset L^2(R^N)$, they are bounded below, and essentially self-adjoint. For the most part we shall be concerned with the cases $N \geqslant 2$, but we may also include $N = 1$ provided $q > -1$. The one-dimensional hydrogen atom ($N = 1, q = -1$) has been extensively studied [16–22] but requires special side conditions not consistent with the class of problems we consider in this paper. For the operators we consider, the essential spectrum is in $(0, \infty)$ and, by using a normalized Gaussian trial function ϕ, it is easy to select a scale so that $(\phi, H\phi) < 0$, thus establishing the existence of a discrete eigenvalue; for $q > 0$, the entire spectrum is discrete [23]. The eigenvalues $E^N_{n\ell}$ for the power-law potential can be labelled by two quantum numbers, the total angular momentum $\ell = 0, 1, 2, \ldots$, and a 'radial' quantum number, $n = 1, 2, 3, \ldots$, which represent 1 plus the number of nodes in the radial part of the wavefunction. These eigenvalues satisfy the relation $E^N_{n\ell} \leqslant E^N_{m\ell}$, $n < m$. With our labelling convention, the eigenvalue $E^N_{n\ell}(q)$ in $N \geqslant 2$ spatial dimensions has degeneracy 1 for $\ell = 0$ and, for $\ell > 0$, the degeneracy is given [24] by the function $\Lambda(N, \ell)$, where

$$\Lambda(N, \ell) = (2\ell + N - 2)(\ell + N - 3)!/\{\ell!(N - 2)!\} \qquad N \geqslant 2 \quad \ell > 0. \tag{1.2}$$

We first review some general elementary results for the power-law eigenvalues [2]. Nieto and Simons [6] have proved that the eigenvalues $E_n = E^1_{n0}$ for the power-law potentials in one dimension increase with the quantum number n at a higher rate when q is greater. However, for any q, this increase never attains n^2, i.e., $\lim_{n\to\infty} E_n/n^2 = 0, q < \infty$. In general, the dependence of the eigenvalues $E^N_{n\ell}$ on the coupling parameter v may be established with the aid of elementary scaling arguments in which r is replaced by σr, where $\sigma > 0$. We find that

$$E^N_{n\ell}(v) = v^{2/(q+2)} E^N_{n\ell}(1). \tag{1.3}$$

Thus, without loss of generality, we may limit further discussion to the case of unit coupling, $v = 1$. We shall henceforth let an expression such as $E(q)$ represent the dependence of an eigenvalue of unit coupling on the power q.

We do have *some* exactly solvable potentials in N dimensions. For example, for the well-known hydrogenic atom and the harmonic oscillator potentials we have for $n = 1, 2, 3, \ldots$.

$$E^N_{n\ell}(-1) = -[2(n + \ell + N/2 - 3/2)]^{-2} \qquad N \geqslant 2 \tag{1.4}$$

and

$$E^N_{n\ell}(2) = 4n + 2\ell + N - 4 \qquad N \geqslant 2 \tag{1.5a}$$

and in one dimension (keeping $n = 1, 2, 3, \ldots$)

$$E_n(2) = 2n - 1 \qquad N = 1. \tag{1.5b}$$

Analytical solutions are also possible for the linear potential in one dimension, and for the S states in three dimensions. For $N = 1$ and $N = 3$ the repulsive $1/r^2$ term in the 'effective potential' $V_{\text{eff}}(r) = (N - 1)(N - 3)/4r^2$, obtained using the transformation $\psi(r) = \phi(r)/r^{(N-1)/2}$, is zero. The exact solution in these cases is in terms of the zeros of Airy's function $\text{Ai}(r)$ in three dimensions and the zeros of the first derivative $\text{Ai}'(r)$ of Airy's function in one dimension. We have

$$E^1_n(v) = v^{\frac{2}{3}} r_{n+1} \qquad \text{Ai}'(-r_{n+1}) = 0 \qquad n = 0, 1, 2, \ldots. \tag{1.6}$$

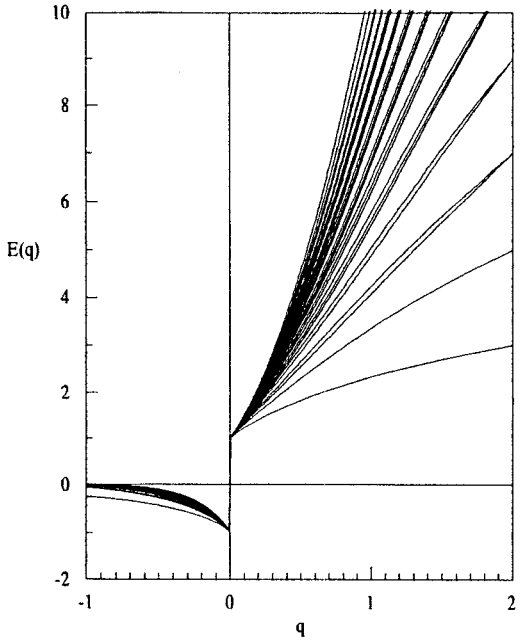

Figure 1. The first 30 eigenvalues $E_{n\ell}(q)$, $1 \leqslant n \leqslant 5, 0 \leqslant \ell \leqslant 5$, corresponding to the power potential $V(r) = \mathrm{sgn}(q)r^q$ in $N = 3$ dimensions. For $q > 0$, the eigenvalues increase with q from 1 to $E_{n\ell}(2) = 4n + 2\ell - 1$; for $q < 0$, they decrease (as q increases) from $E_{n\ell}(-1) = -[2(n+\ell)]^{-2}$ to -1. Both sets of curves increase with n and ℓ.

$$E^3_{n0}(v) = v^{\frac{2}{3}} r_n \qquad \mathrm{Ai}(-r_n) = 0 \qquad n = 1, 2, 3, \ldots. \tag{1.7}$$

Unfortunately, for $N = 2$ or $N > 3$, and for higher angular momenta $\ell > 0$ generally, exact solutions are unavailable at this time. However, by using theorem 1 [25, theorem 2] we have for $N \geqslant 2$ the general correspondence $E^N_{n\ell} = E^{N+2\ell}_{n0}$. In figure 1 we exhibit the graphs of the eigenvalues $E^3_{n0}(q)$ for $n = 1, \ldots, 5$. In the limit $q \to \infty$ the problem is equivalent to an infinite square well with width 1 in N dimensions. Thus we have $\lim_{q\to\infty} |E^3_{n0}(q)| = (n\pi)^2$. For small values of q, the $|E(q)|$ curves are asymptotically like $|E(q)| \sim C|q/2|^{q/2}$ and have infinite slopes in the limit $q \to 0$ [2, 26, 27].

The approach in the present paper is to study a representation for $E_{n\ell}(q)$ which is smoother and easier to approximate than the 'raw' eigenvalues themselves. We shall write many of our equations for the case $N \geqslant 2$: they are also valid for $N = 1$ provided $q > -1$. In both cases we keep the convention $n = 1, 2, 3, \ldots$. We have

$$E^N_{n\ell} = \min_{r>0} \left\{ \left(\frac{P^N_{n\ell}(q)}{r} \right)^2 + \mathrm{sgn}(q) r^q \right\} \qquad q > -2 \quad q \neq 0 \tag{1.8a}$$

and

$$E^N_{n\ell} = \min_{r>0} \left\{ \left(\frac{P^N_{n\ell}(0)}{r} \right)^2 + \ln(r) \right\}. \tag{1.8b}$$

The form of this representation, in which the kinetic energy is represented by P^2/r^2 and the power potential is represented by itself, is what leads us to use the term 'semiclassical' in the

title of the paper: the two parts of the quantum mechanical problem are replaced by simple real functions of r, scaling as the classical terms would scale, and their sum is exactly equal to the quantum mechanical energy. This is a quite different use of the term 'semiclassical' from that describing a reformulation of the quantum mechanical problem itself. Such a method is the JWKB approximation which has been applied to estimate the pure-power spectra [12, 13] and could in principle therefore be employed to approximate $P^N_{n\ell}(q)$: however, this approach would not yield exact analytical information about the P-functions, such as bounds or convexity. The existence of the representation $P(q)$ for $E(q)$ is guaranteed because the functions

$$g(P,q)=\min_{r>0}\left\{\left(\frac{P}{r}\right)^2+\mathrm{sgn}(q)r^q\right\}=\mathrm{sgn}(q)\left(1+\frac{q}{2}\right)\left(\frac{2P^2}{|q|}\right)^{\frac{q}{2+q}} \qquad q>-2 \quad q\neq 0 \tag{1.9a}$$

and

$$g(P,0)=\min_{r>0}\left\{\left(\frac{P}{r}\right)^2+\ln(r)\right\}=\frac{1}{2}(1+\ln(2))+\ln(P). \tag{1.9b}$$

are monotone increasing in P. Indeed we find

$$\frac{\partial g}{\partial P}(P,q)=P^{\frac{q}{2+q}}\left(\frac{|q|}{2P}\right)^{\frac{2}{q+2}}>0 \qquad q>-2 \quad q\neq 0 \tag{1.10a}$$

and

$$\frac{\partial g}{\partial P}(P,0)=\frac{1}{P}>0. \tag{1.10b}$$

From (1.4) and (1.5) we find

$$P^N_{n\ell}(-1)=(n+\ell+N/2-3/2) \qquad N\geqslant 2 \tag{1.11}$$

and

$$P^N_{n\ell}(2)=(2n+\ell+N/2-2) \qquad N\geqslant 2 \tag{1.12a}$$

and in one dimension (keeping $n=1,2,3,\ldots$)

$$P_n(2)=\left(n-\tfrac{1}{2}\right) \qquad N=1. \tag{1.12b}$$

In table 1 we exhibit some numerical values for $P^N_{n\ell}(1)$. The case $q=0$ corresponds *exactly* to the $\ln(r)$ potential [26]. In this paper we shall denote by $E(q)$ and $P(q)$ the ground-state eigenvalues and P-functions in N dimensions.

We now return briefly to the question of considering the log potential as the limit of the family $V(r,q)=(r^q-1)/q$, as $q\to 0$, where we define $V(r,0)=\ln(r)$. A useful feature of the P-representation is that, for a given eigenvalue, only one P-number is required to determine the eigenvalue $\mathcal{E}$ corresponding to the 'scaled' power potential $A+B\,\mathrm{sgn}(q)r^q$, $B>0$. Thus, we may write (exactly)

$$\mathcal{E}^N_{n\ell}(A,B,q)=\min_{r>0}\left\{\left(\frac{P^N_{n\ell}(q)}{r}\right)^2+A+B\,\mathrm{sgn}(q)r^q\right\} \qquad q>-2 \quad q\neq 0 \quad B>0. \tag{1.13}$$

In particular, with $A=-1/q$, $B=1/|q|$ we have

$$V(r,q)=(r^q-1)/q \quad\Rightarrow\quad \mathcal{E}^N_{n\ell}(q)=\min_{r>0}\left\{\left(\frac{P^N_{n\ell}(q)}{r}\right)^2+\frac{r^q-1}{q}\right\} \qquad q>-2 \quad q\neq 0. \tag{1.14}$$

Table 1. The 'input' P-values $P^N_{n0}(1)$ used in the general formula (1.8), for $N = 2, 3, \ldots, 12$. The same data apply to $\ell > 0$ since, by theorem 1, we have $P^N_{n\ell} = P^{N+2\ell}_{n0}$.

N	$n=1$	$n=2$	$n=3$	$n=4$
2	0.9348	2.8063	4.6249	6.4416
3	1.3761	3.1813	4.9926	6.8051
4	1.8735	3.6657	5.4700	7.2783
5	2.3719	4.1550	5.9530	7.7570
6	2.8709	4.6472	6.4398	8.2396
7	3.3702	5.1413	6.9291	8.7251
8	3.8696	5.6367	7.4204	9.2129
9	4.3692	6.1330	7.9130	9.7024
10	4.8689	6.6299	8.4068	10.1932
11	5.3686	7.1274	8.9053	10.7453
12	5.8684	7.6253	9.4045	11.2744

Provided $P(q)$ is continuous, it follows immediately from (1.14) that

$$V(r) = \ln(r) \quad \Rightarrow \quad \mathcal{E}^N_{n\ell} = \min_{r>0}\left\{\left(\frac{P^N_{n\ell}(0)}{r}\right)^2 + \ln(r)\right\}. \tag{1.15}$$

As we mentioned above, the continuity (in fact, monotonicity) of $P^N_{n\ell}(q)$ was proved in [2]. It is our opinion that the advantage of accommodating this limit easily does not justify the concomitant complication of having to work, for example, with a harmonic oscillator having the form $V(r, 2) = (r^2 - 1)/2$.

For $N \geqslant 2$, the P-numbers and the underlying eigenvalues $E^N_{n\ell}$ satisfy the relation $P^N_{n\ell} = P^{N+2\ell}_{n0}$. This result is obtained using the following theorem.

Theorem 1 (25, theorem 2). *Suppose that $H = -\Delta + V(r)$, where $V(r)$ is a central potential in $N \geqslant 2$ dimensions, has a discrete eigenvalue $E^N_{n\ell}$, then $E^N_{n\ell} = E^{N+2\ell}_{n0}$. This theorem expresses the invariance of the eigenvalues with respect to changes in ℓ and N that leave the sum $N + 2\ell$ invariant.*

The advantage of the P-representation is illustrated by comparing figure 1 with figure 2 which show, respectively, the eigenvalues $E_{n\ell}(q)$ and the corresponding P-representations $P_{n\ell}(q)$ for the case $N = 3$. The P-functions of figure 2 are evidently monotone increasing. This property has been proved mathematically by means of the envelope theory [2]: one power q was written as a smooth transformation of another p, and then the limit $p \to q$ was taken in the P-picture. The infinite slopes of $E(q)$ at $q = 0$, mentioned above, are not visible in figure 1 because the approach of the slopes to infinity is very slow for such functions: if, for example, we consider [27] the function $f(q) = |q|^q$, then, although $f'(0) = -\infty$, we have $f'(10^{-5}) \approx -10.51$.

The principal result of the present paper is theorem 4, to the effect that for $N \geqslant 1$, $Q(q) = Z(q)P(q)$ is monotone increasing, where $Z(q) = (1 + q/N)^{\frac{1}{q}}$: this result is stronger than the monotonicity of $P(q)$ because the factor $Z(p)$ is decreasing; thus we know more about $P(q)$ than we did. This theorem is proved in section 2 and principally concerns the power-law potentials, but also treats the log case by the use of the limit $q \to 0$ and continuity. As consequences of theorem 4 we shall be able to derive some specific formulae for upper and lower bounds for the power-law energy eigenvalues, by using nearby comparisons. However,

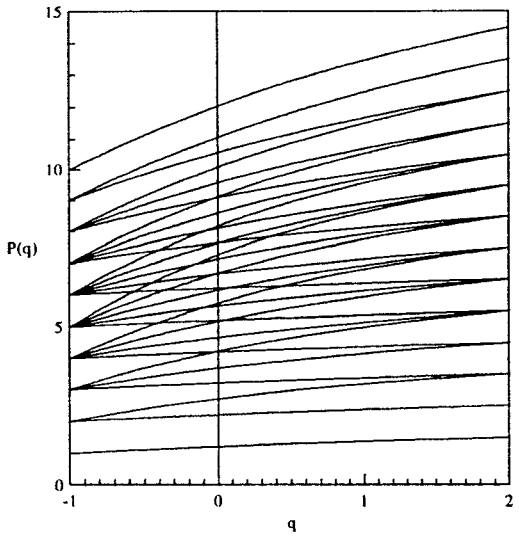

Figure 2. In the P-representation, the same set of 30 eigenvalues shown in figure (1) now lie on monotone smooth curves. The log-power theorem states that the P-values for the log potential are precisely $P_{n\ell}(0)$. As q increases from -1 to 2, the degeneracy of the Coulomb problem $P_{n\ell}(-1) = n + \ell$ evolves into the degeneracy of the harmonic oscillator $P_{n\ell}(2) = 2n + \ell - \frac{1}{2}$.

it should be clearly emphasized at this point that the main purpose of the present paper is to strengthen our knowledge of the monotone function $P(q)$.

Theorem 4 has been made possible by the emergence of generalized comparison theorems that allow comparison potentials to cross over and still predict spectral ordering. In section 2 we restate the generalized comparison theorem (theorem 4, of [25]) which becomes theorem 2 here, and we state theorem 3 (theorem 7, of [25]), which provides explicit sufficient conditions for the application of theorem 3 under a variety of potential crossing schemes. Theorem 3 allows us to prove our main result, theorem 4. In section 3, we use theorem 4 to prove theorem 5 which sharpens the envelope bounds found earlier in [2]. The earlier result used 'envelope theory' based on the 'standard' comparison theorem, which may be written as $V_1 < V_2 \Rightarrow E[V_1] < E[V_2]$. As an illustration of theorem 5 we apply it to generate spectral bounds for the bottom of the spectrum of $-\Delta + r^{\frac{3}{2}}$ in dimensions $N = 3 \ldots 10$.

2. Power-law potentials and generalized comparison theorems

We now discuss the generalized comparison theorems which we shall apply to obtain our main result. We consider the two eigenproblems $(-\Delta + V_1(r))\psi_1(r) = E[V_1]\psi_1(r)$ and $(-\Delta + V_2(r))\psi_2(r) = E[V_2]\psi_2(r)$ in $N \geqslant 1$ dimensions, where $\psi_i(r), i = 1, 2$, are the respective ground states (or the bottoms of angular momentum subspaces labelled by a fixed $\ell \geqslant 0$).

Theorem 2 (25, theorem 4).

$$k(r) = \int_0^r [V_1(t) - V_2(t)]\psi_i(t)t^{N-1}\,dt < 0 \qquad \forall r > 0$$
$$i = 1 \quad \text{or} \quad 2 \Rightarrow E[V_1] < E[V_2]. \tag{2.1}$$

We have stated this theorem (and the following theorem) with strict inequalities: the proofs are essentially the same as given in [25]. It may be difficult to apply theorem 2 in practice since the positivity of the function $k(r)$ depends on the detailed properties of the comparison potentials. Thus, it is helpful to have simpler sufficient conditions, depending on the number and nature of the crossings over of the two comparison potentials. In particular we shall employ the case of two crossings, and sufficient conditions not involving the wavefunction. Thus, we have

Theorem 3 (25, theorem 7). *If the potentials $V_1(r)$ and $V_2(r)$ cross twice for $r > 0$ at $r = r_1, r_2$ $(r_1 < r_2)$ with*

(i) $V_1(r) < V_2(r)$ *for* $0 < r < r_1$ *and*

(ii) $\int_0^{r_2}[V_1(t) - V_2(t)]t^{N-1}\,dt = 0$

then,

$$k(r) = \int_0^r [V_1(t) - V_2(t)]\psi_i(t)t^{N-1}\,dt < 0 \qquad \forall r > 0 \qquad i = 1 \text{ or } 2 \tag{2.2}$$

from which $E[V_1] < E[V_2]$ *follows, by theorem 2.*

Now we shall use the generalized comparison theorems to prove the monotonicity of a new function $Q(q)$, which does not 'vary' so much as the function $P(q)$. As a consequence, we shall be able to derive specific formulae for upper and lower bounds for the power-law energy eigenvalues. We are able to prove the following:

Theorem 4. *$P(q)$ represents via (1.8) the bottom $E(q)$ of the spectrum of $H = -\Delta + \operatorname{sgn}(q)r^q$, where $q \neq 0$, and $q > -2$, in $N \geqslant 2$ dimensions (or $q > -1$ for $N = 1$). Define $Q(q) = (1 + q/N)^{1/q}P(q)$, and $Q(0) = \lim_{q\to 0} Q(q) = e^{1/N}P(0)$, then $Q(q)$ is monotone increasing for $N \geqslant 2$, $q > -2$ (or $N = 1$, $q > -1$).*

Proof. Let $p > q$, $p, q > -2$ for $N \geqslant 2$ and $p, q > -1$ for $N = 1$. We shall first suppose $p \neq 0$ and $q \neq 0$. Our goal is to prove that $Q(p) > Q(q)$. Assume that $V_1(r) = A + B\operatorname{sgn}(p)r^p$ and $V_2(r) = \operatorname{sgn}(q)r^q$. Now, we choose A and B so that the potentials $V_1(r)$ and $V_2(r)$ cross over exactly twice, as illustrated in figure 3. Let A_1 and B_1 represent the absolute values of the areas between the potentials. We vary A and B so that $A_1 = B_1$. Then theorem 3 implies $E[V_1] \leqslant (\geqslant) E[V_2]$ depending, as r increases from zero, on which potential lies beneath the other when they first differ. Without loss of generality, we will assume, in this sense, that V_1 starts above V_2; this leads to an upper bound. Since $V_1(r)$ is designed to intersect $V_2(r)$ exactly twice, we shall have two equations to solve to provide sufficient conditions for a bound

$$V_1(R) = V_2(R) \quad \Rightarrow \quad A + B\operatorname{sgn}(p)R^p = \operatorname{sgn}(q)R^q \tag{2.3a}$$

and

$$\int_0^R [V_1(r) - V_2(r)]r^{N-1}\,dr = 0 \quad \Rightarrow \quad A\frac{R^N}{N} + B\operatorname{sgn}(p)\frac{R^{p+N}}{p+N} - \operatorname{sgn}(q)\frac{R^{q+N}}{q+N} = 0 \tag{2.3b}$$

where R is the second potential intersection point. We let $t = R^{p/q}$ and, solve (2.3a) and (2.3b) for $A(t)$ and $B(t)$, to find

$$A(t) = \frac{\operatorname{sgn}(q)Nt^{q^2/p}(p-q)}{p(q+N)} \tag{2.4}$$

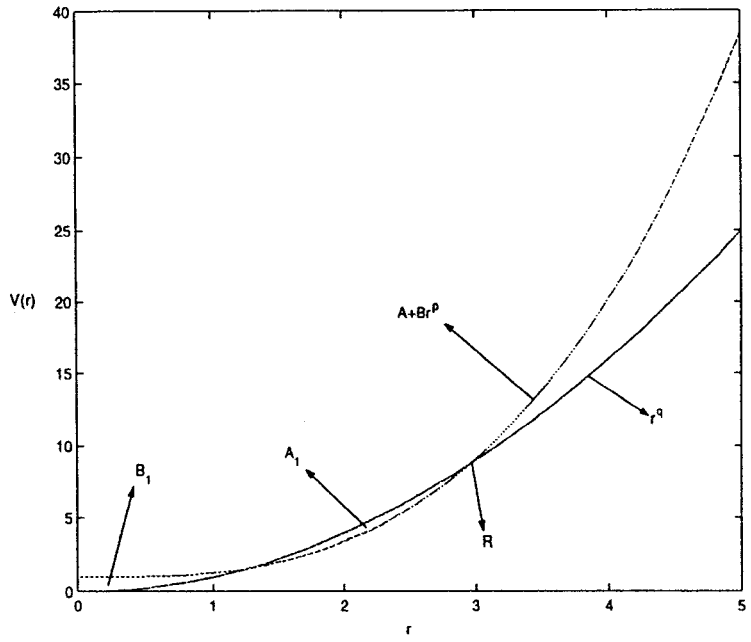

Figure 3. The shifted linear potential $V_1(r) = A + Br^p$ used to estimate an upper bound for the eigenvalues corresponding to the potential $V_2(r) = r^q$. A_1 and B_1 are the absolute values of the inter-potential areas. We vary A and B so that $A_1 = B_1$, where R is the second intersection point. Thereafter, theorem 3 implies that $E[V_2] \leqslant E[V_1]$. This result is used to prove the monotonicity of $Q(q)$.

$$B(t) = \frac{|q|(p+N)}{|p|(N+q)t^{q/p(p-q)}}. \tag{2.5}$$

Without loss of generality, we may consider only the case when p and $q > 0$, since the proof of the other cases is exactly similar. Theorem 3 thus implies that

$$\min_t \left\{ A(t) + B(t)^{\frac{2}{(p+2)}} E(p) \right\} > E(q) \tag{2.6}$$

Optimizing the left-hand side over t, we find the critical point as follows. We define

$$F(t) = A(t) + (B(t))^{\frac{2}{p+2}} E(p) = \frac{Nt^{q^2/p}(p-q)}{p(q+N)} + \left(\frac{q(p+N)}{p(N+q)t^{q/p(p-q)}} \right)^{\frac{2}{p+2}} E(p). \tag{2.7}$$

We now simplify the equation to find the critical point in terms of p and q. We define the following:

$$n = q^2/p \qquad m = \frac{q}{p}(p-q)\left(\frac{2}{2+p}\right) \qquad a_1 = \left(\frac{N(p-q)}{p(q+N)}\right)$$

and

$$b_1 = \left(\frac{q(p+N)}{p(N+q)}\right)^{\frac{2}{2+p}} E(p).$$

Thus we have

$$F(t) = a_1 t^n + b_1 t^{-m} \qquad F'(t) = a_1 n t^{n-1} - b_1 m t^{-m-1}$$

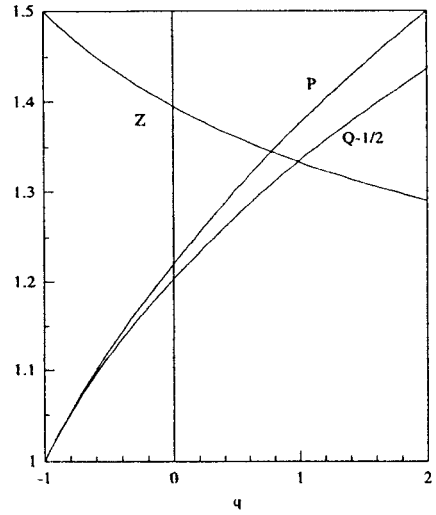

Figure 4. The functions $P(q)$, $Z(q)$ and $Q(q) = P(q)Z(q)$ for the ground state in dimension $N = 3$. Theorem 4 states that for the ground state in all dimensions $N \geqslant 1$, $Q(q)$ is monotone increasing with q.

for which the minimum occurs at $\hat{t} = \left[\frac{b_1 m}{a_1 n}\right]^{\frac{1}{n+m}}$. Meanwhile, the minimum value $F(\hat{t})$ is given by

$$F(\hat{t}) = a_1\left[\frac{b_1 m}{a_1 n}\right]^{\frac{n}{n+m}} + b_1\left[\frac{b_1 m}{a_1 n}\right]^{-\frac{m}{n+m}} = a_1^{\frac{m}{n+m}} b_1^{\frac{n}{n+m}}\left[\frac{m}{n}\right]^{-\frac{m}{n+m}}\left[\frac{m}{n}+1\right] \geqslant E(q).$$

By substituting $F(\hat{t})$ and $E(p)$ given by (1.9) in (2.6), we find that

$$\left(\frac{N(p-q)}{p(q+N)}\right)^{\frac{2(p-q)}{p(q+2)}}\left[\left(\frac{q(N+p)}{p(q+N)}\right)^{\frac{2}{2+p}}\left(\frac{p+2}{2}\right)\left(\frac{2P(p)^2}{p}\right)^{\frac{p}{p+2}}\right]^{\frac{q(2+p)}{p(q+2)}}$$
$$\times\left[\frac{q(p+2)}{2(p-q)}\right]^{\frac{2(p-q)}{p(q+2)}}\left[\frac{p(q+2)}{q(p+2)}\right] > \left(\frac{q+2}{2}\right)\left(\frac{2P(q)^2}{q}\right)^{\frac{q}{2+q}}. \tag{2.8}$$

By simplifying this expression, we find eventually that $Q(q) = (1+q/N)^{1/q}P(q)$ is monotone increasing, that is to say

$$Q(p) > Q(q). \tag{2.9}$$

Now for $N \geqslant 2$, $P(q)$ is continuous, $q > -2$, (or for $N = 1, q > -1$), and, if we define $Z(0) = \lim_{q\to 0} Z(q) = e^{1/N}$, then $Q(0) = Z(0)P(0)$. It follows immediately that $Q(q) = Z(q)P(q)$ is continuous and monotone increasing $q > -2$ (or for $N = 1, q > -1$). □

The three functions $P(q)$, $Z(q)$ and $Q(q)$ are illustrated for $N = 3$ in figure 4: theorem 4 states that in all dimensions $N \geqslant 1$, $Q(q)$ is a monotone increasing function of q.

3. Application

By using the monotonicity of the function $Q(q)$, we now prove a special comparison theorem (a corollary to theorem 4) for the comparison of eigenvalues generated by power-law potentials.

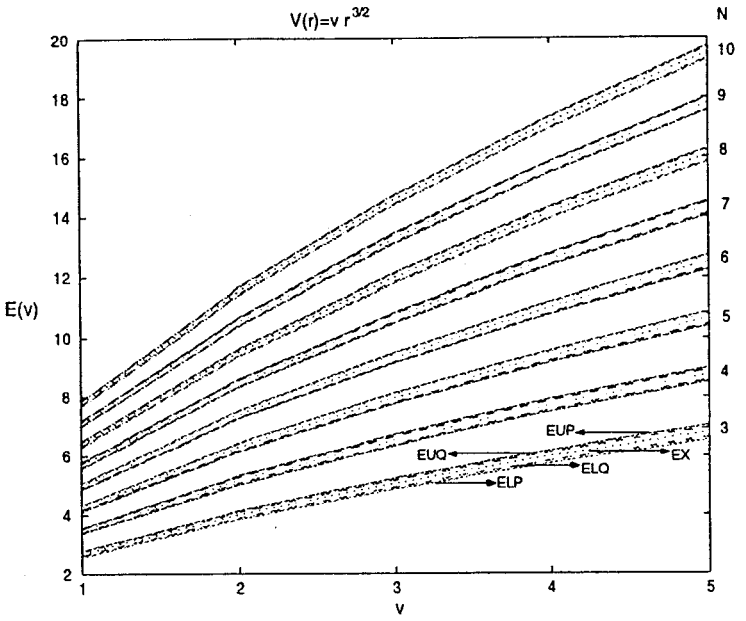

Figure 5. Bounds on the eigenvalues $E^N_{l0}(v)$ corresponding to the power potential $V(r) = vr^{\frac{3}{2}}$ in N dimensions. The upper and lower bounds (full lines) are obtained by harmonic oscillator tangents EUP, and linear tangents ELP (theorem 5 (i), (ii)). The dashed curves EUQ and ELQ represent, respectively, the improved upper and lower bounds (theorem 5 (iii), (iv)). Accurate numerical data (dotted curves) EX are shown for comparison.

Theorem 5. *Consider the power-law potentials* $V_i(r) = \mathrm{sgn}(q_i)r^{q_i}, q_i > -2$, $(q_i > -1,$ *for* $N = 1)$, $i = 1, 2$, *where* $q_1 < q_2$. *Let* $Z(q) = (1 + q/N)^{1/q}$, $Z(0) = \lim_{q\to} Z(q) = \mathrm{e}^{1/N}$, $Q(q) = Z(q)P(q)$ *and* $g(P, q)$ *be given by (1.9a) and (1.9b), then*

(i) $E[V_1] < E_1^U = g(P(q_2), q_1)$

(ii) $E[V_2] > E_1^L = g(P(q_1), q_2)$

(iii) $E[V_1] < E_2^U = g\left(\dfrac{Q(q_2)}{Z(q_1)}, q_1\right) < E_1^U$

(iv) $E[V_2] > E_2^L = g\left(\dfrac{Q(q_1)}{Z(q_2)}, q_2\right) > E_1^L.$

Proof. We first establish the upper bound (iii). We note that the function $Z(q) = (1+q/N)^{1/q}$ is decreasing. Thus $q_1 < q_2$, implies $Z(q_2) < Z(q_1)$, and by using the monotonicity of the functions $P(q)$ [2] and $g(P, q)$, we may conclude that $P(q_1) < Z(q_2)P(q_2)/Z(q_1) = Q(q_2)/Z(q_1) < P(q_2)$, which, in turn, implies $E[V_1] < E_2^U < E_1^U$. This proves (i) and (iii). After a reversal of the inequalities, the proofs for the lower bounds (ii) and (iv) follow similarly. □

We note that theorem 5 includes applications to the log potential. For example, if $q_1 = 0$ and $q_2 = q > 0$, then we have from theorem 5 (iv)

$$E(q) > \min_{r>0}\left\{\left(\frac{Q(0)}{Z(q)r}\right)^2 + \mathrm{sgn}(q)r^q\right\} \qquad q > 0. \tag{3.1}$$

Example: $V(r) = r^{\frac{3}{2}}$. We illustrate theorem 5 by applying it to the potential $V(r) = r^{\frac{3}{2}}$ in $N \geqslant 3$ dimensions. We first use the linear and the harmonic oscillator problems to obtain upper and lower bounds by envelope theory. That is to say, we first use equation (1.9*a*) to give the envelope lower bound ELP given by $g(P(1), 3/2)$, and the envelope upper bound EUP given by $g(P(2), 3/2)$. Then we use theorem 5 (iv) to generate the improved lower bound ELQ given by $g(Q(1)/Z(3/2), 3/2)$, and theorem 5 (iii) to generate the improved upper bound EUQ given by $g(Q(2)/Z(3/2), 3/2)$. These results are shown in figure 5, along with accurate numerical data EX, for $N = 3, \ldots, 10$: they illustrate the improvement obtained in the approximation when Q is used rather then P in the semiclassical energy formulae.

4. Conclusion

The eigenvalues $E(q)$ of $H = -\Delta + \mathrm{sgn}(q)r^q, q > -2, q \neq 0$, may be conveniently represented by the functions $P(q)$, which are known [2] to be positive, continuous and monotone increasing. In the proof of the earlier result, each q-potential was written as a smooth transformation of a p-potential with definite convexity, and then the 'envelope theory' was applied. The envelope method, in turn, depends on the 'standard' comparison theorem of quantum mechanics. In the present paper we use a stronger comparison theorem, valid for node-free states in N dimensions, and we are able thereby to learn more about $P(q)$ for the bottom of each angular momentum subspace ($n = 1$). If $N > 1$ and $\ell > 0$, we use the equivalence $E^N_{1\ell} = E^{2\ell+N}_{10}$. We have shown for all these problems that $Q(q) = P(q)Z(q)$ is monotone increasing, where the factor $Z(q) = (1 + q/N)^{1/q}$ is decreasing. This immediately leads to some sharpened spectral inequalities concerning pairs of power-law Hamiltonians.

The $P(q)$ functions are important for an established general lower bound for potentials which are sums of powers. Thus, if $V(r) = \sum_q a(q)\,\mathrm{sgn}(q)r^q + a(0)\ln(r)$, then we have [1, 31] for the bottom of each angular momentum subspace in $N \geqslant 2$ dimensions

$$E^N_{1\ell} \geqslant \min_{r>0}\left\{\frac{1}{r^2} + \sum_q a(q)\,\mathrm{sgn}(q)\left(P^N_{1\ell}(q)r\right)^q + a(0)\ln\left(P^N_{1\ell}(0)r\right)\right\}.$$

This formula, which is easily extended to smooth mixtures defined by an integral, is exact whenever the non-negative 'weight' $a(q)$ is concentrated on a single term. The lower bound is preserved if the P-numbers are replaced by lower bounds to them. Thus, any information concerning these fundamental numbers for the power-law potentials immediately has application to this general lower bound. These numbers have yielded useful energy bounds also for the many-body problem [32], and for relativistic problems [33, 34].

In spite of the simplicity of the power-law potentials and the attractive scaling properties of the corresponding Schrödinger eigenvalues, general results concerning the unit-coupling eigenvalues $E(q)$ seem to be difficult to obtain. One might expect that the results of the present paper would extend to all the excited states, but we know of no way at present to prove such general results. A proof of the apparent concavity of all the $P(q)$ functions seems to be even more elusive some of which are illustrated for $N = 3$ in figure 2. The establishment of concavity of $P(q)$ (or better, $Q(q)$) would immediately yield a large number of new spectral inequalities arising from the use of tangents and chords to the corresponding graphs.

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Coulomb plus power-law potentials in quantum mechanics

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Abstract

We study the discrete spectrum of the Hamiltonian $H = -\Delta + V(r)$ for the Coulomb plus power-law potential $V(r) = -1/r + \beta\,\mathrm{sgn}(q)r^q$, where $\beta > 0, q > -2$ and $q \neq 0$. We show by envelope theory that the discrete eigenvalues $E_{n\ell}$ of H may be approximated by the semiclassical expression $E_{n\ell}(q) \approx \min_{r>0}\{1/r^2 - 1/(\mu r) + \mathrm{sgn}(q)\beta(\nu r)^q\}$. Values of μ and ν are prescribed which yield upper and lower bounds. Accurate upper bounds are also obtained by use of a trial function of the form, $\psi(r) = r^{\ell+1}\,\mathrm{e}^{-(\alpha r)^d}$. We give detailed results for $V(r) = -1/r + \beta r^q$, $q = 0.5, 1, 2$ for $n = 1, \ell = 0, 1, 2$, along with comparison eigenvalues found by direct numerical methods.

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1. Introduction

In this paper we derive upper and lower bound formulae for the spectrum of a single particle in three dimensions that obeys non-relativistic quantum mechanics and has Hamiltonian

$$H = -\omega\Delta - A/r + B\,\mathrm{sgn}(q)r^q \qquad \omega, A, B > 0 \quad \text{and} \quad q \neq 0, q > -2. \tag{1.1}$$

The Coulomb plus power-law potential is of interest in particle physics where it serves as a non-relativistic model for the principal part of the quark–quark interaction. This class of potentials has been well studied and much work has been done to approximate the eigenvalues, with or without the Coulomb term necessitated by QCD [1–14]. Our goal in this paper is to provide simple formulae for upper and lower energy bounds for this class of potentials. Firstly, we use the 'envelope method' [15, 16] to obtain upper and lower bound formulae for all the discrete eigenvalues. We also use a Gaussian trial function and the 'sum approximation' [17, 18] to improve the bounds for the bottom of each angular-momentum subspace. The

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energy bounds discussed so far may all be expressed in terms of the following semiclassical energy formula:

$$\mathcal{E} \approx \min_{r>0}\left\{\omega\frac{1}{r^2} - \frac{A}{\mu r} + B\,\mathrm{sgn}(q)(\nu r)^q\right\} \tag{1.2}$$

for suitable choices of the parameters $\mu > 0$ and $\nu > 0$. We also apply a variational method used earlier [19] which is based on the exact Coulomb wavefunction and yields accurate upper bounds for the bottom of each angular momentum subspace. We compare all these results with 'exact' eigenvalues computed by direct numerical integration.

For the class of potentials studied some exactly solvable cases exist for suitable values of the couplings ω, A, B, and the power q. For example, for the well-known hydrogenic atom and the harmonic oscillator potentials we have explicitly for $n = 1, 2, 3, \ldots$

$$q = -1 \quad \Rightarrow \quad E_{n\ell} = -\frac{A^2}{4\omega(n+\ell)^2} \tag{1.3}$$

and

$$q = 2 \quad \Rightarrow \quad E_{n\ell} = (\omega B)^{\frac{1}{2}}(4n + 2\ell - 1). \tag{1.4}$$

For $\ell = 0$, exact solutions are also available for the linear potential $q = 1$. We can simplify the coupling problem in general by the use of scaling arguments. If, for each fixed q, we denote the eigenvalues of $H = -\omega\Delta - A/r + Br^q$ by $\mathcal{E}(\omega, A, B)$, and consider a scale change of the form $s = r/\sigma$, and choose the scale $\sigma = \omega/A$, then it is straightforward to show that

$$\mathcal{E}(\omega, A, B) = \left(\frac{A^2}{\omega}\right)\mathcal{E}(1, 1, \beta) \qquad \beta = \left(\frac{B}{\omega}\right)\left(\frac{\omega}{A}\right)^{q+2}. \tag{1.5}$$

Hence, the full problem is now reduced to the simpler one-parameter problem

$$H = -\Delta - 1/r + \beta\,\mathrm{sgn}(q)r^q \qquad E = E(\beta) = \mathcal{E}(1, 1, \beta) \qquad \beta > 0. \tag{1.6}$$

2. Energy bounds by the envelope method and the sum approximation

The comparison theorem tells us that an ordering between potentials implies an ordering between the corresponding eigenvalues. The 'envelope method' [15, 16] is based on this theorem and establishes upper and lower bound formulae for a wide class of attractive spherically-symmetric potentials. We need a solvable model $-\Delta + h(r)$ which provides an 'envelope basis' for the study of the problems of the form $-\Delta + g(h(r))$, where the transformation function g is monotone increasing and of definite convexity: when g is convex, we obtain lower bounds; when g is concave, the theory yields upper bounds. The natural basis in this context is a single power-law potential. The spectrum of a Hamiltonian of the form

$$H = -\Delta + \mathrm{sgn}(q)r^q \qquad \text{where} \quad q > -2 \quad \text{and} \quad q \neq 0 \tag{2.1}$$

may be represented *exactly* by the following semiclassical expression [11, 16]:

$$E_{n\ell} = \min_{r>0}\left\{\frac{1}{r^2} + \mathrm{sgn}(q)(P_{n\ell}(q)r)^q\right\} \tag{2.2a}$$

$$= \mathrm{sgn}(q)\left(1 + \frac{q}{2}\right)\left(\frac{2P_{n\ell}(q)^2}{|q|}\right)^{\frac{q}{2+q}}. \tag{2.2b}$$

The function $P = P_{n\ell}(q)$ is known as the P-representation, for the Schrödinger spectra generated by the power-law potentials. It is convenient to use the P function to study and

Table 1. The 'input' values $P_{n\ell}(\frac{1}{2})$ and $P_{n\ell}(1)$ to be used in the general formula (2.5) for the energies corresponding to the potential $V(r) = -1/r + \beta\,\mathrm{sgn}(q)r^q$. These P-values yield upper bounds when $q \leqslant \frac{1}{2}$, or $q \leqslant 1$, respectively.

n	ℓ	$P_{n\ell}(\frac{1}{2})$	$P_{n\ell}(1)$
1	0	1.302 66	1.376 08
2	0	2.973 87	3.181 31
3	0	4.654 40	4.992 55
4	0	6.337 42	6.805 14
5	0	8.021 49	8.618 23
1	1	2.297 47	2.371 92
2	1	3.939 66	4.155 01
3	1	5.601 54	5.953 00
4	1	7.271 94	7.757 01
5	1	8.946 79	9.564 08
1	2	3.295 35	3.370 18
2	2	4.922 61	5.141 35
3	2	6.570 89	6.929 11
4	2	8.230 22	8.725 15
5	2	9.896 19	10.525 96
1	3	4.294 24	4.369 23
2	3	5.912 40	6.132 98
3	3	7.550 77	7.913 04
4	3	9.201 18	9.702 36
5	3	10.859 29	11.497 48
1	4	5.293 52	5.368 63
2	4	6.905 60	7.127 32
3	4	8.536 58	8.901 48
4	4	10.179 64	10.685 21
5	4	11.831 10	12.475 32

analyse the spectra of these problems mainly because it is known [11] that $P_{n\ell}(q)$ is monotone in q and it is also smoother than $E_{n\ell}$ as a function of q; the case $q = 0$ corresponds exactly to the log potential. From (1.3) and (1.4) we find, in particular, that

$$P_{n\ell}(-1) = n + \ell \tag{2.3}$$

and

$$P_{n\ell}(2) = 2n + \ell + 1/2. \tag{2.4}$$

In table 1 we exhibit some numerical values for $P_{n\ell}(\frac{1}{2})$ and $P_{n\ell}(1)$. We have found the exact eigenvalues for the linear potential in terms of the zeros of the Airy function, but those for $q = \frac{1}{2}$ have to be computed numerically: this use of some isolated numerical input is justified since, for each $\{n, \ell\}$ pair, the resulting approximation formulae include all the potential parameters but depend only on a single 'numerical input'. Envelope theory [12, 17] shows that the eigenvalues of the Coulomb plus power-law potential may be approximated by the following semiclassical expression:

$$\mathcal{E} \approx \min_{r>0}\left\{\frac{1}{r^2} - \frac{1}{\mu r} + \beta\,\mathrm{sgn}(q)(\nu r)^q\right\} \qquad \text{where} \quad \mu, \nu > 0. \tag{2.5}$$

Since $V(r) = g(h(r))$ is at once a convex function of $h(r) = -1/r$ and a concave function of $h(r) = \mathrm{sgn}(q)r^q$, the spectral representation $P_{n\ell}(q)$ allows us to specify upper and lower

bound formulae as follows. If $\mu = \nu = P_{n\ell}(-1)$, then $\mathcal{E}$ is a lower bound for $E_{n\ell}$, and if $\mu = \nu = P_{n\ell}(q)$, then $\mathcal{E}$ is an upper bound. We may improve the lower bound for the bottom of each angular momentum subspace by using the sum approximation [17, 18], which is equivalent to the choice $\mu = P_{1\ell}(-1) = (\ell + 1)$ and $\nu = P_{1\ell}(q)$. For the bottom of the spectrum we can also improve the upper bound by using a Gaussian trial function and minimizing over scale: this is equivalent [12] to using the parameter values

$$\mu = \nu = P_{10}^{U} = \left(\frac{3}{2}\right)^{\frac{1}{2}} \left[\frac{2\Gamma((3+q)/2)}{\sqrt{\pi}}\right]^{\frac{1}{q}}. \tag{2.6}$$

We note that the *same* parameters μ and ν which guarantee that (2.5) yields various energy bounds may also be used in the 'full' semiclassical formula (1.2), including all the original Hamiltonian parameters $\{\omega, A, B\}$. In section 3 we apply (2.5) to the explicit cases $V(r) = -1/r + \beta r^q$ for $\ell = 0, 1, 2$, where $q = 1, 2$ and 0.5.

3. Variational method

The second approach in this paper is to use a trial function explored in previous work [19] to obtain accurate upper bounds for the bottom of each angular momentum subspace. We start with Schrödinger's equation

$$H\psi(r) = \left(-\Delta - \frac{1}{r} + \beta\,\mathrm{sgn}(q) r^q\right)\psi(r) = E_{n\ell}(\beta)\psi(r) \qquad q \neq 0 \quad q > -2. \tag{3.1}$$

This problem is solvable if $\beta = 0$, and the corresponding wavefunction $\psi(r)$ is given by

$$\psi(r) = r^{\ell+1} \mathrm{e}^{-xr} L_n^{2\ell+1}(2xr). \tag{3.2}$$

In order to obtain an upper bound for the bottom of each angular momentum subspace $E_{1\ell}$ for fixed power q we choose $\psi(r)$ to be of the following form

$$\psi(r) = r^{\ell+1} \mathrm{e}^{-(xr)^d} \tag{3.3}$$

and define $\mathcal{E}$ by $\mathcal{E}(\beta, x, d) = \frac{\langle\psi, H\psi\rangle}{\langle\psi,\psi\rangle}$, where x and d are variational parameters. Now, we minimize $\mathcal{E}$ with respect to x and d. The necessary conditions for a critical point are $\frac{\partial\mathcal{E}}{\partial x} = 0$ and $\frac{\partial\mathcal{E}}{\partial d} = 0$. Consequentially, using (3.1) and (3.3), we obtain the following upper bound formula for the eigenvalues $E_{1\ell}$

$$\mathcal{E}_{1\ell}(\beta, d, x) = a_1 x^2 - a_2 x + a_3 x^{-q} \tag{3.4}$$

where a_1, a_2 and a_3 are as given below

$$a_1 = 2^{\frac{2-2d}{d}} \frac{(2\ell+1)(2\ell+d+1)\Gamma\left(\frac{2\ell+1}{d}\right)}{\Gamma\left(\frac{2\ell+3}{d}\right)}$$

$$a_2 = 2^{\frac{1}{d}} \frac{\Gamma\left(\frac{2\ell+2}{d}\right)}{\Gamma\left(\frac{2\ell+3}{d}\right)}$$

$$a_3 = \mathrm{sgn}(q)\beta 2^{\frac{-q}{d}} \frac{\Gamma\left(\frac{2\ell+q+3}{d}\right)}{\Gamma\left(\frac{2\ell+3}{d}\right)}.$$

By using (3.4) we derive the following equation for x:

$$x^{q+2} - \frac{a_2}{2a_1} x^{q+1} - \frac{q a_3}{2a_1} = 0. \tag{3.5}$$

After solving (3.5) to obtain x from the numerical solution of $\frac{\partial\varepsilon}{\partial d} = 0$ we find d for $n = 1$ and $\ell = 0$ and then we use the same d value for all ℓ.

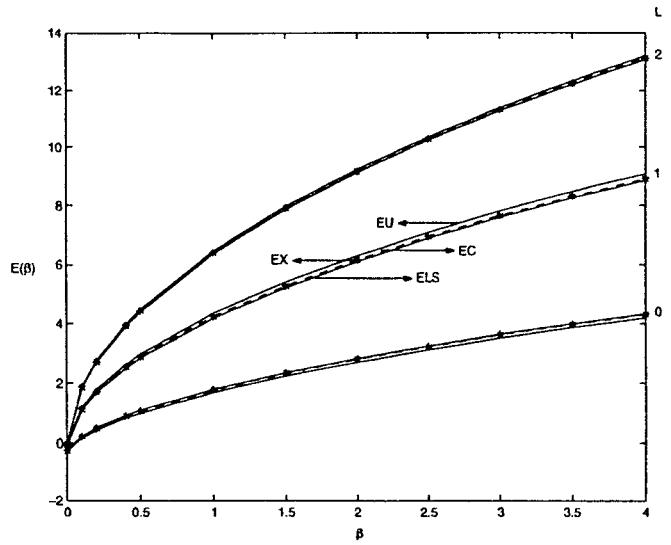

Figure 1. The eigenvalues $E(\beta)$ of the Hamiltonian $H = -\Delta - 1/r + \beta r^2$ for $N = 3$, $n = 1$, and $\ell = 0, 1, 2$. The continuous curves show the upper bound EU given by the envelope formula (2.5) with $\nu = \mu = P_{1\ell}(2)$, for $\ell = 1, 2$ and the lower bound ELS by the sum approximation given by the same formula but with $\nu = P_{1\ell}(2)$ and $\mu = P_{1\ell}(-1)$. The upper bound for $\ell = 0$ is calculated using $\nu = P^U_{1\ell}(2)$ and $\mu = P^U_{1\ell}(-1)$ in formula (2.5). The dashed curve EC represents the upper bound by formula (3.4). The stars EX represent accurate numerical data.

4. Results and conclusion

We have found general semiclassical energy formulae (1.2) and (2.5) for the eigenvalues generated by the Coulomb plus power-law potentials. Specific values for the parameters μ and ν are given which guarantee that the formulae yield bounds for all the discrete energies. By using a more finely tuned wavefunction, we have also derived an improved upper bound (3.4) valid for the bottom of each angular momentum subspace. We may rewrite (2.5) in the form of a pair of parametric equations for the curve $\{\beta, E(\beta)\}$. For fixed $q > -1$ we obtain

$$\beta = \frac{1}{|q|(\nu r)^q}\left(\frac{2}{r^2} - \frac{1}{\mu r}\right) \qquad E(\beta) = \frac{1+2/q}{r^2} - \frac{1+1/q}{\mu r}. \tag{4.1}$$

By envelope theory, we know that these parametric equations yield a lower bound if $\mu = \nu = P_{n\ell}(-1) = (n + \ell)$, and an upper bound when $\mu = \nu = P_{n\ell}(q)$. For the bottom of each angular momentum subspace the prescription $\mu = P_{1\ell}(-1) = (\ell + 1)$, $\nu = P_{1\ell}(q)$ yields an improved lower bound. An improved upper bound for the bottom of the spectrum is given by using the 'Gaussian' P-numbers (2.6). In figures 1–3, we plot the function $E(\beta)$ for $n = 1$, $\ell = 0, 1, 2$ for the Coulomb plus harmonic oscillator ($q = 2$), Coulomb plus linear ($q = 1$) and Coulomb plus $r^{0.5}$ potentials, along with the corresponding accurate variational bounds using (3.4) (dashed line), and some comparison numerical values represented as stars. The advantage of the semiclassical formulae is that they describe in approximate analytical form how the eigenvalues depend on all the parameters of the problem.

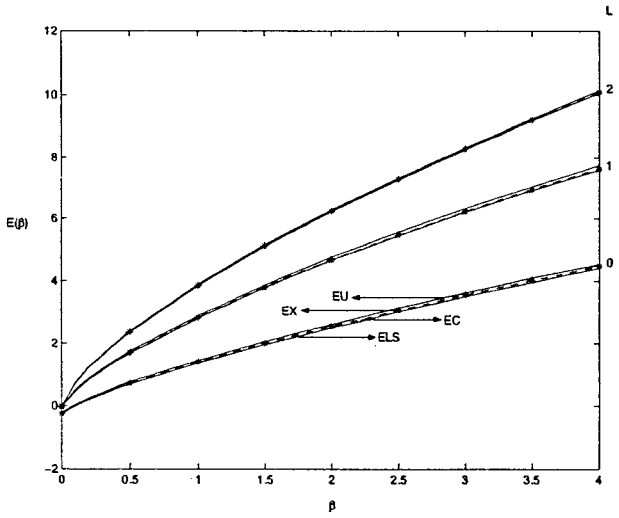

Figure 2. The eigenvalues $E(\beta)$ of the Hamiltonian $H = -\Delta - 1/r + \beta r$ for $N = 3, n = 1$, and $\ell = 0, 1, 2$. The continuous curves show the upper bound EU given by the envelope formula (2.5) with $\nu = \mu = P_{1\ell}(2)$, and the lower bound ELS by the sum approximation given by the same formula but with $\nu = P_{1\ell}(1)$ and $\mu = P_{1\ell}(-1)$. The upper bound for $\ell = 0$ is calculated using $\nu = P^U_{1\ell}(1)$ and $\mu = P^U_{1\ell}(-1)$ in formula (2.5). The dashed curve EC represents the upper bound by formula (3.4). The stars EX represent accurate numerical data.

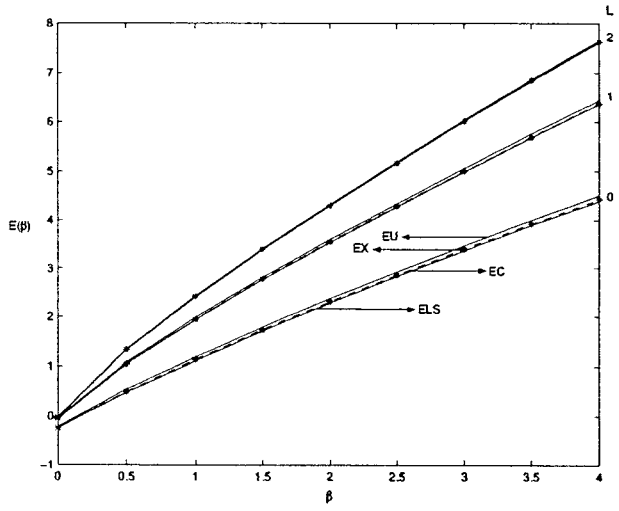

Figure 3. The eigenvalues $E(\beta)$ of the Hamiltonian $H = -\Delta - 1/r + \beta r^{0.5}$ for $N = 3, n = 1$ and $\ell = 0, 1, 2$. The continuous curves show the upper bound EU given by the envelope formula (2.5) with $\nu = \mu = P_{1\ell}(0.5)$, and the lower bound ELS by the sum approximation given by the same formula but with $\nu = P_{1\ell}(0.5)$ and $\mu = P_{1\ell}(-1)$. The upper bound for $\ell = 0$ is calculated using $\nu = P^U_{1\ell}(0.5)$ and $\mu = P^U_{1\ell}(-1)$ in formula (2.5). The dashed curve EC represents the upper bound by formula (3.4). The stars EX represent accurate numerical data.

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