

SPECTRAL BISECTION ALGORITHM FOR SOLVING SCHRÖDINGER EQUATION USING UPPER AND LOWER SOLUTIONS

QUTAIBEH DEEB KATATBEH

ABSTRACT. This paper establishes a new criteria for obtaining a sequence of upper and lower bounds for the ground state eigenvalue of Schrödinger equation $-\Delta\psi(r) + V(r)\psi(r) = E\psi(r)$ in N spatial dimensions. Based on this proposed criteria, we prove a new comparison theorem in quantum mechanics for the ground state eigenfunctions of Schrödinger equation. We determine also lower and upper solutions for the exact wave function of the ground state eigenfunctions using the computed upper and lower bounds for the eigenvalues obtained by variational methods. In other words, by using this criteria, we prove that the substitution of the lower(lower) bound of the eigenvalue in Schrödinger equation leads to an upper(lower) solution. Finally, two proposed iteration approaches lead to an exact convergent sequence of solutions. The first one uses Raielgh-Ritz theorem. Meanwhile, the second approach uses a new numerical spectral bisection technique. We apply our results for a wide class of potentials in quantum mechanics such as sum of power-law potentials in quantum mechanics.

1. INTRODUCTION

In quantum mechanics, many comparison theorems have been proved for the spectrum of schrödinger equations of the form [9, 12, 13, 14],

$$-\Delta\psi(r) + V(r)\psi(r) = E\psi(r), \quad \text{where } r = \|\mathbf{r}\|, \mathbf{r} \in \mathbb{R}^N. \quad (1.1)$$

The standard comparison theorem of quantum mechanics states that the ordering $V_1 < V_2$ of the potentials implies the ordering $E_1 < E_2$ of the eigenvalues. Hall in [13], proved a new comparison theorem by allowing the potentials to intersect and to keep the ordering of the eigenvalues. In [9], we have generalized the comparison theorem for higher dimensions and proved it for higher angular momentum $\ell > 0$. In all previous works in the literature, the researchers were interested in using these comparison theorems to improve the upper and lower bounds for the eigenvalues of Schrödinger equations without any information about the corresponding wave function. For example, using min-max principles [22] and the envelope method [15, 16], we can find analytical upper and lower bounds for the eigenvalue without

2000 *Mathematics Subject Classification.* 34L16, 81Q10.

Key words and phrases. Schrödinger equation; lower solution; upper solution; spectral bounds; envelope method.

©2007 Texas State University - San Marcos.

Submitted July 18, 2007. Published October 4, 2007.

any information about the corresponding wave function. Many authors [1, 2, 6, 18, 19, 20, 21, 26, 27] have developed iterative methods to solve differential equations of first order, second order and higher orders. Throughout this paper, we use the spectral bounds obtained by spectral approximation methods for monotone increasing potentials having discrete spectrum in quantum mechanics, to find upper and lower solution for schrödinger equation for the ground state eigenfunction. We say that $\phi(r)$ is an upper (lower) solution to an eigenvalue problem $H\psi(r) = E\psi(r)$, where H is a differential operator if and only if $\phi(r) \geq (\leq) \psi(r)$ for all r .

We propose here two iterative approaches which yield to an exact convergent sequence of solutions. The first one uses a modified and generalized Raielgh-Ritz theorem. Meanwhile, the second approach uses a new numerical bisection technique. Our results for Schrödinger equations allow us to prove the modified Rayleigh-Ritz theorem which connects the upper bound for the eigenvalue of the ground state with the corresponding solutions for their eigenvalues. This paper is organized as follows: In section 2, we recall some of the methods available in the literature to find upper and lower solutions for the eigenvalues, such as variational methods and the envelope method. In section 3, we prove the new comparison theorem for the upper and lower solution of schrödinger equation. In section 4, we apply our method to anharmonic oscillator potential in quantum mechanics to verify the proposed criteria. More specifically, we modify the old version of Rayleigh-Ritz and generalize it in a way that our iterative algorithm together with the well-known variational methods such as the envelope method yields to a more efficient approximation method. In section 5, we introduce the spectral bisection algorithm and explain how it can be applied. Finally, in section 6, we apply our results to some examples of sum of power-law potentials.

2. UPPER AND LOWER BOUNDS FOR THE EIGENVALUES OF SCHÖDINGER EQUATIONS

Upper bounds are easy to find over finite dimensional spaces. In [7], we have developed new variational methods using different kinds of bases to find bounds for the eigenvalues for a sum of power-law potentials. Furthermore, we use comparison theorems based on solvable models, to find upper and lower bounds for the eigenvalues.

Moreover, in [3, 8, 10, 11, 24], we have developed the envelope method and used it widely in finding upper and lower bound for wide range of unsolvable potentials in quantum mechanics. The min-max principal [22] plays an important rule in obtaining the formula for the upper and lower bounds for the eigenvalues in the envelope method. The minimization is performed over two stages: first we fix the mean of the kinetic energy $(\psi, -\Delta\psi) = s$, then we minimize over $s > 0$. The mean of the potential energy under the constrain $(\psi, -\Delta\psi) = s$ is called the 'kinetic potential' $\bar{V}(s)$ associated with the potential $V(r)$. Accordingly, the eigenvalues can be written in the form,

$$E = \min_{s>0} \{s + \bar{V}(s)\}, \quad (2.1)$$

where,

$$\bar{V}(s) = \inf \{(\psi, V\psi) : \psi \in \mathcal{D}(H), (\psi, \psi) = 1, (\psi, -\Delta\psi) = s\}. \quad (2.2)$$

The kinetic potential can be derived using the coupling of the potential in the original problem and can be found using Legendre transformation [5],

$$H\psi = -\Delta\psi + V(r)\psi = E\psi. \quad (2.3)$$

For simplicity, let $E = F(v)$; then $s = F(v) - vF'(v)$ and $\bar{V}(s) = F'(v)$. It is worth to mention that Kinetic potentials are applicable to find upper or lower bounds for the eigenvalues in case of concave or convex transformation of a solvable model. We can apply this method to find upper and lower bounds for many examples, such as Hamiltonian of the form

$$H = -\Delta + \sum_q a(q)r^q, \quad q > 0. \quad (2.4)$$

In fact, the energy bounds can be expressed in natural way using the P-representation [8, 9] by minimizing over r , so we have obtained new formulation for the energy in terms of the potential $V(r)$,

$$E = \min_{r>0} \{K^{(V)}(r) + vV(r)\} \quad (2.5)$$

where

$$K^{(V)}(r) = (\bar{V}^{-1}oV)(r). \quad (2.6)$$

This function is known concretely for certain potentials. For example, if we consider the pure power $V(r) = \text{sgn}(q)r^q$ in N dimensional space, we find that

$$K^{(q)}(r) = (P(q)/r)^2, \quad (2.7)$$

[8, 9], where

$$P(q) = |E(q)|^{(2+q)/2q} \left[\frac{2}{2+q} \right]^{1/q} \left[\frac{|q|}{2+q} \right]^{1/2}, \quad q \neq 0. \quad (2.8)$$

Therefore, (2.1) can be written in the form

$$E = \min_{r>0} \left\{ \left(\frac{P(q)}{r} \right)^2 + V(r) \right\}. \quad (2.9)$$

We established in our previous work [3, 8, 9], how to choose the suitable values for the $P(q)$ to obtain upper and lower bounds for the eigenvalues for the power-law potentials in quantum mechanics.

In the next section, we prove our main new comparison theorem for the upper and lower solution corresponding to the ground state of Schrödinger equation in quantum mechanics.

3. UPPER AND LOWER BOUNDS FOR THE SOLUTION OF SCHÖDINGER EQUATION

We need to prove some results before we derive the new method for finding envelope for the solutions of Schrödinger equation in Theorem 3.3.

Theorem 3.1. *Consider the eigenvalue problem*

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

subject to $\psi(0) = 1$ and $\psi'(0) = 0$. If $H\phi = \lambda\phi$, where $E \neq \lambda$, then

$$\int_0^\infty \phi(r)\psi(r)r^{n-1}dr = 0.$$

Proof. First let ϕ and ψ be solutions of

$$-\Delta\psi(r) + V(r)\psi(r) = E\psi(r), \quad (3.1)$$

$$-\Delta\phi(r) + V(r)\phi(r) = \lambda\phi(r). \quad (3.2)$$

Multiply (3.1) by ϕ and (3.2) by ψ . After subtracting, we obtain

$$\Delta\phi(r)\psi(r) - \Delta\psi(r)\phi(r) = (E - \lambda)\phi(r)\psi(r). \quad (3.3)$$

Integrating equation (3.3) from 0 to ∞ , we get that the left hand side is zero and the result follows directly. \square

In [9], we proved the following lemma which plays an important rule in our proof.

Lemma 3.2 ([9]). *Suppose that $\psi = \psi(r)$, $r = \|\mathbf{r}\|$, $\mathbf{r} \in \mathbb{R}^N$, satisfies Schrödinger's equation:*

$$H\psi(r) = (-\Delta + V(r))\psi(r) = E\psi(r), \quad (3.4)$$

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

Assume now that upper and lower bounds for the eigenvalues of Schrödinger equation have been found as discussed earlier in section 2, then we can state our main theorem for the first eigenfunction as follows:

Theorem 3.3. *Consider a Schrödinger equation in N spatial dimensions,*

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

subject to $\psi(0) = 1$ and $\psi'(0) = 0$. If $E^L < E_1 < E^U$, then

- (1) The solution of $H\phi = E^U\phi$, subject to the same boundary conditions is a lower solution for $\psi(r)$; i.e., $\phi(r) \leq \psi(r)$.
- (2) The solution of $H\phi = E^L\phi$, subject to the same boundary conditions is an upper solution for $\psi(r)$; i.e., $\phi(r) \geq \psi(r)$.

Proof. First, let ϕ and ψ be solutions of

$$-\Delta\psi(r) + V(r)\psi(r) = E\psi(r), \quad (3.5)$$

$$-\Delta\phi(r) + V(r)\phi(r) = E^U\phi(r). \quad (3.6)$$

We prove the first part of the theorem; the second part can be proved similarly. Suppose that there exists $a \in \mathbb{R}$ such that $\phi(a) > \psi(a)$. Suppose first that the solution of $H\phi = E^U\phi$ is less than ψ for $0 < r < r_0 < a$, where r_0 is the intersection point. Then, by expressing $\Delta\psi(r)$ by $\psi''(r) + \frac{(N-1)}{r}\psi(r)$ in N spatial dimensions, multiplying (3.5) by ϕ and (3.6) by ψ , we obtain after subtracting

$$\phi''(r)\psi(r) - \psi''(r)\phi(r) = (E - E^U)\phi(r)\psi(r) = -\epsilon\psi(r)\phi(r) \quad (3.7)$$

for some $\epsilon > 0$. Now, integrating equation (3.7) from 0 to r_0 (the intersection point), we obtain:

$$\psi(r_0)\phi'(r_0) - \phi(r_0)\psi'(r_0) = -\epsilon \int_0^{r_0} \psi(t)\phi(t)dt. \quad (3.8)$$

In this step, we have to deal with two cases:

First case: If $\phi'(r_0) > 0$, this contradicts the fact that the first eigenfunction of the Schrödinger equation is always decreasing i.e $\psi'(r_0) < 0$. Since we will have

$$0 < \frac{\psi(r_0)\phi'(r_0) + \epsilon \int_0^{r_0} \psi(t)\phi(t)dt}{\phi(r_0)} = \psi'(r_0) < 0. \quad (3.9)$$

Second case: If $\phi'(r_0) < 0$, we have to note first that $\phi(r)$ intersects $\psi(r)$ at r_0 , only if $\phi'(r_0)$ is greater than $\psi'(r_0)$. Now, using equation (3.8) and the fact that $\psi(r_0) = \phi(r_0)$, we can take a common factor $\psi(r_0)$ in the left hand side to get:

$$0 < (\phi'(r_0) - \psi'(r_0)) = -\frac{\epsilon \int_0^{r_0} \psi(t)\phi(t)dt}{\psi(r_0)} < 0 \quad (3.10)$$

which is a contradiction.

The other case, if $\phi(r) > \psi(r)$ for $0 < r < r_0$: since it can not be greater than $\psi(r)$ for all r , then this contradicts the fact that $0 = \int_0^\infty \psi(r)\phi(r)dr > \int_0^\infty \psi^2(r)dr > 0$ (see Theorem 3.1 (orthogonality)). Consequently, we have only to consider $\phi(r) > \psi(r)$ for $0 < r < r_0$. Using the Mean Value Theorem, there exists $0 < c < r_0$ such that $\phi'(c) = \psi'(c)$. Now similarly, integrating equation (3.7) from 0 to c , we obtain,

$$\psi(c)\phi'(c) - \phi(c)\psi'(c) = -\epsilon \int_0^c \psi(t)\phi(t)dt. \quad (3.11)$$

Since $\alpha = \phi'(c) = \psi'(c) < 0$, we get

$$\alpha(\psi(c) - \phi(c)) = -\epsilon \int_0^c \psi(t)\phi(t)dt \quad (3.12)$$

and $(\psi(c) - \phi(c)) < 0$. This implies that $\int_0^c \psi(t)\phi(t)dt < 0$ which contradicts the fact that $\psi\phi > 0$ for $0 < r < c$. This completes the proof of our main theorem. \square

Next, we will use this theorem to develop two algorithms to approximate the solution for the ground state eigenfunction and its corresponding eigenvalue. We should emphasize the fact that the monotonicity behavior of the wave function of the ground state allows us to develop these two algorithms. It can not be applied to higher eigenfunctions in this paper to approximate higher eigenvalues problems.

4. AN ITERATIVE METHOD TO CONSTRUCT A SEQUENCE CONVERGES TO THE EXACT EIGENFUNCTION AND THE EXACT EIGENVALUE

The Rayleigh-Ritz theorem is the most well-known theorem to find upper bounds for the first eigenvalue. We restrict the operator to a finite dimensional subspace, then we approximate the eigenvalues of the Hamiltonian by the eigenvalues of the constrained operator.

Now, after proving Theorem 3.3, we can state a generalized modified form for Rayleigh-Ritz theorem, where the proof can be directly deduced from the standard Rayleigh-Ritz theorem and Theorem 3.3.

Theorem 4.1 (Modified Rayleigh-Ritz Theorem). *For an arbitrary function ψ in $\mathcal{D}(H)$, the expectation value (mean value) of H in the state ψ is such that*

$$E = \frac{(\psi, H\psi)}{(\psi, \psi)} \geq E_1, \quad (4.1)$$

where the equality holds if and only if ψ is the eigenstate of H with the eigenvalue E_1 . Moreover, the corresponding solution ϕ for $H\phi = E\phi$, is a lower bound for the exact eigenfunction, i.e $\phi \leq \psi_{\text{exact}}$.

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

$$\psi = \sum_{i=1}^n c_i \phi_i, \quad (4.2)$$

the restriction of the eigenvalue problem of H to the n -dimensional subspace \mathcal{D}_n yields to a good approximate solutions for the eigenvalue problem. If $\mathcal{D}_n = \text{span}\{\phi_1, \phi_2, \dots, \phi_n\} \subset \mathcal{D}(H)$, then in a sense, we reduce the problem to a matrix problem $HC = EC$, where H is the $n \times n$ matrix $H_{ij} = (\phi_i, H\phi_j)$ with eigenvalues $\{\mathcal{E}_1, \mathcal{E}_2, \dots\}$ such that $\mathcal{E}_1 \leq \mathcal{E}_2 \dots \leq \mathcal{E}_n$. So, we obtain upper bounds using the following theorem.

Theorem 4.2 (Generalized Ritz Theorem [22]).

- (1) $E_i \leq \mathcal{E}_i^{(n)}$, $i = 1, \dots, n$ provided the E_i exist.
- (2) $\lim_{n \rightarrow \infty} \mathcal{E}_i^{(n)} = E_i$, provided $\text{span}\{\phi_n : n \in N\}$ is dense in $\mathcal{D}(H)$.

A consequent practical result from the above theorems is the convergence of the monotone sequence of solutions to the exact wave function corresponding to the ground state eigenvalue.

5. COMPUTING EIGENVALUES USING UPPER AND LOWER SOLUTIONS

Based on the previous analysis and proposed theorems, a new converging numerical criteria is proposed as follows:

Numerical Convergence criteria. The sequence of upper bounds for the first eigenvalue obtained using Ragileh-Ritz method, generate a monotone sequence of lower solutions to the exact eigenvalue problem and converges to the exact eigenfunction for Schrödinger equation.

This criteria provides us with a simple numerical technique to construct a sequence of monotone solutions for eigenvalue problems which converges to the exact solution for a wide class of potentials of interest in quantum mechanics. Having upper and lower bounds for the eigenvalues provides us with lower and upper bounds for the solutions for the eigenfunction. These results connect the spectral results obtained in quantum mechanics, such as, the envelope method, and many other variational methods. Theorems 3.3, 4.1, and 4.2 considered the first step to generate monotone sequences for the corresponding solution for Schrödinger equations.

This method combined with the envelope method is powerful and improves spectral approximation bounds for the eigenvalues see [8, 15, 16, 24]. Now, our bounds have a meaning in terms of upper and lower solution. The second algorithm is explained as follows:

Spectral Bisection Algorithm (SBA) to approximate the bottom of the spectrum of Schrödinger equation.

Input E^L and E^U : Lower and Upper bounds for the eigenvalue calculated using the envelope method or the generalized comparison theorems, or any other variational approach.

x_b : Large number to solve the problem in the given domain.

Nmax: Maximum number of iterations.

Tol: Tolerance

Step 1: $i = 1$

Step 2: While $i \leq N_{\text{max}}$ or $|E^U - E^L| > \text{Tol}$ do step 3-6

Step 3: Let $E_m = \frac{(E^L + E^U)}{2}$

Step 4: Solve the differential equation $H\phi^{(m)} = E_m\phi^{(m)}$

Step 5: If $\phi(x_b) < 0$, then $E^U = E_m$ else $E^L = E_m$

Step 6: $i = i + 1$

Step 7: If $i > N_{\text{max}}$, then Print [“Method Fail to get accurate approximation for the eigenvalue within N_{max} iterations”, $E_{\text{app}} = E_m$], else Print [$E_{\text{app}} = E_m$]

Step 8: End.

We can develop many forms of algorithms based on our new comparison theorem, where we can transform our eigenvalue problem to a simple algebraic problem.

The Spectral Bisection Algorithm always converges to the exact eigenvalue. The following theorem allows us to obtain accurate number of iterations needed to compute the eigenvalue within a given error bound.

Theorem 5.1. Suppose that $H\phi = E\phi$, where $E \in [E^L, E^U]$ is the ground state eigenvalue for Schrödinger equation in N spatial dimensions. The Spectral Bisection Algorithm generates a sequence $\{E_n\}$ approximating the exact eigenvalue with

$$|E_n - E| \leq \frac{E^U - E^L}{2^n}, \quad n \geq 1. \quad (5.1)$$

Proof. For each $n \geq 1$, we have

$$E_n^U - E_n^L = \frac{E^U - E^L}{2^{n-1}} \quad (5.2)$$

and $E \in (E_n^L, E_n^U)$. Because $E_n = \frac{E_n^L + E_n^U}{2}$ for all $n \geq 1$. Therefore,

$$|E_n - E| \leq \frac{1}{2}(E_n^U - E_n^L) = \frac{E^U - E^L}{2^n}. \quad (5.3)$$

It is clear that the generated sequence converges to the exact eigenvalue E with rate of convergence $O(1/2^n)$. \square

We can determine the number of iterations needed to approximate the ground state eigenvalue within given accuracy for wide class of problems in quantum mechanics. For the anharmonic oscillator, if $\text{Tol} = 10^{-6}$ using Theorem 5.1 with $E^L = 1$ and $E^U = 1.4$ we can iterate to approximate the eigenvalue of $-\psi''(x) + x^4\psi(x) = E\psi(x)$, where the exact eigenvalue (using the shooting method) is given by $E_x = 1.06303600$. We find that $E_{18}(\text{app}) = 1.0603622$ with absolute error less than 1.66953×10^{-6} . If we choose $x_{\text{large}} = 15$, we achieve this result after 18 steps using our algorithm. Similarly for all potentials in N spatial dimensions, with discrete spectrum, Mathematica software or any other Mathematical softwares can be used to write the above algorithm, generate and analyze these spectral properties for Schrödinger equation in quantum mechanics.

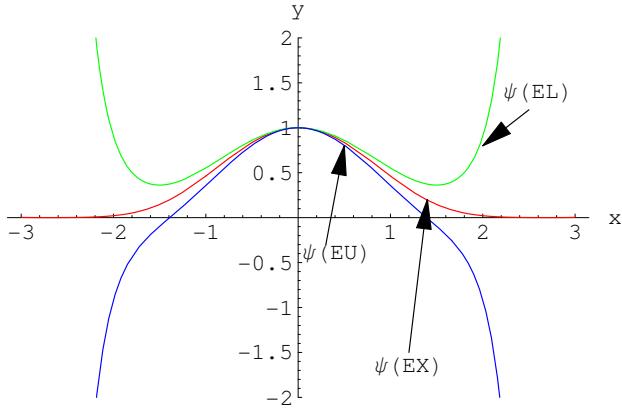


FIGURE 1. Upper and lower solutions for $-\psi''(x) + (x^2 + x^4)\psi(x) = E\psi(s)$ using the upper and lower bounds for the eigenvalues calculated using envelope method. The exact eigenvalue is $EX = 1.39235$ calculated using shooting method, $EL = 1.18226$ and $EU = 1.65098$ obtained using envelope method

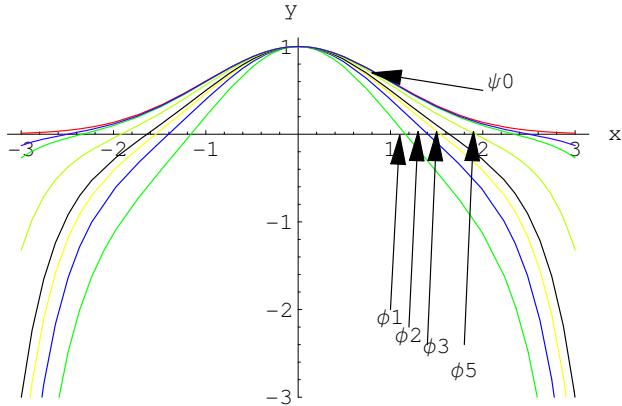


FIGURE 2. Upper solutions $\{\phi_n, n \in N\}$ for the wave function of $-\psi''(x) + x^4\psi(x) = E_0\psi(x)$ for E_0 calculated using Theorem 3.3, using $El^{(n)}$, $n \in N$ calculated using generalized Rayleigh-Ritz sequence of upper bounds in finite dimensional subspace. ψ_0 denotes the exact wave function corresponds to the bottom of the spectrum of the anharmonic oscillator

6. APPLICATIONS

Schrödinger's equations with power-law potentials have enjoyed wide attention in the literature of quantum mechanics [3, 4, 7, 8, 9, 15, 16, 17, 22, 23, 24, 25, 28, 29, 30]. We can apply this method to find a lower and upper solutions for a wide class of non-solvable problems in quantum mechanics in N spatial dimensions as well as to approximate the eigenvalue using SBA. The form for such Hamiltonian

TABLE 1. Approximation for the first eigenvalue E_1 for $-\Delta + x + x^2$. Linear potential using the second numerical Algorithm (Spectral Bisection Algorithm) as an application for the new comparison theorem. The exact eigenvalue using shooting method is $Ex = 1.52789748$. In the right column, appears $\text{Sign}(\phi^{(m)}(x_b))$.

i	E^L	$E^m = \frac{(E^U+E^L)}{2}$	E^U	Sign
1	1.0000000000000000	1.3500000000000000	1.7000000000000000	+1
2	1.3500000000000000	1.5250000000000000	1.7000000000000000	+1
3	1.5250000000000000	1.6125000000000000	1.7000000000000000	+1
4	1.5250000000000000	1.5687499999999999	1.6125000000000000	-1
5	1.5250000000000000	1.5468800000000000	1.5687499999999999	-1
6	1.5250000000000000	1.5359375000000000	1.5468750000000000	-1
10	1.5277343749999999	1.5284179687500000	1.5291015624999999	-1
15	1.527862548828124	1.527883911132812	1.52790527347499	+1
20	1.527897262573242	1.527897930145263	1.527898597717285	-1
25	1.527897471189498	1.527897492051124	1.527897512912750	+1
30	1.527897498570382	1.527897499222308	1.527897499874234	+1

is given by,

$$-\Delta\psi(r) + \sum_q a(q)r^q\psi(r) = E(q)\psi(r), \quad q > 0, \quad (6.1)$$

where $r = \|\mathbf{r}\|$, $\mathbf{r} \in \mathbb{R}^N$.

We can apply our method to find upper and lower solutions using the envelope method for anharmonic oscillator model: $-\psi''(x) + (x^2 + x^4)\psi(x) = \lambda\psi(x)$, subject to $\psi(0) = 1$ and $\psi'(0) = 0$, as we see in Figure 1. As another application for our results, we can generate a sequence of lower bounds that converges to the exact solution for a Hamiltonian of the form $-\psi''(x) + x^4\psi(x) = \lambda\psi(x)$, with the use of variational methods to obtain a sequence of upper bounds as we see in Figure 2.

Now, for a wide class of potentials studied in the literature, we can use the obtained upper and lower bounds for the eigenvalues to obtain lower and upper bounds for the corresponding solutions. Moreover, the Spectral Bisection Algorithm can be used efficiently to approximate the ground state eigenvalues for the corresponding eigenvalues, as it is clear in Table 1. Transforming our spectral problem to a problem similar to an algebraic problem, is the first step in spectral analysis to find the first eigenvalue as well eigenfunctions using simple algebraic algorithm in quantum mechanics.

Extensions and further remarks. Upper and lower sequence of solutions that converge to the exact solution for Schrödinger equation can be constructed easily using our new comparison theorem. We can use the upper and lower bounds using modified Rayleigh-Ritz theorem, envelope method to find lower and upper solutions for the first eigenfunction. This method is efficient and reliable in solving eigenvalue problems in quantum mechanics. Numerical applications and iterative methods are recognized to be useful in computing the eigenvalues and verifying the analytical results. Many applications and interesting examples can be applied and analyze the solutions of Schrödinger equations in N spatial dimensions.

In a forthcoming work, we will generalize this iterative method to approximate the eigenvalues and eigenfunctions for higher states. Moreover, we will combine the proved comparison theorems with the sum approximation [9] and the generalized Temple's bounds to develop a new algebraic approach for the eigenvalue problem.

REFERENCES

- [1] S. Breuer and D. Gottlieb; *Upper and lower bounds on solutions of initial value problems*, Journal of Mathematical Analysis and Applications, **36**, 283-300 (1971).
- [2] A. Cabada; *The method of lower and upper solutions for second, third, fourth, and higher order boundary value problem*, Journal of Mathematical Analysis and Applications, **185**, 302-320 (1994).
- [3] H. Ciftci, R. L. Hall, and Q. D. Katatbeh; *Coulomb Plus power-law potentials in quantum mechanics*, J. Phys. A, **36**, 7001-7007 (2003).
- [4] L. C. Detwiler and J. R. Klauder; *Supersingular quantum perturbations*, Phys. Rev. 11, (1975), 1436.
- [5] I. M. Gel'fand and S. V. Fomin; *Calculus of Variations*, Prentic-Hall, Englewood Cliffs, NJ, 1963.
- [6] J. R. Haddock, M. N. Nkashama; *Periodic boundary value problems and monotone iterative methods for functional differential equations*, Nonlinear Anal., **22**, 267-276 (1994).
- [7] R. L. Hall, Q. D. Katatbeh, and N. Saad; *A basis for variational calculations in d dimensions*, J. Phys. A, **37**, 11629-11644 (2004).
- [8] R. L. Hall and Q. D. Katatbeh; *Semiclassical energy formulae for power-law and log potentials in quantum mechanics*, J. Phys. A, **36**, 7173-7184 (2003).
- [9] R. L. Hall and Q. D. Katatbeh; *Generalized comparison theorems in quantum mechanics*, J. Phys. A, **35**, 8727-8742 (2002).
- [10] R. L. Hall and Q. D. Katatbeh; *Spectral bounds for the cutoff Coulomb potential*, Phys. Lett. A, **294**, 163-167 (2002).
- [11] R. L. Hall and Q. D. Katatbeh; *Spectral bounds for the Hellmann potential*, Phys. Lett. A, **287**, 183-186 (2001).
- [12] R. L. Hall; *Spectral comparison theorem for the Dirac equation*, Phys. Rev. Lett., **83**, 468-471 (1999).
- [13] R. L. Hall; *Refining the comparison theorem of quantum mechanics*, J. Phys. A, **25**, 4459-4469 (1992).
- [14] R. L. Hall and N. Saad; *Eigenvalue comparisons for quantum systems in a box*, Phys. Lett. A, **237**, 107-112 (1998).
- [15] R. L. Hall; *A geometrical theory of energy trajectories in quantum mechanics*, J. Math. Phys, **24**, 324 (1983).
- [16] R. L. Hall; *Kinetic potentials in quantum mechanics*, J. Math. Phys, **25**, 2708 (1984).
- [17] E. M. Harrell; *Singular Perturbation Potentials*, Ann. Phys. (NY), **105**, 379 (1977).
- [18] D. Jiang, Juan J. Nieto ,and W. Zuo; *On monotone method for first and second order periodic boundary value problems and periodic solutions of functional differential equations*, Journal of Mathematical Analysis and Applications, **289**, 691-699 (1985).
- [19] G. Ladde, V. Lakshmikantham, A. Vatsale; *Monotone Iterative Techniques for Nonlinear Differential Equations*, Pitman Advanced Publishing Program (1985).
- [20] W. Leighton; *Upper and lower bounds for eigenvalues*, Mathematical Analysis and Applications, **35**, 381-388 (1971).
- [21] C. V. Pao; *Accelerated monotone iterations for numerical solutions of nonlinear elliptic boundary value problems*, Computers and Mathematics with Applications, **46**, 1535-1544 (2003).
- [22] M. Reed and B. Simon; *Methods of Modern Mathematical Physics IV: Analysis of Operators*, Academic, New York, 1978. The min-max principle for the discrete spectrum is discussed on p.75.
- [23] A. K. Roy; *Calculation of the spiked harmonic oscillators through a generalized pseudospectral method*, Phys. lett. A, **321**, 231 (2004).
- [24] N. Saad, Richard L. Hall, Q. D. Katatbeh; *Study of anharmonic singular potentials*, J. Math. Phys., **46**, 022104 (2005).

- [25] Wai-Yee Keung, Eve Kovacs, and Uday P. Sukhatme; *Supersymmetry and Double-Well Potentials*, Phys. Rev. Lett., **60**, 41 (1988).
- [26] M. Yebdri, S. M. Bouguima and O. Arino; *An iterative method for functional differential equations*, Applied Mathematics and Computation, **161**, 265-269 (2005).
- [27] Q. Zhang, S. Chen and J. Lü; *Upper and lower solution method for fourth-order four-point boundary value problems*, Journal of Computational and Applied Mathematics, **196**, 387-393 (2006).
- [28] M. Znojil; *Singular potentials with quasi-exact Dirac bound states*, Phys. Lett. A, **255**, 1 (1999).
- [29] M. Znojil; *Spiked harmonic oscillators and Hill determinants*, Phys. Lett. A , **169**, 415 (1992).
- [30] M. Znojil; *Elementary bound states for the power-law potentials*, J. Phys. A: Math. Gen., **15**, 2111 (1982).

QUTAIBEH DEEB KATATBEH
DEPARTMENT OF MATHEMATICS AND STATISTICS, JORDAN UNIVERSITY OF SCIENCE AND TECHNOLOGY, IRBID, JORDAN 22110

E-mail address: qutaibeh@yahoo.com