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GEOMETRICAL APPROXIMATION METHODS FOR THE DISCRETE SPECTRA OF SCHRÖDINGER OPERATORS

Nasser Saad

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ABSTRACT

Nasser Saad, Ph. D.

Concordia University, 1998

We study a concrete class of eigenvalue problems in mathematical physics, which arise from non-relativistic quantum mechanics and the Sturm-Liouville theory. We develop practical techniques to obtain reliable bounds for the eigenvalues of the Schrödinger operator $H = -\Delta + V(r), r = |\mathbf{r}| \in \mathbf{R^n}$.

We introduce a three-parameter variational function, to determine an upper bound to the ground-state energy, of the supersingular spiked harmonic oscillator potentials $V(x) = x^2 + \frac{\lambda}{x^\alpha} \quad (\alpha \geq 1, \lambda > 0)$. The entire parameter range $\lambda > 0$ and $\alpha \geq 1$ is treated by a single formulation. We employ the method of potential envelopes to derive a simple energy lower bound formula, valid for all parameter ranges $\lambda > 0$ and $\alpha \geq 1$, and for all the discrete eigenvalues.

The standard method of envelope potentials is extended and applied to analyse the discrete spectrum of the generalized singular potentials $V(x) = \mu x^\beta + \frac{\lambda}{x^\alpha}$, where $\mu, \lambda > 0$, α and $\beta > 0$ are arbitrary positive parameters. We analyse also the discrete spectrum of of the generalized Kratzer's potentials $V(r) = -\frac{\lambda}{r} + \frac{\mu}{r^\beta} \quad (\lambda, \mu > 0, \beta > 1)$. We obtain lower and upper bound expressions to the eigenvalues which are valid for all dimensions $N \geq 2$.

We introduce the h-method to study smooth transformations $V(r) = h_0(r) + g(h(\beta r))$, of the potentials $V_0(r) = h_0(r) + h(\beta r)$, for which exact bound-state solutions of the Schrödinger equation are known for certain values of the positive parameter β. Eigenvalue approximation formulae thereby obtained provide lower or upper energy bounds, depending on whether the transformation function g is convex or concave. This enables us to give lower and upper bound expressions to the perturbed Coulomb potential $V(r) = -\frac{1}{r} + \mu r + \lambda r^2$, with arbitrary coefficients $\{\mu, \lambda\}$.

Several new comparison theorems for the eigenvalues of a pair of Schrödinger equations $-u'' + Q_i(t)u = \lambda u, \ t \in [-l, l], \ i = 1, 2$, are introduced. These theorems allow the comparison function $Q_i \ (i = 1, 2)$ to intersect at a finite number of points within $[-l, l]$, while maintaining the eigenvalue comparisons. The extension to more general Sturm-Louvile problems is also discussed.

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To the Memory of my Parents

Contents

List of Tables x
List of Figures xi
Introduction 1

Chapter I: Min-Max Principle and the method of potential envelopes 5
I. 1. Min-Max Principle 6
I. 2. The Method of Potential Envelopes 11
References 14

Chapter II: Energy Bounds For The Spiked Harmonic Oscillator 16
II. 1. Introduction and Main Results 16
II. 2. The Domain Problem 19
II. 3. Variational Method 20
II. 4. The Envelope Method 22
II. 5. Numerical Results 24
II. 6. On the numerical integration of Schrödinger equation with singular potential 26
II. 7. Conclusion 26
References 35

Chapter III: Eigenvalue bounds for a class of Singular Potentials 37
III. 1. Introduction and Main Results 37
III. 2. Transformed Potentials 40
III. 3. Numerical Results 42
III. 3. 1. The potential $V(x) = \lambda x^\beta + \frac{\mu}{x^\alpha}$ 42

III. 3. 2. The spiked harmonic oscillator potential 43
III. 3. 3. The potential $V(x) = \lambda x^3 + \frac{\mu}{x^\alpha}, \alpha = 3$ 44
References 51

Chapter IV: Smooth Transformations of Kratzer's Potential in N Dimensions 54
IV. 1. Introduction and Main Results 54
IV. 2. Transformed Potentials 57
IV. 3. Numerical Results 59
IV. 3. 1. The potential $V(r) = -\frac{a}{r} + \frac{b}{r^2}$ 59
IV. 3. 2. The potential $V(r) = -\frac{\mu}{r}[1 - \frac{ar}{1+r}] + \frac{b}{r^2}$ 60
References 68

Chapter V: Eigenvalues bounds for transformations of quasi-exactly soluble potentials 70
V. 1. Introduction and Main Results 70
V. 2. Perturbed Coulomb Potentials 72
V. 3. Transformed Potentials 74
V. 4. Numerical Results 77
V. 4. 1. The potential $V(r) = -\frac{1}{r} + \mu r + \lambda r^2$ 78
V. 4. 2. The potential $V(r) = -\frac{1}{r} + \mu \ln(r + r^2)$ 79
V. 4. 3. The potential $V(r) = -\frac{1}{r} + \mu e^{\lambda(r+r^2)}$ 79
References 84

Chapter VI: Eigenvalues Comparisons for Quantum Systems in a box 86
VI. 1. Introduction 86
VI. 2. New Comparison Theorems 87
VI. 3. Practical Method 92
VI. 4. Applications 93
VI. 5. Elementary Results for a System of Sturm-Liouville 96

VI. 6. Applications to Sturm-Liouville Problems 99
References 104

Conclusion 105
Appendix: Publications 107

Lists of Tables

Tables **Page**

II.1 Upper bounds for $H = -\frac{d^2}{dx^2} + x^2 + \frac{\lambda}{|x|^{5/2}}$ with different values of λ. The values E^G were evaluated by formula (II.3), and for E^H we used formula (II.2). E_0^L is from inequality (II.16) of the present work. The 'exact' values were obtained by direct numerical integration 28

II.2 Upper and lower bounds for the $H = -\frac{d^2}{dx^2} + x^2 + \frac{1000}{|x|^\alpha}$ with different values of α, by inequality (II.16) and the formulas (II.4-5) 29

II.3 A comparison between the results E^F of Fernández [27], and the results E_0^U of the present work obtained from the inequality (II.16) for $\alpha = 4$ and 6 and various values for the coupling λ 29

III.1 Some lower bounds E_0^L and upper bounds E_0^U using (III.8) and (III.9) for $H = -\frac{d^2}{dx^2} + x^2 + \frac{1000}{x^\alpha}$. The "exact" values E_0^N were obtained by direct numerical integration of the Schrödinger equation 46

III.2 Comparison between the ground-state energy E_{II} obtained by (II.4) and the eigenvalues E_{III} obtained by (III.8-9) of the present chapter, along with the "exact" values E_0^N obtained by direct numerical integration of the Schrödinger equation. 47

III.3 Upper bounds E_n^U using (III.19) for $H = -\frac{d^2}{dx^2} + \lambda x^{1.9} + \frac{\mu}{x^{1.9}}$ with different values of n. The "exact" values E_n^N were obtained by direct numerical integration of the Schrödinger equation. 48

III.4 lower bounds E_n^L using (III.17) for $H = -\frac{d^2}{dx^2} + \lambda x^{2.1} + \frac{\mu}{x^{2.1}}$ with different values of n. The "exact" values E_n^N were obtained by direct numerical integration of the Schrödinger equation. 49

IV.1 Some lower bounds E_{01}^{L} and upper bounds E_{01}^{U} using (IV.20) for $H = -\Delta - \frac{5}{r} + \frac{1}{r^2}$ in 3-dimensions with $l = 1$. The "exact" values E_{01} were obtained by direct numerical integration of Schrödinger's equation 62

IV.2 lower bounds E_{00}^{L} using (IV.20) for $H = -\Delta - \frac{1}{r} + \frac{1}{r^{2.1}}$ for dimension $N = 2$ to 10. The "exact" values E_{00} were obtained by direct numerical integration of Schrödinger's equation 63

IV.3 lower bounds E_{00}^{L} using (IV.20) for $H = -\Delta - \frac{5}{r} + \frac{1}{r^{2.1}}$ for dimension $N = 2$ to 10. The "exact" values E_{00} were obtained by direct numerical integration of Schrödinger's equation 64

IV.4 Upper bounds E_{00}^{U} using (IV.23) for $H = -\Delta - \frac{5}{r}\left[1 - \frac{0.5r}{1+r}\right] + \frac{1}{r^2}$ for dimension $N = 2$ to 10. The "exact" values E_{00} were obtained by direct numerical integration of Schrödinger's equation 65

V.1 Eigenvalues of $H = -\frac{1}{2}\Delta - \frac{1}{r} + \mu r + \lambda r^2$ for different values of μ and λ. Comparison between results E^{B} of Bessis *et al* [13], using the moment method, and the present work which yields the lower bound E^{L} 80

V.2 Eigenvalues of $H = -\Delta - \frac{1}{r} + \mu r + \lambda r^2$ for different values of μ and λ. Comparison between the lower bound E^{L} given by formulas (V.25) and (V.26) and accurate values E^{N} found by direct numerical integration 81

V.3 Eigenvalues of $H = -\Delta - \frac{1}{r} + \mu \ln(r + r^2)$ for different values of μ. Comparison between the upper bound E^{U} given by (23) and accurate values E^{N} found by direct numerical integration 82

Lists of Figures

Figure **Page**

II.1 The spiked harmonic oscillator potential $V(x) = x^2 + \lambda|x|^{-\alpha}$ for $\alpha = 3$ and λ =0.001, 1 and 10 30

II.2 Family of 'tangent' potentials $V^{(t)}(x)$, for different values of t along with the graph of spiked harmonic oscillator for $\lambda = 1$ and $\alpha = 5/2$ 31

II.3 Comparison between the result of the present chapter with the result of Harrell (II.2) and of Aguilera et al (II.3) 32

II.4 A comparistion between the variational results (II.16) for $\alpha = \frac{5}{2}$ and the 'exact' solutions found by direct numerical integration of Schrödinger's equation 33

II.5 The graph of the variation wave function (II.26) 34

II.6 The graph of the variation wave function (II.27) 34

III.1 Potential envelopes $V^{(s,t)}(x)$ for $V(x) = x^{2.1} + \frac{1}{x^{2.1}}$ 3

IV.1 Graph of $\epsilon(t) = \epsilon_{01}(t)$ along with the exact eigenvalue E and corresponding unnormalized wavefunction in 3-dimensions 66

IV.2 The graph of the lower bound E_{00}^L obtained by (IV.20) as a function of the parameter b, along with some exact eigenvalues E_{00} obtained by direct numerical integration 67

V.1 Two parametric regions: if $\mu < \sqrt{\lambda}$, the formulas (V.25-26) yield a lower bound for the ground-state energy of the Hamiltonian $H = -\triangle - \frac{1}{r} + \mu r + \lambda r^2$, while $\mu > \sqrt{\lambda}$ yields an upper bound. 83

VI.1 The potentials $t^2 + \frac{s}{10}\sin(4t^2)$, where $s \in \{-1.0, 1\}$. If the lowest 'even' eigenvalues are written $\lambda_0(s)$, theorem (1) implies $\lambda_0(-1) \leq \lambda_0(0) \leq \lambda_0(1)$.102

VI.2 The potentials $t^2 + \frac{s}{10}\sin(4t^2)/t^2$, where $s \in \{-1.0, 1\}$. If the lowest 'odd' eigenvalues are written $\lambda_1(s)$, theorem (3) implies $\lambda_1(-1) \leq \lambda_1(0) \leq \lambda_1(1)$103

Introduction

This thesis deals with a concrete class of eigenvalue problems which arose in the literature of mathematical physics in the past two decades and traces the origin of the problem to non-relativistic quantum mechanics, and the Sturm-Liouville theory. Continuing this approach, we develop herein practical techniques for obtaining reliable bounds for the eigenvalues of the Schrödinger operator

$$H = -\Delta + V(r), \tag{0.1}$$

whose action is defined on a suitable dense linear manifold of $L^2(\mathbf{R}^n)$.

The Schrödinger operator (0.1) appears throughout quantum mechanics as well as in applications of the Sturm-Liouville theory. Since the eigenvalues are not explicitly ascertainable in most cases, several approximation schemes have been devised and improved over many decades. For concrete past examples, as well as the history (although incomplete) of this problem, the reader is refered to the references mentioned in [1].

It is well established [2-10] that, for suitable $V(r)$, this operator (0.1) is essentially self-adjoint on the space of infinitely differentiable functions with compact support $C_0^\infty(\mathbf{R}^n)$ and can be defined as a sum of quadratic forms. Physically, it represents the Hamiltonian (energy) operator of the particles in non-relativistic quantum mechanics, after the centre of mass motion has been removed.

Adhering to the quotation of Weinstein et al [1], "these connections between theories and concrete problems proved to be most fruitful", we emphasize these connections in this thesis; in particular, we develop our constructive techniques out of ideas behined concrete problems that have appeared in the literature.

In chapter II we study the supersingular spiked harmonic oscillator potentials

$$V(x) = x^2 + \frac{\lambda}{x^\alpha} \quad (\alpha \geq 1, \lambda > 0). \tag{0.2}$$

We introduce a three-parameter variational trial function to determine an upper bound to the ground-state energy. The entire parameter range $\lambda > 0$ and $\alpha \geq 1$ is treated by means of a single formulation. Further, we employ the method of

potential envelopes [11,12] to derive a simple energy lower bound formula valid for all parameter ranges $\lambda > 0$ and $\alpha \geq 1$, and all the discrete eigenvalues.

In chapter III we extend the standard method of envelope potentials to obtain more reliable and general energy bounds. We develop this technique through the analysis of the discrete spectrum of the singular potentials

$$V(x) = x^2 + \frac{\lambda}{x^2}, \ \lambda > 0. \tag{0.3}$$

Utilizing the eigenvalues expression, we derive an effective procedure for computing more precise lower potentials (0.2), as well as that of the generalized singular potentials

$$V(x) = \mu x^{\beta} + \frac{\lambda}{x^{\alpha}}, \tag{0.4}$$

where $\mu, \lambda > 0$, α and $\beta > 0$, are arbitrary positive parameters.

In chapter IV we use the exact solution of Kratzer's potential

$$V(r) = -\frac{\lambda}{r} + \frac{\mu}{r^2} \tag{0.5}$$

in N-dimensional real space. We apply the new technique developed in chapter III to investigate the discrete spectrum of the potentials

$$V(r) = g(-\frac{1}{r}) + f(\frac{1}{r^2}) \tag{0.6}$$

in N-dimensions, where g and f are smooth transformations of $-\frac{1}{r}$ and $\frac{1}{r^2}$ respectively. Consequently we obtain a simple algorithm to ascertain a bound for the spectra of the generalized Kratzer's potentials

$$V(r) = -\frac{\lambda}{r} + \frac{\mu}{r^{\beta}} \quad (\lambda, \mu > 0, \beta > 1) \tag{0.7}$$

and for the perturbed Coulomb potential

$$V(r) = -\frac{v}{r}[1 - \frac{ar}{1+r}] + \frac{b}{r^2} \quad (0 < a \leq 1, b > 0) \tag{0.8}$$

valid for all dimensions $N \geq 2$.

In chapter V we introduce the h-method to study smooth transformations

$$V(r) = h_0(r) + g(h(\beta r)) \tag{0.9}$$

of the potentials

$$V_0(r) = h_0(r) + h(\beta r), \tag{0.10}$$

for which exact bound-state solutions of the Schrödinger equation exist, for certain parameter values β. Eigenvalue approximation formulae are obtained and provide lower or upper energy bounds depending on whether the transformation function g is convex or concave. This enables us to give lower and upper bound expressions to the potential

$$V(r) = -\frac{1}{r} + \mu r + \lambda r^2 \tag{0.11}$$

with arbitrary coefficients $\{\mu, \lambda\}$. We obtain, as a consequence of the h-method developed, energy bounds for the potential

$$V(r) = -\frac{1}{r} + \mu \ln(r + r^2). \tag{0.12}$$

Chapter VI is devoted to Sturm-Liouville theory, where several new comparison theorems for the eigenvalues of a pair of Schrödinger equations

$$\begin{cases} -u'' + Q_1(t)u = \lambda_1 u, \\ -v'' + Q_2(t)v = \lambda_2 v, \end{cases}$$

are introduced ($t \in [-l, l]$). These theorems allow the comparison function Q_i ($i = 1, 2$) to intersect at finite number of points within $[-l, l]$, while upholding the eigenvalue comparisons. The extension to *regular* Sturm-Louville problems is also discussed. In the next chapter we review basic concepts from operator theory that are needed, and introduce the standard method of potential envelopes.

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CHAPTER I

Min-Max Principle and the method of potential envelopes

The majority of problems in non-relativistic quantum mechanics cannot be exactly solved. The usual approach is to use some approximation as a substitute for the exact solution. It is, indeed, common in most of quantum mechanics texts to include several chapters dealing with approximation methods. Some methods even preceded the actual birth of quantum mechanics (Perturbation theory, Variational and WKB approximation among others). Some are quite recent, such as the Padé approximation [1], the approximation based on Hill determinants [2] or continued fractions [3], the Self-Similar approximation [4] and the method of potential envelopes [5-8]. Among all these approximations, the variational method and the method of potential envelopes both provide definite bounds. This is no coincidence, because the envelope method employs the variationally obtained eigenvalues with the advantage that it can contribute lower and upper bounds. The accurate estimate of discrete eigenvalues of the non-relativistic Schrödinger Hamiltonian

$$H = -\Delta + V(r) \tag{I.1}$$

requires, in principle, the calculation of a reliable lower bound, to complement a variational upper bound. In practice however, all known procedures for computing lower bounds are both more cumbersome, and less accurate, than the variational procedure for upper bounds. In particular, many standard expressions for lower bounds involve matrix elements of H^2, and restrict the choice of admissible trial functions. Furthermore, a priori knowledge of the spectrum H is always required. On other hand, the variational method requires the computation of a matrix element of H, with a suitable trial wave function of many parameters, to ensure the accuracy of the upper bounds. The main advantage of the envelope method is that it yields analytic expressions, obtained by simple extremization over one or two variables, as shown below.

I.1. The Min-Max Principle

Since the reader has some familiarity with the theory of unbounded operators, we will briefly review some essential basic definitions without comment. For a comprehensive introduction to unbounded operator, refer to Refs.[9-18]. Herein the following notation is adhered to throughout. $\mathcal{H}$ denotes a complex separable Hilbert space. The symbols $\mathbf{N}$, $\mathbf{R}$, $\mathbf{C}$ and $\mathbf{R}^n$ stand for the set of natural, real and complex numbers and n-dimensional real space respectively. Further H and V are (possible unbounded) operators on a suitable domain $D(H)$ in $\mathcal{H}$ - i.e. $H : D(H) \to \mathcal{H}$.

An linear *operator* H *in* the Hilbert space $\mathcal{H}$ is defined as a linear transformation $H : D(H) \to \mathcal{H}$, where the domain $D(H)$ of H is a linear manifold of $\mathcal{H}$. The domain $D(H)$ of H is assumed to be dense in $\mathcal{H}$ unless otherwise indicated. In this case we call H densely defined in $\mathcal{H}$. Further, for densely defined bounded H the domain $D(H)$ is identical with $\mathcal{H}$.

The *graph* $\Gamma(H)$ *of the operator* H is the set of all ordered pairs

$$\Gamma(H) = \{\{\phi, H\phi\} | \phi \in D(H)\}$$

and is a submanifold of $\mathcal{H} \times \mathcal{H}$. An operator H in $\mathcal{H}$ is called *closed*, if $\Gamma(H)$ is closed in $\mathcal{H} \times \mathcal{H}$ (Cartesian product of two Hilbert spaces). Related to the concept of closedness of an operator is the *adjoint* H^* of the operator H. The operator H^* in $\mathcal{H}$ - i.e. $H^* : D(H^*) \to \mathcal{H}$ - is defined as

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

If H_1 and H are operators in $\mathcal{H}$ and $\Gamma(H_1) \subset \Gamma(H)$, then H is called an *extension of* H_1 and we write $H_1 \subset H$. Also, H_1 is called *restriction of* H to $D(H_1)$, which is written as $H|_{D(H_1)}$. An operator H is called *closable* if it has a closed extension. The smallest closed extension is called the *closure of* H and is written as $\bar{H}$.

An operator H in $\mathcal{H}$ is called *Hermitian* if

$$D(H) \subset D(H^*) \quad \text{and} \quad H\phi = H^*\phi \quad \forall \phi \in D(H).$$

Alternatively, we can also say H is Hermitian iff $H \subset H^*$. A Hermitian operator H in $\mathcal{H}$ is called *positive* if

$$(\phi, H\phi) \geq 0 \quad \forall \phi \in D(H).$$

If $(\phi, H\phi) > 0 \quad \forall \phi \in D(H),\ \phi \neq 0$, then the operator H is called *positive definite.* Moreover, we say that operator H is *self-adjoint* if

$$D(H) = D(H^*) \quad \text{and} \quad H = H^*.$$

As previously H is self-adjoint iff $H \subset H^*$ and $H^* \subset H$. Bringing in the idea of closure, a Hermitian operator H is *essentially self-adjoint* if its closure is self-adjoint. Furthermore, if H is a closed operator, the subset $D_c \subset D(H)$ is called a *core* or *domain of essential self-adjointness* if $\overline{H|_{D_c}} = H$.

A number $z \in \mathbf{C}$ is called eigenvalue of H if there exists a non-trivial $\phi \in D(H)$ such that $H\phi = z\phi$. The *resolvent operator* $R(z, H)$ *of* H *in* $\mathcal{H}$ *at* z is

$$R(z, H) = (zI - H)^{-1}.$$

$$\rho(H) = \{z \in C |\ R(z, H) \in B(\mathcal{H})\}$$

is called the *resolvent set* of H, where $B(\mathcal{H})$ denote Banach-algebra of bounded linear operators *on* $\mathcal{H}$. It follows that the *spectrum* $\sigma(H)$ is the complement of the resolvent set $\rho(H)$ in $\mathbf{C}$. For Hermitian operators H, $\sigma(H)$ is a subset of $(-\infty, \infty)$. The *essential spectrum* $\sigma_e(H)$, of a self adjoint operator H, is the set of points of $\sigma(H)$, that are either accumulation points of $\sigma(H)$ or isolated eigenvalues of infinite geometrical multiplicity (the dimension of the eigenspace=∞). Therefore, the set $\sigma_d(H) = \sigma(H) \setminus \sigma_e(H)$ is called the *discrete spectrum* of H. The operator H in $\mathcal{H}$ has a pure discrete spectrum if $\sigma_e(H)$ is empty.

Given the quadratic form q, which is a map $q : D(q) \to \mathbf{C}$, where the linear manifold $D(q)$ in $\mathcal{H}$ is the *form domain*, we write $q(\psi)$ for the evaluation of q at $\psi \in D(q)$. However, since every quadratic form is detemined by a sesquilinear form and vica versa, we write also q for the sesquilinear form determined by the quadratic form q, although we now mean $q : D(q) \times D(q) \to \mathbf{C}$ - i.e. $q(\phi, \psi) \in \mathbf{C}\ \forall\ \phi$ and

$\psi \in D(q)$. For the positive definite operator H in $\mathcal{H}$, the sesquilinear form q_H is a map $D(q_H) \times D(q_H) \to \mathbf{C}$ defined by

$$q_H(\phi, \psi) = (H^{\frac{1}{2}}\phi, H^{\frac{1}{2}}\psi)$$

on $D(q_H)$, where the form domain $D(q_H)$ is the dense linear subset of $\mathcal{H}$ consisting of all $\phi \in \mathcal{H}$ such that $\|H^{\frac{1}{2}}\phi\| < \infty$. Notice that the operator domain $D(H)$ of a self-adjoint operator H consists of all ϕ in $\mathcal{H}$ such that $\|H\phi\| < \infty$. Consequently, because of

$$\|H^{\frac{1}{2}}\phi\|^2 \leq \|H\phi\|\|\phi\|,$$

the form domain $D(q_H)$ of a positive self-adjoint operator H is larger than its operator domain $D(H)$ - i.e. $D(H) \subset D(q_H)$ in the sense of set inclusion.

For H_0 and V positive self-adjoint operators in $\mathcal{H}$, we write $H = H_0 + \lambda V$ with $D(H) = D(H_0) \cap D(V)$. If $D(H)$ is dense in $\mathcal{H}$, then *the form sum* $(H_0 + \lambda V)$ is defined as

$$q'_H(\phi, \psi) = (H_0^{\frac{1}{2}}\phi, H_0^{\frac{1}{2}}\phi) + \lambda(V^{\frac{1}{2}}\psi, V^{\frac{1}{2}}\psi)$$

$\forall\, \phi \in D(H_0)$ and $\forall \psi \in D(V)$. This form sum concept is used in defining the domain of the supersingular spiked harmonic oscillator operator in Chapter II.

A common thread running through all works dealing with properties of Hamiltonian operators (I.1), is the min-max principle.

Theorem I.1.: (Weyl, Fischer and Courant)
Given a complex, separable Hilbert space $\mathcal{H}$ with norm $(\cdot,\cdot)^{\frac{1}{2}}$, we consider a self-adjoint operator H in $\mathcal{H}$ bounded below with spectrum $E_{n+1} \geq E_n$(counting multiplicities). If $\mathcal{D}_n$ denotes the family of all n-dimensional subspaces D_n of $\mathcal{H}$, then the eigenvalues of $\{E_n\}_{n\in\mathbf{N}}$ can be calculated in following four ways[1]:

$$E_n = \inf_{\mathcal{D}_n} \sup_{\psi \in D_n \cap D(H)} \frac{(\psi, H\psi)}{(\psi, \psi)}, \tag{I.2}$$

[1] The ratio $\frac{(\psi, H\psi)}{(\psi, \psi)}$ is called the Rayleigh quotient. The values $\{E_n\}_{n\in\mathbf{N}}$ are called the eigenvalues of Rayleight quotient. They are defined wherever (ψ, ψ) is non-zero and the quotient $\frac{(\psi, H\psi)}{(\psi, \psi)}$ is bounded below.

$$E_n = \min_{\mathcal{D}_n} \max_{\psi \in D_n \cap D(H)} \frac{(\psi, H\psi)}{(\psi, \psi)}, \tag{I.3}$$

$$E_n = \sup_{\mathcal{D}_{n-1}} \inf_{\psi \in D_{n-1}^{\perp} \cap D(H)} \frac{(\psi, H\psi)}{(\psi, \psi)}, \tag{I.4}$$

$$E_n = \max_{\mathcal{D}_{n-1}} \min_{\psi \in D_{n-1}^{\perp} \cap D(H)} \frac{(\psi, H\psi)}{(\psi, \psi)}. \tag{I.5}$$

Equation (I.2) and (I.3) occur most frequently in the literature of mathematical physics [11,14,17,19,20]. Their equivalence follows if we write the function ψ in Eq.(I.2) as a linear combination of appropriate basis elements $\{\psi_i\}_{n=1}^{n}$ of D_n. It is important to note at this point that the mini-max principle is valid even if the spectrum $\sigma(H)$ is not purely discrete. If the number of eigenvalues $E_n < E_*$ is finite, where n counts multiplicities and E_* is the infimum of the essential spectrum of H, then each of (I.2-5) must be interpreted as $E_k \equiv E_* \ \forall k \geq n$.

The stated result of Theorem I.1 makes it possible to estimate the eigenvalues of H by means of finite-dimensional approximations, which is the basic idea of the so-called *Rayleigh-Ritz method* or *variation method*. If $D_n \subset D(H)$, then the eigenvalues

$$E_1(D_n) \leq E_2(D_n) \leq \ldots \leq E_n(D_n)$$

of the matrix representing H in D_n provide upper bounds $E_1(D_n) \geq E_1$. In quantum theory, the subspaces $\mathcal{D}_n$ are generally unknown. In addition, there are some quantum numbers associated with constants of motions, whose eigenfunctions have known structure. This happens for example with angular momentum. Under these circumstances, it is practical to choose trial functions with this quantum number fixed so that the Rayleigh quotients of the Hamiltonian H are not lower than the energy of the levels with this quantum number.

There are many other highly regarded important consequences of the minimax principle in quantum theory, among these we consider the following theorems.

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

Proof: Ref.[11], page 100.

Note that in the case of $n \geq 3$, the operator $-\Delta + \lambda V$ acting on $L^2(\mathbf{R}^n)$ where V is purely attractive (i.e. assuming nonpositive values only), may have no bound state at all if the interaction is weak enough [11].

Theorem I.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

$$\int V(x)dx \leq 0.$$

Proof: Ref.[11], page 338.

Theorem I.4.: Let $V \in L^1_{loc}(\mathbf{R}^n)$ 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.

Proof: Ref.[11], page 249.

Theorem I.5.: If $V \in L^2_{loc}(\mathbf{R}^n)$ is positive and

$$\lim_{|x| \to 0} V(x) = \infty,$$

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

Proof: Ref.[11], page 207.

On the other Hand, if V is allowed to be very singular, then $-\Delta + V$, defined as a sum of quadratic forms, can have a degenerate ground state.

Theorem I.6.: If $V \in L^2_{loc}(\mathbf{R})$ and satisfies

$$\int_a^{a+1} |V(x)|^2 dx \to 0, \text{ as } |a| \to \infty, \tag{I.6}$$

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

Proof: Ref.[15], page 53.

Theorem I.7.: For V_1, $V_2 \in L^2_{loc}(\mathbf{R})$ satisfying

$$\sup_a \int_a^{a+1} |V_1(x)|^2 dx < 0 \tag{I.7}$$

and

$$\int_a^{a+1} |V_2(x)|^2 dx \to 0 \text{ as } |a| \to \infty, \tag{I.8}$$

we have

$$\sigma_e(-\frac{d^2}{dx^2} + V_1 + V_2) = \sigma_e(-\Delta + V_1). \tag{I.9}$$

Proof: Ref.[15], page 56.

Theorem I.8.: If $\sigma_e(H) = [0, \infty)$ and $V(x) \leq 0$ for $x \leq a$, for some $a \geq 0$ with

$$\int_a^{\infty} V(x)dx = -\infty,$$

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

Proof: Ref.[15], page 71.

Theorem I.9.: If S, T are self-adjoint operators such that $S \leq T$, in the sense that $D(T) \subset D(S)$ 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.

$$E_n[S] \leq E_n[T] \ (n = 1, 2, \ldots), \tag{I.10}$$

where $E_n[S]$ denotes the *n-th* eigenvalues of S in ascending order.

This is known as The Comparison Theorem (or Monotonicity Principle) of quantum mechanics, see Ref.[11,14,17,19,20] for the proof of this theorem and for an interesting refinement Ref.[21].

Theorem I.10.: (Sum of Operators)[11,22-23]

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

$$E_{k+l-1}[S + T] \leq E_k[S] + E_l[T]. \tag{I.11}$$

Unfortunately this result is weak [24] for $k, l > 1$.

I.2. The method of Potential Envelopes

The method of potential envelopes is a very general technique for approximating the spectrum of an operator. A brief account for our application follows

(for a complete account and further developement consult Refs.[5-8]). We suppose that the energy trajectories[2] $F_{nl}(v)$ of the Schrödinger Hamiltonian $-\Delta + vh(r)$ are exactly known, where h is the shape of a central potential. The energy trajectory functions $F_{nl}(v)$ are restricted, if necessary, to only values of the coupling parameter v sufficiently large for the corresponding discrete eigenvalues to exist. The quantum number n counts the eigenvalues in each angular-momentum subspace; eigenvalues so labelled have degeneracy of exactly $(2l+1)$.

We now consider a new Hamiltonian $-\Delta + V(r)$, whose potential V is a smooth transformation

$$V(r) = g(h(r))$$

of the potential h. We assume the transformation function $g(h)$ is monotone increasing and either convex or concave, that is to say $g'' > 0$ or $g'' < 0$. These cases give rise respectively to lower and upper energy bounds [5]. This sitution can be summarized by the following two expression

$$-\Delta + vh(r) \to F_{nl}(v), \tag{I.12}$$

$$-\Delta + V(r) \to E_{nl}. \tag{I.13}$$

For definiteness, we suppose that g is concave - i.e. $g'' < 0$. Because of the concavity of g, we know that the tangent lines to g (as a function of h) all lie above g, and thus we write

$$V(r) = g(h(r)) \leq A + vh(r). \tag{I.14}$$

By calculus we have

$$\begin{cases} A = g(h(t)) - h(t)g'(h(t)), \\ v = g'(h(t)), \quad t \in (0, \infty), \end{cases} \tag{I.15}$$

where $h(t)$ is the point of contact of $V(r)$ with its tangent potential

$$V^{(t)}(r) = A(t) + v(t)h(r). \tag{I.16}$$

[2] Energy trajectory: Curve describing how the energy E depends on the potential's coupling v, which we write as $E = F(v)$.

This family of 'tangent' potentials generates the so-called envelope representation for $V(x)$ expressed by

$$V(x) = \underset{t>0}{\text{Envelope}} \left\{ V^{(t)}(x) \right\}. \tag{I.17}$$

Since the Hamiltonians are self adjoint and bounded below, we can employ the variational characterization of eigenvalues to derive the comparison theorem (I.9) of quantum mechanics, which tells us that the potential inequality (I.14) implies the corresponding spectral inequality

$$E_{nl} \leq A(t) + F_{nl}(v(t)). \tag{I.18}$$

This means:

$$E_{nl} \leq g(h(t)) - h(t)g'(h(t)) + F_{nl}(g'(h(t)). \tag{I.19}$$

We now minimize the right-hand side of inequality (I.17) by differentiation with respect to t to obtain the best upper bound. That is

$$E_{nl} \leq \min_{t>0}\{g(h(t)) - h(t)g'(h(t)) + F_{nl}(g'(h(t))\}. \tag{I.20}$$

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CHAPTER II

Energy Bounds For The Spiked Harmonic Oscillator

In this chapter we introduce a three-parameter variational trial function to determine an upper bound to the ground state energy of the spiked harmonic oscillator Hamiltonian (II.1). The entire parameter range $\lambda > 0$ and $\alpha \geq 1$ is treated in a single formulation. We also apply the method of potential envelopes to derive a lower bound formula valid for all discrete eigenvalues.

II.1 Introduction and main results

Since the pioneering paper of Case [1], an extensive literature has developed on the subject of singular potentials [1-27]. Detwiler and Klauder [10], on their early work of singular potential theory, introduced the term supersingular to distinguish a potential that is so singular that the first nontrivial correction to the energy (i.e. the matrix element) diverges. They investigated the so-called spiked harmonic oscillator Hamiltonian

$$H = -\frac{d^2}{dx^2} + x^2 + \frac{\lambda}{|x|^\alpha}, \tag{II.1}$$

where the constant λ is a positive coupling parameter which measures the strength of the perturbative potential and α is positive constant. The importance of the spiked harmonic oscillator Hamiltonian (II.1) is that it helps understand the behavior of nonrenormalizable field theory and is a prototype for Klauder's phenomenon [10-12], namely sufficiently singular potentials V cannot be turned off ($\lambda = 0$) in the Hamiltonian $H = H_0 + \lambda V$ to restore the free Hamiltonian H_0. The phenomenon of supersingularity for (II.1) occurs for $\alpha \geq 5/2$. Its name comes from the shape of the graph of the full potential which shows a pronounced peak near the origin for $\lambda > 0$. An illustration of the potential for $\alpha = 3$ and $\lambda = 0.01, 1$, and 10 is shown in Fig. II.1.

The Hamiltonian (II.1) has fascinating properties from the point of view of mathematical physics. First of all, there is no dominance of either of the two terms

of the interaction potential x^2 and $\frac{\lambda}{x^\alpha}$. Thus, for all values of $\lambda > 0$, $\lambda \neq 0$, $\frac{\lambda}{x^\alpha}$ always adds an infinite repulsive barrier near the origin; on the other hand, one can never neglect the x^2 term, the potential being like a wide valley extending to ∞. Potentials of this type are of relevance in a wide range of physical situations, namely chemical, nuclear and particle physics.

Although the Rayleigh-Schrödinger perturbation series for the eigenvalues of the operator H, regarded as a harmonic oscillator operator $H_0 = -\frac{d^2}{dx^2} + x^2$ perturbed by $\frac{\lambda}{|x|^\alpha}$, diverges, a number of research papers [10,13-19] have been devoted to the study of a modified perturbation series for the eigenvalues and eigenfunctions. Detwiler and Klauder [10] realized that normal perturbation theory could not be applied for values of $\alpha \geq 5/2$, however, they were able to predict the kind of dependence of the ground state energy $E = E(\lambda)$, for small values of the coupling λ, by investigating the asymptotic behavior of the lowest eigenvalue of H. They discovered that $E(\lambda)$ is proportional to $\lambda \ln(\lambda)$ ($\alpha = 3$) and to $\lambda^{\frac{1}{\alpha-2}}$ ($\alpha > 3$). Therefore, they conclude that when the perturbation $\lambda r^{-\alpha}$ is turned off ($\lambda \to 0$) vestigial effects of the interaction remain. Using some elegant results of Kato's work on the perturbation theory of linear operators [28] and approximation techniques for differential equations, Harrell [13] was able to derive explicit expressions for the lower-order corrections to the eigenvalues of H when λ is sufficiently small. For example, his expression for the spiked harmonic oscillator ground state energy with $\alpha = \frac{5}{2}$ reads,

$$E(\alpha = \frac{5}{2}, \lambda) = 3 + \frac{2\Gamma(\frac{1}{4})}{\Gamma(\frac{1}{2})}\lambda + \frac{16}{\Gamma(\frac{1}{2})}\lambda^2 \ln(\lambda) + O(\lambda^2) \qquad \text{(II.2)}$$

for small values of λ. Aguilera et al [14], motivated by Harrell's results, have developed a large-coupling perturbative expansion for the ground state energy and they present an approximate analytic expression valid for $\alpha < 3$. Their expression for the ground state energy when $\alpha = \frac{5}{2}$ reads

$$E(\alpha = \frac{5}{2}, \lambda) = \frac{9}{5}(\frac{5\lambda}{4})^{\frac{4}{9}} + (\frac{9}{2})^{\frac{1}{2}} + \frac{77}{288}(\frac{4}{5\lambda})^{\frac{4}{9}} - \frac{1967}{27648}(\frac{9}{2})^{\frac{1}{2}}(\frac{4}{5\lambda})^{\frac{8}{9}} + \ldots \qquad \text{(II.3)}$$

for large λ.

In addition to analytical approximations for the ground-state energy of the spiked harmonic oscillator Hamiltonian, direct numerical integration methods have been used to compute eigenvalues for (II.1). Killingbeck [20-22] provided an integration method based on improvement of the finite difference algorithm. He was critical of the numerical results of Detwiler and Klauder using the Milne method. His conclusions confirmed the result of Korsch and Laurent [23]. W. Solano-Torres et al [24] used the Lanczos/grid method [25] to integrate the radial Schrödinger equation for the Hamiltonian H. They introduced some errors in their application of Harrell's formulas for $\alpha = 4$ and $\alpha = 6$. For example, if $\lambda = 0.01$ and $\alpha = 4$, then formula (4) of Ref. [24] yields $E = 3.225\ 68$ not $3.075\ 22$, Table (2); if $\lambda = 0.01$ and $\alpha = 6$, then formula (5) yields $E = 3.482\ 41$ not $3.096\ 48$, in Table (3); and similarily for other values of λ. These corrections demonstrate that formulas (4) and (5) of [24], correctly reproduced from Harrell [13], yield results which are better than Tables (2) and (3) of [24] would suggest.

The variety of approaches, and the complication using different approximation formulas for different ranges of α and λ, raises the following question: is it possible to devise a reliable uniform treatment to cover all cases? Section (II.3) answers this question: we describe a simple three-parameter variational wave function that estimates $E(\alpha, \lambda)$ for the ground-state energy of H, for all values of α and λ. In addition, in section (II.4), the method of potential envelopes is employed to derive a complementary energy lower-bound formula

$$\epsilon_n(\alpha, \lambda; \hat{t}) = \frac{\lambda}{\hat{t}^\alpha}\left(\frac{\alpha}{2} + 1\right) + \frac{(4n+3)^2}{2\hat{t}^2}, \tag{II.4}$$

where $\hat{t}$ is *the* positive real root of

$$4t^4 - 2\alpha\lambda t^{2-\alpha} - (4n+3)^2 = 0, \quad n = 0, 1, 2, \ldots \tag{II.5}$$

valid for all the discrete eigenvalues $\{E_n\}_{n=0}^{\infty}$. In section (II.5) we describe our numerical results and compare them with previous work. In the next section we discuss the domain problem associated with the spiked harmonic oscillator.

II.2 The domain problem

We may write the Hamiltonian associated with the spiked harmonic oscillator as

$$H(\alpha,\lambda) = -\frac{d^2}{dx^2} + x^2 + \lambda|x|^{-\alpha} \equiv H_0 + \lambda V, \tag{II.6}$$

where H_0 is the simple harmonic oscillator Hamiltonian, and $V = |x|^{-\alpha}$. The domain, denoted by D, of $H(\alpha,\lambda)$ is $D(H) = D(H_0) \cap D(V)$. To identify $D(H)$ explicitly we notice that

$$D(V) = \{\psi \in L^2(R,dx) | \int_R x^{-\alpha}|\psi(x)|^2 dx < \infty\}. \tag{II.7}$$

But the condition $\int_R x^{-\alpha}|\psi(x)|^2 dx < \infty$ for $\alpha \geq 1$ requires that $\psi \in D(H_0)$ must satisfy the Dirichlet boundary condition, namely

$$\psi(0) = 0. \tag{II.8}$$

Thus the domain of the potential $V(x)$ can be defined as

$$D(V) = \{\psi \in L^2(R,dx) | \int_R x^{-\alpha}|\psi(x)|^2 dx < \infty,\ \psi(0) = 0\}. \tag{II.9}$$

This domain is not the whole domain of $D(H_0)$, indeed there are functions of $D(H_0)$ that are not in the $D(V)$, for example the functions satisfying $\psi'(0) = 0$. In this case when $\lambda \to 0^+$, α fixed, the operator $H(\alpha,\lambda)$ does not converges to H_0 but converges to an operator formally equal to the harmonic oscillator supplemented by Dirichlet boundary condition (II.8). This is known as Klauder's phenomenon. We may then identify the domain of $H(\alpha,\lambda)$ as

$$D(H) = \{\psi \in D(H_0) | \int_R x^{-\alpha}|\psi(x)|^2 dx < \infty, \psi(0) = 0\}.$$

Another problem is that the harmonic oscillator Hamiltonian H_0 with Dirichlet boundary condition (II.8) has a spectrum consisting of twofold degenerated eigenvalues. The degeneracy arises from the effective decoupling of the two half lines

$(-\infty, 0)$ and $(0, \infty)$. To remove this degeneracy, the operator $H(\alpha, \lambda)$ will be restricted to space $L^2([0, \infty), dx)$, with $\psi(0) = 0$. This avoids problems stemming from the degeneracy of the spectrum. Thus

$$D(H) = \{\psi \in D(H_0) | \int_0^\infty x^{-\alpha} |\psi(x)|^2 dx < \infty, \psi(0) = 0\}.$$

The situation that the domain of the quadratic form need not be the whole space guides us to search for a meaning of + in $H_0 + \lambda V$ (11.6) in the realm of quadratic forms [11-12.20]. So we can interpret the sum of H_0 and λV as the sum of quadratic forms defined on functions ψ in $L^2([0, \infty. dx)$ that satisfy $\psi(0) = 0$ and for which $(\psi, H\psi) < \infty$.

II.3 Variational method

One advantage of the variational method is that it deals with analytic expressions and is therefore amenable to symbolic manipulation employing existing software. Since the variational wave function discussed in this section may serve as a starting point for further refined techniques. we present detailed calculations. We consider the following three-parameter trial function

$$\psi(x) = x^{p+\epsilon} \exp(-\beta x^q), \qquad 0 \leq x < \infty. \tag{II.10}$$

which satisfies the Dirichlet boundary condition $\psi(0) = 0$, and vanishes at infinity. The ϵ, β and q are three positive variational parameters. The parameter p will be determined shortly. We have found that the optimal q is usually sufficiently different from 2 , the value normally used for the harmonic oscillator wave function, to justify the added computational difficulty. Convergence of the expectation value $(\psi, -\Delta\psi)$ for the kinetic energy of (II.1) is immediately assured. Indeed, the expectation value reads for the wave function (II.10):

$$\begin{aligned}(\psi, -\frac{d^2\psi}{dx^2}) =& (\frac{1}{2\beta})^{\frac{2p+2\epsilon-1}{q}} \{(2p+q+2\epsilon-1)\Gamma(\frac{2p+q+2\epsilon-1}{q}) \\ &- \frac{2}{q}(p+\epsilon)(p+\epsilon-1)\Gamma(\frac{2p+2\epsilon-1}{q}) \\ &- \frac{q}{2}\Gamma(\frac{2p+2q+2\epsilon-1}{q})\},\end{aligned} \tag{II.11}$$

where $\Gamma(a)$ is the gamma function.

The constant $p \geq 0$ can be determined as follows. Since it is necessary that the wave function (II.10) be in $D(H)$, the convergence of the expectation value of the spiked harmonic oscillator potential

$$V(x) = x^2 + \frac{\lambda}{|x|^\alpha} \tag{II.12}$$

may be used to determine p in terms of α. Since there is no convergence difficulty for large x, a sufficient condition for the convergence of $(\psi, V\psi)$ is $\int_0^1 x^{-\alpha}\psi^2(x)\,dx < \infty$. This in turn is guaranteed if

$$\int_0^1 x^{2p+2\epsilon-\alpha}\,dx < \infty \text{ or } \quad 2p + 2\epsilon - \alpha > -1$$

for $\epsilon > 0$. Thus the minimum value of p (i.e. $\epsilon \to 0$) for an acceptable wave function is given by

$$p = \frac{\alpha - 1}{2}. \tag{II.13}$$

This criterion guarantees that ψ will be in $D(H)$ for each value of α. Thus the expectation value of the potential (II.12) now reads as

$$\begin{aligned}(\psi, V(x)\psi) =& (\frac{2}{q})(\frac{1}{2\beta})^{\frac{2p+2\epsilon+3}{q}}\Gamma(\frac{2p+2\epsilon+3}{q}) \\ &+ \frac{2\lambda}{q}(\frac{1}{2\beta})^{\frac{2p+2\epsilon-\alpha+1}{q}}\Gamma(\frac{2p+2\epsilon-\alpha+1}{q}),\end{aligned} \tag{II.14}$$

where p given by (II.13). Finally,

$$(\psi, \psi) = (\frac{2}{q})(\frac{1}{2\beta})^{\frac{2p+2\epsilon+1}{q}}\Gamma(\frac{2p+2\epsilon+1}{q}).$$

The variational method provides an upper bound E_0^U for the lowest eigenvalue E_0 of the Hamiltonian H. From this we obtain for the function (II.10)

$$E_0 \leq E_0^U = \min_{\epsilon,\beta,q\geq 0} E_0^{(\epsilon,\beta,q)}(\lambda,\alpha), \tag{II.15}$$

where the variational integral is

$$\begin{aligned}E_0^{(\epsilon,\beta,q)}(\lambda,\alpha) &= \frac{(\psi, H\psi)}{(\psi,\psi)} \\ &= \Big[\frac{q}{2}(2\beta)^{\frac{2}{q}}[(2p+q+2\epsilon-1)g_1 - \frac{2}{q}(p+\epsilon)(p+\epsilon-1)g_2 \\ &\quad - \frac{q}{2}g_3] + (\frac{1}{2\beta})^{\frac{2}{q}}g_4 + \lambda(2\beta)^{\frac{\alpha}{q}}g_5\Big]/g_6\end{aligned} \tag{II.16}$$

and

$$g_1 = \Gamma(\frac{2p+q+2\epsilon-1}{q}), \quad g_2 = \Gamma(\frac{2p+2\epsilon-1}{q}),$$
$$g_3 = \Gamma(\frac{2p+2q+2\epsilon-1}{q}), \quad g_4 = \Gamma(\frac{2p+2\epsilon+3}{q}), \tag{II.17}$$
$$g_5 = \Gamma(\frac{2p+2\epsilon-\alpha+1}{q}), \quad g_6 = \Gamma(\frac{2p+2\epsilon+1}{q}).$$

Note that $g_5 = \Gamma(\frac{2\epsilon}{q})$ because of (II.13). Inequality (II.16) is general enough to compute an upper bound for the lowest eigenvalue of the Hamiltonian H for all $\alpha \geq 1$. The single inequality (II.16) also allows us to estimate E_0 for all positive values of the coupling λ. It is desirable to derive an analytic expression for the variational energy as $\lambda \to 0$. Thus we expand the minimum of the variational integral (II.14) about $\lambda = 0$, which yields

$$E_0^{(0.250308,\ 0.500067,\ 1.999484)}(\lambda, \alpha = \frac{5}{2}) = 3 + 4.08521\lambda. \tag{II.18}$$

Similar analytic expressions can be generated for different values of α and λ in the following way. For arbitrary values of α and λ we minimize formula (II.16) over ϵ, β and q, we then substitute these variational values back in (II.16) to find an analytic expression for the bound state energy in terms of λ. Such an analytic expression will be valid for λ's sufficiently small.

II.4 The envelope method

In the light of the comparison theorem discussed in the previous chapter, we know that the ordering between potentials implies a corresponding ordering of the eigenvalues. This observation is an essential feature of solving many problems in quantum mechanics. The envelope method [29,30] makes use of this comparison theory and provides simple formulas for lower and upper bounds. To use the envelope method we need some kind of a solvable model that best fits the problem at hand and proves itself useful as a comparison potential. The shape of the spiked harmonic oscillator potential (see Fig. 1), for large x, suggests the harmonic oscillator potential $h(x) = x^2$ as comparison potential. Therefore, we represent

$$V^t(x) = a + bh(x), \quad h(x) = x^2 \tag{II.19}$$

where the variables a and b are chosen such that the graph of the potential $V(x)$ lies entirely above the graph of the potential $h(x)$, but is tangential to it at a point, say t, where $V(t) = h(t)$ and $V'(t) = h'(t)$. Therefore we can say

$$V^t(x) = a(t) + b(t)x^2. \tag{II.20}$$

Elementary differentiation of $V^t(x)$ with respect to x implies

$$\begin{cases} a(t) = (1 + \frac{\alpha}{2})\frac{\lambda}{t^\alpha}, \\ b(t) = 1 - \frac{\alpha\lambda}{2t^{\alpha+2}}. \end{cases}$$

which leads to

$$V^t(x) = \frac{\lambda}{t^\alpha}(\frac{\alpha}{2} + 1) + (1 - \frac{\alpha\lambda}{2t^{\alpha+2}})x^2. \tag{II.21}$$

This one-parameter family of 'tangent' potentials (Fig. II.2) generates the so-called envelope representation for $V(x)$ expressed by

$$V(x) = \underset{t>0}{\text{Envelope}} \left\{ V^{(t)}(x) \right\}. \tag{II.22}$$

A simple calculation shows that the eigenvalues of Schrödinger's equation with the potential (II.21) are

$$\epsilon_n(\alpha, \lambda; t) = \frac{\lambda}{t^\alpha}\left(\frac{\alpha}{2} + 1\right) + (4n + 3)\left(1 - \frac{\alpha\lambda}{2t^{\alpha+2}}\right)^{1/2}. \tag{II.23}$$

where $n = 0, 1, 2, 3, \ldots$ counts the *odd* eigen-states of the harmonic oscillator in agreement with the Dirichlet condition $\psi(0) = 0$. The envelope theory provides lower bounds for all the energies of the spiked harmonic oscillator Hamiltonian H because

$$V^{(t)}(x) \leq V(x) \; \forall \; t > 0$$

and our claim follows from the application of the comparison theorem. We obtain the greatest lower bound by maximizing over the contact point t, namely

$$E_n(\alpha, \lambda) \geq E_n^L = \max_{t>0} \epsilon_n(\alpha, \lambda; t). \tag{II.24}$$

The maximization condition

$$\frac{\partial \epsilon_n(\alpha, \lambda; t)}{\partial t} = 0$$

implies that the optimal positive $\hat{t}$ must satisfy the equation

$$4t^4 - 2\alpha\lambda t^{2-\alpha} - (4n+3)^2 = 0 \quad n = 0, 1, 2, \ldots \ . \tag{II.25}$$

This equation has only one positive root for any $\alpha > 2$ because the left hand side tends to $-\infty$ as $t \to 0^+$ and tends to ∞ as $t \to \infty$ and it is monontone increasing on the open interval $(0, \infty)$. For $\alpha < 2$, the left hand side of (II.25) has only one minimum occurring at $\left(\frac{\alpha}{8}(2-\alpha)\right)^{\frac{1}{2+\alpha}}$. Moreover, it tends to $-(4n+3)^2$ as $t \to 0$ and tends to ∞ as $t \to \infty$, therefore we conclude again that the equation (II.25) has only one positive root for any $0 < \alpha < 2$.

By solving (II.25) for t^α and substituting this value into (II.23), we obtain the simpler form of the energy spectrum

$$\begin{cases} \epsilon_n(\alpha, \lambda; \hat{t}) = \dfrac{\lambda}{\hat{t}^\alpha}\left(\dfrac{\alpha}{2} + 1\right) + \dfrac{(4n+3)^2}{2\hat{t}^2}, \\ \hat{t} \text{ is root of } \quad 4t^4 - 2\alpha\lambda t^{2-\alpha} - (4n+3)^2 = 0. \end{cases}$$

Equations (II.4) and (II.5) establish the energy bounds of the spiked harmonic oscillator Hamiltonian (II.1). Indeed solving (II.5) with respect to t yields the optimal solution $\hat{t}$ and consequently $\epsilon_n(\alpha, \lambda; \hat{t})$ in (II.4) gives lower bounds for arbitrary α and λ.

A similar technique utilizing the square well potential, for example, as comparison potential provides us with an upper bound for all the eigenvalues of H. For the most important case, however, namely the ground-state, the variational argument of section (II.3) is much more accurate.

II.5 Numerical results

An accurate eigenvalue analytic expansion, as suggested by Aguilera et al [15] should involve two different expansions according to the values of the coupling parameter λ: a non power series expansion given by Harrell [13] when λ is small, and a large coupling perturbative expansion given by them when λ is large. For intermediate

values of $\lambda(\approx 1)$ W Solano-Torres et al [24] claimed that they have constructed an approximant to represent the energy in this region using a single Padé extrapolant. They did not present any numerical results for eigenvalues in this case, however. In this section we discuss the numerical results for the upper bound E_0^U (by (II.16)) and lower bound E_0^L (by (II.4-5)) of the ground-state energy of the spiked harmonic oscillator Hamiltonian (II.1). These bounds are valid for small, intermediate and large values of the coupling parameter λ. In Fig.(II.3) we illustrate the difference between our variational approach and the work of Harrell [13] and of Aguilera et al [15]. Fig.(II.4) illustrate the comparison between the variational results and the exact solutions derived by direct numerical integration of Schrödinger equation.

A simple method to compute the upper bound E_0^U from inequality (II.16) is to fix one or two of the parameters (β, ϵ, q) and then minimize with respect to the remining free parameters. We found that the most convenient approach was to explore the parameter space (β, ϵ, q) by using the downhill simplex method of Nelder and Mead [31]. The initial simplex points for this method may be chosen with the aid of few preliminary calculations. As an example, consider $\alpha = 5/2$ and $\lambda = 1000$, simple loops over fixed ranges of ϵ and q give for the minimization of the right hand side of inequality (II.16) $\beta = 0.89$ and $E_0^U = 44.955\ 66$ when $\epsilon = 27.6$ and $q = 1.80$. With these values of (β, ϵ, q) as a base for the simplex method, the other three initial points can be chosen close to it. The downhill simplex method now gives the more accurate eigenvalue $E_0^U = 44.955\ 49$. In Table (1) we exhibit the results of our computations of the upper bounds for different values of the coupling parameter λ, where α is fixed at $5/2$. For comparison, we include the partial results given by the formulas of Harrell E^H (II.2) and of Aguilera et al E^G (II.3), and the 'exact' numerical results obtained by direct numerical integration.

In Table (2) we present some sample ground state energy eigenvalues of the spiked harmonic oscillator Hamiltonian H for fixed λ and different values of α. The results for $\lambda = 1000$ cannot be possible by any of the earlier analytic approximations mentioned in the introduction. Similar tables can of course be constructed using the inequalities (II.16) and (II.24) and any desired values for $\lambda > 0$ and $\alpha \geq 1$. The lower bounds given by (II.24) are weak, especially for small λ, but the formula is simple

and valid for *all* the discrete eigenvalues $n = 0, 1, 2, \ldots$. Examples for $\alpha = 5/2$ (as in Table (1)) are: $\lambda = 1000$, $E_0^L = 42.917$; $\lambda = 10$, $E_0^L = 6.228$; $\lambda = 1$, $E_0^L = 3.529$. The idea of using a trial wave function to determine variational upper bounds to the eigenvalues of the ground-state of H for positive even integers α was used by Guardiola et al [26] and Fernández [27]. In Table (3) we report a comparison between the ground-state eigenvalues of H using formula (9) of reference [27] and inequality (II.16) of the present work.

II.6 On the numerical integration of Schrödinger equation with a singular potential

The divergence of the singular potential at the origin leads to many difficulties with the standard methods of numerical integration of the Schrödinger equation. In this case one should usually start the integration far from the origin with a careful adjustment for the step-size of the numerical method to ensure the accuracy of the eigenvalues. How far may we go so that the start of our integration does not affect the calculation of the eigenvalues? The variational wave function we introduced in the previous sections helps to answer this question. In Fig.(II.5) and (II.6) we plot the variational wave functions

$$\psi(x) = x^{10.613} e^{-0.773 x^{1.826}} \tag{II.26}$$

for the ground state of the Hamiltonian (II.1) with $\lambda = 100$ and $\alpha = \frac{5}{2}$ and

$$\psi(x) = x^{11.032} e^{-1.223 x^{1.735}} \tag{II.27}$$

for the ground state of the Hamiltonian (II.1) with $\lambda = 1000$ and $\alpha = 6$, respectively. The interesting point in these graphs is the shifting to the right of the wave functions along the $x-$axis: this shows where to start the numerical integration.

II.7 Conclusion

The significance of the contribution made in the present chapter is that upper and lower bounds are simply and uniformly obtainable for all values of the potential parameters. The upper bound (II.16) for the ground-state energy is accurate and

also yields a trial wave function for which has already been used to estimate effective starting points for numerical solution; other interesting applications could also be considered for this useful by-product. The lower bounds we provide are not very accurate for small λ, but they are in the form of simple formulas (II.4-5), which is valid for all values of the potential parameters and for all the discrete eigenvalues.

Table(II.1): Upper bounds for $H = -\frac{d^2}{dx^2} + x^2 + \frac{\lambda}{|x|^{5/2}}$ with different values of λ. The values E^G were evaluated by formula (II.3), and for E^H we used formula (II.2). E_0^U is from inequality (II.16) of the present work. The 'exact' values were obtained by direct numerical integration.

$\alpha = 5/2$				
λ	E^G	E^H	E_0^U	**Exact**
1000	44.955 49	...	44.955 49	44.955 49
100	17.541 92	...	17.541 92	17.541 89
10	7.735 58	...	7.735 32	7.735 11
5	6.297 55	...	6.296 85	6.296 47
1	4.323 60	...	4.318 54	4.317 31
0.5	3.860 53	3.481 27	3.850 32	3.848 55
0.1	...	3.201 25	3.269 28	3.266 87
0.05	...	3.136 95	3.154 50	3.152 43
0.01	...	3.036 75	3.037 43	3.036 73
0.005	...	3.019 26	3.019 47	3.019 14
0.001	...	3.004 03	3.004 04	3.004 02

Table(II.2): Upper and lower bounds for the $H = -\frac{d^2}{dx^2} + x^2 + \frac{1000}{|x|^\alpha}$ with different values of α, by inequality (II.16) and the formulas (II.4-5).

$\lambda = 1000$		
α	E_0^U	E_0^L
2.5	44.955 49	42.917 48
3	33.316 78	31.186 55
3.5	26.108 98	23.894 13
4	21.370 26	19.076 98
4.5	18.102 87	15.737 60
5	15.763 56	13.330 60
5.5	14.036 26	11.539 28
6	12.725 65	10.170 24

Table(II.3): A comparison between the results E^F of Fernández [27], and the results E_0^U of the present work obtained from the inequality (II.16) for $\alpha = 4$ and 6 and various values for the coupling λ.

	$\alpha = 4$		$\alpha = 6$	
λ	E^F	E_0^U	E^F	E_0^U
1000	21.384 46	21.370 26	12.737 60	12.725 65
100	11.292 41	11.265 86	8.422 60	8.420 96
10	6.649 78	6.609 66	6.016 4	6.014 94
5	5.832 05	5.788 89	5.527 51	5.528 09
1	4.548 79	4.504 16	4.676 88	4.684 97
0.1	3.626 44	3.600 44	4.019 15	4.042 84
0.01	3.237 75	3.249 80	3.524 93	3.580 70

Fig. II.1 The spiked harmonic oscillator potential $V(x) = x^2 + \lambda|x|^{-\alpha}$ for $\alpha = 3$ and λ =0.001, 1 and 10.

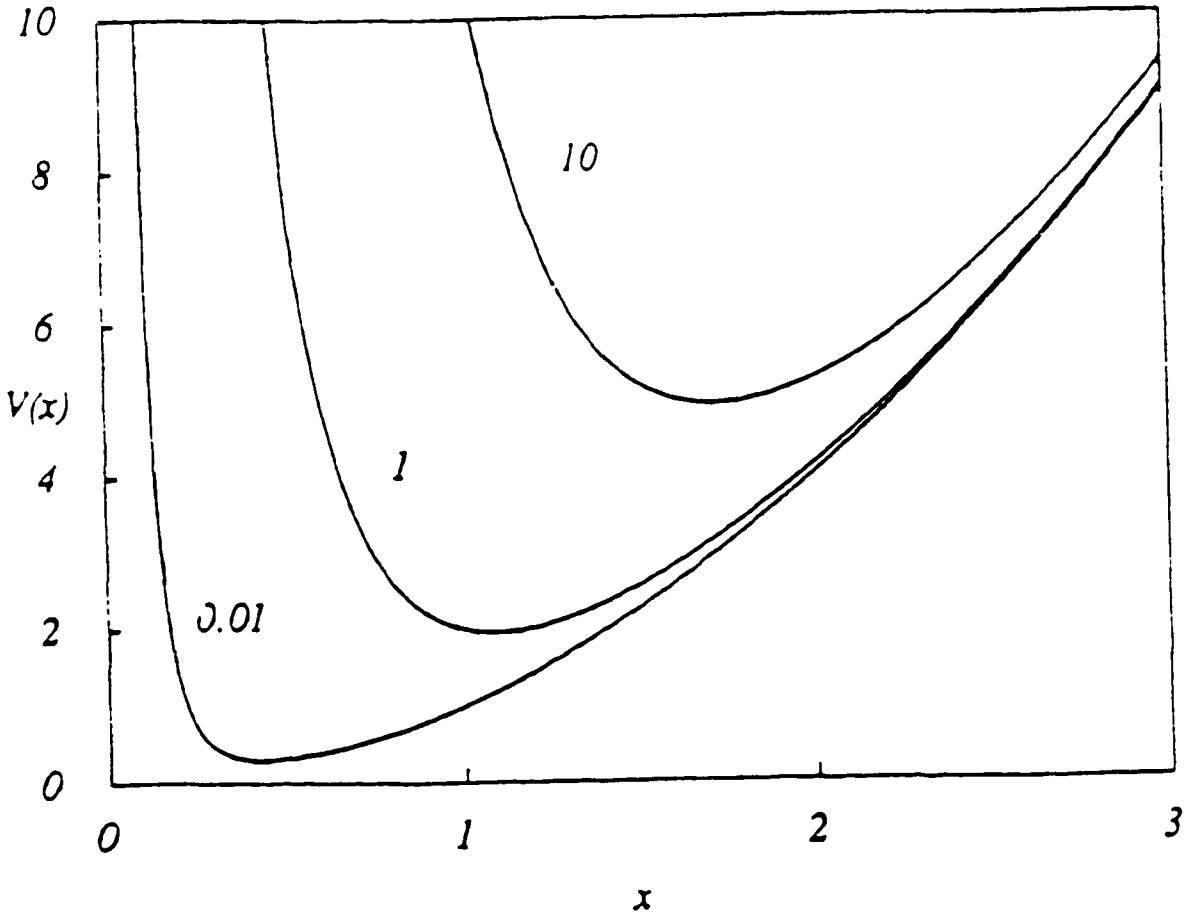


Fig. II.2 Family of 'tangent' potentials $V(x) = \overset{\text{Envelope}}{t>0} \left\{V^{(t)}(x)\right\}$, for different values of t along with the graph of spiked harmonic oscillator for $\lambda = 1$ and $\alpha = 5/2$.

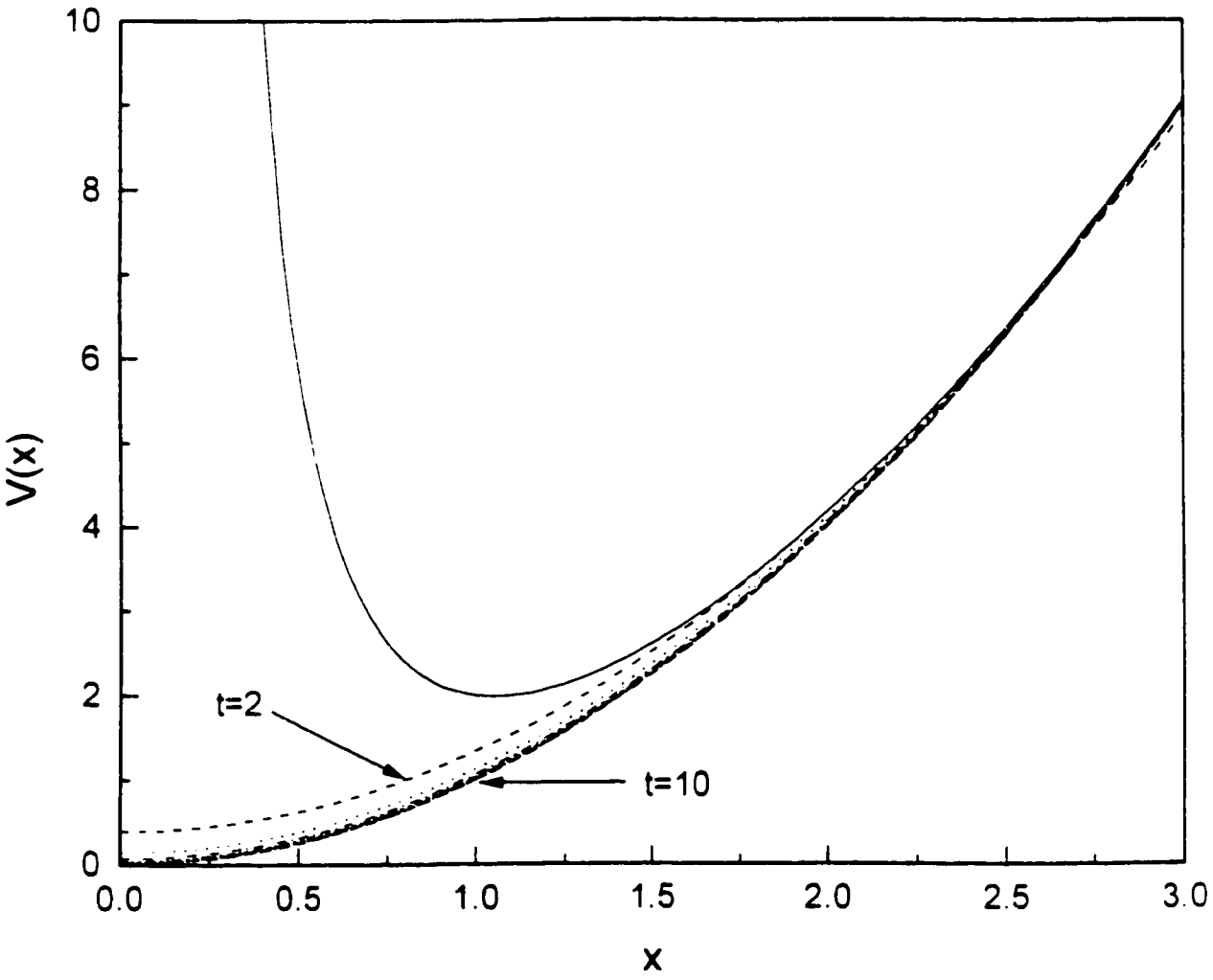


Fig. II.3 Comparison between the result of the present chapter with the result of Harrell (II.2) and of Aguilera et al (II.3).

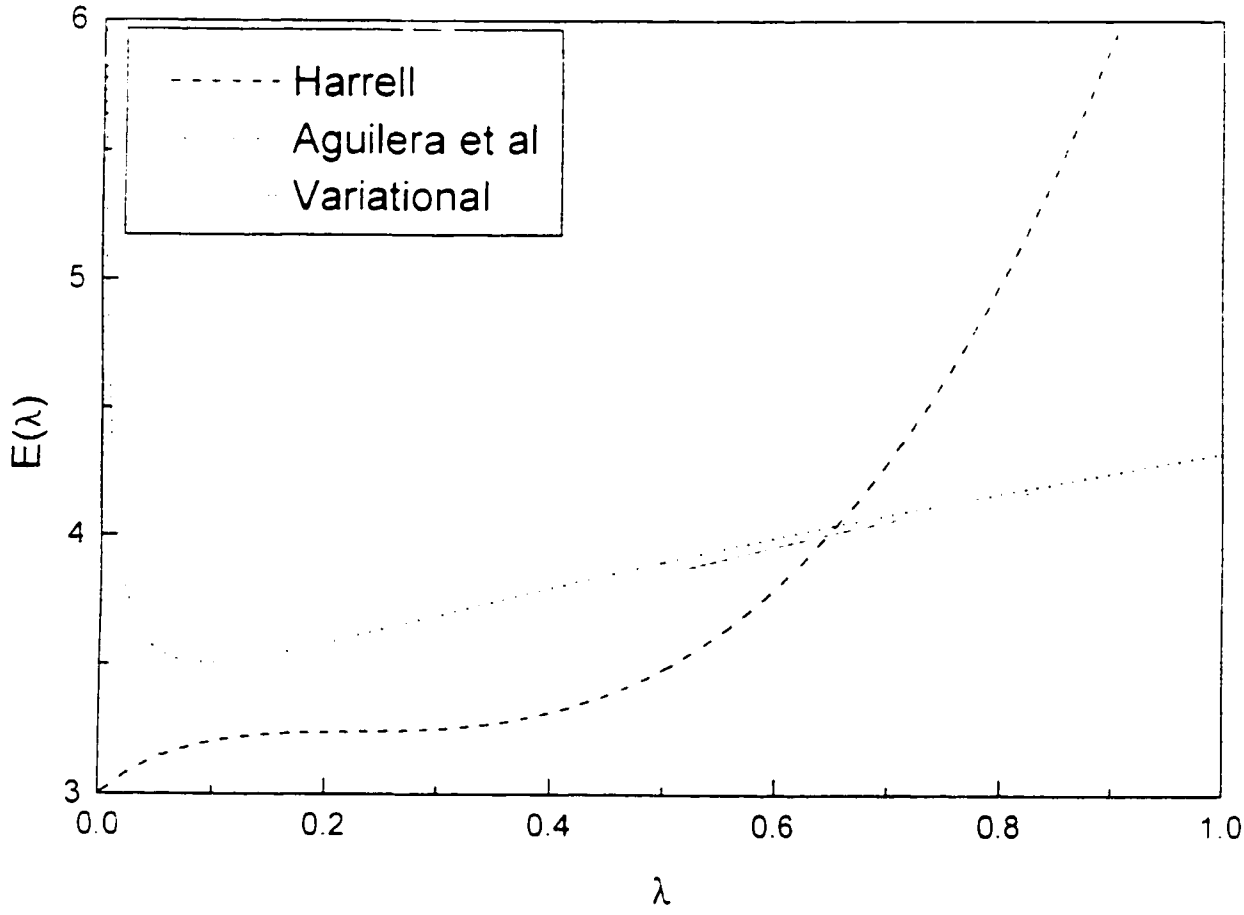


Fig. II.4 A comparistion between the variational results (II.16) for $\alpha = \frac{5}{2}$ and the 'exact' solutions found by direct numerical integration of Schrödinger's equation.

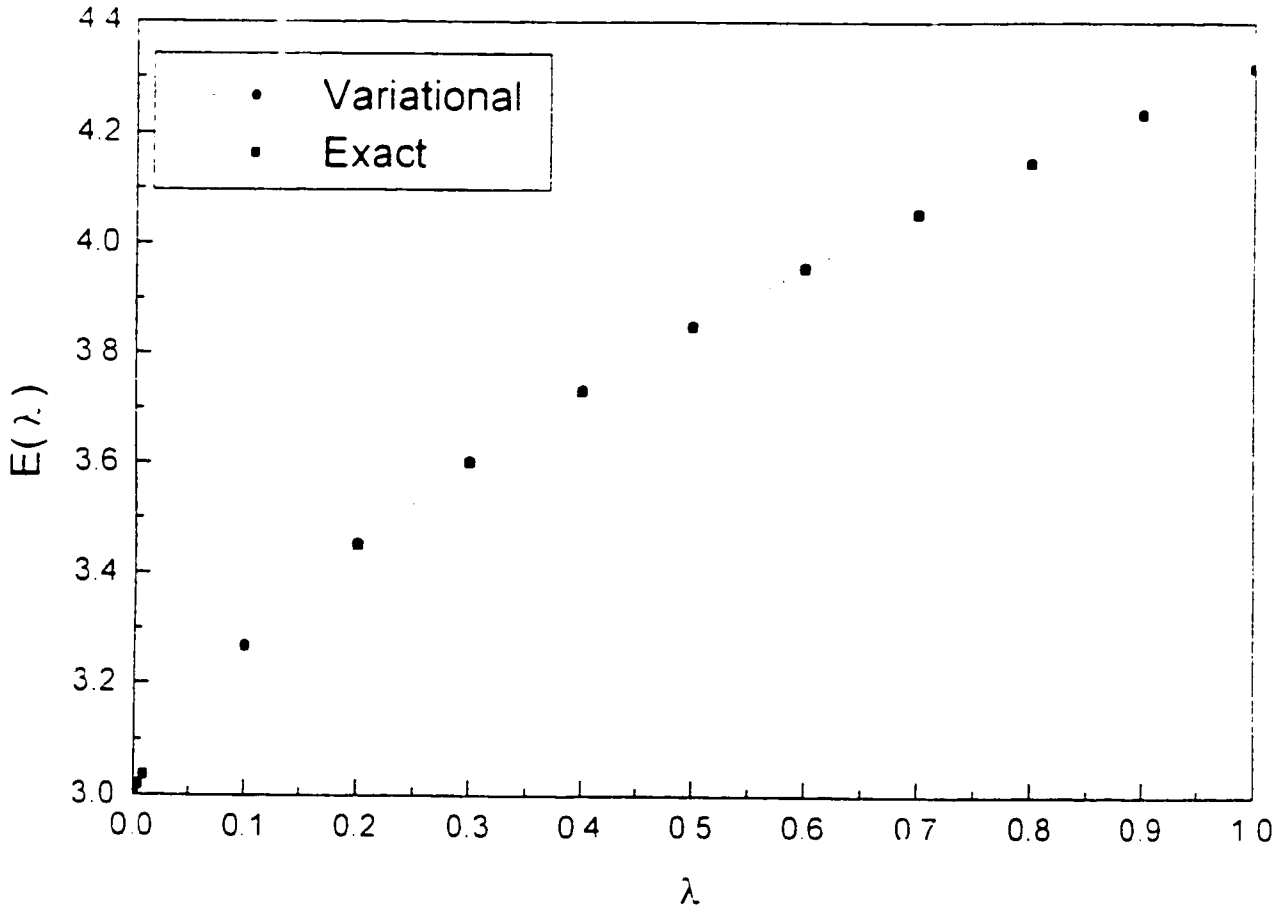


Fig. II.5 The graph of the variation wave function (II.26).

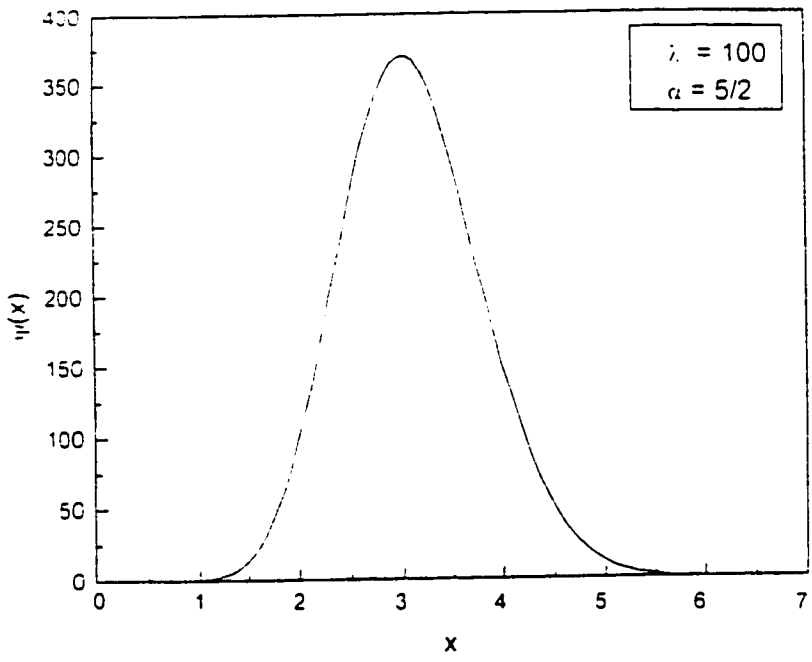
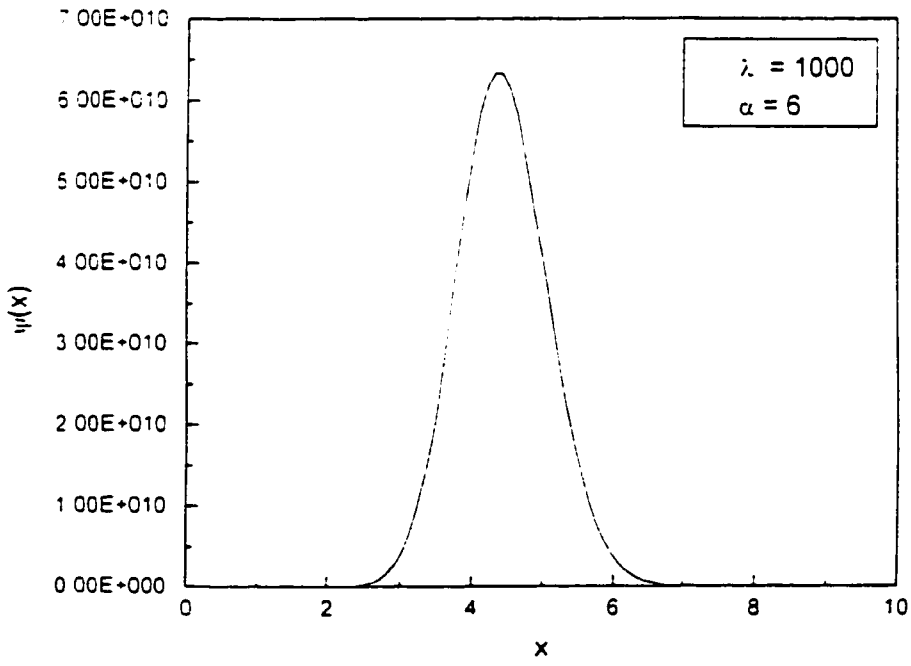


Fig. II.6 The graph of the variation wave function (II.27).



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CHAPTER III

Eigenvalue bounds for a class of of singular potentials

In the previous chapter we applied the method of envelope representation to obtain lower-bound expressions for the spiked harmonic oscillator

$$H = -\Delta + x^2 + \lambda/x^\alpha, \ (\alpha \geq 1, \lambda > 0).$$

Although the lower-bound formulas obtained were simple in formulation and applied to *all* energy levels, the eigenvalues were not sufficiently accurate for small λ. This of course is easy to predict, because as $\lambda \to 0$, the term $\frac{\lambda}{x^\alpha}$ adds an infinite repulsive barrier near the origin and, therefore, it cannot be expressed by the comparison potential, the harmonic oscillator (II.19). In this chapter we introduce a new technique that gives to sharper and more general.

III.1 Introduction and main results

We consider the one-dimensional Schrödinger equation (in units $\hbar = 2m = 1$)

$$-\psi'' + V(x)\psi = E\psi$$

where $V(x)$ is continuous everywhere, except that $|V(x)| \to \infty$ as $x \to 0^+$. The potentials $V(x)$, then, can be classified into three classes.

i. A class of mildly singular potentials where

$$\lim_{\epsilon \to 0} \int_\epsilon^a V(x)dx < 0.$$

ii. A class of singular potentials where

$$\lim_{\epsilon \to 0} \int_\epsilon^a x|V(x)|dx < 0$$

but

$$\lim_{\epsilon \to 0} \int_\epsilon^a V(x)dx \to \infty.$$

iii. A class of supersingular (SS) potentials with

$$\lim_{\epsilon \to 0} \int_{\epsilon}^{a} x|V(x)|dx$$

divergent.

Recently, the SS potential class has attracted many researchers for the following two reasons:

1. In mathematics, the standard perturbation theory [1,2] fails badly in the sense that the first or the second order correction to the energy either diverges or does not exist. Thus a modified perturbation theory to deal with singular potentials is highly desirable [3-10].

2. In physics, one often encounters phenomenological potentials which are strongly singular at the origin; for example: the Lennard-Jones potential, the potential $V(x) = x^2 + e^{\frac{1}{x^2}}$, the potential $V(x) = ax^2 + \frac{b}{x^4} + \frac{c}{x^6}(a, b, c > 0)$, and certain types of nucleon-nucleon potentials, singular models of fields in zero dimensions, etc [11-35].

In the literature very few SS type potentials give exact values for the energy. These exact values of energy are either restricted to the ground state, or to several excited states, provided certain constraints between the potential parameters are satisfied.

Exactly soluble problems [36-47] in non-relativistic quantum mechanics provide simple and effective models, illustrating the most relevant features of actual physical phenomena. Further, they may provide a starting point for more accurate approximations, based on a variational or perturbative method. In the method of envelope representation, exactly soluble models play a fundamental role in the development of the energy-approximation expressions. Gol'dman and Krivchenkov [37], for example, have provided a clear description of the exact solution of the following one-dimensional Schrödinger equation (in units $\hbar = 2m = 1$)

$$-\psi'' + V_0\left(\frac{a}{x} - \frac{x}{a}\right)^2 \psi = E_n \psi, \qquad x \in [0, \infty) \tag{III.1}$$

and ψ satisfies Dirichlet boundary condition $\psi(0) = 0$. They showed that the energy spectrum, in terms of the parameters V_0 and a, is given by

$$E_n = \frac{4}{a}\sqrt{V_0}\left\{n + \frac{1}{2} + \frac{1}{4}\left(\sqrt{4V_0a^2 + 1} - 2a\sqrt{V_0}\right)\right\}. \qquad \text{(III.2)}$$

To simplify the notation, we introduce the parameters $\lambda = \frac{V_0}{a^2}$ and $\mu = V_0a^2$, and obtain an exact solution to the Schrödinger equation with a singular potential

$$V(x) = \lambda x^2 + \frac{\mu}{x^2}, \qquad \lambda > 0, \mu > 0, \qquad \text{(III.3)}$$

where the energy spectrum is now in terms of the parameters λ and μ,

$$\mathcal{E}_n = \sqrt{\lambda}(4n + 2 + \sqrt{4\mu + 1}), \quad n = 0, 1, 2, \ldots. \qquad \text{(III.4)}$$

The wave functions have the form

$$\psi_n(x) = C_n x^{\frac{1}{2}(1+\sqrt{4\mu+1})} e^{-\frac{1}{2}\sqrt{\lambda}x^2} {}_1F_1(-n, \frac{1}{2}\sqrt{4\mu + 1} + 1; \sqrt{\lambda}x^2)$$

where ${}_1F_1$ is the confluent hypergeometric function

$${}_1F_1(a, b; z) = \sum_k \frac{(a)_k z^k}{(b)_k k!}.$$

and the constant C_n can be found from the normalization conditions. The Pochhammer's symbol $(a)_k$ is given by

$$(a)_k = a(a + 1)(a + 2)\ldots(a + k - 1) = \frac{\Gamma(a + k)}{\Gamma(a)}.$$

where $\Gamma(a)$ is the gamma function.

We notice from the energy expression (III.4) that the exact solutions for (III.3) depend on the existence of the harmonic oscillator term x^2. Secondly, the Schrödinger equation with the potential $\frac{\mu}{x^2}(\mu > 0)$ alone is exactly solvable, but supports no bound state energy, that is, no discrete eigenvalue [47].

In this chapter we shall use such exact solutions (III.4) to investigate the spectrum $\{E_n\}_{n=0}^{\infty}$ of the Schrödinger equation

$$-\psi'' + V(x)\psi = E_n\psi, \quad \psi(0) = 0, \qquad \text{(III.5)}$$

where

$$V(x) = g(x^2) + f(\frac{1}{x^2}) \tag{III.6}$$

is a sum of two C^2-transformations of x^2 and $\frac{1}{x^2}$ respectively. We shall show in section III.3 that E_n can be approximated by the expression

$$E_n \approx \epsilon_n = \left\{ g(s^2) - s^2 g'(s^2) + f(\frac{1}{t^2}) - \frac{1}{t^2} f'(\frac{1}{t^2}) + \sqrt{g'(s^2)}(4n + 2 + \sqrt{4f'(\frac{1}{t^2}) + 1}) \right\}, \; n = 0, 1, 2, \ldots. \tag{III.7}$$

This simple formula provides a lower bound ($\approx = \geq$) or an upper bound ($\approx = \leq$) to the exact eigenvalues, depending on whether the transformation functions g and f are both convex ($g''(x), f''(x) > 0$) or concave ($g''(x), f''(x) < 0$). This allows us, for example, to obtain simple expressions which bound the spectrum of the spiked harmonic oscillator potential

$$V(x) = \lambda x^2 + \frac{\mu}{x^\alpha}, \; \alpha \geq 1, n = 0, 1, 2, \ldots.$$

Indeed, formula (III.7) implies that the energy of spiked harmonic oscillator can be approximated by

$$E_n \approx \epsilon_n(\hat{t}) = (1 - \frac{\alpha}{2})\frac{\mu}{\hat{t}^\alpha} + 2\lambda \hat{t}^2 + 2\sqrt{\lambda}(2n + 1), \tag{III.8}$$

where $\hat{t}$ is the real positive root of

$$4\lambda t^4 - 2\mu\alpha t^{2-\alpha} - 1 = 0. \tag{III.9}$$

Here $\epsilon_n(\hat{t})$ is lower bound to E_n, when $\alpha > 2$, and an upper bound, when $\alpha < 2$.

III.2 Transformed Potentials

Our aim is to construct an approximation method which allows us to obtain lower and upper bounds to the Schrödinger Hamiltonian

$$H = -\frac{d^2}{dx^2} + g(x^2) + f(\frac{1}{x^2}), \tag{III.10}$$

where g and f are C^2-transformations of x^2 and $\frac{1}{x^2}$ respectively. The method of potential envelopes might suggest the following approach to deal with a Hamiltonian of the form (III.10). We might approximate the shape of the potential $V(x)$ as a smooth transformation G of the soluble base potential $x^2 + 1/x^2$. that is to say

$$V(x) = G(x^2 + \frac{1}{x^2}).$$

When G has definite convexity, this would lead to energy bounds, as found in Chapter II. Now, instead of approximating $V(x)$ by a single potential, we use the tangent approximation for $g(x^2)$ and $f(\frac{1}{x^2})$, separately. That is replace g and f by their corresponding tangent approximations

$$\begin{aligned} g^{(s)}(x^2) &= a(s) + b(s)x^2, \\ f^{(t)}(\frac{1}{x^2}) &= c(t) + \frac{d(t)}{x^2} \end{aligned} \tag{III.11}$$

respectively, where s is a contact point between $g(x^2)$ and its tangent approximation $g^{(s)}(x^2)$, and t is a contact point between $f(\frac{1}{x^2})$ and its tangent approximation $f^{(t)}(\frac{1}{x^2})$. Elementary differentiation with respect to s and t repectively leads to

$$\begin{cases} a(s) = g(s^2) - s^2 g'(s^2), \\ b(s) = g'(s^2), \end{cases} \tag{III.12}$$

and

$$\begin{cases} c(t) = f(\frac{1}{t^2}) - \frac{1}{t^2} f'(\frac{1}{t^2}), \\ d(t) = f'(\frac{1}{t^2}). \end{cases} \tag{III.13}$$

Therefore, $V(x)$ in (III.5) can be approximated by

$$V^{(s,t)}(x) = g(s^2) - s^2 g'(s^2) + f(\frac{1}{t^2}) - \frac{f'(\frac{1}{t^2})}{t^2} + g'(s^2)x^2 + \frac{f'(\frac{1}{t^2})}{x^2}. \tag{III.14}$$

This two-parameter family of 'tangent' potentials generate the so-called 'envelope representation' for $V(x)$ expressed by

$$V(x) = \underset{s,t>0}{\text{Envelope}} \left\{ V^{(s,t)}(x) \right\}.$$

With this representation of $V(x)$, we may use the results of (III.3) and (III.4) for expressing the eigenvalues of the Schrödinger equation

$$-\psi'' + V^{(s,t)}(x)\psi = \epsilon_n(s,t)\psi, \tag{III.15}$$

namely

$$\begin{aligned}\epsilon_n(s,t) =& g(s^2) - s^2 g'(s^2) + f(\frac{1}{t^2}) - \frac{1}{t^2} f'(\frac{1}{t^2}) \\ &+ \sqrt{g'(s^2)}\left(4n + 2 + \sqrt{4f'(\frac{1}{t^2}) + 1}\right) \quad n = 0, 1, 2, \ldots .\end{aligned} \tag{III.16}$$

Theorem III.1. The eigenvalues E_n of the Schrödinger equation (III.5) satisfy

(a) $E_n \leq \epsilon_n(s,t)$ if g and f are both convex,

(b) $E_n \geq \epsilon_n(s,t)$ if g and f are both concave.

Proof: For definiteness, we consider case (a). Since g and f are convex, their graphs lie above their tangents. Consequently, from (III.14), $V^{(s,t)}(x) \leq V(x)$ for $s, t > 0$. Case (a) then follows by an application of the comparison theorem. Case (b) is proved in analogous way if 'convex' is replaced by 'concave'.

It is appropriate to mention here, that the conclusions of this theorem follow even if either of f and g in (III.14) is the identity transformation. It is also appropriate to mention that if the transformations f and g are both the identity transformation, then (III.16) exactly corresponds to the exact solution (III.4). These bounds (III.16) may, of course, be sharpened by optimization [48] with respect to s and t, and are furthermore valid for the entire discrete spectrum $n \geq 0$.

III.3 Numerical results

An interesting point concerning the bounds just obtained (III.16), is the large variety of approximations made possible by different choices of the transformations g and f.

III.3.1 The potential $V(x) = \lambda x^\beta + \frac{\mu}{x^\alpha}$

For the Schrödinger equation (III.15) consider the singular potential

$$V(x) = \lambda x^\beta + \frac{\mu}{x^\alpha}, \tag{III.17}$$

or $g(x^2) = \lambda x^\beta$ and $f(\frac{1}{x^2}) = \frac{\mu}{x^\alpha}$ $(\alpha, \beta > 0)$ in (III.14), for which it follows that

$$V^{(s,t)}(x) = \lambda(1 - \frac{\beta}{2})s^\beta + (1 - \frac{\alpha}{2})\frac{\mu}{t^\alpha} + \frac{\lambda\beta}{2}s^{\beta-2}x^2 + \frac{\mu\alpha}{2x^2}\frac{1}{t^{\alpha-2}}. \qquad \text{(III.18)}$$

The graph of these enevelopes for $\lambda = \mu = 1$ and $\alpha = \beta = 2.1$ is displayed in Fig.(III.1) for some arbitrary values of s and t, accompanied by the graph of the potential $V(x) = x^{2.1} + \frac{1}{x^{2.1}}$. The energy formula (III.16) reads in this case

$$\epsilon_n(s,t) = \lambda(1 - \frac{\beta}{2})s^\beta + (1 - \frac{\alpha}{2})\frac{\mu}{t^\alpha} + \sqrt{\frac{\lambda\beta s^{\beta-2}}{2}}\left(4n + 2 + \sqrt{\frac{2\mu\alpha}{t^{\alpha-2}} + 1}\right). \qquad \text{(III.19)}$$

While theorem III.1 entails

$$E_n \leq \epsilon_n(s,t) \quad \text{if} \quad \alpha \leq 2, \beta \leq 2,$$

and

$$E_n \geq \epsilon_n(s,t) \quad \text{if} \quad \alpha \geq 2, \beta \geq 2.$$

The best upper or lower bound can be obtained by any optimization procedure [37]. Indeed, using the conditions

$$\frac{\partial\epsilon_n(s,t)}{\partial s} = 0, \quad \frac{\partial\epsilon_n(s,t)}{\partial t} = 0$$

We complete part of the search for the optimum, leaving the task to optimize (III.16) over t only since we find

$$s^2 = t^2(2\mu\alpha t^{2-\alpha} + 1)^{-\frac{1}{2}}(4n + 2 + \sqrt{2\mu\alpha t^{2-\alpha} + 1})$$

$$\epsilon_n(s,t) = g(s^2) - s^2 g'(s^2) + f(\frac{1}{t^2}) - \frac{1}{t^2}f'(\frac{1}{t^2}) + \sqrt{g'(s^2)}\left(4n + 2 + \sqrt{4f'(\frac{1}{t^2}) + 1}\right) \quad n = 0, 1, 2, \ldots.$$

III.3.2 The spiked harmonic oscillator potential

Since, for the spiked harmonic oscillator $\beta = 2$, it follows from (III.18) and (III.19) that

$$V^{(t)}(x) = (1 - \frac{\alpha}{2})\frac{\mu}{t^\alpha} + \lambda x^2 + \frac{\mu\alpha}{2x^2}\frac{1}{t^{\alpha-2}} \qquad \text{(III.20)}$$

and

$$\epsilon_n(t) = (1 - \frac{\alpha}{2})\frac{\mu}{t^\alpha} + \sqrt{\lambda}\left(4n + 2 + \sqrt{\frac{2\mu\alpha}{t^{\alpha-2}} + 1}\right). \qquad \text{(III.21)}$$

If $\alpha > 2$, then $\max_{t>0} \epsilon_n(t)$ is a lower bound, whereas for $\alpha < 2$ we have $\min_{t>0} \epsilon_n(t)$ is an upper bound. We can simplify this optimization further by differentiating (III.20) and solving for t. In this case, the optimal positive t must satisfy the equation

$$4\lambda t^4 - 2\mu\alpha t^{2-\alpha} - 1 = 0. \qquad \text{(III.22)}$$

It is not hard to prove for an optimal t, that there is only one positive real root given by (III.22). If we let $h(t) = 4\lambda t^4 - 2\mu\alpha t^{2-\alpha} - 1$, then for $\alpha < 2$: $h(t) \to -1$ as $t \to 0$ and $h(t) \to \infty$ as $t \to \infty$. On the interval $(0, \infty)$ the function $h(t)$ has only one minimum at

$$t_{\min} = \left(\frac{\mu\alpha(2-\alpha)}{8\lambda}\right)^{\frac{1}{2+\alpha}}$$

Consequently for $\alpha < 2$, Eq.(III.22) has only one real positive root. For $\alpha > 2$, $h(t) \to -\infty$ as $t \to 0^+$ and tends to ∞ as $t \to \infty$. On the interval $(0, \infty)$, $h(t)$ is monontone, increasing on the open interval $(0, \infty)$, and we conclude that (III.22) has only one real positive solution for all α. Now solving equation (III.22) for $t^{\alpha-2}$ and substiting it in (III.21), we arrive at the simplified algorithm to compute the energy bounds

$$\begin{cases} \epsilon_n(\hat{t}) = (1 - \frac{\alpha}{2})\frac{\mu}{\hat{t}^\alpha} + 2\lambda\hat{t}^2 + 2\sqrt{\lambda}(2n+1), \\ \hat{t} \text{ is the root of } \quad 4\lambda t^4 - 2\mu\alpha t^{2-\alpha} - 1 = 0. \end{cases}$$

In Tables 1 and 2 we exhibit results of the lower bounds obtained by use of this algorithm for different values of α and for $\lambda = 1$ as well as different values of the coupling parameter μ, along with some accurate values determined by the numerical integration of Schrödinger's equation. We also present in Table 2 a comparison between the results obtained by standard envelope method discussed in chapter II, namely (II.4) and (II.5), with the results of the new approximation method developed in this chapter, namely (III.8) and (111.9).

III.3.3 The potential $V(x) = \lambda x^{\beta} + \frac{\mu}{x^{\alpha}}, \alpha = \beta$

For the potential

$$V(x) = \lambda x^{1.9} + \frac{\mu}{x^{1.9}} \tag{III.23}$$

we let $\beta = 1.9$ and $\alpha = 1.9$ in formula (III.17), which provides upper bounds in this case because of Theorem III.1. A comparison of some results for eleven energy levels obtained by formula (III.19), and the corresponding results obtained by direct numerical integration are presented in Table 3. Table 4 reports the corresponding results for the case $\beta = 2.1$ and $\alpha = 2.1$, that is to say, for the potential

$$V(x) = \lambda x^{2.1} + \frac{\mu}{x^{2.1}}. \tag{III.24}$$

Table(III.1): Some lower bounds E_0^L and upper bounds E_0^U using (III.8) and (III.9) for $H = -\frac{d^2}{dx^2} + x^2 + \frac{1000}{x^\alpha}$. The "exact" values E_0^N were obtained by direct numerical integration of the Schrödinger equation.

$\lambda = 1000$			
α	E_0^L	E_0^N	E_0^U
0.5	– – – –	415.889 79	416.309 77
1	– – – –	190.723 31	190.992 13
1.5	– – – –	104.410 22	104.539 93
1.9	– – – –	71.061 58	71.086 86
2	65.253 46	65.253 46	65.253 46
2.1	60.127 04	60.152 01	– – – –
2.5	44.833 49	44.955 49	– – – –
3	33.079 40	33.316 76	– – – –
3.5	25.762 04	26.108 85	– – – –
4	20.918 65	21.369 64	– – – –
4.5	17.552 18	18.101 83	– – – –
5	15.117 58	15.761 13	– – – –
5.5	13.298 42	14.031 07	– – – –
6	11.901 53	12.718 62	– – – –

Table(III.2): Comparison between the ground-state energy E_{II} obtained by (II.4) and the eigenvalues E_{III} obtained by (III.8-9) of the present chapter, along with the "exact" values E_0^N obtained by direct numerical integration of the Schrödinger equation.

$\alpha = 5/2$			
λ	E_{II}	E_{III}	E_0^N
1000	42.917 47	44.833 49	44.955 49
100	15.651 17	17.419 00	17.541 89
10	6.227 67	7.611 69	7.735 11
5	4.977 67	6.173 94	6.296 47
1	3.529 31	4.204 53	4.317 31
0.5	3.280 67	3.746 16	3.848 55
0.1	3.059 32	3.204 95	3.266 87
0.05	3.029 89	3.109 54	3.152 43
0.01	3.006 01	3.023 36	3.036 70
0.005	3.003 01	3.011 78	3.019 05
0.001	3.000 60	3.002 37	3.003 97

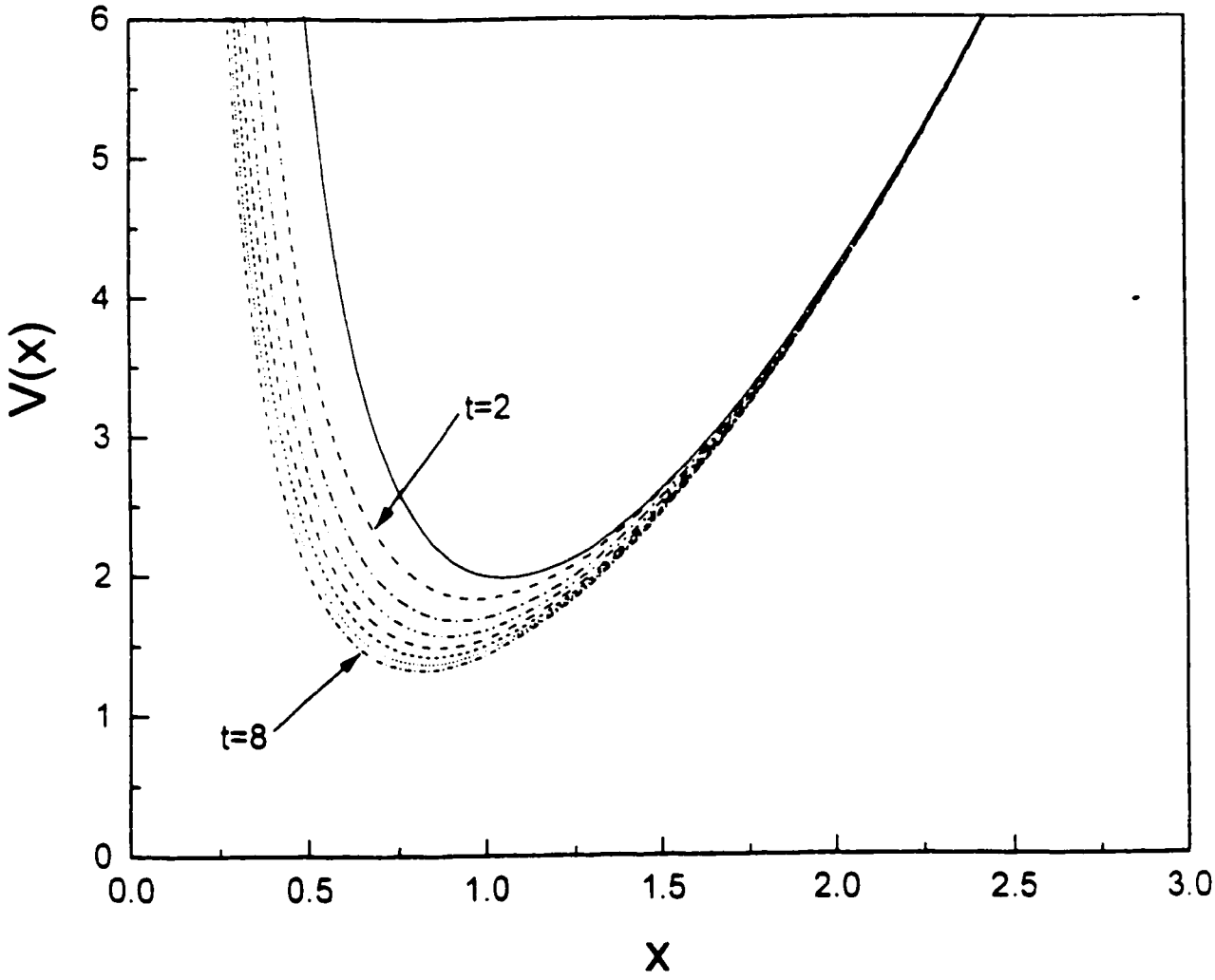
Table(III.3): Upper bounds E_n^U using (III.19) for $H = -\frac{d^2}{dx^2} + \lambda x^{1.9} + \frac{\mu}{x^{1.9}}$ with different values of n. The "exact" values E_n^N were obtained by direct numerical integration of the Schrödinger equation.

$\mu = \mu = 1$		
n	E_n^U	E_n^N
0	4.160 38	4.116 28
1	7.946 96	7.850 41
2	11.684 36	11.544 96
3	15.389 87	15.211 95
4	19.071 75	18.857 79
5	22.734 85	22.486 48
6	26.382 39	26.100 75
7	30.016 64	29.702 60
8	33.639 30	33.293 52
9	37.251 69	36.874 71
10	40.854 86	40.447 12

Table(III.4): lower bounds E_n^L using (III.17) for $H = -\frac{d^2}{dx^2} + \lambda x^{2.1} + \frac{\mu}{x^{2.1}}$ with different values of n. The "exact" values E_n^N were obtained by direct numerical integration of the Schrödinger equation.

$\lambda = \mu = 1$		
n	E_n^L	E_n^N
0	4.309 42	4.356 98
1	8.519 89	8.626 97
2	12.782 43	12.940 00
3	17.079 60	17.283 55
4	21.402 86	21.650 81
5	25.747 12	26.037 51
6	30.108 94	30.440 71
7	34.485 90	34.858 23
8	38.876 13	39.288 42
9	43.278 21	43.729 98
10	47.690 99	48.181 84

Fig. III.1 Potential envelopes $V^{(t)}(x)$ for $V(x) = x^2 + \frac{1}{x^{2.5}}$ for $t = 2, 3, \ldots, 8$.



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CHAPTER IV

Smooth Transformations of Kratzer's Potential in N Dimensions

Using the exact solution of Kratzer's potential $-\frac{\lambda}{r}+\frac{\mu}{r^2}$ in N-dimensional real space, we study smooth transformations $V(r)=g(-\frac{1}{r})+f(\frac{1}{r^2})$ for $N\geq 2$ spatial dimensions. We obtain eigenvalue approximation formulas, which provide lower or upper energy bounds for all the discrete eigenvalues E_{nl} and all $N\geq 2$, corresponding to the cases that the transformation functions g and f are either both convex or both concave respectively. Detailed results are presented for $V(r)=-\frac{a}{r}+\frac{b}{r^3}$ and $V(r)=-\frac{v}{r}[1-\frac{ar}{1+r}]+\frac{b}{r^2}$ $(a\in(0,1], b>0)$.

IV.1. Introduction and main results

There is considerable interest in Kratzer's potential [1] as a model to describe internuclear vibrations [2-4]. This potential can be expressed in the form

$$U(r)=-\frac{\lambda}{r}+\frac{\mu}{r^2},\quad \lambda,\mu>0. \tag{IV.1}$$

The model contains two parameters and the corresponding eigenvalue equation can be solved in closed form [5,10]. Unlike the Morse potential, which has exact solutions restricted to the zero rotation state, Kratzer's potential has exact solutions even when the rotational effects are taken into account. The Kratzer potential also differs from the Morse potential having an infinite number of bound states, while the Morse has a finite number of bound states. Applications of Kratzer's potential to various molecular problems have been given by von Hooydonk [11]. Another interesting application of the Kratzer potential is to use its eigenfunctions, in perturbative or variational calculations of energy levels, for more realistic potentials [12,13]. For example, Requena et al [12] developed a perturbative treatment of the perturbed Kratzer potential based upon commutation relations, and the successive energy corrections are obtained recursively.

The radial Schrödinger equation with Kratzer's potential (in units $\hbar=2m=1$) can written in the form

$$\left[-\frac{d^2}{dr^2}+\frac{l(l+1)+\mu}{r^2}-\frac{\lambda}{r}\right]\psi=E_{nl}\psi, \tag{IV.2}$$

where l is the angular momentum quantum number (rotational state). For $\mu = 0$, the hydrogenic equation is obtained. As μ increases, the relative impotance of the centrifugal term diminishes, and the rotating oscillator is obtained in the limit $\mu \to \infty$.

Since Eq.(IV.2) has the form of a hydrogenic equation, characterized by an effective angular momentum number s given by

$$l(l+1) + \mu = s(s+1), \tag{IV.3}$$

the problem presents no special difficulties other than those arising from the possibility that s is not integer. We introduce the usual substitutions for ψ to obtain a power-series expansion for ψ, with the property that the ratio between any pair of adjacent terms is known. The termination of the series yields the eigenvalues

$$E_{nl} = -\frac{\lambda^2}{4(n+s+1)^2}, \quad n = 0, 1, 2, \ldots \tag{IV.4}$$

where s is the positive solution of Eq. (IV.3) and therefore

$$E_{nl} = -\frac{\lambda^2}{\left(2n+1+\sqrt{(2l+1)^2+4\mu}\right)^2}, \quad n, l = 0, 1, 2, \ldots. \tag{IV.5}$$

The reason for choosing the positive solution of s, is that the admissible wavefunction ψ in (IV.2) must be square integrable, and must vanish at zero. The eigenfunctions are given in terms of confluent hypergeometric functions [5-10].

Another method to solve Eq.(IV.2) was proposed by Landau and Lifshitz [8]. They compared Eq.(IV.2) with the radial Schrödinger equation of the hydrogen atom with the angular momentum number s satisfying Eq.(III.3); consequently, they immediately obtained the eigenvalue formula (IV.5). Mavromatis [14] on the other hand extended the exact solutions of hydrogen atom to the N dimensional case, replaced the angular momentum number s by $s + \frac{N}{2} - \frac{3}{2}$, and derived the eigenvalue formula for a Coulomb potential in N-dimensions. An interesting observation can be stated: If Schrödinger's equation with arbitrary potential $U(r)$ is exactly solvable

in 3-dimensions, then it is also solvable if we add a term $\frac{\mu}{r^2}(\mu > 0)$ to the $U(r)$, and is consequently solvable in N dimensions (and obviously vice versa), namely:

$$U(r) + \frac{\mu}{r^2}(\lambda > 0) \Leftrightarrow \ 3 - \text{dim. case} \Leftrightarrow \ \text{N} - \text{dim. case.}$$

We should take into account the restriction of r to the interval $[0, \infty)$ in the one-dimensional case to avoid the degeneracy arising from effective decoupling of the two half lines $(-\infty, 0)$ and $(0, \infty)$.

Another interesting case arises when $\mu < 0$ in (IV.1). Although the potential in this case is a superposition of the two terms, such that in both the extreme cases $\mu = 0$ and $\lambda = 0$ the complete three-dimensional Schrödinger equation becomes exactly solvable [15-16], however the potential $V(r) = -\frac{\lambda}{r} - \frac{|\mu|}{r^2}$ does not support the existence of ground states $(n = 0, l = 0)$. This follows from the condition that $l(l+1)$ must be greater than μ to guarantee the existence of such eigenvalues.

Thus the exact solutions of Eq.(IV.2) can be generated by means of the well known solutions of a Coulomb potential, using the following two simple transformations: first replace the angular momentum s in the Coulomb energy expression by $-\frac{1}{2} + \sqrt{(l+\frac{1}{2})^2 + \mu}$, and then replace l with $l + \frac{N}{2} - \frac{3}{2}$. Thus the exact eigenvalues of the N-dimensional Schrödinger equation with the Kratzer's potential (IV.1) are

$$\mathcal{E}_{nl}^{(N)} = -\frac{\lambda^2}{4\left(n + \frac{1}{2} + \sqrt{(l + \frac{N}{2} - 1)^2 + \mu}\right)^2}, \ n, l = 0, 1, 2, \ldots . \qquad \text{(IV.6)}$$

In this equation we notice that the discrete spectrum $\mathcal{E}_{nl}^{(N)}$ is monotone increasing in N and bounded above by zero energy. Therefore, for large N, the energy levels get closer and closer to the minimum element 0 of the essential spectrum. Secondly, the existence of bound states for (IV.1) depends on the existence of the Coulomb potential term $-\frac{\lambda}{r}(\lambda > 0)$.

The aim of this chapter is to use the eigenvalue formula (IV.6) to investigate the discrete spectrum $E_{nl}^{(N)}$ of the Schrödinger equation

$$[-\Delta + V(r)]\psi = E_{nl}^{(N)}\psi, \qquad \text{(IV.7)}$$

where

$$V(r) = g(-\frac{1}{r}) + f(\frac{1}{r^2}) \tag{IV.8}$$

is a sum of two smooth transformations of $-\frac{1}{r}$ and $\frac{1}{r^2}$ respectively ($r = |\mathbf{r}|$, $\mathbf{r} \in \mathbf{R}^N$). We shall prove in the next section that $E_{nl}^{(N)}$ can be approximated by the expression

$$E_{nl}^{(N)} \approx \epsilon_{nl}^{(N)}(s,t) = g(-\frac{1}{s}) + \frac{g'(-\frac{1}{s})}{s} + f(\frac{1}{t^2}) - \frac{f'(\frac{1}{t^2})}{t^2} - \frac{[g'(-\frac{1}{s})]^2}{4\left(n + \frac{1}{2} + \sqrt{(l + \frac{N}{2} - 1)^2 + f'(\frac{1}{t^2})}\right)^2} \tag{IV.9}$$

valid for all $N \geq 2$, where the extreme value (min or max) provides a lower bound or an upper bound to the exact eigenvalues, depending on whether the transformation functions g and f are both convex, or both concave. This allows us, for example, to obtain simple expressions which bound the discrete spectrum of the potential

$$V(r) = -\frac{a}{r} + \frac{b}{r^\beta} \quad (\beta > 0) \tag{IV.10}$$

for all dimensions $N \geq 2$, a problem which is of considerable interest [17-24]. Indeed, formula (IV.9) implies in this case that the energy of $V(r)$ can be approximated by

$$\epsilon_{nl}^{(N)}(t) = (1 - \frac{\beta}{2})\frac{b}{t^\beta} - \frac{a^2}{4(n + \frac{1}{2} + \sqrt{(l + \frac{N}{2} - 1)^2 + \frac{\beta b}{2t^{\beta-2}}})^2} \quad (t > 0). \tag{IV.11}$$

Here $\epsilon_{nl}^{(N)}(t)$ is lower bound to $E_{nl}^{(N)}$, when $\beta > 2$, and an upper bound, when $\beta < 2$.

IV.2. Transformed Potentials

We consider the Schrödinger equation

$$[-\Delta + V(r)]\psi_{nl} = E_{nl}\psi_{nl}, \quad V(r) = g(-\frac{1}{r}) + f(\frac{1}{r^2}), \tag{IV.12}$$

in N-dimensions, where g and f are smooth transformations of $-\frac{1}{r}$ and $\frac{1}{r^2}$ respectively. For example, when g and f are the identity transformations, the problem

has the exact solution (IV.6) for all n, l, and arbitrary positive values of λ and μ in all dimensions.

The core of the approximation method lies in noticing that each term of the potential $V(r)$ can be approximate by its tangential approximation. That is to say, we approximate the transformations g and f in $V(r)$ by

$$\begin{aligned} g^{(s)}(-\frac{1}{r}) &= a(s) - \frac{b(s)}{r}, \\ f^{(t)}(\frac{1}{r^2}) &= c(t) + \frac{d(t)}{r^2} \end{aligned} \tag{IV.13}$$

respectively, where s is a contact point between $g(-\frac{1}{r})$ and its tangent approximation $g^{(s)}(\frac{1}{r^2})$, and t is a contact point between $f(\frac{1}{r^2})$ and its tangent approximation $f^{(t)}(\frac{1}{r^2})$. Elementary differentiation of (IV.13) with respect to s and t repectively implies

$$\begin{cases} a(s) = g(-\frac{1}{s}) + \frac{1}{s}g'(-\frac{1}{s}), \\ b(s) = g'(-\frac{1}{s}) \end{cases} \tag{IV.14}$$

and

$$\begin{cases} c(t) = f(\frac{1}{t^2}) - \frac{1}{t^2}f'(\frac{1}{t^2}), \\ d(t) = f'(\frac{1}{t^2}). \end{cases} \tag{IV.15}$$

Therefore, $V(r)$ in (IV.12) can be approximated by

$$V^{(s,t)}(r) = g(-\frac{1}{s}) + \frac{g'(-\frac{1}{s})}{s} + f(\frac{1}{t^2}) - \frac{f'(\frac{1}{t^2})}{t^2} - \frac{g'(-\frac{1}{s})}{r} + \frac{f'(\frac{1}{t^2})}{r^2}. \tag{IV.16}$$

This two-parameter family of 'tangent' potentials generates the so-called 'envelope representation' for $V(r)$ expressed by

$$V(r) = \underset{s,t>0}{\text{Envelope}} \left\{ V^{(s,t)}(r) \right\}.$$

To this representation of $V(r)$, we may apply the energy expression (IV.6) for the eigenvalues of Schrödinger equation

$$[-\Delta + V^{(s,t)}(r)]\psi = \epsilon_{nl}(s,t)\psi, \tag{IV.17}$$

which entails that $\epsilon_{nl}(s,t)$ is given by

$$\epsilon_{nl}(s,t) = g(-\frac{1}{s}) + \frac{g'(-\frac{1}{s})}{s} + f(\frac{1}{t^2}) - \frac{f'(\frac{1}{t^2})}{t^2} - \frac{[g'(-\frac{1}{s})]^2}{4\left(n+\frac{1}{2}+\sqrt{(l+\frac{N}{2}-1)^2+f'(\frac{1}{t^2})}\right)^2}. \qquad \text{(IV.18)}$$

Now, since functions with definite convexity lie on one side of their tangents, an application of the comparison theorem in quantum mechanics allows us to conclude the following. For the eigenvalues E_{nl} of the Schrödinger equation (IV.12), we have

(a) $E_{nl} \leq \epsilon_{nl}(s,t)$ if g and f are both convex,

(b) $E_{nl} \geq \epsilon_{nl}(s,t)$ if g and f are both concave.

The proof of this claim is similar to Theorem (III.1). It is appropriate to mention here, that the conclusions follow for the special cases where either f or g is the identity transformation. These bounds may, of course, be sharpened by optimization with respect to s and t, and moreover they are valid for the entire discrete spectrum $n, l \geq 0$, and for all dimensions $N \geq 2$.

IV.3. Numerical results

One of the interesting points concerning the bounds we have obtained in the previous section is the large variety of approximations made possible by different choices of the transformations g and f.

IV.3.1 The potential $V(r) = -\frac{a}{r} + \frac{b}{r^\beta}$

We consider the case where $g(-\frac{1}{r}) = -\frac{a}{r}$ and $f(\frac{1}{r^2}) = \frac{b}{r^\beta}$, which yields the generalized Kratzer potential

$$V(r) = -\frac{a}{r} + \frac{b}{r^\beta}.$$

The envelope representations of this potential using (IV.16) now reads

$$V^{(t)}(r) = (1-\frac{\beta}{2})\frac{b}{t^\beta} - \frac{a}{r} + \frac{\frac{\beta b}{2t^{\beta-2}}}{r^2}, \qquad \text{(IV.19)}$$

whereas the energy formula (IV.18) reads in this case

$$\epsilon_{nl}^{(N)}(t) = (1 - \frac{\beta}{2})\frac{b}{t^\beta} - \frac{a^2}{4\left(n + \frac{1}{2} + \sqrt{(l + \frac{N}{2} - 1)^2 + \frac{\beta b}{2t^{\beta-2}}}\right)^2}. \qquad \text{(IV.20)}$$

This function is convex in t for $\beta > 2$, its maximum provides a lower energy bound for the Schrödinger Hamiltonian with the generalized Kratzer potential, and concave for $\beta < 2$, its minimum yields an upper energy bound. In Table 1 we exhibit some results of the upper and lower bounds derived from (IV.20) for the potential

$$V(r) = -\frac{5}{r} + \frac{1}{r^{2.1}} \qquad \text{(IV.21)}$$

in 3-dimensional space with $n = 0, l = 1$ and different values of β, along with some accurate values obtained by direct numerical integration of the Schrödinger equation. The graph of $\epsilon_{01}(t)$ is displayed in Fig.(IV.1) along with the exact eigenvalue E obtained by direct numerical integration, and also the corresponding unnormalized wavefunction in 3-dimensions, for Schrödinger's equation with $V(r)$ given by (IV.21). In Fig.(IV.2), we plot the lower bound obtained by (IV.20) as a function of the parameter b, along with some exact eigenvalues obtained by direct numerical integration. The main advantage of an analytic approximation such as (IV.20) is, that questions to do with the dependence of the eigenvalues on the potential parameters are easy to answer. In Table 2 and Table 3 we exhibit the results of the lower bounds, obtained by use of formula (IV.20), for $\beta = 2.1$ with $a = 1$ and $b = 1$ as well as $a = 5$ and $b = 1$ respectively, for the dimensions N ranging from 2 to 10, along with some accurate values obtained by direct numerical integration of Schrödinger's equation.

IV.3.2 The potential $V(r) = -\frac{v}{r}[1 - \frac{ar}{1+r}] + \frac{b}{r^2}$

For this potential, we consider $g(-\frac{1}{r}) = -\frac{v}{r}[1 - \frac{ar}{1+r}]$ where v and a are positive parameters with $a \leq 1$ and $f(\frac{1}{r^2}) = \frac{b}{r^2}$. In this case g is the well known screened Coulomb potential [25-27], which is almost Coulombic everywhere, because it is like $-\frac{v}{r}$ for small r and like $-\frac{v(1-a)}{r}$ for large r. Therefore, it is very effective in representing the screened Coulomb potential as a smooth (concave) transformation of

$-\frac{1}{r}$. For this choice of g and f we have from (IV.16) that the envelope representation is

$$V^{(s)}(r) = \frac{av}{(1+s)^2} - \frac{v[1-\frac{as^2}{(1+s)^2}]}{r} + \frac{b}{r^2}. \qquad \text{(IV.22)}$$

The energy formula (IV.18) is

$$\epsilon_{nl}(s) = \frac{av}{(1+s)^2} - \frac{v^2[1-\frac{as^2}{(1+s)^2}]^2}{4\left(n+\frac{1}{2}+\sqrt{(l+\frac{N}{2}-1)^2+b}\right)^2}. \qquad \text{(IV.23)}$$

which is concave in s. Moreover, $\epsilon_{nl}(s)$ leads to a simple upper-bound energy formula valid for all n, l and arbitrary dimension $N \geq 2$. These upper bounds indicate approximately how the eigenvalues E_{nl} depend on all the potential parameters. We display some results obtained by formula (IV.22) in Table (3) for $v = 5$, $a = 0.5$ and $b = 1$ for dimension N ranging from 2 to 10. It is approparite to mention here that in the limit as $b \to 0$ we recover the Coulomb envelopes used in [28] for the special case $N = 3$.

For the bottom of each angular-momentum subspace, the bounds we have obtained can be improved by the use of a refined version of the comparison theorem [29]. However, the main point of the approach described in this chapter is to provide a way to generate simple general approximate formulas to be used for exploratory purposes and for 'seeding' direct numerical methods.

Table(1): Some lower bounds E_{01}^L and upper bounds E_{01}^U using (IV.20) for $H = -\Delta - \frac{5}{r} + \frac{1}{r^\beta}$ in 3-dimensions with $l = 1$. The "exact" values E_{01} were obtained by direct numerical integration of Schrödinger's equation.

β	E_{01}^L	E_{01}	E_{01}^U
1.5	– – – –	−1.111 34	−1.073 66
1.6	– – – –	−1.127 68	−1.097 39
1.7	– – – –	−1.142 44	−1.119 66
1.8	– – – –	−1.155 77	−1.140 56
1.9	– – – –	−1.167 79	−1.160 19
2	−1.178 63	−1.178 63	−1.178 63
2.1	−1.195 96	−1.188 38	– – – –
2.2	−1.212 28	−1.197 18	– – – –
2.3	−1.227 65	−1.205 08	– – – –
2.4	−1.242 14	−1.212 19	– – – –
2.5	−1.255 81	−1.218 58	– – – –

Table(2): lower bounds E_{00}^{L} using (IV.20) for $H = -\Delta - \frac{1}{r} + \frac{1}{r^{2.1}}$ for dimension $N = 2$ to 10. The "exact" values E_{00} were obtained by direct numerical integration of Schrödinger's equation.

N	E_{00}^{L}	E_{00}
2	−0.120 49	−0.116 90
3	−0.102 997	−0.100 70
4	−0.072 63	−0.071 78
5	−0.049 50	−0.049 19
6	−0.034 68	−0.033 40
7	−0.025 27	−0.024 01
8	−0.019 09	−0.015 81
9	−0.014 87	−0.012 60
10	−0.011 89	−0.007 55

Table(3): lower bounds E_{00}^{L} using (IV.20) for $H = -\Delta - \frac{5}{r} + \frac{1}{r^{2.1}}$ for dimension $N = 2$ to 10. The "exact" values E_{00} were obtained by direct numerical integration of Schrödinger's equation.

N	E_{00}^{L}	E_{00}
2	−2.728 16	−2.650 75
3	−2.371 92	−2.319 71
4	−1.720 24	−1.699 15
5	−1.195 96	−1.188 39
6	−0.847 88	−0.844 98
7	−0.622 07	−0.620 84
8	−0.472 00	−0.471 43
9	−0.368 78	−0.368 49
10	−0.295 33	−0.295 17

Table(4): Upper bounds E_{00}^U using (IV.23) for $H = -\Delta - \frac{5}{r}\left[1 - \frac{0.5r}{1+r}\right] + \frac{1}{r^2}$ for dimension $N = 2$ to 10. The "exact" values E_{00} were obtained by direct numerical integration of Schrödinger's equation.

N	E_{00}	E_{00}^U
2	−1.598 63	−1.502 02
3	−1.296 02	−1.213 58
4	−0.808 11	−0.754 90
5	−0.481 10	−0.452 67
6	−0.300 88	−0.286 88
7	−0.201 54	−0.194 66
8	−0.143 49	−0.139 97
9	−0.107 23	−0.105 33
10	−0.083 20	−0.082 12

FIG.(IV.1) Graph of $\epsilon(t) = \epsilon_{01}(t)$ along with the exact eigenvalue E and corresponding unnormalized wavefunction in 3-dimensions.

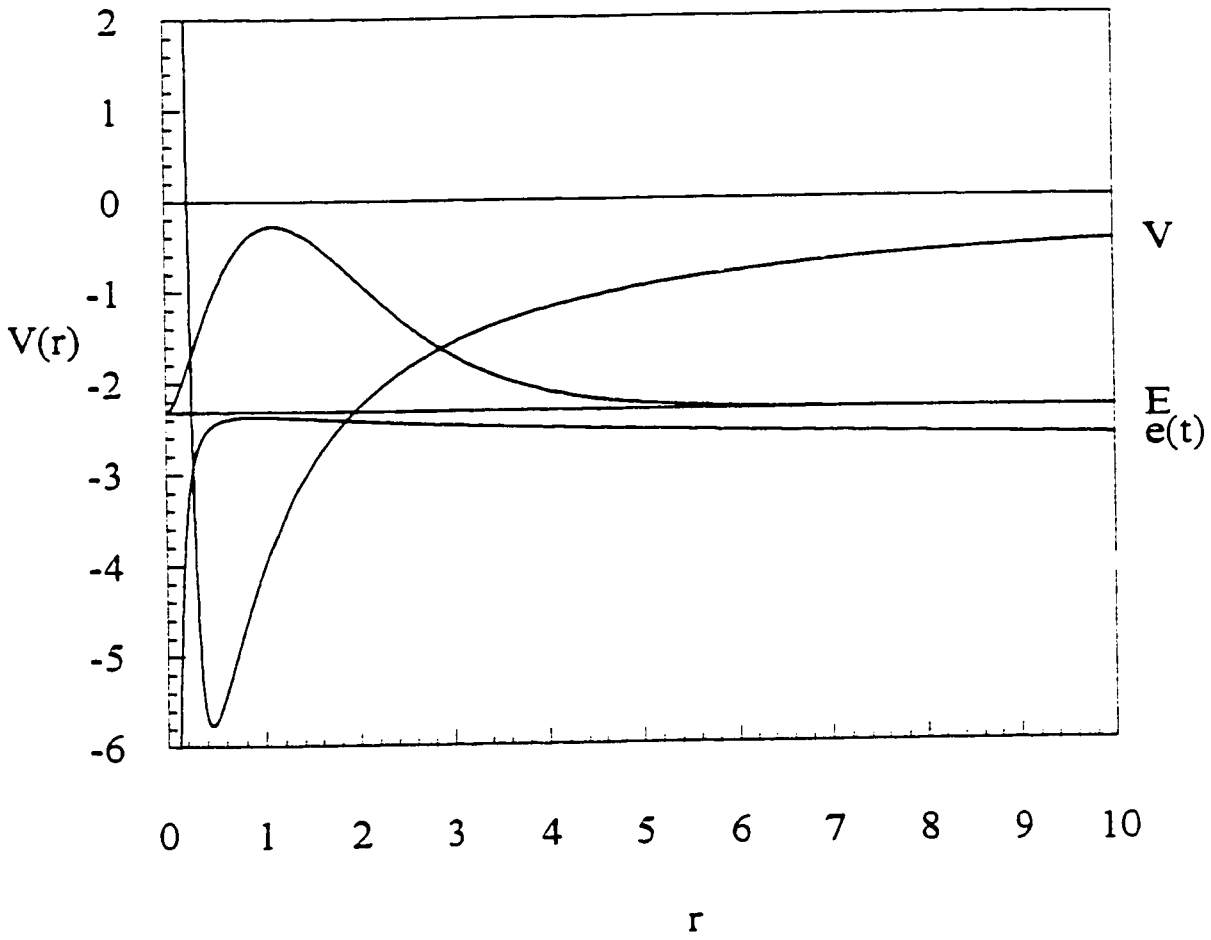
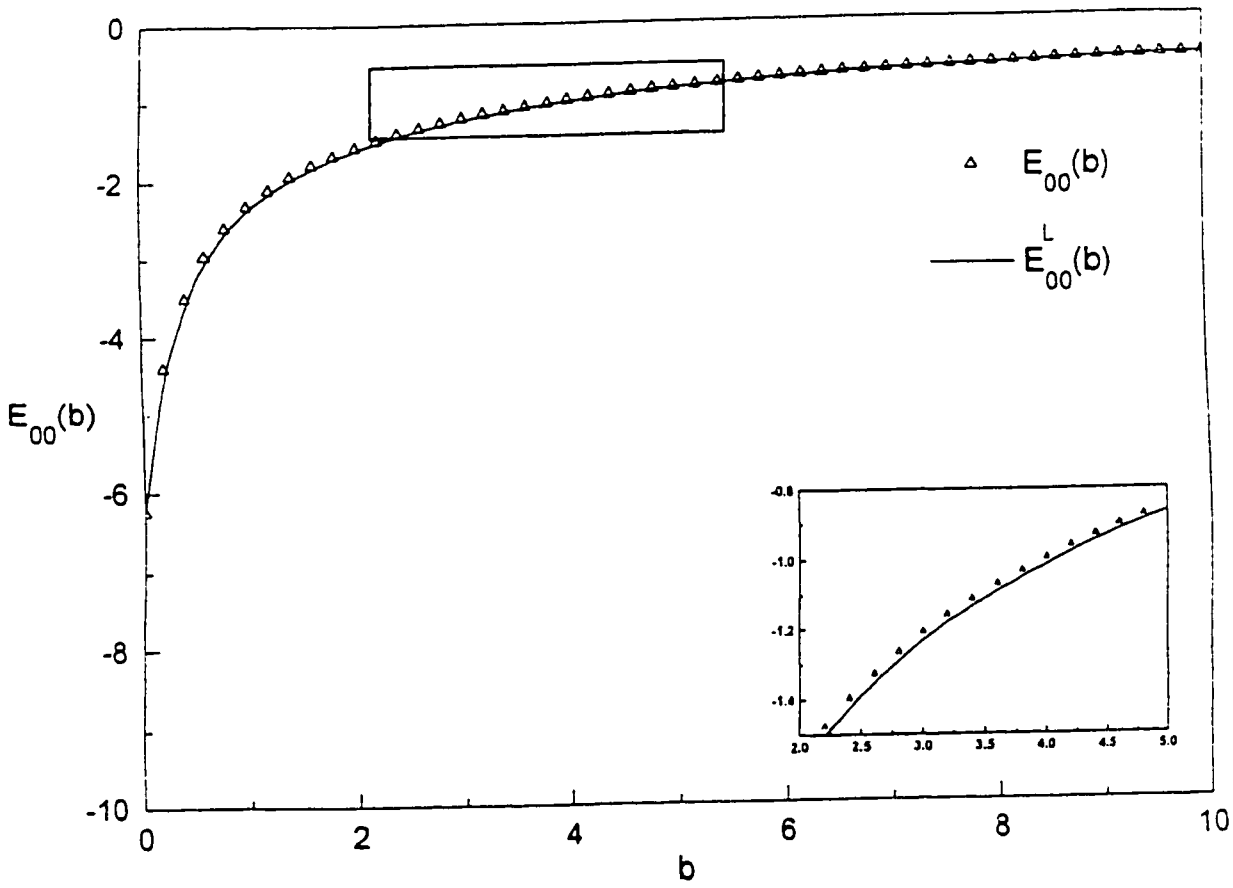


FIG.(IV.2) The graph of the lower bound E_{00}^{L} obtained by (IV.20) as a function of the parameter b, along with some exact eigenvalues E_{00} obtained by direct numerical integration.



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CHAPTER V

Eigenvalue bounds for transformations of quasi-exactly soluble potentials

The potentials in non-relativistic quantum mechanics can be classified, according to the solvability of the corresponding Schrödinger equation, into four categories.
1. Exactly soluble potentials. The best-known examples of this category are Coulomb and harmonic oscillator potentials. Several others are also known [1-15].
2. Conditionally exactly soluble potentials are those potentials for which the entire spectra can be obtained in an algebraic manner, provided one of the potential parameters is assigned a fixed negative value [16-18].
3. Quasi-exactly soluble potentials are those potentials that are soluble for one or two energy levels, if a certain constraint between the parameters of the potentials is satisfied [19-38].
4. Non-soluble potentials.

The method of envelope representations deals mainly with two classes of this category. The class of exactly soluble potentials represents the base potentials for the envelope method, which approximates the spectra of the non-soluble potentials. In 1981, Hall and Satpathy [39] introduced the envelope method to the class of quasi-exactly soluble potentials. In this chapter we continue their approach and introduce a new method, called h-theory, which utilizes the known spectrum of certain Schrödinger operators for construction of a simple algorithm to bound the eigenvalues of more complicated potentials.

V.1. Introduction and main results

Wigner [40] introduced an interesting method to generate exact expressions for the eigenvalues by applying the kinetic energy operator, to an appropriate wave function, and then constructed the Schrödinger equation which would correspond to the result. For example, if we choose the wave function for the bottom of the Y_l^m angular momentum subspace to be

$$\psi(r) = r^l e^{-\frac{1}{2}(r+\beta r^2)} Y_l^m(\theta, \phi), \tag{V.1}$$

then Schrödinger's equation

$$H\psi = (-\Delta + V)\psi = E\psi$$

is satisfied if

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

This gives us the exact solution to the problem of the hydrogen atom (in its s-states) perturbed by the potential $\beta r + (\beta r)^2$. Such exact eigenvalues are certainly useful, but they stop short of treating, for example, the more general problem

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

in which the coefficients $\{A, B, D\}$ are *arbitrary*.

In this chapter we use exact eigenvalues, such as (V.2), to estimate the spectrum corresponding to a potential $V(r)$, of the form,

$$V(r) = -\frac{1}{r} + g(\beta r + (\beta r)^2). \tag{V.4}$$

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

$$E \approx \epsilon_{0l}(t) = f(t) - h(\frac{t^2 f'(t)}{2l+3}) + tf'(t) - \frac{1}{4},$$

where

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

This formula provides a lower bound, or an upper bound, to the exact ground-state energy E according as the transformation function g is convex ($\approx = \geq$) or concave ($\approx = \leq$). This allows us, for example, to estimate the spectrum corresponding to $V(r) = -D/r + Br + Ar^2$ for arbitrary $\{A, B, D\}$. At the expense of more complicated conditions on the coefficients, the collection (V.2) of exact eigenvalues may be extended to certain excited states including $\ell \neq 0$. In the next section we summarize the more detailed exact results for the perturbed Coulomb case (V.3).

Since similar results may be obtained for other families of potentials, such as $V(r) = ar^2 + br^4 + cr^6$, we formulate the h-theory approximation, in Section (V.3), in a general framework suitable for application to all exact solutions of this general type. In Section (V.4) we present numerical results for a number of specific examples, some of which are compared with known results by other methods.

V.2. Perturbed Coulomb Potentials

In his interesting work of solving Dirac's equations in the presence of a magnetic field, Hautot [19-20] introduced some methods for solving certain second-order differential equations. One of these methods deals with the radial Schrödinger equation with the potential energy operator:

$$V(r) = -\frac{D}{r} + Br + Ar^2 \quad (A \neq 0). \tag{V.5}$$

The author obtained [20] exact solutions only for certain relations between the constants A, B and D. He achieved this by applying the kinetic energy operator to an appropriate wave function and used the standard procedure of comparing the coefficients of the induced recurrence relations.

More precisely, introducing

$$\psi(r) = \exp(-\frac{1}{2}(\sqrt{A}r^2 + \frac{B}{\sqrt{A}}r)) \sum_{k=0}^{n} a_k r^{k+l} \quad (n = 0, 1, 2, \ldots) \tag{V.6}$$

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

$$\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{l(l+1)}{r^2} + [E + \frac{D}{r} - Br - Ar^2]\right)\psi(r) = 0 \tag{V.7}$$

we obtain, after some algebraic manipulations, the following three-term recursion relation between the coefficients

$$\begin{aligned}[(k+2)(k+2l+3)]a_{k+2} + [D - \frac{B}{\sqrt{A}}(k+2+l)]a_{k+1} \\ + [E - \sqrt{A}(2k+2l+3) + \frac{B^2}{4A}]a_k = 0.\end{aligned} \tag{V.8}$$

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

$$E = E_{nl} = \sqrt{A}(2n + 2l + 3) - \frac{B^2}{4A}. \tag{V.9}$$

Equations (V.9) and (V.10) give the following $(n+1) \times (n+1)$ determinant which provides the relations between A, B and D (for a given value of n) to ensure the existence of the solutions of (5) (note that $a_{-m} = 0, m = 1, 2, \ldots$), namely

$$\begin{vmatrix} a_0 & b_0 & & & & & \\ c_1 & a_1 & b_1 & & & & \\ & c_2 & a_2 & b_2 & & & \\ & & \cdot & \cdot & \cdot & & \\ & & & \cdot & \cdot & \cdot & \\ & & & & c_{n-1} & a_{n-1} & b_{n-1} \\ & & & & & c_n & a_n \end{vmatrix} = 0, \tag{V.10}$$

where

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

For example: if $n = 0$ (s-states), then

$$E = \sqrt{A}(2l + 3) - \frac{B^2}{4A} \quad (D = \frac{B}{\sqrt{A}}(l+1)): \tag{V.11}$$

if $n = 1$, then

$$E = \sqrt{A}(2l + 5) - \frac{B^2}{4A} \tag{V.12}$$

with

$$(D - \frac{B}{\sqrt{A}}(l+1))(D - \frac{B}{\sqrt{A}}(l+2)) - 2\sqrt{A}(2l+2) = 0:$$

and if $n = 2$, then

$$E = \sqrt{A}(2l + 7) - \frac{B^2}{4A} \tag{V.13}$$

with

$$(D - \frac{B}{\sqrt{A}}(l+3))[(D - \frac{B}{\sqrt{A}}(l+1))(D - \frac{B}{\sqrt{A}}(l+2)) - 2\sqrt{A}(2l+2)]$$
$$- 4\sqrt{A}(D - \frac{B}{\sqrt{A}}(l+1))(2l+3) = 0.$$

Since this early work, the technique of generating exact solutions for a Schrödinger operator has been widely applied either to obtain some interesting potential functions with known eigenvalues, or to investigate the quality of perturbation theory. This technique was used, for example, by Killingbeck [39] to prove that the Rayleigh-Schrödinger perturbation series terminated after the first-order approximation for the Hamiltonian

$$H = -\frac{1}{2}\triangle - \frac{1}{r} + 2\lambda r + 2\lambda^2 r^2 \quad (\beta > 0). \tag{V.14}$$

Extending Killingbeck's work, Saxena *et al* [26-27] investigated the case $\lambda < 0$, and explained why the Rayleigh-Schrödinger series was invalid for $\lambda < 0$ and successfully constructed instead a perturbation series in powers of $|\lambda|^{-\frac{1}{2}}$ valid for $\lambda < 0$. Although Plesset [41] proved that the second-order differential equation has no exact solution in terms of elementary functions, if the potential has the form $V(r) = \sum_{k=-m}^{n} \alpha_k r^k$ with *arbitrary* constants α_k, the problem of solving Schrödinger's equation approximately with the potential (V.3), where the parameters are no longer constrained, has fascinated many physicists. Bessis *et al* [28], used the moment method to bound the ground-state energy for arbitrary D, B and positive A. Roychoudhury *et al* [29] examined the shifted $1/N$ expansion to obtain accurate eigenvalues for arbitrary l. In the next section, we construct a simple and straightforward approximation to bound the eigenvalues of (V.3) for arbitrary D, B and A, using the exact solution (V.2).

V.3. Transformed Potentials

To give a general framework to the approximation method we consider a Schrödinger Hamiltonian of the form

$$H = -\triangle + h_0(r) + f(r), \tag{V.15}$$

where $h_0(r)$ is a fixed potential term and $f(r)$ is a smooth transformation $g(h(\beta r))$ of a second scaled potential term $h(\beta r)$ with $\beta > 0$. Such a transformation always exists because of the monotonicity of h. For example, when $h_0(r) = -\frac{1}{r}$ and $h(\beta r) = \beta r + (\beta r)^2$ and g is the identity transformation, the problem is exactly

solvable for $n = 0$. Indeed, in this case, we have from (V.9) and (V.10) that E_{0l} is given by (V.2).

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

$$H = -\Delta - \frac{l+1}{r} + g(h(\beta r)), \tag{V.16}$$

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

$$\alpha(t) + h(\beta(t)r) = f^{(t)}(r), \tag{V.17}$$

where t is the point of contact between $h(\beta r)$ and $f(r) = g(h(\beta r))$. The parameters $\alpha(t)$ and $\beta(t)$ are determined as follows. Suppose that ϕ is an invertible function defined by

$$\phi(t\beta(t)) = tf'(t), \tag{V.18}$$

where $'$ denotes differentiation with respect to t. Then, using (V.17), we have

$$\begin{cases} \beta(t) = \frac{1}{t}\phi^{-1}(tf'(t)) \\ \alpha(t) = f(t) - h(\phi^{-1}(tf'(t))). \end{cases} \tag{V.19}$$

Differentiation of (V.19) with respect to t gives

$$\frac{\alpha'(t)}{\beta'(t)} = -th'(t\beta(t)). \tag{V.20}$$

The energy formula (V.2) with (V.17) leads to

$$\epsilon_{0l}(t) = \alpha(t) + \beta(t)(2l+3) - \frac{1}{4}. \tag{V.21}$$

By differentiating (V.21) with respect to t and using the extreme condition $\epsilon'_{nl}(t) = 0$, we get

$$\frac{\alpha'(t)}{\beta'(t)} = -(2l+3). \tag{V.22}$$

Now, since

$$\phi(t\beta(t)) = tf'(t) = t\beta(t)h'(t\beta(t)), \tag{V.23}$$

we have from (V.20), (V.22) and (V.23) that

$$\beta(t) = \frac{tf'(t)}{2l+3}, \tag{V.24}$$

$$\begin{aligned} \alpha(t) &= f(t) - h(t\beta(t)) \\ &= f(t) - h(\frac{tf'(t)}{2l+3}); \end{aligned} \tag{V.25}$$

whence it follows that

$$th'(\frac{t^2 f'(t)}{2l+3}) = (2l+3). \tag{V.26}$$

Finally we obtain using (V.19), (V.24) and (V.21) that

$$\epsilon_{0l}(t) = f(t) - h(\frac{t^2 f'(t)}{2l+3}) + tf'(t) - \frac{1}{4}. \tag{V.27}$$

Equations (V.26) and (V.27) establish the energy bounds of the Hamiltonian (V.15). Indeed, solving (V.26) with respect to t, for any smooth function $f(r) = g(h(\beta r))$, yields the optimal solution $\hat{t}$; therefore, $\epsilon_{0l}(\hat{t})$ gives [16] lower bounds when the transformation g is convex, and upper bounds when g is concave.

Equations (V.26) and (V.27) represent a complete recipe for obtaining a bound to the lowest eigenvalue ($n = 0$) of any Coulomb problem perturbed by a smooth transformation $g(h)$ of $h(\beta r) = \beta r + (\beta r)^2$. Although we shall not develop the more general case in detail here, the method for $n > 0$ works as follows. If we consider the Schrödinger equation (V.7) with $A = B^2$, we then have from (V.9) that

$$E_{nl} = B(2n + 2l + 3) - \frac{1}{4}.$$

The parameter D is related to B through a recurrence relation, which can be obtained by expanding the determinant (V.10) about the last row or column and using $A = B^2$, namely

$$\begin{aligned} D_k = [D - (k+l+1)]D_{k-1} - 2Bk(k+2l+1)D_{k-2} \\ (k = 0, 1, 2, \ldots \quad D_{-2} = 0,\ D_{-1} = 1). \end{aligned} \tag{V.28}$$

For example, $D_0 = D - (l+1)$ which implies the condition $D = l+1$. As discussed above, we obtain the corresponding formulas (V.26) and (V.27), but instead of the term $(2l+3)$, we have in general $(2n+2l+3)$; that is to say

$$th'(\frac{t^2 f'(t)}{2n+2l+3}) = (2n+2l+3) \tag{V.29}$$

and

$$\epsilon_{nl}(t) = f(t) - h(\frac{t^2 f'(t)}{2n+2l+3}) + tf'(t) - \frac{1}{4}. \tag{V.30}$$

Of physical interest is the case [42] when $n = 1$ and B approaches 0. In this case, we have from (V.28) that $D \approx l+2$, and this allows us to keep the potential $h_0(r) = -D/r$ as a fixed term. Hence, we have

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

$$\epsilon_{1l}(t) = f(t) - h(\frac{t^2 f'(t)}{2l+5}) + tf'(t) - \frac{1}{4}.$$

which gives a bound to the first excited state of

$$H = -\triangle - \frac{l+2}{r} + g(h(\beta r)),$$

where g is any smooth tranformation of h.

V.4. Numerical Results

It is interesting that a variety of approximations is possible by different choices of the transformation g. For example, we can let $f(r) = g(h(\beta r)) = \mu r + \lambda r^2$ or $f(r) = g(h(r)) = \mu e^{\lambda(r+r^2)}$, for arbitrary μ and λ etc., where in each case equations (V.26) and (V.27) give us a bound. A second point is the possibility of using the approximation with different base functions h. For example, if we consider $h_0(r) = r^2$ and $h(r) = -1/r + r$ and use an appropriate smooth transformation, then the method we have discussed readily gives a bound for the eigenvalues of the Harmonic Oscillator Hamiltonian perturbed by $f(r) = g(h(r))$. This particular example can be discussed in terms of the theory presented in Ref.[39], but the present method is much simpler and more general. It is simpler in that its derivation and the formulas it produces are simple. It is more general in that, given an arbitrary smooth transformation g, formulas (V.26) and (V.27) provide an eigenvalue bound directly.

V.4.1 The potential $V(r) = -\frac{1}{r} + \mu r + \lambda r^2$

Our first example is

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

where μ and λ are arbitrary real parameters. We consider $h_0(r) = -\frac{1}{r}$ and $f(r) = \mu r + \lambda r^2$. It is clear that the transformation g exists for such an f. Equation (V.26) yields

$$4\lambda t^4 + 2\mu t^3 + (2l+3)t - (2l+3)^2 = 0, \tag{V.31}$$

while the energy formula (V.27) leads to

$$\epsilon_{0l}(t) = 3\lambda t^2 + 2\mu t - \frac{\mu t^2 + 2\lambda t^3}{2l+3}\left(1 + \frac{\mu t^2 + 2\lambda t^3}{2l+3}\right) - \frac{1}{4}. \tag{V.32}$$

For arbitrary λ, μ and l, equations (V.31) and (V.32) give the required approximation. We may use any root finding method [43] to solve (V.31) for $\hat{t}$, and substitute this in (V.31), to abtain the approximate eigenvalue. The natural question which arises is whether $\epsilon_{0l}(\hat{t})$ is an upper or lower bound? The answer depends on the convexity of $f(r) = g(h(r))$. Indeed, if $\mu < \sqrt{\lambda}$, then $f(r) > f^{(t)}(r)$ and therefore, $\epsilon_{0l}(\hat{t})$ is a lower bound for the Schrödinger Hamiltonian with potential $-1/r + \mu r + \lambda r^2$; and if $\sqrt{\lambda} < \mu$, then $f(r) < f^{(t)}(r)$ and $\epsilon_{0l}(\hat{t})$ is an upper bound. In figure (1) we graph these two independent regions and note that along the curve $\lambda = \mu^2$ we have the exact solution. By means of a scale transformation (to remove the $\frac{1}{2}$ in front of the Laplacian in $H = -\frac{1}{2}\Delta - \frac{1}{r} + \mu r + \lambda^2 r^2$), we can compare our bounds E^L through the relation

$$E^B(\mu, \lambda) \approx 2E^L(\frac{\mu}{4}, \frac{\lambda}{8}),$$

with the results E^B of Bessis et al [28] as shown in Table (V.1). These results show that our simple formulas can be used to obtain a satisfactory bound for a class of potentials generated by g, without the lengthy derivations required in each case by the moment method [28], or the shifted $1/N$ expansion [29]. In Table (V.2) we present our results, using (V.26) and (V.27), for a range of values of μ and λ and for the sake of comparison, the corresponding accurate results obtained by direct numerical integration of (V.15).

V.4.2. The potential $V(r) = -\frac{1}{r} + \mu \ln(r + r^2)$

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

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

and the formulas (V.26) and (V.27) provide an upper bound if $\mu > 0$, or a lower bound if $\mu < 0$. We have in this case

$$4\mu t^3 + (2\mu + 2l + 3)t^2 - (2l + 2)(2l + 3)t - (2l + 3)^2 = 0,$$

and

$$\begin{aligned} \epsilon_{0l}(t) = \mu \ln(t + t^2) + \mu \left(\frac{1 + 2t}{1 + t} \right) \\ - \frac{\mu}{2l + 3} \left(\frac{t + 2t^2}{1 + t} \right) \left(1 + \frac{\mu}{2l + 3} \frac{t + 2t^2}{1 + t} \right) - \frac{1}{4}. \end{aligned} \tag{V.33}$$

A comparison of some results obtained by this formula and the corresponding results obtained by direct numerical integration are in Table (V.3).

V.4.3. The potential $V(r) = -\frac{1}{r} + \mu e^{\lambda(r+r^2)}$

Our final example is $f(r) = \mu e^{\lambda(r+r^2)}$, where λ and μ are arbitrary real. The formulas (V.25) and (V.26) provide an upper bound if $\lambda, \mu > 0$, and lower bound if $\lambda < 0$, μ arbitrary real. The formulas (V.25) and (V.26) imply

$$2\lambda\mu t^3(1 + 2t)e^{\lambda(t+t^2)} + (2l + 3)t - (2l + 3)^2 = 0 \tag{V.34}$$

and

$$\begin{aligned} \epsilon_{0l} = \mu e^{\lambda(t+t^2)} - \frac{\lambda\mu(t^2 + 2t^3)e^{\lambda(t+t^2)}}{2l + 3} \\ - \frac{\lambda\mu t^4(1 + 2t)^2 e^{2\lambda(t+t^2)}}{(2l + 3)^2} + \lambda\mu(t + 2t^2)e^{\lambda(t+t^2)} - \frac{1}{4}. \end{aligned} \tag{V.35}$$

The essence of the approach described, in this chapter, is to provide a means to generate simple approximate formulas for exploratory purposes. Once the appropriate ranges of the potential parameters are established, then the present direct numerical methods can be used to estimate the eigenvalues more accurately.

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

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

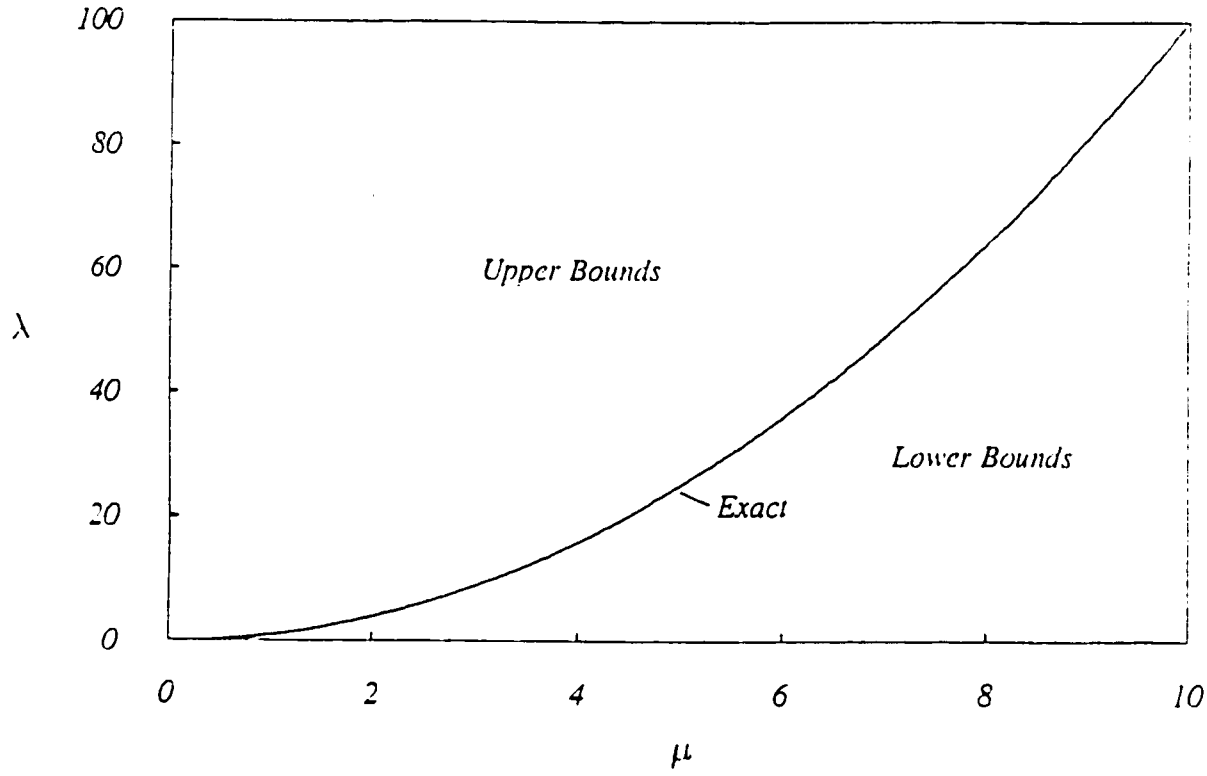
Table (V.2): Eigenvalues of $H = -\triangle - \frac{1}{r} + \mu r + \lambda r^2$ for different values of μ and λ. Comparison between the lower bound E^L given by formulas (V.25) and (V.26) and accurate values E^N found by direct numerical integration.

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

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

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

Figure(1). Two parametric regions: if $\mu < \sqrt{\lambda}$, the formulas (V.25-26) yield a lower bound for the ground-state energy of the Hamiltonian $H = -\Delta - \frac{1}{r} + \mu r + \lambda r^2$, while $\mu > \sqrt{\lambda}$ yields an upper bound.



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CHAPTER VI

Eigenvalue Comparisons for Quantum Systems in a box

We provide several comparison theorems for the first even and odd solutions of Schrödinger's equation

$$-v'' + Q(t)v = \lambda v, \ -l \leq t \leq l$$

with boundary conditions $v(-l) = v(l) = 0$. These theorems allow the comparison function Q_i $(i = 1,2)$ to intersect at a finite number of points within $[-l,l]$, while maintaining the eigenvalue comparisons. Immediate extensions are discused for a more general class of Sturm-Liouville problems, as well as for problems in unbounded regions.

VI.1. Introduction

We consider the pair of Schrödinger equations

$$-u'' + Q_1(t)u = \lambda_1 u, \tag{VI.1}$$

$$-v'' + Q_2(t)v = \lambda_2 v, \tag{VI.2}$$

where the exact solutions $u(t)$ and $v(t)$ satisfy the boundary conditions $u(\pm l) = v(\pm l) = 0$ and $Q_i(t)$ $(i = 1,2)$ are symmetric and monotone increasing on the half interval $[0,l]$. It is known from the Sturm comparison theorem [1,2] that $\lambda_1 \geq \lambda_2$ if $Q_1(t) \geq Q_2(t)$ for all $t \in [-l,l]$. Further, as a consequence of Leighton's criterion [2,3], $\lambda_1 \geq \lambda_2$ if

$$\int_{-l}^{l} (Q_1(t) - Q_2(t))u^2(t)dt \geq 0. \tag{VI.3}$$

This result follows immediately, if u is applied as a 'trial function' for (VI.2). Our purpose is to provide several comparison theorems that allow us to order the *first* even and odd eigenvalues of the pair of Schrödinger equations (VI.1) and (VI.2),

even if the functions $Q_i(t)$, $i = 1, 2$, intersect at a finite number of points within $(-l, l)$. Consider, for example, the following problems (illustrated in Fig.(VI.1))

$$-u'' + (t^2 + s\ a\ m(t)\sin(bt^2))u = \lambda(s)u \quad (-l \leq t \leq l), \tag{VI.4}$$

where: $s \in \{-1, 0, 1\}$, a and b are positive, $ab \leq 0.5$ and $m(t)$ is a monotone symmetric non-increasing function with $m(t) \leq 1/b$. By means of the theorems we prove, we shall be able to show that $\lambda_0(-1) \leq \lambda_0(0) \leq \lambda_0(1)$ for the first even eigenvalue of (VI.4). The idea behind our comparison theorems is to replace the condition $Q_1 > Q_2$ of Sturm's theorem with the weaker condition $U_1 > U_2$, where $U_i = \int_0^t Q_i(x)\rho(x)dx$, $0 \leq t \leq l$, and ρ is a suitable positive non-increasing function. These theorems, developed in the next section, allow the prediction of spectral ordering, even when the comparison functions intersect. We present in section VI.3 a simplified expression of our results for use in quantum mechanics. In section VI.4 some examples using the known exact solutions of the square-well potential are discussed. An extension to more general Sturm-Liouville problems is provided in the section VI.5 and VI.6.

VI.2. New Comparison Theorems:

We start by utilizing the results of Sturm-Liouville theory [4-5] for a boundary value problem. The spectrum of the differential equation

$$-v'' + Q(t)v = \lambda v, \ -l \leq t \leq l, \tag{VI.5}$$

is an unbounded sequence of increasing eigenvalues $\{\lambda_n\}_{n=0}^{\infty}$. Further, each eigenvalue has a unique eigenfunction $v_n(t)$ with precisely n zeros in the given interval. The eigenfunctions $v_n(t)$ are even or odd functions according as n is even or odd. Consequently, the eigenvalues of (VI.5) can be obtained by solving the given equation on the half-domain $[0, l]$ with *one* of the conditions

$$v'(0) = 0, \ v(0) = 0 \tag{VI.6}$$

for the even and odd (subscripted) eigenvalues respectively. We consider first the case of the lowest even eigenfunction. Since $v(t) = v_0(t)$ has no node, we may assume v to be positive on $(-l, l)$.

Lemma VI.1.: The first even wavefunction $v(t)$ of Schrödinger's equation (VI.4) satisfies

$$v'(t) \leq 0, \quad 0 \leq t \leq l. \tag{VI.7}$$

Proof: First the case where the eigenvalue lies above the function $Q(t)$, when equation (VI.5) implies $v(t)$ is concave, and from $v'(0) = 0$ it follows that $v(t)$ is monotone decreasing on $[0, l]$. Secondly, if the eigenvalue lies within $[Q_{\min}, Q_{\max}]$, then (VI.5), and the monotonicity of $Q(t)$, imply that $v''(t) = 0$ for some unique point, say a, in the interval $[0, l]$. Thus, $v''(t) < 0$ and $v'(t) \leq 0$ on the interval $[0, a]$. Since $v(t) > 0$, and $v''(t) \neq 0$ for $t \in (a, l]$, and $v(l) = 0$, it follows that $v'(t) \leq 0$ for $t \in (a, l]$. This proves (VI.7)∎

Multiplying Eq.(VI.1) by v and Eq.(VI.2) by u, and subtracting the resulting equations leads to

$$J = \int_0^l (uv'' - vu'')dt + \int_0^l (Q_1(t) - Q_2(t))uvdt = (\lambda_1 - \lambda_2) \int_0^l uvdt.$$

The term $\int_0^l (uv'' - vu'')dt$ is equal to zero, because of (VI.6), and the boundary conditions $u(l) = v(l) = 0$; Therefore,

$$J = \int_0^l (Q_1(t) - Q_2(t))uvdt = (\lambda_1 - \lambda_2) \int_0^l uvdt. \tag{VI.8}$$

Consequently

$$Q_2(t) \leq Q_1(t) \ (0 \leq t \leq l) \qquad \text{implies} \quad \lambda_2 \leq \lambda_1.$$

The idea behind our comparison theorem is to replace the condition $Q_2(t) < Q_1(t)$ with the weaker condition $U_2 < U_1$, where $U_i(t) = \int_0^t Q_i(x)\rho(x)dx$ $(0 \leq t \leq l, \ i = 1, 2)$ and ρ is a suitable positive non-increasing function. For the first even eigenvalue we choose $\rho = 1$, and $\rho = u(t)$ *or* $v(t)$, where $u(t)$ and $v(t)$ are the eigenfunctions corresponding to differential equations (VI.1) and (VI.2) respectively. The first choice of ρ leads to our first result, whereas the second allows us to recover Leighton's condition (VI.3) in a more general form.

Theorem (VI.1): If the functions $Q_1(t)$ and $Q_2(t)$ in the Schrödinger equations (VI.1) and (VI.2) are monotonically increasing on $[0, l]$, then

$$g(t) = \int_0^t (Q_1(x) - Q_2(x))dx \geq 0 \qquad (0 \leq t \leq l) \tag{VI.9}$$

implies $\lambda_1 \geq \lambda_2$.

Proof: Integration by parts of the left-hand side of (VI.8) yields

$$J = [g(t)uv]_0^l - \int_0^l g(t)(uv)'(t)dt. \tag{VI.10}$$

However $g(0) = 0$ and the vanishing of the eigenfunctions $u(t)$ and $v(t)$ at l makes the first term of the right-hand side of (VI.10) vanish. From the hypothesis $g(t) \geq 0$ and from (VI.7) we know that $(uv)'(t) \leq 0$ for all $t \in [0, l]$ and thus $J \geq 0$. We conclude $\lambda_1 \geq \lambda_2$ as a result of (VI.8)■

An immediate illustration of this theorem is provided by the pair of differential equations

$$-u'' = \lambda_1 u$$

and

$$-v'' - (\cos 2t)v = \lambda_2 v$$

for $t \in [-\pi/2, \pi/2]$. Using (VI.9),

$$\int_0^t \cos(2x)dx = \frac{1}{2}\sin(2t) \geq 0$$

for $t \in [0, \pi/2]$ and this non-negative expression implies the inequality $\lambda_1 > \lambda_2$. This result can also be derived using Leighton's criterion which requires the exact solution of the problem $-u'' = \lambda_1 u$.

A more interesting example is the eigenvalue comparison of the pair of differential equations:

$$-u'' - (\cos 2t)u = \lambda_1 u$$

and

$$-v'' + (t^2 - 1)v = \lambda_2 v.$$

where $t \in [-\pi/2, \pi/2]$. Again, simple calculations using (VI.9) show

$$\int_0^t (-\cos(2x) - x^2 + 1)dx = t - \frac{1}{3}t^3 - \frac{1}{2}\sin(2t) \geq 0 \quad (0 \leq t \leq \pi/2),$$

which yields the eigenvalue inequality $\lambda_1 \geq \lambda_2$. By numerical integration of the coresponding Schrödinger equation $\lambda_1 = 0.470$ and $\lambda_2 = 0.305$, which results confirm our conclusion.

Theorem (VI.2.): If the functions $Q_1(t)$ and $Q_2(t)$ in the Schrödinger equations (VI.1) and (VI.2) are monotonically increasing on $[0, l]$, then from

$$h(t) = \int_0^t (Q_1(x) - Q_2(x))\rho(x)dx \geq 0, \quad (0 \leq t < l) \tag{VI.11}$$

it follows that $\lambda_1 \geq \lambda_2$, where $\rho(t) = u(t)$ or $v(t)$.

The proof of the theorem follows the same argument as theorem (VI.1). We observe here that theorem (VI.1) is stronger than theorem (VI.3), because the condition of theorem (VI.2) is weaker, although it utilizes one of the exact solutions u or v. This is evident because u *or* v is decreasing on $[0, l]$ and therefore, the functions $Q_1(t)$ and $Q_2(t)$ can intersect each other 'even further' and still yield $\lambda_1 \geq \lambda_2$. This result, however is more general than Leighton's criterion (IV.3).

We now turn to the first odd eigenfunction of Eq.(VI.5).

Theorem (VI.3): If the functions $Q_1(t)$ and $Q_2(t)$ in the Schrödinger equations (VI.1) and (VI.2) are monotonically increasing on $[0, l]$, then

$$k(t) = \int_0^t (Q_1(x) - Q_2(x))x^2 dx \geq 0 \quad (0 \leq t \leq l) \tag{VI.12}$$

implies $\lambda_1 \geq \lambda_2$ for the first odd eigenvalue.

To prove this theorem we shall need to use the following monotonicity property for the first odd eigenfunction. A result of this type was first obtained by Common [10].

Lemma (VI.2): The first odd eigenfunction v of Schrödinger equation (VI.5) satisfies

$$(\frac{v(t)}{t})' \leq 0 \quad (0 \leq t \leq l). \tag{VI.13}$$

Proof: For the first odd eigenfunction of (VI.5), from (VI.6), $v(0) = 0$, and further $v(l) = 0$ from the hypothesis. Without loss of generality, we assume that $v(t) > 0$ $(0 < t < l)$. Rolle's theorem guarantees the existence of a point η in $(0, l)$, at which $v'(\eta) = 0$. On the interval $[0, \eta]$, v is concave and therefore its lies below its tangents and above its chords; consequently, $0 < v'(t) < \frac{v(t)}{t}$. Differentiating $\frac{v(t)}{t}$ and using $v'(t) < \frac{v(t)}{t}$ establishes the lemma■

Proof of theorem (VI.3): Notice first that $u(0) = v(0) = 0$ for the first odd eigenvalue and because the solutions of (VI.5) have only simple zeros [5], it further follows that $u'(0) \neq 0$ and $v'(0) \neq 0$. Thereafter, application of l'Hôpital's rule shows that

$$\lim_{t \to 0^+} \frac{u(t)v(t)}{t^2} = u'(0)v'(0)$$

has finite value, and thus the left-hand side of (VI.8) can be written as

$$J = \int_0^l (Q_1(t) - Q_2(t))t^2 \frac{u(t)v(t)}{t^2} dt.$$

Integrating this expression by parts with respect to the function k, as defined by (VI.12), and making use of $u(l) = v(l) = 0$, leads to

$$J = -\int_0^l k(t)(\frac{u(t)v(t)}{t^2})' dt.$$

Since $k(t) \geq 0$ by hypothesis and $(\frac{u(t)v(t)}{t^2})' \leq 0$ from (VI.13), then $J \geq 0$; consequently, (VI.8) lets $\lambda_1 \geq \lambda_2$ ■

By an exactly similar argument we may also demonstrate

Theorem (VI.4): If the functions $Q_1(t)$ and $Q_2(t)$ in the Schrödinger equations (VI.1) and (VI.2) are monotonically increasing on $[0, l]$, then

$$k(t) = \int_0^t (Q_1(x) - Q_2(x))x\rho(x)dx \geq 0 \ (0 \leq t \leq l) \tag{VI.14}$$

implies $\lambda_1 \geq \lambda_2$ for the first odd eigenvalue, where $\rho(t) = u(t)$ or $v(t)$.

Example (The Schrödinger problem with ripple perturbations)

Consider the example mentioned in the introduction

$$-u'' + (t^2 + s\ a\ m(t)\sin(bt^2))u = \lambda(s)u \quad (-l \leq t \leq l),$$

where: $s \in \{-1, 0, 1\}$, a and b are positive, $ab \leq 0.5$ and $m(t)$ is a monotonic symmetric non-increasing function with $m(t) \leq 1/b$. Condition (VI.9) implies

$$\int_0^t a\ m(x)\sin(bx^2)dx \geq 0.$$

This follows because the successive positive and negative areas of the integrand decrease monotonically in absolute value. Therefore, by theorem (IV.1)

$$\lambda(-1) < \lambda(0) < \lambda(1)$$

for the first even eigenvalue. More specifically, if $l = 2$, $b = 4$, $a = 0.1$ and $m(t) = 1$ (Fig. VI.1), then by direct numerical solution $\lambda(-1) = 1.043$, $\lambda(0) = 1.075$ and $\lambda(1) = 1.107$.

Similarly, if $l = 2$, $b = 4$, $a = 0.1$ and $m(t) = 1/t^2$ (Fig. VI.2), because $\int_0^t a\ \sin(bx^2)dx \geq 0$, and with theorem (VI.3), $\lambda(-1) < \lambda(0) < \lambda(1)$ for the first odd eigenvalue of the differential equations

$$-u'' + (t^2 + s\ a\ \frac{\sin(bt^2)}{t^2})u = \lambda(s)u, \quad (-l \leq t \leq l).$$

Meanwhile, direct numerical solution yields $\lambda(-1) = 3.439$, $\lambda(0) = 3.530$ and $\lambda(1) = 3.616$.

VI.3. Practical Method:

If the two functions $Q_1(t)$ and $Q_2(t)$ of Eq.(VI.1) and Eq.(VI.2) do not intersect each other in a very complicated way on the interval $[0, l]$, we can greatly simplify conditions (VI.9) and (VI.12) for the ordering of the eigenvalues. Such simplifications are useful in practical applications. For example, if we let a and b be

the only two points of intersection of $Q_1(t)$ and $Q_2(t)$ in $[0,l]$ with $Q_1(l) > Q_2(l)$, then for $\int_0^t (Q_1(x) - Q_2(x))dx \geq 0$, $(0 \leq t \leq l)$ to hold in theorem (VI.1), it is sufficient that

$$\int_0^a (Q_1(x) - Q_2(x))dx + \int_a^b (Q_1(x) - Q_2(x))dx \geq 0. \qquad \text{(VI.15)}$$

Similarly, for $\int_0^t (Q_1(x) - Q_2(x))x^2 dx \geq 0$ $(0 \leq t \leq l)$ to hold in theorem (VI.3), it is sufficient that

$$\int_0^a (Q_1(x) - Q_2(x))x^2 dx + \int_a^b (Q_1(x) - Q_2(x))x^2 dx \geq 0. \qquad \text{(VI.16)}$$

The significance of inequalities (VI.15) and (VI.16) is that they reduce the condition for ordering the eigenvalues, to the problem of comparing (signed and weighted) areas between the points of intersection of the functions $Q_1(t)$ and $Q_2(t)$ inside $[0,l]$. Indeed, if A and B represent the (signed) areas between the two functions $Q_1(t)$ and $Q_2(t)$ on the interval $[0,a]$ and $[a,b]$ respectively, then inequality (VI.15) or (VI.16) is equivalent to the condition $A + B \geq 0$. This technique extends readily to the case of any finite number of intersections. In the more general case of n intersections $(n > 1)$, we obtain a sufficient condition comprising $(n-1)$ area inequalities.

VI.4 Applications:

Using the technique introduced previously, we can calculate bounds on the first even and odd eigenvalues for the class of Schrödinger problems of the type discussed in section (VI.2). Consider the square-well problem

$$-u'' + V(t)u = \lambda u \ (-l \leq t \leq l)$$

where

$$V(t) = \begin{cases} -U & \text{for} \quad |t| \leq a, \\ d & \text{for} \quad a < |t| \leq l. \end{cases} \qquad \text{(VI.17)}$$

Flügge [6] provides the following transcendental expression for the eigenvalues λ_n $(n = 0, 1, 2, \ldots)$ within $[-U, d]$:

for *even* eigenvalues ($n = 0, 2, \ldots$)

$$\sqrt{U + d - \epsilon_n} \tan(a\sqrt{U + d - \epsilon_n}) = \sqrt{\epsilon_n} \coth((l - a)\sqrt{\epsilon_n}) \qquad \text{(VI.18)}$$

and for *odd* eigenvalues ($n = 1, 3, \ldots$)

$$\sqrt{U + d - \epsilon_n} \cot(a\sqrt{U + d - \epsilon_n}) = -\sqrt{\epsilon_n} \coth((l - a)\sqrt{\epsilon_n}), \qquad \text{(VI.19)}$$

where $\epsilon_n = -\lambda_n + d$. The existence of such eigenvalues depends on the well-depth $U + d$ as indicated by these formulae [7]. For example, if $d = 0$ and $0 \leq U \leq 0.74$, then there is no eigenvalue within the interval $[-U, 0]$; consequently, the spectrum is entirely nonnegative [7]. In this case, Flügge [6] provides the following expressions for the eigenvalues that lie within $[d, \infty)$:
for *even* eigenvalues ($n = 0, 2, \ldots$)

$$\sqrt{U + d - \epsilon_n} \tan(a\sqrt{U + d - \epsilon_n}) = \sqrt{\epsilon_n} \cot((l - a)\sqrt{\epsilon_n}) \qquad \text{(VI.20)}$$

and for *odd* eigenvalues ($n = 1, 3, \ldots$)

$$\sqrt{U + d - \epsilon_n} \cot(a\sqrt{U + d - \epsilon_n}) = -\sqrt{\epsilon_n} \cot((l - a)\sqrt{\epsilon_n}). \qquad \text{(VI.21)}$$

where $\epsilon_n = -\lambda_n + d$.

Consider an arbitrary Schrödinger problem of the type discussed in Section VI.2 and let

$$U = \min\{|Q(t)| \ : -l \leq t \leq l\}$$

and

$$d = \max\{Q(l) : -l \leq t \leq l\}.$$

We introduce a square-well problem (VI.16) for comparison as follows. The value of a is chosen so that the area between $Q(t)$ and $V(t)$ on the intervals $[0, a]$ and $[a, l]$ coincide; thus expression (VI.18) yields a lower bound for the first even eigenvalue. On the other hand, if we introduce a square-well problem with a minimum exceeding the minimum of $Q(t)$, then the square-well function (VI.17) intersects $Q(t)$ in the two points a and b, where b is chosen such that the area between $Q(t)$ and $V(t)$ on

the intervals $[0, a]$ and $[a, b]$ coincide. Hence, the expression (VI.18) yields an upper bound for the Schrödinger problem. The same argument can be used to obtain a lower and upper bound to the first-odd eigenvalue. This technique provides us with a condition guaranteeing that the spectrum of an arbitrary Schrödinger problem (VI.5) lies within $[d, \infty)$. In particular, it follows that the minimum of the function $Q(t)$ of (VI.5) cannot exceed

$$v_c = \frac{8(U+d)}{A(4l(U+d)-A)}, \tag{VI.22}$$

where $A = 2dl - \int_{-l}^{l} Q(t)dt$. To prove this condition, let $Q(x) = vf(x)$ with $vf(0) = d + U$, and define A to be the area between $d = Q(l)$ and the shape $f(x)$. Since we required $vA = 2(d+U)a$, thus we have

$$A = \int_{-l}^{l} [d - vf(x)]dx = 2(d+U)a. \tag{VI.23}$$

Because $\theta \cot\theta \geq 1$, the following inequality

$$1 + \frac{\theta^2}{2} < \theta\cot\theta + \theta^2 \quad (\forall\theta > 0) \tag{VI.24}$$

holds. Let $\theta = a\sqrt{d+U}$, then we have from (VI.18) as $\epsilon_0 \to 0$ that

$$\theta \tan\theta = \frac{a}{l-a}$$

or

$$(l-a)\theta = a\cot\theta$$

multiply by θ and thereby obtain

$$\begin{aligned}\theta^2 + \theta\cot\theta &= \frac{\theta^2 l}{a} \\ &= a(d+U)l \\ &= \frac{Avl}{2}.\end{aligned}$$

Therefore (VI.24) implies

$$v \geq v_c = \frac{8(U+d)}{A(4l(U+d)-A)}$$

with $A = 2dl - \int_{-l}^{l} Q(t)dt$.

Furthermore, the interesting exact solution of the rectangular potential hole between two walls (VI.17) allows us to obtain an estimate of the number of the eigenvalues that lie within $[-U, d]$. Indeed from the horizontal asymptotes of the tangent function in (VI.18) let us write

$$\frac{n^2\pi^2}{4a^2} \leq \epsilon_n + (U + d) \leq \frac{(n+1)^2\pi^2}{4a^2} \quad (n = 0, 1, 2, \ldots).$$

As $\epsilon_n \to 0$, this yields

$$\frac{2a}{\pi}\sqrt{U+d} - 1 \leq n \leq \frac{2a}{\pi}\sqrt{U+d}.$$

VI.5. Elementary results for a system of Sturm-Liouville

We present, in this section, two elementary comparison theorems for the eigenvalues of the self-adjoint second-order linear differential equations

$$-(p_1(x)u_1')' + q_1(x)u_1 = \lambda_1 u_1 \tag{VI.25}$$

$$-(p_2(x)u_2')' + q_2(x)u_2 = \lambda_2 u_2, \tag{VI.26}$$

where: $p_i(x) > 0$, $p_i'(x)$ and $q_i(x)$ are continuous functions on a closed interval $[a, b]$ $(i = 1, 2)$, and a and b are two consecutive zeros of the solutions $u_1(x)$ and $u_2(x)$. The simplest Sturm comparison theorem [1], dating back to 1836, demonstrates that if $p_1(x) = p_2(x)$ and $q_1(x) \geq q_2(x)$ in the differential equations (VI.25) and (VI.26), then $\lambda_1 \geq \lambda_2$. It took almost a century for this result to be modified for the case where $p_1(x)$ is different from $p_2(x)$. This modification, due to Picone [2], states:

if $p_1(x) \geq p_2(x)$ and $q_1(x) \geq q_2(x)$, then $\lambda_1 \geq \lambda_2$.

As an immediately consequence of Sturm-Picone's theorem for

$$-(p(x)u')' + q(x)u = \lambda u \tag{VI.27}$$

with $m_p \leq p(x) \leq M_p$ and $m_q \leq q(x) \leq M_q$ for all x in $[a, b]$, the eigenvalue bounds

$$\frac{(n+1)^2\pi^2}{(b-a)^2}m_p + m_q \leq \lambda_n \leq \frac{(n+1)^2\pi^2}{(b-a)^2}M_p + M_q \quad (n = 0, 1, 2, \ldots)$$

holds.

Since Sturm-Picone's theorem was stated, the question of the ordering of the eigenvalues λ_1 and λ_2 has been raised for the case [2] when the functions $p_1(x)$ and $p_2(x)$ or $q_1(x)$ and $q_2(x)$ of equations (VI.25) and (VI.26) have common zeros on the *open* interval (a, b). This question was partially solved by Leighton [3] using a variational lemma based on an elementary identity. He derived the following sufficiency condition:

$$\int_a^b [(p_1(x) - p_2(x))u_1'^2 + (q_1(x) - q_2(x))u_1^2]dx \geq 0 \qquad \text{(VI.28)}$$

for $\lambda_1 \geq \lambda_2$. The proof of this condition is based on Picone's identity

$$\frac{d}{dx}[\frac{u}{v}(p_1(x)vu' - p_2(x)uv')] = (\lambda_2 - \lambda_1)u^2 + (q_1(x) - q_2(x))u^2 + (p_1(x) - p_2(x))u'^2 + p_2(x)(u' - \frac{uv'}{v})^2.$$

Integrating both side from a to b and using

$$\frac{u}{v}(P_1(x)vu' - P_2(x)uv')|_a^b = 0$$

yields

$$(\lambda_1 - \lambda_2)\int_a^b u^2 dx \geq \int_a^b [(q_1(x) - q_2(x))u^2 + (p_1(x) - p_2(x))u'^2]dx.$$

To illustrate this result we consider an example. Let $p_1(x) = p_2(x) = 1$, $q_1(x) = 0$ and $q_2(x) = -\cos(2x)$. It is known that $u_1(x) = \sqrt{2/\pi}\cos(x)$ is a solution of equation (VI.25) with $\lambda_1 = 1$ and $[a, b] = [-\pi/2, \pi/2]$. Condition (VI.28) now reads as

$$\frac{4}{\pi}\int_0^{\pi/2} \cos(2x)\cos^2(x)dx = 0.5 > 0,$$

which implies $\lambda_1 > \lambda_2$. Indeed, a numerical integration of $-u_2'' - \cos(2x)u_2 = \lambda_2 u_2$ yields $\lambda_2 = 0.470$. Leighton's result (VI.28) is certainly useful, but it stops short of treating many differential equations because of the lack of exact solutions required by (VI.28). We first present two elementary results that do predict the ordering of

eigenvalues without appealing to the exact solutions. The proofs employ variational methods.

Theorem II.5.: If in the differential equations (VI.25) and (VI.26) $p_1(x) = p_2(x) + f(x)$ and $q_1(x) = q_2(x) + g(x)$ where $f(x) \geq m_f \geq 0$, and $g(x) \geq m_g$,, then

$$\lambda_1 \geq \lambda_2 + \frac{\pi^2}{(b-a)^2} m_f + m_g. \tag{VI.29}$$

Proof: After substituting $p_1(x) = p_2(x) + f(x)$ and $q_1(x) = q_2(x) + g(x)$ in equation (VI.25), multiplying it by $u_1(x)$ and integrating over $[a, b]$, we obtain

$$\begin{aligned} \int_a^b [-u_1(p_2(x)u_1')' + q_2(x)u_1^2]dx + \int_a^b [-u_1(f(x)u_1')' + g(x)u_1^2]dx \\ = \lambda_1 \int_a^b u_1^2 dx. \end{aligned} \tag{VI.30}$$

It is a well known consequence of the min-max characterization [6] of the Sturm-Liouville problem, that the first integral of (VI.30) is greater than $\lambda_2 \int_a^b u_1^2 dx$. Integration by parts in the second integral of (VI.30) leads to

$$\int_a^b [-u_1(f(x)u_1')' + g(x)u_1^2]dx \geq (\frac{\pi^2}{(b-a)^2} m_f + m_g) \int_a^b u_1^2 dx$$

since $f(x) \geq m_f$ and $g(x) \geq m_g$■

Here we note that if we restrict our comparison to the case of $p_2(x) = 1$ and $q_2(x) = 0$, then theorem VI.5 reduces to the known result of Smirnov [8] for asymptotic expression of the eigenvalues of boundary value problems.

Theorem VI.6.: If $p_1(x) = f(x)p_2(x)$ and $q_1(x) = g(x)q_2(x)$ where $f(x) \geq m_f > 0$, $g(x) \geq m_g$, $p_2(x) \geq m_{p_2}$, and $q_2(x) \geq m_{q_2}$ in differential equations (VI.25) and (VI.26), then

$$\lambda_1 \geq \lambda_2 + \frac{\pi^2}{(b-a)^2}(m_f - 1)m_{p_2} + (m_g - 1)m_{q_2}. \tag{VI.31}$$

Proof: By means of the substitution $p_1(x) = f(x)p_2(x)$ and $q_1(x) = g(x)q_2(x)$ in equation (VI.25) followed by multiplication by $u_1(x)$ and thereafter by integration.

we obtain

$$\begin{aligned}\lambda_1 \int_a^b u_1^2 dx &= \int_a^b [-u_1(f(x)p_2(x)u_1')' + g(x)q_2(x)u_1^2]dx \\ &\geq (m_f - 1)\int_a^b p_2(x){u_1'}^2 dx + (m_g - 1)\int_a^b q_2(x)u_1^2 dx \\ &+ \int_a^b (p_2(x){u_1'}^2 + q_2(x)u_1^2)dx \\ &\geq (\frac{\pi^2}{(b-a)^2}(m_f - 1)m_{p_2} + (m_g - 1)m_{q_2} + \lambda_2)\int_a^b {u_1}^2 dx.\end{aligned}$$

which implies (VI.31)■

We illustrate this theorem by considering the following example. Let $p_1(x) = p_2(x) = 1$, $q_1(x) = x$, $q_2(x) = x^2$, $[a,b] = [0.5, 1.5]$, consequently $f(x) = 1$ and $g(x) = 1/x$ or $f(x) = 1$ and $g(x) = x$. A straightforward calculation from (VI.31) shows $\lambda_2 + 0.125 \geq \lambda_1 \geq \lambda_2 - 0.08$ or equivalently, the difference $-0.125 \leq \Delta\lambda = \lambda_2 - \lambda_1 \leq 0.08$. The comparison condition (VI.28) of Leighton cannot be applied to this example.

IV. Application to Sturm-Liouville problems

We have obtained some comparison theorems for the *first* even and odd eigenvalues of Schrödinger's equation

$$-v'' + Q(t)v = \lambda v, \ -l \leq t \leq l,$$

with the boundary conditions $v(-l) = v(l) = 0$. These theorems allow the comparison functions $Q(t)$ to intersect at a finite number of points within $[-l, l]$. It is clear that the results derived by Nehari [9] for a pair of differential equations of the form $u'' + \lambda q(x)u = 0$ are radically different: neither set of results can be derived from the other.

The comparison theorems we have derived herein also provide eigenvalue comparisons for *regular* Sturm-Liouville problems of the type we introduced in section (VI.2), namely

$$-(p(x)u')' + q(x)u = \lambda u, \quad -a \leq x \leq a, \tag{VI.32}$$

where $p(x) > 0$ and both $p(x)$ and $q(x)$ are continuous symmetric with respect to the midpoint of $[-a, a]$, $u(-a) = u(a) = 0$, and two further conditions are met.

It is straightforward to show that equation (IV.32) can be transformed, using Liouville transformations [5], into the *Liouville normal form*, that is to say *the one-dimensional Schrödinger equation*

$$-v'' + Q(t)v = \lambda v, \ -l \leq t \leq l, \tag{VI.33}$$

where

$$l = \int_0^a \frac{1}{\sqrt{p(z)}} dz, \quad t = \int_0^x \frac{1}{\sqrt{p(z)}} dz, \ v = \sqrt[4]{p(x)}u$$

and the transformed function

$$Q(t) = q(x) + \frac{1}{\sqrt[4]{p(x)}} \frac{d^2}{dt^2} \sqrt[4]{p(x)}.$$

To apply the theorems we have developed in section (VI.2), the following condition must be satisfied. The expression

$$q(x) - \frac{[p'(x)]^2}{16p(x)} + \frac{1}{4}p''(x) \tag{VI.34}$$

must be monotone increasing on $[0, a]$, and further the functions $p(x)$ and $q(x)$ be symmetric on the interval $[-l, l]$. These conditions guarantee that the transformed function $Q(t)$ is monotone increasing on the right half of the interval $[0, a]$. Our results can thus be applied to such a pair of Sturm-Liouville problems (VI.1) and (VI.2) without any further change. The comparison results are, of course, invariant with respect to vertical and horizontal shifts in space. Results of this type may also be obtained for Schrödinger's equation in an unbounded region [11]. Thus the ripple examples discussed in section VI.3 here also apply to the problem in $\mathbf{R}$. Other illustrations of this type are straightforward to construct. For example if

$$Q_1 = t^2$$

and

$$Q_2 = t^2 + a\frac{sin(bt)}{t} \ (0 < ab^3 < 6),$$

then it follows that Q_1 and Q_2 are symmetric and monotone on each half line. moreover

$$\int_0^t \frac{\sin(t')}{t'} dt' > 0 \quad \forall\, t > 0.$$

Hence the ground state generated by Q_2 is above that corresponding to Q_1 for any value of l.

Fig. VI.1. The potentials $t^2 + \frac{s}{10}\sin(4t^2)$, where $s \in \{-1, 0, 1\}$. If the lowest 'even' eigenvalues are written $\lambda_0(s)$, theorem (VI.1) implies $\lambda_0(-1) \leq \lambda_0(0) \leq \lambda_0(1)$.

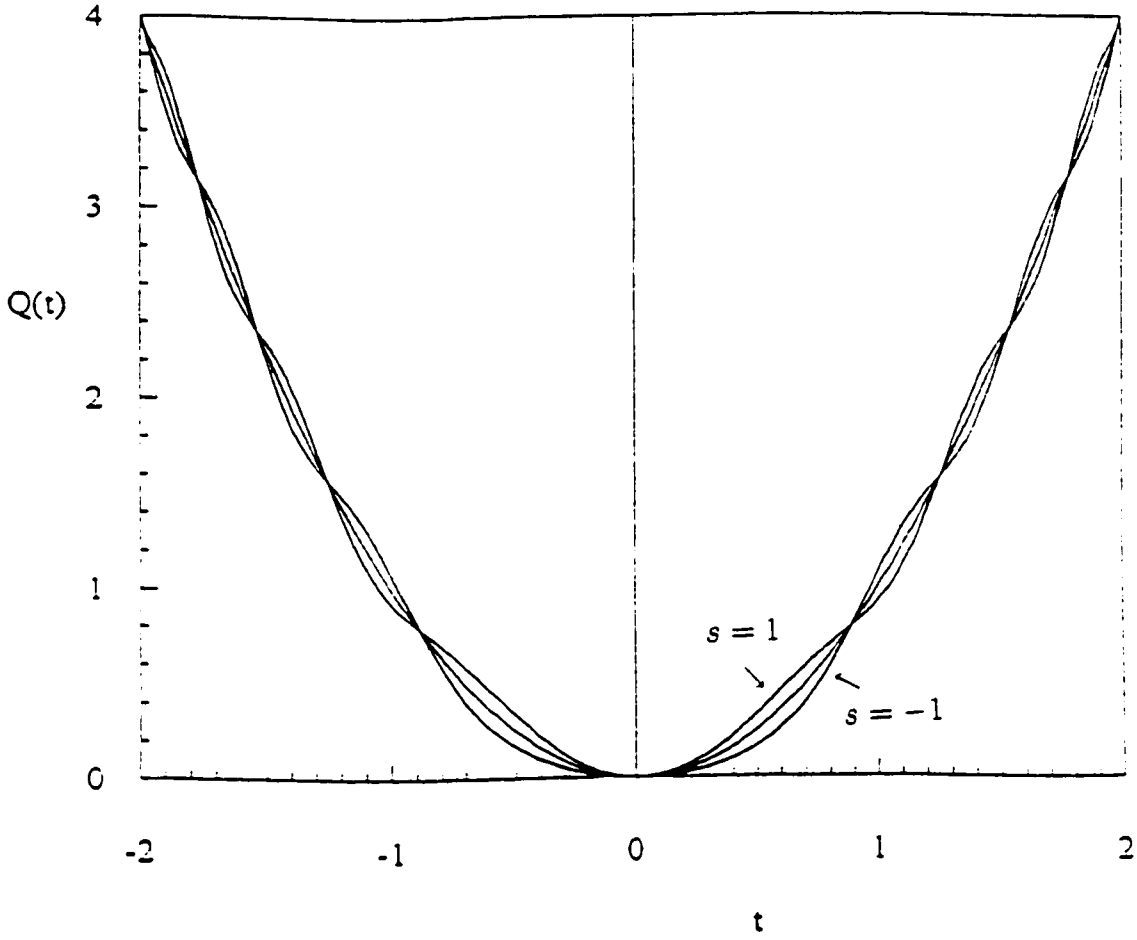
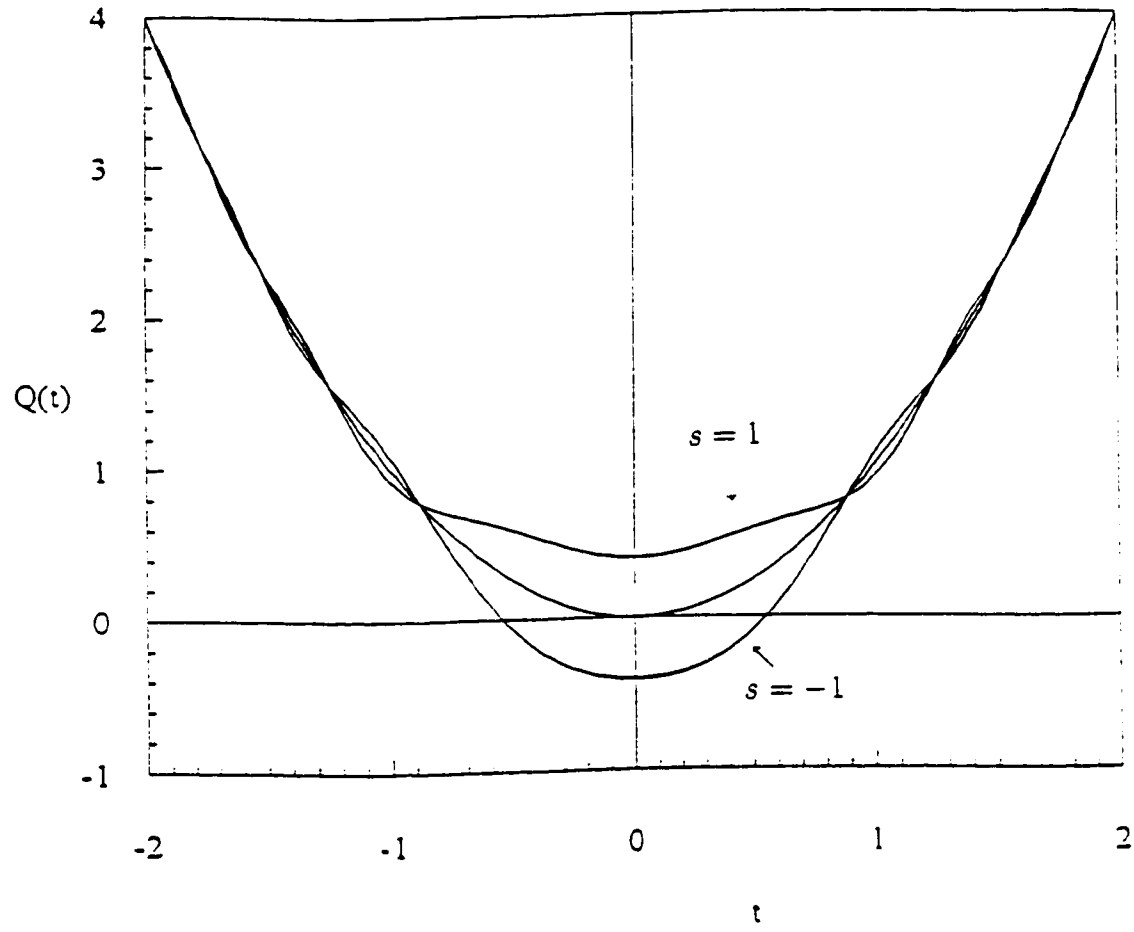


Fig. VI.2. The potentials $t^2 + \frac{s}{10}\sin(4t^2)/t^2$, where $s \in \{-1, 0, 1\}$. If the lowest 'odd' eigenvalues are written $\lambda_1(s)$, theorem (VI.3) implies $\lambda_1(-1) \leq \lambda_1(0) \leq \lambda_1(1)$.



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Conclusion

We have presented in this thesis a collection of practical techniques to obtain energy bounds for Schrödinger Hamiltonians of the form

$$H = -\Delta + V(r).$$

The main theory behind some of these techniques is the method of potential envelopes which is discussed in first chapter of the thesis. If we represent the potential $V(r)$ as a transformation g of a soluble base potential $h(r)$, and the convexity of the transformation function g is definite, then the method of potential envelopes yields energy bounds. Further, if $h_1(r)$ and $h_2(r)$ are two base potentials, then the method we presented in Chapters III and IV yields eigenvalue bounds for a wider class of potentials of the form

$$V(r) = g(h_1(r)) + f(h_2(r))$$

where again the convexity of the transformation functions g and f yields definite upper or lower bounds according to theorem (III.1). This idea can be used, for example, to obtain general energy bounds to the generalized supersingular potentials

$$V(r) = \lambda r^{\delta} + \frac{\mu}{r^{\alpha}}$$

valid for all dimensions $N \geq 1$. The method discussed in Chapters III and IV is general and always yields analytical information concerning the dependence of the eigenvalues on the components of the potential and the various parameters which enter its definition. The exact wave functions of the singular potential (as presented in Chapter III)

$$V(x) = \lambda r^2 + \frac{\mu}{r^2}$$

can be extended to the corresponding exact solution in N-dimensions, and can be used to compute the diagonal elements of the Hamiltonian matrix for a potential consisting of both positive and negative powers, without necessitating use of the wavefunction. A promising direction for future work would be to develop all of the

integrals necessary to perform first order perturbation theory on oscillators with an interaction potential consisting of positive and negative powers. The method extend naturally to sums with any finite number of terms.

Although the application of the envelope method to the class of quasi-exact soluble potentials is rather limited by the parametric constraints necessary for solubility, we have presented an effective and simple method in Chapter V to dealt with such a class of potentials. The method, for example, enables us to obtain bounds for all the eigenvalues at the bottoms of angular-momentum subspaces of the perturbed Coulomb potential

$$V(r) = -\frac{1}{r} + \mu r + \lambda r^2.$$

These energy bounds are valid for arbitrary values of the positive parameters μ and λ. The h-method can be applied equally well to the interesting potential

$$V(r) = ar^2 + br^4 + cr^6$$

for which exact solutions are only available when special relations exist between the parameters: h-theory would allow us to reach beyond these limitations.

For Schrödinger systems in a box, we have developed some methods to obtain eigenvalue comparisons for the first even and odd solutions. It would be very interesting to extended these comparison theorems to higher eigenvalues. However, because these theorems depend on the monotonic behaviour inherited by the wavefunction from the potential, we suspect that the generalization of the theorems to higher eigenvalues, beyond the first two, may not easily be achieved.

Appendix
Publications

Energy bounds for the spiked harmonic oscillator

Richard L. Hall and Nasser Saad

Abstract. A three-parameter variational trial function is used to determine an upper bound to the ground-state energy of the spiked harmonic-oscillator Hamiltonian $H = -\frac{d^2}{dx^2} + x^2 + \frac{\lambda}{|x|^\alpha}$. The entire parameter range $\lambda > 0$ and $\alpha \geq 1$ is treated in a single elementary formulation. The method of potential envelopes is also employed to derive a complementary energy lower bound formula valid for all the discrete eigenvalues.

Résumé. On utilise une fonction d'essai variationnelle à trois paramètres pour déterminer une limite supérieure de l'énergie de l'état fondamental de l'hamiltonien $H = -\frac{d^2}{dx^2} + x^2 + \frac{\lambda}{|x|^\alpha}$ de l'oscillateur harmonique à pointes. Tout l'intervalle $\lambda > 0$ et $\alpha \geq 1$ est traité en une seule formulation élémentaire. On emploie aussi la méthode des enveloppes de potentiel pour obtenir une formule complémentaire donnant une limite inférieure de l'énergie pour toutes les valeurs propres discrètes.

[Traduit par la rédaction]

1. Introduction

In early work on singular potential theory, Detwiler and Klauder [1] introduced the term supersingular to distinguish a potential that is so singular that every matrix element of the potential is infinite. An example that has been given special attention because of its importance in nonrenormalizable field theory [2] and as a prototype for the Klauder phenomenon [3, 4] is the so-called spiked harmonic-oscillator Hamiltonian

$$H = -\frac{d^2}{dx^2} + x^2 + \frac{\lambda}{x^\alpha} \qquad (1)$$

where λ is a positive coupling parameter that measures the strength of the perturbative potential, and $\alpha \geq 1$ is a constant. The phenomenon of supersingularity occurs for $\alpha > 2$. An illustration of the potential for $\alpha = 3$ and $\lambda = 0.01$, 1, and 10 is shown in Fig. 1.

Although the Rayleigh–Schrödinger perturbation series for the eigenvalues of the operator H, regarded as harmonic-oscillator operator $H_0 = -d^2/dx^2 + x^2$ perturbed by λ/x^α, diverges, a number of papers [1, 5–11] have been devoted to the study of a modified perturbation series for the eigenvalues and eigenfunctions. Detwiler and Klauder [1] discussed the asymptotic behavior of the lowest eigenvalue of H for small values of the coupling λ. They discovered that $E(\lambda)$ is proportional to $\lambda \ln(\lambda)$ when $\alpha = 3$, and proportional to $\lambda^{1/\alpha-2}$ when $\alpha > 3$. Using some elegent results of Kato's work on the perturbation theory of linear operators [12] and approximation techniques for differential equations, Harrell [5] was able to derive explicit expressions for the lower order corrections to the eigenvalues of H when λ is sufficiently small. Aguilera-Navarro et al. [6] developed a large-coupling perturbative expansion for the ground-state energy and they present an approximate analytic expression valid for $\alpha < 3$.

Apart from the analytical approximations for the ground-state energy of the spiked harmonic-oscillator Hamiltonian, direct numerical integration methods have been used to compute eigenvalues for H. Killingbeck [13] provided an integration method based on his improvement of the finite-difference algorithm. Killingbeck was critical of the numerical results obtained by Detwiler and Klauder using the Milne method. These conclusions were later confirmed by Korsch and Laurent [14]. Solano-Torres et al. [15] used the Lanczos or grid method to integrate the radial Schrödinger equation for the Hamiltonian H. They have evidently introduced some errors in their application of Harrell's formulas for $\alpha = 4$ and 6. For example, if $\lambda = 0.01$ and $\alpha = 4$, then formula (4) of ref.

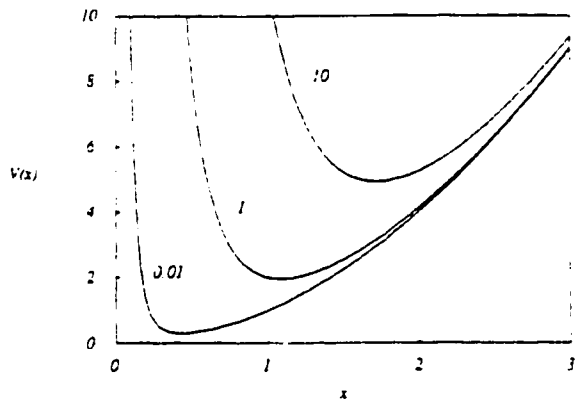

Fig. 1. The spiked harmonic oscillator potential $V(x) = x^2 + \lambda x^{-\alpha}$ for $\alpha = 3$ and $\lambda = 0.01$, 1, and 10.

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15 yields $E = 3.225\ 68$ not $3.075\ 22$, as quoted in Table 2 of ref. 15; if $\lambda = 0.01$ and $\alpha = 6$, then formula (5) yields $E = 3.482\ 41$ not $3.096\ 48$, as quoted in Table 3 of ref. 15; and similarly of other values of λ. These corrections demonstrate that formulas (4) and (5) of ref. 15, correctly reproduced from Harrell [5], yield results that are better than Tables 2 and 3 of ref. 15 would suggest.

The variety of approaches and the complication of having to use different approximation formulas for different ranges of α and λ raises the following question: is it possible to devise a secure uniform treatment to cover all cases? Section 2 of this paper is devoted to answering this question: we describe a simple three-parameter variational wave function that estimates $E(\alpha, \lambda)$ for the ground-state energy of H for all values of α and λ. In addition, in Sect. 3, we apply the envelope method [16] to generate a lower bound to the ground-state energy of H. In Sect. 4 we report our numerical results in detail.

2. Variational method

In view of the work of Simon [3] and DeFacio and Hammer [4] on the domain problem of the spiked harmonic-oscillator Hamiltonian (1), we conclude that an appropriate domain for H, considered as a quadratic form, is the subset $D(H)$ of functions ψ in $L_2([o, \infty), dx)$ that satisfy the Dirichlet boundary condition $\psi(0) = 0$ and for which $(\psi, H\psi) < \infty$. We consider in particular the following three-parameter trial function

$$\psi(x) = x^{p-\varepsilon} \exp(-\beta x^q), \qquad 0 \le x < \infty \tag{2}$$

where the constant $p \ge 0$ will be determined shortly, and ε, β, and q are three positive variational parameters. We find that the optimal q is usually sufficiently different from 2 to justify the added computational difficulty. Convergence of the expectation value $(\psi, -\Delta\psi)$ for the kinetic energy of H is immediately assured. Since it is necessary that $\psi \in D(H)$, the convergence of the expectation value of the spiked harmonic potential

$$V(x) = x^2 + \frac{\lambda}{x^\alpha} \tag{3}$$

may be used to determine p in terms of α. Since there is no convergence difficulty for large x, a sufficient condition for the convergence of $(\psi, V\psi)$ is $\int_0^1 x^{-\alpha}\psi^2(x)\,dx < \infty$. This in turn is guaranteed if $\int x^{2(p-\varepsilon)-\alpha}\,dx < \infty$, for $\varepsilon > 0$. Thus, the minimum value of p for an acceptable wave function is given by

$$p = \frac{\alpha - 1}{2} \tag{4}$$

This criterion guarantees that ψ will be in $D(H)$ for each value of $\alpha \ge 1$. The variational method provides an upper bound for the lowest eigenvalue E_0 of the Hamiltonian H. Thus, by a long calculation by hand, we obtain

$$\begin{aligned} E_0 \le E_0^U &= \min_{\varepsilon,\beta,q\ge 0} \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} \\ &= \min_{\varepsilon,\beta,q\ge 0} \left[\frac{q}{2}(2\beta)^{2/q}\left[(2p+q+2\varepsilon-1)g_1 - \frac{2}{q}(p+\varepsilon)(p+\varepsilon-1)g_2 - \frac{q}{2}g_3\right] + \left(\frac{1}{2\beta}\right)^{2/q} g_4 + \lambda(2\beta)^{\alpha/q} g_5\right]/g_6 \end{aligned} \tag{5}$$

where

$$\begin{aligned} g_1 &= \Gamma\left(\frac{2p+q+2\varepsilon-1}{q}\right), \quad g_2 = \Gamma\left(\frac{2p+2\varepsilon-1}{q}\right), \quad g_3 = \Gamma\left(\frac{2p+2q+2\varepsilon-1}{q}\right) \\ g_4 &= \Gamma\left(\frac{2p+2\varepsilon+3}{q}\right), \quad g_5 = \Gamma\left(\frac{2p+2\varepsilon-\alpha+1}{q}\right), \quad g_6 = \Gamma\left(\frac{2p+2\varepsilon+1}{q}\right) \end{aligned} \tag{6}$$

This inequality is general enough to compute an upper bound for the lowest eigenvalue of the Hamiltonian H for all $\alpha \ge 1$; V is supersingular [1] only when $\alpha > 2$. The single inequality (5) also allows us to estimate E_0 for all positive values of the coupling λ.

3. The envelope method

The fact that ordering between potentials implies corresponding ordering of the eigenvalues is an essential feature of solving many problems in quantum mechanics. The envelope method [16,17] makes use of this comparison theory and provides simple formulas for lower and upper bounds. The shape of the spiked harmonic-oscillator potential (3) for large x suggest the harmonic-oscillator potential $h(x) = a + bx^2$ as a comparison potential where the variables a and b are chosen such that the graph of the potential $V(x)$ lies entirely above the graph of the potential $h(x)$, but is tangential to it at a point, say t, where $h(t) = V(t)$ and $h'(t) = V'(t)$. A simple calculation shows that the eigenvalues of such a harmonic-oscillator Hamiltonian with potential h are

$$\varepsilon_n(\alpha, \lambda; t) = \frac{\lambda}{t^\alpha}\left(\frac{\alpha}{2} + 1\right) + (4n+3)\left(1 - \frac{\alpha\lambda}{2t^{\alpha+2}}\right)^{1/2} \tag{7}$$

where $n = 0, 1, 2, 3, \ldots$ counts the *odd* eigenstates of the harmonic oscillator, in agreement with the Dirichlet condition $\psi(0) = 0$. The envelope theory provides lower bounds for all the energies of the spiked harmonic-oscillator Hamiltonian H. We obtain the best lower bound by maximizing over the contact point t. Thus

$$E_n(\alpha, \lambda) \ge E_n^L = \max_{t>0} \varepsilon_n(\alpha, \lambda; t) \tag{8}$$

Table 1. Upper and lower bounds for $H = -\frac{d^2}{dx^2} + x^2 + \frac{\lambda}{|x|^{5/2}}$ for different values of λ. The values E^G were evaluated by formula (4.33) of ref. 6, and those of E^H, we used formula (5.1) from ref. 5. E_0^U and E_0^L are from inequalities (5) and (8) of the present work. The "exact" values were obtained by direct numerical integration [6].

$\alpha = 5/2$				
λ	E^G	E^H	E_0^U	Exact
1000	44.955 49	—	44.955 49	44.955 49
100	17.541 92	—	17.541 92	17.541 89
10	7.735 58	—	7.735 32	7.735 11
5	6.297 55	—	6.296 85	6.296 47
1	4.323 60	—	4.318 54	4.317 31
0.5	3.860 53	3.481 27	3.850 32	3.848 55
0.1	—	3.201 25	3.269 28	3.266 87
0.05	—	3.136 95	3.154 50	3.152 43
0.01	—	3.036 75	3.037 43	3.036 73
0.005	—	3.019 26	3.019 47	3.019 14
0.001	—	3.004 03	3.004 04	3.004 02
0.000 156 25	—	3.000 64	3.000 64	—

A similar technique with the use of a square-well potential as a comparison potential, for example, can also be used to provide an upper bound for all the eigenvalues of H. However, for the most important case, the ground-state, the variational argument used in Sect. 2 is much more accurate.

4. Numerical results

For an accurate analytic eigenvalue expansion, Aguilera-Navarro et al. [6] suggest considering two different expansions according to the values of the coupling parameter λ, a nonpower series expansion given by Harrell [5] when λ is small, and a large coupling perturbative expansion given by them when λ is large.

For intermediate values of $\lambda(\approx 1)$ Solano-Torres et al. [15] claim that they have constructed an approximant to represent the energy in this region using a single Padé extrapolant. However, they do not present any numerical results for eigenvalues in this case.

In this section we discuss the numerical results for the upper bound E_0^U (by (5)) and lower bound E_0^L (by (8)) of the ground-state energy of the spiked harmonic-oscillator Hamiltonian (1): these bounds are valid for small, intermediate, and large values of the coupling parameter λ.

Table 2. Upper and lower bounds for the $H = -\frac{d^2}{dx^2} + x^2 + \frac{1000}{|x|^\alpha}$ with different values of α, by inequalities (5) and (8).

$\lambda = 1000$		
α	E_0^U	E_0^L
3	33.316 78	31.186 55
3.5	26.108 98	23.894 13
4	21.370 26	19.076 98
4.5	18.102 87	15.737 60
5	15.763 56	13.330 60
5.5	14.036 26	11.539 28
6	12.725 65	10.170 24

A simple method to compute the upper bound E_0^U from inequality (5) is to fix one or two of the parameters (β, ε, q) and then minimize with respect to the free parameters. However, we found that the most convenient approach was to explore the parameter space (β, ε, q) by using the downhill simplex method of Nelder and Mead [20]. The initial simplex points for this method may be chosen with the aid of a few preliminary calculations. As an example, consider $\alpha = 5/2$ and $\lambda = 1000$, simple loops over fixed ranges of ε and q give for the minimization of the right-hand side of inequality (5) $\beta = 0.89$ and $E_0^U = 44.955\ 66$ when $\varepsilon = 27.6$ and $q = 1.80$. With these values of (β, ε, q) as a base for the simplex method, the other three initial points can be chosen close to it. The downhill simplex method gives now the more accurate eigenvalue $E_0^U = 44.955\ 49$.

In Table 1 we exhibit the results of our computations of the upper bounds for different values of the coupling parameter λ, where α is fixed at 5/2. For comparison, the partial results given by the formulas of Harrell E^H [5] and Aguilera-Navarro et al. E^G [6], and the "exact" numerical results of Aguilera-Navarro et al. [6] are also included. It is clear from these data that the wave function (2) provides an excellent approximation for the ground-state energy of the spiked harmonic-oscillator for all values of the potential parameters.

Lower bounds by (8) are weak, especially for small λ, but the formula is simple and valid for *all* the discrete eigenvalues. Examples for $\alpha = 5/2$ (as in Table 1) are: $\lambda = 1000$. $E_0^L = 42.917$; $\lambda = 10$. $E_0^L = 6.228$; and $\lambda = 1$. $E_0^L = 3.529$.

In Table 2 we present some sample ground-state energy eigenvalues of the spiked harmonic-oscillator Hamiltonian H for fixed λ and different values of α. The results for $\lambda = 1000$ are not possible by any of the earlier analytic approximations mentioned in the introduction. Similar tables can of course be constructed by using the inequalities (5) and (8) and any desired values for $\lambda > 0$ and $\alpha \geq 1$.

The idea of using a trial wave function to approximate the upper bound eigenvalues of the ground state of H variationally for α, a positive even integer, was used by Guardiola

Table 3. A comparison between the results E^F of Fernández [19], and the results E_0^L of the present work obtained from the inequality (5) for $\alpha = 4$ and 6 and various values for the coupling λ.

	$\alpha = 4$		$\alpha = 6$	
λ	E^F	E_0^L	E^F	E_0^L
1000	21.384 46	21.370 26	12.737 60	12.725 65
100	11.292 41	11.265 86	8.422 60	8.420 96
10	6.649 78	6.609 66	6.016 4	6.014 94
5	5.832 05	5.788 89	5.527 51	5.528 09
1	4.548 79	4.504 16	4.676 88	4.684 97
0.1	3.626 44	3.600 44	4.019 15	4.042 84
0.01	3.237 75	3.249 80	3.524 93	3.580 70

and Ros. [18] and Fernández [19]. In Table 3 we report a comparison between the ground-state eigenvalues of H using formula (9) of ref. 19 and inequality (5) of the present work.

5. Conclusion

The spiked harmonic-oscillator Hamiltonian is interesting for two principal reasons: it has played an important rôle as a model for non-renormalizable interactions used in field theories; and it has provided a useful model for a certain class of curious difficulties, which may arise in perturbation theory. The key feature of this potential, leading to the so-called "Klauder phenomenon," is that if the limit is taken to zero perturbation ($\lambda = 0$), there is a dramatic change in the possible interpretation of the operator (or quadratic form).

The significance of the contribution made in the present paper is that upper and lower bounds are provided simply and uniformly for all values of the potential parameters. The upper bound (5) for the ground-state energy is accurate and yields also a trial wave function whose possible further use has not been explored in the present paper. The lower bounds we provide are not very tight for small λ, but they are in the form of a simple formula (8), which is valid for all values of the potential parameters and for all the discrete eigenvalues.

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Eigenvalue bounds for a class of singular potentials

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Abstract. We study smooth transformations $V(x) = g(x^2) + f(\frac{1}{x^2})$ of the solvable potentials $\lambda x^2 + \frac{\mu}{x^2}$. Eigenvalue approximation formulae are obtained which provide lower or upper energy bounds for all the discrete energy eigenvalues E_n, $n = 0, 1, 2, \ldots$, accordingly as the transformation functions g and f are both convex or both concave. Detailed results are presented for the special case of two-term singular potentials of the form $V(x) = \lambda x^\beta + \frac{\mu}{x^\alpha}$, $\alpha, \beta > 0$, and also for the potentials $V(x) = \lambda x^{1.9} + \frac{\mu}{x^{1.9}}$ and $V(x) = \lambda x^{2.1} + \frac{\mu}{x^{2.1}}$, $\lambda > 0$, $\mu > 0$, for $0 \leqslant n \leqslant 10$.

1. Introduction and main result

In many cases the exactly solvable problems in non-relativistic quantum mechanics provide simple and effective models illustrating the most relevant features of actual physical phenomena. Further, they may provide a starting point for more accurate approximations based on a variational or perturbation method, or on geometric properties of the Hamiltonian involved [1, 2]. In envelope theory [3], for example, the exactly solvable models play a basic role in the development of the energy approximation expressions. There are many excellent sources available in the literature for exactly solvable models in quantum mechanics [4–10]. Gol'dman and Krivchenkov [5], for example, have provided a clear description of the exact solution for the following one-dimensional Schrödinger equation (in units $\hbar = 2m = 1$):

$$-\psi'' + (\lambda x^2 + \frac{\mu}{x^2})\psi = \mathcal{E}_n\psi \qquad \psi(0) = 0 \qquad \lambda > 0,\ \mu > 0. \tag{1}$$

They showed that the energy spectrum of (1) is given by

$$\mathcal{E}_n = \sqrt{\lambda}\left(4n + 2 + \sqrt{4\mu + 1}\right) \qquad n = 0, 1, 2, \ldots. \tag{2}$$

The purpose of the paper is to use such solutions to investigate the spectrum of the Schrödinger equation:

$$-\psi'' + V(x)\psi = E_n\psi \qquad \psi(0) = 0 \tag{3}$$

where

$$V(x) = g(x^2) + f\left(\frac{1}{x^2}\right) \tag{4}$$

is a sum of two smooth transformations respectively of x^2 and $\frac{1}{x^2}$, and E_n is the eigenvalue. We shall show that E_n can be approximated by the expression

$$E_n \approx \epsilon_n = \min_{s,t>0}\left\{g(s^2) - s^2g'(s^2) + f\left(\frac{1}{t^2}\right) - \frac{1}{t^2}f'\left(\frac{1}{t^2}\right)\right.$$

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$$+\sqrt{g'(s^2)}\left(4n+2+\sqrt{4f'\left(\frac{1}{t^2}\right)+1}\right)\Bigg\} \qquad n=0,1,2,\ldots. \tag{5}$$

This formula provides a lower bound ($\approx=\geqslant$) or an upper bound ($\approx=\leqslant$) to the exact eigenvalues according to whether the transformation functions g and f are both convex or both concave. This allows us, for example, to obtain simple expressions which bound the spectrum of the spiked harmonic oscillator potential $V(x) = \lambda x^2 + \frac{\mu}{x^\alpha}$, $\alpha \geqslant 1$, $n = 0, 1, 2, \ldots$, a problem which is of considerable interest [11–18]. Indeed, formula (5) implies that the energy of spiked harmonic oscillator can be approximated by

$$E_n \approx \epsilon_n(\hat{t}) = \left(1-\frac{\alpha}{2}\right)\frac{\mu}{\hat{t}^\alpha} + 2\lambda\hat{t}^2 + 2\sqrt{\lambda}(2n+1) \tag{6}$$

where $\hat{t}$ is the real root of

$$2\mu\alpha t^{2-\alpha} - 4\lambda t^4 + 1 = 0.$$

Here $\epsilon_n(\hat{t})$ is lower bound to E_n when $\alpha > 2$ and an upper bound when $\alpha < 2$.

2. Transformed potentials

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

$$H = -\frac{d^2}{dx^2} + g(x^2) + f\left(\frac{1}{x^2}\right) \tag{7}$$

where g and f are smooth transformations of x^2 and $\frac{1}{x^2}$, respectively. For example, when g and f are identity transformations, the problem has the exact solution (2) for all n and arbitrary positive values of λ and μ. Standard envelope theory [3] suggests the following approach to treat a Hamiltonian of the form (7). We may approximate the shape of $V(x) = g(x^2) + f(\frac{1}{x^2})$ by some suitable potential, called base potential, with known spectrum. Using the well known comparison theorem (or refinements thereto [19]) for $V(x)$ with this base potential, we can obtain eigenvalue bounds for H. This method has been applied to obtain a simple lower bound formula for eigenvalues of the spiked harmonic oscillator $V(x) = x^2 + 1/x^\alpha$, $\alpha \geqslant 1$ using a harmonic oscillator as a base potential [18].

Here we add a new idea which leads to energy bounds which are both more general and sharper. Instead of approximating $V(x)$ by a single potential, as in [18], we use the tangent approximation for $g(x^2)$ and $f(\frac{1}{x^2})$, separately. That is to say, we replace g and f by their corresponding tangent approximations

$$\begin{aligned} g^{(s)}(x^2) &= a(s) + b(s)x^2 \\ f^{(t)}\left(\frac{1}{x^2}\right) &= c(t) + \frac{d(t)}{x^2} \end{aligned} \tag{8}$$

respectively, where s is a contact point between $g(x^2)$ and its tangent approximation $g^{(s)}(x^2)$, and t plays a similar role for f. Elementary analysis implies that $V(x)$ in (4) can thus be approximated by

$$V^{(s,t)}(x) = g(s^2) - s^2g'(s^2) + g'(s^2)x^2 + f\left(\frac{1}{t^2}\right) - \frac{f'(\frac{1}{t^2})}{t^2} + \frac{f'(\frac{1}{t^2})}{x^2}. \tag{9}$$

With this approximation for $V(x)$, we may use the result of Gol'dman and Krivchenkov (2) for the eigenvalues of Schrödinger equation

$$-\psi'' + V^{(s,t)}(x)\psi = \epsilon_n(s,t)\psi. \tag{10}$$

Table 1. Some lower bounds E_0^L and upper bounds E_0^U using (6) for $H = -\frac{d^2}{dx^2} + x^2 + \frac{1000}{x^6}$. The 'exact' values E_0^N were obtained by direct numerical integration of Schrödinger's equation.

	$\mu = 1000$		
α	E_0^L	E_0^N	E_0^U
0.5	—	415.889 79	416.309 77
1	—	190.723 31	190.992 13
1.5	—	104.410 22	104.539 93
1.9	—	71.061 58	71.086 86
2	65.253 46	65.253 46	65.253 46
2.1	60.127 04	60.152 01	—
2.5	44.833 49	44.955 49	—
3	33.079 40	33.316 76	—
3.5	25.762 04	26.108 85	—
4	20.918 65	21.369 64	—
4.5	17.552 18	18.101 83	—
5	15.117 58	15.761 13	—
5.5	13.298 42	14.031 07	—
6	11.901 53	12.718 62	—

Table 2. lower bounds E_0^L using (6) for $H = -\frac{d^2}{dx^2} + x^2 + \frac{\mu}{x^{5/2}}$ with different values of μ. The 'exact' values E_0^N were obtained by direct numerical integration of Schrödinger's equation.

	$\alpha = \frac{5}{2}$	
μ	E_0^L	E_0^N
1000	44.833 49	44.955 49
100	17.419 00	17.541 89
10	7.611 69	7.735 11
5	6.173 94	6.296 47
1	4.204 53	4.317 31
0.5	3.746 16	3.848 55
0.1	3.204 95	3.266 87
0.05	3.109 54	3.152 43
0.01	3.023 36	3.036 70
0.005	3.011 78	3.019 05
0.001	3.002 37	3.003 97

Thus we have

$$\epsilon_n(s,t) = g(s^2) - s^2 g'(s^2) + f\left(\frac{1}{t^2}\right) - \frac{1}{t^2} f'\left(\frac{1}{t^2}\right) + \sqrt{g'(s^2)}\left(4n + 2 + \sqrt{4f'\left(\frac{1}{t^2}\right) + 1}\right). \tag{11}$$

For the eigenvalues of Schrödinger equation (3), we have

(a) $E_n \leqslant \epsilon_n(s,t)$ if g and f are both convex.

(b) $E_n \geqslant \epsilon_n(s,t)$ if g and f are both concave.

The proof is obtained by the following simple argument. For definiteness we consider case (a). Since g and f are convex, their graphs lie above their tangents. Consequently, we have from (9) that $V^{(s,t)}(x) \leqslant V(x)$. Case (a) then follows by an application of the

Table 3. Upper bounds E_n^U using (12) for $H = -\frac{d^2}{dx^2} + \lambda x^{19} + \frac{\mu}{x^{19}}$ with different values of n. The 'exact' values E_n^N were obtained by direct numerical integration of Schrödinger's equation.

	$\lambda = \mu = 1$	
n	E_n^U	E_n^N
0	4.160 38	4.116 28
1	7.946 96	7.850 41
2	11.684 36	11.544 96
3	15.389 87	15.211 95
4	19.071 75	18.857 79
5	22.734 85	22.486 48
6	26.382 39	26.100 75
7	30.016 64	29.702 60
8	33.639 30	33.293 52
9	37.251 69	36.874 71
10	40.854 86	40.447 12

Table 4. Lower bounds E_n^L using (12) for $H = -\frac{d^2}{dx^2} + \lambda x^{21} + \frac{\mu}{x^{21}}$ with different values of n. The 'exact' values E_n^N were obtained by direct numerical integration of Schrödinger's equation.

	$\lambda = \mu = 1$	
n	E_n^L	E_n^N
0	4.309 42	4.356 98
1	8.519 89	8.626 97
2	12.782 43	12.940 00
3	17.079 60	17.283 55
4	21.402 86	21.650 81
5	25.747 12	26.037 51
6	30.108 94	30.440 71
7	34.485 90	34.858 23
8	38.876 13	39.288 42
9	43.278 21	43.729 98
10	47.690 99	48.181 84

comparison theorem. Case (b) is proven in an analogous way if 'convex' is replaced by 'concave'. It is appropriate to mention here that the conclusions follow even if either f or g is the identity transformation. These bounds may, of course, be sharpened by optimization with respect to s and t, and moreover they are valid for the entire discrete spectrum $n \geqslant 0$.

3. Numerical results and conclusion

One of the interesting points concerning the bounds we have obtained, in section 2, is the large variety of approximations made possible by different choices of the transformations g and f. We consider, for example, the case where $g(x^2) = \lambda x^\beta$ and $f(\frac{1}{x^2}) = \frac{\mu}{x^\alpha}$. From (11) it follows that

$$\epsilon_n(s, t) = \lambda\left(1 - \frac{\beta}{2}\right)s^\beta + \left(1 - \frac{\alpha}{2}\right)\frac{\mu}{t^\alpha} + \sqrt{\frac{\lambda\beta s^{\beta-2}}{2}}\left(4n + 2 + \sqrt{\frac{2\mu\alpha}{t^{\alpha-2}} + 1}\right). \tag{12}$$

For the spiked harmonic oscillator $\beta = 2$ and therefore it follows from (12) that the eigenvalue approximation is given by (6). In tables 1 and 2 we exhibit the results of the lower bounds obtained by using formula (6) for different values of α and for $\lambda = 1$ and different values of the coupling parameter μ, along with some accurate values obtained by direct numerical integration of Schrödinger equation.

For the potential $V(x) = \lambda x^{1.9} + \frac{\mu}{x^{1.9}}$, we take $\beta = 1.9$ and $\alpha = 1.9$ in formula (12), which provides upper bounds in this case. A comparison of some results obtained by this formula and the corresponding results obtained by direct numerical integration, for 11 energy levels, are reported in table 3. In table 4, we report the corresponding results for the case $\beta = 2.1$ and $\alpha = 2.1$, that is to say, for the potential $V(x) = \lambda x^{2.1} + \frac{\mu}{x^{2.1}}$. Similar numerical results could also be obtained by using perturbation methods such as the renormalized hypervirial perturbation method of Killingbeck [20].

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

Acknowledgments

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Eigenvalue bounds for transformations of solvable potentials

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

1. Introduction

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

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

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

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

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

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

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

where

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

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

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

2. Perturbed Coulomb potentials

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

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

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

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

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

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

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

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

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

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

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

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

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

where

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

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

3. Transformed potentials

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

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

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

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

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

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

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

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

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

Differentiation of (12) with respect to t gives

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

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

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

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

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

Now, since

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

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

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

Thus

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

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

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

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

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

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

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

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

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

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

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

4. Numerical results and conclusion

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

Our first example is

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

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

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

while the energy formula (19) gives

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

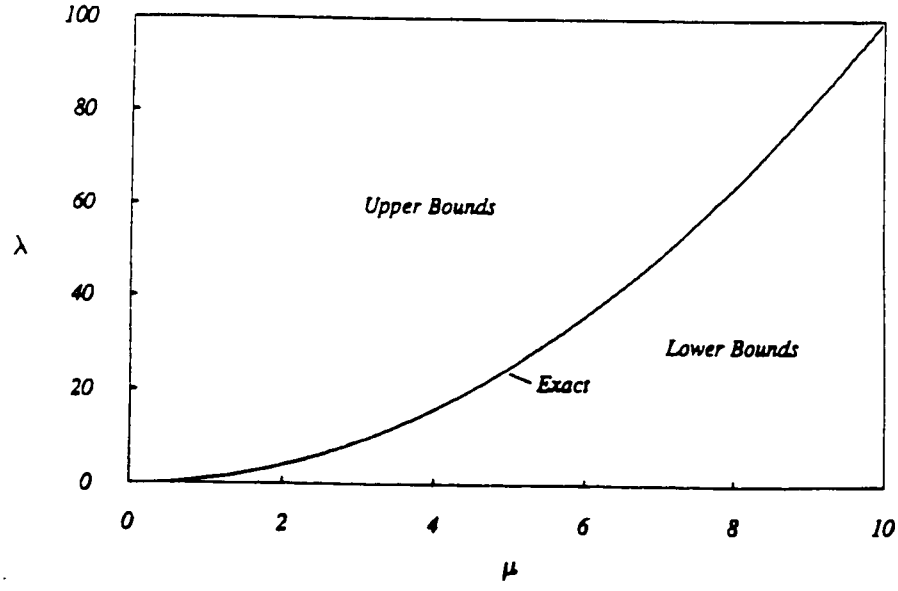

Figure 1. Two parametric regions: if $\mu < \sqrt{\lambda}$, the formulae (21) and (22) yield a lower bound for the ground-state energy of the Hamiltonian $H = -\Delta - \frac{1}{r} + \mu r + \lambda r^2$, while $\mu > \sqrt{\lambda}$ yields an upper bound.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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Eigenvalue comparisons for quantum systems in a box

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Abstract

Comparison theorems are obtained for the first even and odd solutions of Schrodinger's equation $-v'' + Q(t)v = \lambda v$, $-l \leqslant t \leqslant l$ with boundary conditions $v(-l) = v(l) = 0$. The comparison functions $Q_i(t)$, $i = 1, 2$, may intersect at a finite number of points within $[-l, l]$. Immediate extensions are possible for a more general class of Sturm–Liouville problems, and for problems in unbounded regions. © 1998 Published by Elsevier Science B.V.

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1. Introduction

We consider the pair of Schrödinger equations

$$-u'' + Q_1(t)u = \lambda_1 u, \tag{1}$$

$$-v'' + Q_2(t)v = \lambda_2 v, \tag{2}$$

where the exact solutions $u(t)$ and $v(t)$ satisfy the boundary conditions $u = v = 0$, $t = \pm l$ and $Q_i(t)$, $i = 1, 2$, are symmetric and monotone increasing on the half-interval $[0, l]$. It is known from the Sturm comparison theorem [1,2] that $\lambda_1 \geqslant \lambda_2$ if $Q_1(t) \geqslant Q_2(t)$ for all $t \in [-l, l]$. Further, as a consequence of Leighton's criterion [2,3], $\lambda_1 \geqslant \lambda_2$ if

$$\int_{-l}^{l} (Q_1(t) - Q_2(t))u^2(t)\,dt \geqslant 0. \tag{3}$$

This result follows immediately if u is applied as a "trial function" for (2). The purpose of this Letter is to provide several comparison theorems that allow us to order the *first* even and odd eigenvalues of the pair of Schrödinger equations (1) and (2), even if the functions $Q_i(t)$, $i = 1, 2$, intersect at a finite number of points. Consider, for example, the following problems (illustrated in Fig. 1),

$$-u'' + (t^2 + s\,a\,m(t)\sin(bt^2))u = \lambda(s)u \tag{4}$$

$$(-l \leqslant t \leqslant l),$$

where $s \in \{-1, 0, 1\}$, a and b are positive, $ab \leqslant 0.5$ and $m(t)$ is a monotone symmetric non-increasing function with $m(t) \leqslant 1/b$. By means of the theorems we prove, we shall be able to show that $\lambda_0(-1) \leqslant \lambda_0(0) \leqslant \lambda_0(1)$ for the first even eigenvalue of (4). The idea behind our comparison theorems is to replace the condition $Q_1 > Q_2$ of Sturm's theorem with the weaker condition $U_1 > U_2$, where $U_i = \int_0^t Q_i(x)\rho(x)\,dx$, $0 \leqslant t \leqslant l$, and ρ is a suitable pos-

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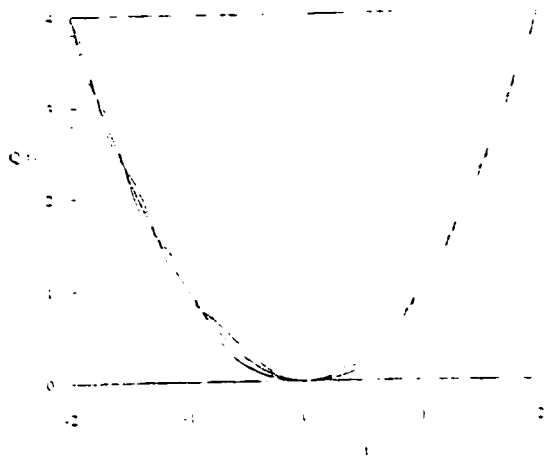

Fig. 1. The potentials $r^2 + (s/10)\sin(4r^2)$, where $s \in \{-1, 0, 1\}$. If the lowest "even" eigenvalues are written $\lambda_0(s)$, Theorem 1 implies $\lambda_0(-1) \leqslant \lambda_0(0) \leqslant \lambda_0(1)$.

itive non-increasing function. These theorems, developed in Section 2, allow the prediction of spectral ordering even when the comparison functions intersect. We present in Section 3 a simplified expression of our results for use in quantum mechanics. In Section 4 some examples using the known exact solutions of the square-well potential are presented. An extension to more general Sturm–Liouville problems is discussed in the conclusion.

2. New comparison theorems

We utilize the results of the Sturm–Liouville theory [4,5] for a boundary value problem. The spectrum of the differential equation

$$-v'' + Q(t)v = \lambda v, \quad -l \leqslant t \leqslant l, \tag{5}$$

is an unbounded sequence of increasing eigenvalues $\{\lambda_n\}_{n=0}^{\infty}$. Further, each eigenvalue has a unique eigenfunction $v_n(t)$ with precisely n zeros in the given interval. The eigenfunctions $v_n(t)$ are even or odd functions according to whether n is even or odd. Consequently, the eigenvalues of (5) can be obtained by solving the given equation on the half-domain $[0, l]$ with *one* of the conditions

$$v'(0) = 0, \quad v(0) = 0 \tag{6}$$

for the even and odd (subscripted) eigenvalues, respectively.

We consider first the case of the lowest even eigenfunction. Since $v(t) = v_0(t)$ has no node, we may assume v to be positive on $(-l, l)$. Moreover, we claim that $v(t)$ is monotone decreasing on $[0, l]$, that is to say

$$v'(t) \leqslant 0, \quad 0 \leqslant t \leqslant l. \tag{7}$$

To prove this, we consider first the case where the eigenvalue lies above the function $Q(t)$, in which case Eq. (5) implies that $v(t)$ is concave, and from $v'(0) = 0$ it follows that $v(t)$ is monotone decreasing on $[0, l]$. Secondly, if the eigenvalue lies within $[Q_{\min}, Q_{\max}]$, then (5) and the monotonicity of $Q(t)$ imply that $v''(t) = 0$ for some unique point, say a, in the interval $[0, l]$. Thus, $v''(t) < 0$ and $v'(t) \leqslant 0$ on the interval $[0, a]$. Since $v(t) > 0$, and $v''(t) \neq 0$ for $t \in (a, l]$, and $v(l) = 0$, it follows that $v'(t) \leqslant 0$ for $t \in (a, l]$. This proves (7).

Multiplying Eq. (1) by v and Eq. (2) by u, and subtracting the resulting equations, we obtain

$$J = \int_0^l (Q_1(t) - Q_2(t))uv\,\mathrm{d}t$$

$$= (\lambda_1 - \lambda_2)\int_0^l uv\,\mathrm{d}t. \tag{8}$$

The term $\int_0^l (uv'' - vu'')\,\mathrm{d}t$ is zero because of (6) and the boundary conditions $u(l) = v(l) = 0$. Consequently, from (8) we see that $Q_2(t) \leqslant Q_1(t)$, $0 \leqslant t \leqslant l$, implies $\lambda_2 \leqslant \lambda_1$. The idea behind our comparison theorem is the replacement of the condition $Q_2(t) < Q_1(t)$ with the weaker condition $U_2 < U_1$, where $U_i(t) = \int_0^t Q_i(x)\rho(x)\,\mathrm{d}x$, $0 \leqslant t \leqslant l$, $i = 1, 2$, and ρ is a suitable positive non-increasing function. For the first even eigenvalue we use the choices $\rho = 1$ and $\rho = u(t)$ or $v(t)$, where $u(t)$ and $v(t)$ are the eigenfunctions corresponding to differential equations (1) and (2), respectively. The first choice of ρ leads to our first result, whereas the second allows us to recover Leighton's condition (3) in a more general form.

Theorem 1. If the functions $Q_1(t)$ and $Q_2(t)$ in the Schrödinger equations (1) and (2) are monotonically increasing on $[0,l]$, then

$$g(t) = \int_0^t (Q_1(x) - Q_2(x))\,dx \geqslant 0, \qquad (9)$$

$$0 \leqslant t \leqslant l,$$

implies $\lambda_1 \geqslant \lambda_2$.

Proof Integration by parts of the left-hand side of (8) yields

$$J = [g(t)uv]_0^l - \int_0^l g(t)(uv)'(t)\,dt. \qquad (10)$$

However $g(0) = 0$ and the vanishing of the eigenfunctions $u(t)$ and $v(t)$ at l makes the first term of the right-hand side of (10) vanish. From the hypothesis $g(t) \geqslant 0$ and from (7) we know that $(uv)'(t) \leqslant 0$ for $t \in [0,l]$ and thus $J \geqslant 0$. We conclude $\lambda_1 \geqslant \lambda_2$ as a result of (8).

An immediate illustration of this theorem is provided by the pair of differential equations $-u'' = \lambda_1 u$ and $-v'' - (\cos 2t)v = \lambda_2 v$ for $t \in [-\pi/2, \pi/2]$. We have, using Theorem 1, that $\int_0^t \cos(2x)\,dx = \frac{1}{2}\sin(2t) \geqslant 0$ for $t \in [0, \pi/2]$ and this non-negative number implies the inequality $\lambda_1 > \lambda_2$. This result can also be derived by the use of Leighton's criterion. However, unlike the latter, our argument does not require the exact solution of the problem $-u'' = \lambda_1 u$. A more interesting example is the eigenvalue comparison of the following pair of differential equations: $-u'' - (\cos 2t)u = \lambda_1 u$ and $-v'' + (t^2 - 1)v = \lambda_2 v$ $(-\pi/2 \leqslant t \leqslant \pi/2)$. Again, simple calculations show that

$$\int_0^t (-\cos(2x) - x^2 - 1)\,dx = t - \tfrac{1}{3}t^3 - \tfrac{1}{2}\sin(2t) \geqslant 0.$$

$$0 \leqslant t \leqslant \pi/2.$$

which yield the eigenvalue inequality $\lambda_1 \geqslant \lambda_2$. Indeed, by numerical solution we find $\lambda_1 = 0.470$ and $\lambda_2 = 0.305$.

Theorem 2. If the functions $Q_1(t)$ and $Q_2(t)$ in the Schrödinger equations (1) and (2) are monotonically increasing on $[0,l]$, then

$$h(t) = \int_0^t (Q_1(x) - Q_2(x))\rho(x)\,dx \geqslant 0 \qquad (11)$$

$$(0 \leqslant t \leqslant l)$$

implies $\lambda_1 \geqslant \lambda_2$, where $\rho(t) = u(t)$ or $v(t)$.

The proof follows by the same argument as Theorem 1. We observe here that Theorem 2 is stronger than Theorem 1, because the condition of Theorem 2 is weaker, although it utilizes one of the exact solutions u or v. This is evident because u or v is decreasing on $[0,l]$ and therefore, the functions $Q_1(t)$ and $Q_2(t)$ can intersect each other "even further" and still yield $\lambda_1 \geqslant \lambda_2$. We now turn to the first odd eigenfunction of (1) and (2).

Theorem 3. If the functions $Q_1(t)$ and $Q_2(t)$ in the Schrödinger equations (1) and (2) are monotonically increasing on $[0,l]$, then

$$k(t) = \int_0^t (Q_1(x) - Q_2(x))x^2\,dx \geqslant 0, \qquad (12)$$

$$0 \leqslant t \leqslant l,$$

implies $\lambda_1 \geqslant \lambda_2$ for the first odd eigenvalue.

To prove this theorem we shall need to use the following monotonicity property for the first odd eigenfunction. A result of this type was first obtained by Common [10].

Lemma 1. The first odd eigenfunction v of the Schrödinger equation (5) satisfies

$$\left(\frac{v(t)}{t}\right)' \leqslant 0, \quad 0 \leqslant t \leqslant l. \qquad (13)$$

Proof. For the first odd eigenfunction of (5) we have from (6) that $v(0) = 0$ and further $v(l) = 0$ from the hypothesis. Therefore, without loss of generality, we may assume that $v(t) > 0$, $0 < t < l$. Rolle's theorem gives us a point η in $(0,l)$, at which $v'(\eta) = 0$. On the interval $[0,\eta]$ v is concave and therefore, v

lies below its tangents and above its chords. Consequently, $0 < v'(x) < v(t)/t$. Differentiating $v(t)/t$ and using $v'(t) < v(t)/t$ establishes the lemma.

Proof of Theorem 3. We notice first that $u(0) = v(0) = 0$ for the first odd eigenvalue and because the solutions of (5) have only simple zeros [5], it further follows that $u'(0) \neq 0$ and $v'(0) \neq 0$. Thereafter, an application of l'Hôpital's rule shows

$$\lim_{t\to 0} \frac{u(t)v(t)}{t^2} = u'(0)v'(0)$$

has finite value, and thus the left-hand side of (8) can be written as

$$J = \int_0^l (Q_1(t) - Q_2(t))t^2 \frac{u(t)v(t)}{t^2}\,dt.$$

Integrating this expression by parts with respect to the function k as defined by (12) and using $u(l) = v(l) = 0$, leads to

$$J = -\int_0^l k(t)\left(\frac{u(t)v(t)}{t^2}\right)'\,dt.$$

Since $k(t) \geq 0$ by hypothesis and $(u(t)v(t)/t^2)' \leq 0$ from (13), we conclude that $J \geq 0$. Consequently, from (8), we have $\lambda_1 \geq \lambda_2$.

By an exactly similar argument we may also prove

Theorem 4. If the functions $Q_1(t)$ and $Q_2(t)$ in the Schrödinger equations (1) and (2) are monotonically increasing on $[0, l]$, then

$$k(t) = \int_0^t (Q_1(x) - Q_2(x))x\rho(x)\,dx \geq 0 \qquad (14)$$

$$(0 \leq t \leq l)$$

implies $\lambda_1 \geq \lambda_2$ for the first odd eigenvalue, where $\rho(t) = u(t)$ or $v(t)$.

Example (Schrödinger problem with ripple perturbations). We consider the example mentioned in the Introduction (4) and observe that $\int_0^t a\,m(x)\sin(bx^2)\,dx \geq 0$. This follows because the successive

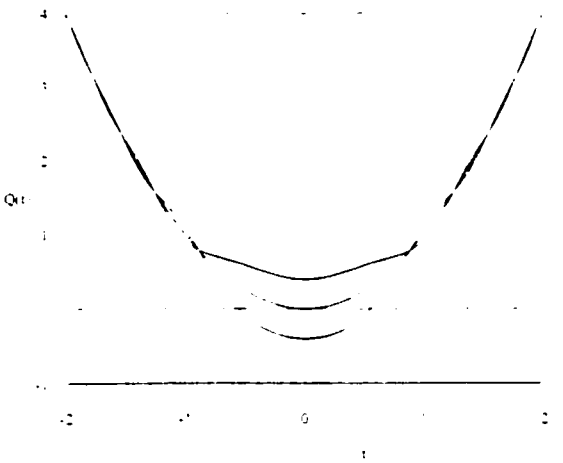

Fig. 2. The potentials $t^2 + (s/10)\sin(4t^2)/t^2$, where $s \in \{-1.0, 1\}$. If the lowest "odd" eigenvalues are written $\lambda_1(s)$, Theorem 3 implies $\lambda_1(-1) \leq \lambda_1(0) \leq \lambda_1(1)$.

positive and negative areas of the integrand decrease monotonically in absolute value. Therefore, by Theorem 1 we have $\lambda(-1) < \lambda(0) < \lambda(1)$ for the first even eigenvalue. More specifically, if we choose $l = 2$, $b = 4$, $a = 0.1$ and $m(t) = 1$ (Fig. 1), then we obtain by direct numerical solution $\lambda(-1) = 1.043$, $\lambda(0) = 1.075$ and $\lambda(1) = 1.107$.

Similarly, if we have $l = 2$, $b = 4$, $a = 0.1$ and $m(t) = 1/t^2$ (Fig. 2), we obtain, because of $\int_0^t a\sin(bx^2)\,dx \geq 0$ and Theorem 3, that $\lambda(-1) < \lambda(0) < \lambda(1)$ for the first odd eigenvalue of the differential equations

$$-u'' + \left(t^2 + sa\frac{\sin(bt^2)}{t^2}\right)u = \lambda(s)u, \quad -l \leq t \leq l.$$

Meanwhile, direct numerical solution in this case yields $\lambda(-1) = 3.439$, $\lambda(0) = 3.530$ and $\lambda(1) = 3.616$.

3. Practical method

If the two functions $Q_1(t)$ and $Q_2(t)$ of (1) and (2) do not intersect each other in a very complicated way on the interval $[0, l]$, we can greatly simplify conditions (9) and (12) for the ordering of the eigenvalues. Such simplifications are useful in practical applications. For example, if we let a and b be the only two points of intersection of $Q_1(t)$ and $Q_2(t)$ in $[0, l]$ with

$Q_1(t) > Q_2(t)$, then for $\int_0^t (Q_1(x) - Q_2(x))\,dx \geqslant 0$, $0 \leqslant t \leqslant l$, to hold in Theorem 1, it is sufficient that

$$\int_0^a (Q_1(x) - Q_2(x))\,dx - \int_a^b (Q_1(x) - Q_2(x))\,dx \geqslant 0. \tag{15}$$

Similarly, for $\int_0^t (Q_1(x) - Q_2(x))x^2\,dx \geqslant 0$, $0 \leqslant t \leqslant l$, to hold in Theorem 3, it is sufficient that

$$\int_0^a (Q_1(x) - Q_2(x))x^2\,dx - \int_a^b (Q_1(x) - Q_2(x))x^2\,dx \geqslant 0. \tag{16}$$

The significance of inequalities (15) and (16) is that they reduce the condition for ordering the eigenvalues to the problem of comparing (signed and weighted) areas between the points of intersection of the functions $Q_1(t)$ and $Q_2(t)$ inside $[0, l]$. Indeed, if A and B represent the (signed) areas between the two functions $Q_1(t)$ and $Q_2(t)$ on the interval $[0, a]$ and $[a, b]$ respectively, then inequality (15) or (16) is equivalent to the condition $A + B \geqslant 0$. This technique extends to the case of any finite number of intersections. In the more general case of n intersections ($n > 1$), we obtain a sufficient condition comprising $(n-1)$ area inequalities.

4. Applications

By means of the technique we introduced in the previous section, we can calculate bounds on the first even and odd eigenvalues for the class of Schrödinger problems of the type discussed in Section 2. We consider the square-well problem

$$-u'' + V(t)u = \lambda u, \quad -l \leqslant t \leqslant l,$$

where

$$V(t) = -U \quad \text{for } |t| \leqslant a,$$
$$= d \quad \text{for } a < |t| \leqslant l. \tag{17}$$

Flügge [6] provides the following transcendental expression for the eigenvalues λ_n, $n = 0, 1, 2, \ldots$, within $[-U, d]$: for *even* eigenvalues ($n = 0, 2, \ldots$)

$$\sqrt{U + d - \epsilon_n}\tan(a\sqrt{U + d - \epsilon_n}) = \sqrt{\epsilon_n}\coth((l-a)\sqrt{\epsilon_n}) \tag{18}$$

and for *odd* eigenvalues ($n = 1, 3, \ldots$)

$$\sqrt{U + d - \epsilon_n}\cot(a\sqrt{U + d - \epsilon_n}) = -\sqrt{\epsilon_n}\coth((l-a)\sqrt{\epsilon_n}), \tag{19}$$

where $\epsilon_n = -\lambda_n + d$. The existence of such eigenvalues depends on the well-depth $U + d$ as indicated by these formulae [7]. For example, if $d = 0$ and $0 \leqslant U \leqslant 0.74$, then there is no eigenvalue within the interval $[-U, 0]$ and consequently, the spectrum is entirely non-negative [7]. In this case, Flügge [6] provides the following expressions for the eigenvalues that lie within $[d, \infty)$: for *even* eigenvalues ($n = 0, 2, \ldots$)

$$\sqrt{U + d - \epsilon_n}\tan(a\sqrt{U + d - \epsilon_n}) = \sqrt{\epsilon_n}\cot((l-a)\sqrt{\epsilon_n}) \tag{20}$$

and for *odd* eigenvalues ($n = 1, 3, \ldots$)

$$\sqrt{U + d - \epsilon_n}\cot(a\sqrt{U + d - \epsilon_n}) = -\sqrt{\epsilon_n}\cot((l-a)\sqrt{\epsilon_n}), \tag{21}$$

where $\epsilon_n = -\lambda_n + d$.

Consider an arbitrary Schrödinger problem of the type discussed in Section 2 and let $U = \min\{|Q(t)| : -l \leqslant t \leqslant l\}$ and $d = \max\{Q(t) : -l \leqslant t \leqslant l\}$. We introduce a square-well problem (17) for comparison as follows. The value of a is chosen so that the area between $Q(t)$ and $V(t)$ on the intervals $[0, a]$ and $[a, l]$ coincide; thus expression (18) yields a lower bound for the first even eigenvalue. On the other hand, if we introduce a square-well problem with a minimum exceeding the minimum of $Q(t)$, then the square-well function (17) intersects $Q(t)$ in the two points a and b, where b is chosen such that the area between $Q(t)$ and $V(t)$ on the intervals $[0, a]$ and $[a, b]$ coincide. Hence, the expression (18) yields an upper bound for the Schrödinger problem. The same argument can be used to obtain a lower and upper bound to the first odd eigenvalue. This technique provides us with a condition that guarantees that the spectrum of an arbitrary

Schrödinger problem (2) lies within $[d, \infty)$. In particular, it follows that the minimum of the function $Q(t)$ of (2) cannot exceed

$$t_c = \frac{8(L-d)}{A(4(L+d)-A)}, \tag{22}$$

where $A = 2dl - \int_{-l}^{l} Q(t)\,dt$.

5. Conclusion

We have obtained some comparison theorems for the *first* even and odd eigenvalues of Schrödinger's equation $-v'' + Q(t)v = \lambda v$, $-l \leqslant t \leqslant l$, with the boundary conditions $v(-l) = v(l) = 0$. These theorems allow the comparison functions $Q(t)$ to intersect at a finite number of points within $[-l, l]$. It is clear that the results derived by Nehari [9] for a pair of differential equations of the form $u'' + \lambda q(x)u = 0$ are radically different; neither set of results can be derived from the other.

The comparison theorems we have derived herein also provide eigenvalue comparisons for *regular* Sturm–Liouville problems of the form

$$-(p(x)u')' + q(x)u = \lambda u, \quad -a \leqslant x \leqslant a, \tag{23}$$

where $p(x) > 0$ and both $p(x)$ and $q(x)$ are continuous symmetric with respect to the midpoint of $[-a, a]$, $u(-a) = u(a) = 0$, and two further conditions are met. Firstly (A) the expression

$$q(x) - \frac{[p'(x)]^2}{16p(x)} + \tfrac{1}{4}p''(x)$$

must be monotone increasing on $[0, a]$. It is straightforward to show that Eq. (23) can be transformed, using Liouville transformations [8], into the *Liouville normal form*, that is to say *the one-dimensional Schrödinger equation*

$$-v'' + Q(t)v = \lambda v, \quad -l \leqslant t \leqslant l, \tag{24}$$

where

$$l = \int_0^a \frac{1}{\sqrt{p(z)}}\,dz, \quad t = \int_0^x \frac{1}{\sqrt{p(z)}}\,dz,$$

$$v = \sqrt[4]{p(x)}\,u$$

and the transformed function

$$Q(t) = q(x) + \frac{1}{\sqrt[4]{p(x)}} \frac{d^2}{dt^2} \sqrt[4]{p(x)}.$$

Condition (B) is that the Q so constructed is symmetric and monotone increasing on the right half of $[-l, l]$. Our results can thus be applied to such a pair of Sturm–Liouville problems (24) without any further change. The comparison results are, of course, invariant with respect to vertical and horizontal shifts in space. Results of this type may also be obtained for Schrödinger's equation in an unbounded region [11]. Thus the ripple examples discussed in Section 2 here also apply to the problem in $\mathbb{R}$. Other illustrations of this type are straightforward to construct. For example if $Q_1 = t^2$ and

$$Q_2 = t^2 + a\frac{\sin(bt)}{t}, \quad 0 < ab^3 < 6,$$

then it follows that Q_1 and Q_2 are symmetric, and monotone on each half line; moreover,

$$\int_0^t \frac{\sin(t')}{t'}\,dt' > 0 \quad \forall\, t > 0.$$

Hence the ground state generated by Q_2 is above that corresponding to Q_1 for any value of l. We are indebted to the Referee for suggesting this illustration.

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