

THE SHOOTING METHOD FOR SOLVING EIGENVALUE PROBLEMS

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ABSTRACT. The *shooting method* is a numerically effective approach to solving certain eigenvalue problems, such as that arising from the Schrödinger equation for the two-dimensional hydrogen atom with logarithmic potential function. However, no complete proof of its rationale and correctness has been given until now. This paper gives the proof, in a generalized form.

1. INTRODUCTION

One of the eigenvalue problems addressed in this paper is that derived from the Schrödinger equation for the two-dimensional hydrogen atom with logarithmic potential function. In its simplest form, this problem requires that we solve

$$\frac{d^2 R}{du^2} - \left(\frac{l^2}{4} + \sigma u e^u \right) R = 0 \quad (1)$$

(where l and σ are physical constants), subject to

$$\int_{-\infty}^{\infty} |R(u)|^2 e^u du < \infty. \quad (2)$$

The system (1)-(2) has been extensively studied, and an efficient numerical method for its solution, the **shooting method**, was introduced in [5]. Briefly, the shooting method first finds, for each λ , the solution of (1) which is bounded on the right side of the real line — that is, the solution $R_\lambda(u)$ which satisfies

$$\int_0^{\infty} |R_\lambda(u)|^2 e^u du < \infty.$$

It then finds the infinite sequence $\lambda_1 < \lambda_2 < \dots$ such that the number of zeros of $R_\lambda(u)$ jumps at each λ_i .

In [2], it is proved that every λ_i is an eigenvalue of the system (1)-(2); but the converse — that the sequence $\lambda_1 < \lambda_2 < \dots$ contains every eigenvalue of the system — was left open. This paper resolves this question affirmatively (in a more general setting), and gives examples

of the application of the shooting method to a larger class of eigenvalue problems derived from the Schrödinger equation.

Suppose $I = [a, b]$ is a closed interval, and $Q(v, \lambda)$ is defined and continuous everywhere on $(-\infty, \infty) \times I$. The **generalized eigenvalue problem** is to find all pairs (λ, R_λ) , where $\lambda \in I$ and R_λ is nontrivial and bounded, satisfying

$$\frac{d^2 R}{dv^2} = Q(v, \lambda)R, \quad (3)$$

and we will call such λ 's and corresponding R_λ 's eigenvalues and eigenfunctions of (3), respectively, under the boundedness condition.

However, since it does not make much sense to ask for solutions for arbitrary Q , in this paper we will always impose on Q one or more of three additional conditions.

- A1.** $Q(v, \lambda)$ has a continuous partial derivative with respect to λ , and $\frac{\partial Q(v, \lambda)}{\partial \lambda} \leq 0$ for all $v \in (-\infty, \infty)$ and $\lambda \in I$.
- A2.** The set $\{\lambda \in I : \frac{\partial Q(v, \lambda)}{\partial \lambda} = 0 \text{ for all } v \in (-\infty, \infty)\}$ is of measure zero.
- A3.** $\int_{-\infty}^{\infty} |v|Q_-(v, \lambda)dv < \infty$ for all $\lambda \in I$, where

$$Q_-(v, \lambda) = \begin{cases} -Q(v, \lambda) & \text{if } Q(v, \lambda) < 0; \\ 0 & \text{if } Q(v, \lambda) \geq 0. \end{cases}$$

For the sake of convenience, we will call a function defined on $(-\infty, +\infty)$ **left-bounded** if it is bounded on $(-\infty, 0]$, and **right-bounded** if it is bounded on $[0, +\infty)$. Now we are ready to state our main results.

2. MAIN RESULTS

Theorem 2.1. *If Q satisfies A3, then for every $\lambda \in I$, there exists a nontrivial right-bounded solution and a nontrivial left-bounded solution to (3), both unique up to a nonzero constant factor.*

Let $Z(\lambda)$ be the number of zeros of the right-bounded solution to (3) for $\lambda \in I$. We see from the previous theorem that $Z(\lambda)$ is well defined provided Q satisfies A3.

Theorem 2.2. *If Q satisfies A1 and A3, then every discontinuity of $Z(\lambda)$ is an eigenvalue of (3).*

Theorem 2.3. *If Q satisfies A1, A2 and A3, then every eigenvalue of (3) is a discontinuity of $Z(\lambda)$.*

Theorem 2.4. *If Q satisfies A1 and A3, then Z is nondecreasing.*

Theorem 2.4 may seem at first to be unrelated to the other three; but, as we will see later, it actually elucidates the structure of $D(Z)$, the set of all discontinuities of Z or equivalently, the eigenvalues of (3), provided Q satisfies A1, A2 and A3 (Theorems 2.2 and 2.3).

An important note: The boundedness condition we impose on the generalized eigenvalue problem is not, in general, equivalent to the square integrable condition from which (2) is derived. However, they are the same in the class of eigenvalue problems we consider here. (We will return to this point in Sec. 4.)

3. PROOFS OF THEOREMS 2.1-2.4

While not deep, the following two lemmas will be helpful.

Lemma 3.1. *Let ϕ and ψ be nontrivial solutions on $[v_0, \infty)$ to $y'' = p(v)y$ and $y'' = q(v)y$, respectively, satisfying the same initial conditions, i.e., $\phi(v_0) = \psi(v_0)$ and $\phi'(v_0) = \psi'(v_0)$. If $p(v) \leq q(v)$ and $\phi(v) > 0$ for all $v > v_0$, then*

- (i) $\frac{\psi(v)}{\phi(v)}$ is nondecreasing in v on (v_0, ∞) ;
- (ii) $\psi(v) \geq \phi(v)$ for all $v > v_0$.

Proof. The Wronskian [8, p. 39] of ϕ and ψ is $W(v) = \phi(v)\psi'(v) - \phi'(v)\psi(v)$. Differentiating, we obtain

$$\frac{dW}{dv} = \phi(v)\psi(v)[q(v) - p(v)].$$

Since $\phi(v) > 0$ for all $v > v_0$, either $\psi(v_0) = \phi(v_0) > 0$ or $\psi(v_0) = 0$ and $\psi'(v_0) = \phi'(v_0) > 0$. If $\psi(v)$ has a non-positive value at some $v > v_0$, it must have at least one zero in (v_0, ∞) . Let a be its smallest zero in (v_0, ∞) . It is easy to derive $\psi'(a) < 0$ and $\psi(v) > 0$ for all $v_0 < v < a$. Then $W'(v) \geq 0$ for all $v_0 < v < a$. But $W(v_0) = 0$ and $W(a) = \phi(a)\psi'(a) < 0$, a contradiction. So $\psi(v) > 0$ for all $v > v_0$. Then $W'(v) \geq 0$ and $W(v) \geq 0$ for all $v > v_0$. So

$$\frac{\psi'(v)}{\psi(v)} \geq \frac{\phi'(v)}{\phi(v)}$$

if $v > v_0$. Integrating both sides yields

$$\log[\psi(v)] - \log[\psi(v_1)] \geq \log[\phi(v)] - \log[\phi(v_1)],$$

where $v > v_1 > v_0$, and so $\frac{\psi(v)}{\phi(v)} \geq \frac{\psi(v_1)}{\phi(v_1)}$ for all $v > v_1 > v_0$. Then since $\lim_{v_1 \rightarrow v_0} \frac{\psi(v_1)}{\phi(v_1)} = 1$, we get $\psi(v) \geq \phi(v)$ for all $v > v_0$. \square

Lemma 3.2. *Let $q(v)$ be a non-positive continuous function defined on $[v_0, \infty)$ which satisfies $\int_{v_0}^{\infty} |(v - v_0)q(v)|dv < 1$ and let $R(v)$ be the solution to $R'' = q(v)R$ satisfying the initial conditions $R(v_0) = 0$ and $R'(v_0) = 1$. Then*

$$k(v - v_0) \leq R(v) \leq (v - v_0) \text{ for all } v > v_0,$$

where $k = 1 - \int_{v_0}^{\infty} |(v - v_0)q(v)|dv$.

Proof. Let (v_0, a) be the greatest interval in which $R(v)$ is positive. Since $R'(v_0) = 1$, we must have $v_0 < a$. It is easy to see $R'(v) \leq 1$ if $v \in (v_0, a)$ since $R'' \leq 0$ on (v_0, a) ; thus $|R(v)| \leq v - v_0$ if $v \in [v_0, a]$. Therefore

$$\begin{aligned} R'(v) &= R'(v_0) + \int_{v_0}^v q(t)R(t)dt \\ &\geq 1 - \int_{v_0}^{\infty} |(v - v_0)q(v)|dv = k \end{aligned}$$

if $v \in (v_0, a)$. So $k(v - v_0) \leq R(v) \leq v - v_0$ for all $v \in (v_0, a)$. It is then clear that a must be ∞ . \square

Suppose Q satisfies A3. For every $\lambda \in I$, there exists a positive number $v_0 = v_0(\lambda)$ such that

$$\int_{v_0}^{\infty} vQ_-(v, \lambda)dv < \frac{1}{2}.$$

Let F_λ and G_λ be the solutions to (3) satisfying the initial conditions $F_\lambda(v_0) = 1$, $F'_\lambda(v_0) = 0$ and $G_\lambda(v_0) = 0$, $G'_\lambda(v_0) = 1$, respectively. Compare G_λ with g_λ , the solution to

$$\frac{d^2R}{dv^2} = -Q_-(v, \lambda)R$$

satisfying the initial conditions $g_\lambda(v_0) = 0$, $g'_\lambda(v_0) = 1$.

Since $\int_{v_0}^{\infty} (v - v_0)Q_-(v, \lambda)dv \leq \int_{v_0}^{\infty} vQ_-(v, \lambda)dv \leq \frac{1}{2}$, we have (from Lemma 3.2)

$$\frac{v - v_0}{2} \leq g_\lambda(v) \leq v - v_0 \text{ for all } v > v_0,$$

and also (from Lemma 3.1)

$$\frac{v - v_0}{2} \leq g_\lambda(v) \leq G_\lambda(v) \text{ for all } v > v_0 \text{ and } \lambda \in I.$$

Thus $\int_v^\infty G_\lambda^{-2}(w)dw < \infty$ for all $v > v_0$. Now define

$$R_\lambda(v) = G_\lambda(v) \int_v^\infty G_\lambda^{-2}(w)dw \text{ for } v \in (v_0, \infty).$$

From Lemma 3.1,

$$\frac{G_\lambda(v_2)}{g_\lambda(v_2)} \geq \frac{G_\lambda(v_1)}{g_\lambda(v_1)} \geq 1 \text{ for all } v_2 > v_1 > v_0.$$

Therefore

$$\frac{\int_v^\infty g_\lambda^{-2}(w)dw}{\int_v^\infty G_\lambda^{-2}(w)dw} \geq \frac{G_\lambda^2(v)}{g_\lambda^2(v)} \geq \frac{G_\lambda(v)}{g_\lambda(v)} \geq 1 \text{ for all } v > v_0,$$

and thus

$$\begin{aligned} R_\lambda(v) &= G_\lambda(v) \int_v^\infty G_\lambda^{-2}(w)dw \\ &\leq g_\lambda(v) \int_v^\infty g_\lambda^{-2}(w)dw \\ &\leq (v - v_0) \int_v^\infty \frac{4}{(t - v_0)^2} dt = 4, \text{ for all } v > v_0, \end{aligned}$$

namely, R_λ is right-bounded. It is not difficult to check that R_λ is a solution to (3) on (v_0, ∞) . Extending it to a solution on all of \mathbb{R} , we get a right-bounded solution to (3). Consequently, to every $\lambda \in I$ there corresponds a nontrivial right-bounded solution to (3). On the other hand, suppose that S_λ is a right-bounded solution to (3). Let $S_\lambda(v) = c_1 F_\lambda(v) + c_2 G_\lambda(v)$. Obviously, $c_1 \neq 0$. Since S_λ is right-bounded and $G_\lambda(v) \rightarrow \infty$ as $v \rightarrow \infty$, $\lim_{v \rightarrow \infty} \frac{S_\lambda(v)}{G_\lambda(v)} = 0$. So $\lim_{w \rightarrow \infty} \frac{F_\lambda(w)}{G_\lambda(w)}$ exists and has

the value $-c_2/c_1$. Therefore, $S_\lambda(v) = c_1 \left[F_\lambda(v) - G_\lambda(v) \lim_{w \rightarrow \infty} \frac{F_\lambda(w)}{G_\lambda(w)} \right]$ and the right-bounded solution to (3) is unique up to a nonzero constant factor. Symmetrically, we can draw the same conclusions regarding left-bounded solutions of (3), and we have Theorem 2.1.

Let $T_\lambda(v) = F_\lambda(v) - G_\lambda(v) \lim_{w \rightarrow \infty} \frac{F_\lambda(w)}{G_\lambda(w)}$. Note that $Z(\lambda)$ is the number of zeros of T_λ . Obviously, T_λ and G_λ are linearly independent, so every solution of (3) can be expressed as their linear sum. The next lemma follows immediately.

Lemma 3.3. *Suppose Q satisfies A3, and let R and S be two nontrivial solutions of (3) for a fixed λ . If $R(v)$ is not right-bounded, then*

- (i) $|R(v)|$ tends to infinity as $v \rightarrow +\infty$;
- (ii) $\lim_{v \rightarrow +\infty} \frac{S(v)}{R(v)}$ exists;
- (iii) $\lim_{v \rightarrow +\infty} \frac{S(v)}{R(v)} = 0$ if and only if $S(v)$ is right-bounded.

Further, the above implication remains true if, throughout, “right-bounded” is changed to “left-bounded”, and $+\infty$ is changed to $-\infty$.

Although we have introduced the function Z , we cannot take it for granted that Z is a finite function everywhere. But if Q satisfies A3 then, since G_λ has finitely many zeros in $[0, \infty)$, according to Sturm’s Separation Theorem [3, p. 223] T_λ must have finitely many zeros in $[0, \infty)$, too; symmetrically, T_λ has finitely many zeros in $(-\infty, 0]$. In summary, Z is finite everywhere in I provided Q satisfies A3.

Notice that the choice of v_0 depends on λ in our arguments. It is hard to obtain properties of F_λ , G_λ and T_λ as functions of λ . However, if Q satisfies both A1 and A3, we can choose a constant $v_0 > 0$ such that

$$\int_{v_0}^{\infty} vQ_-(v, \lambda)dv < \frac{1}{2} \text{ for all } \lambda \in I = [a, b],$$

and in fact, we can simply choose $v_0 > 0$ such that

$$\int_{v_0}^{\infty} vQ_-(v, b)dv < \frac{1}{2}.$$

Since for every fixed v , $Q(v, \lambda)$ is a nonincreasing function of $\lambda \in I$, it must be that $Q_-(v, \lambda)$ is nondecreasing in λ . Consequently, for all $\lambda \in I$,

$$\int_{v_0}^{\infty} vQ_-(v, \lambda)dv \leq \int_{v_0}^{\infty} vQ_-(v, b)dv < \frac{1}{2}.$$

Lemma 3.4. *If Q satisfies A1 and A3, and v_0 , F_λ and G_λ are chosen and defined as above, then the function $\lim_{v \rightarrow \infty} \frac{F_\lambda(v)}{G_\lambda(v)}$ is continuous for all $\lambda \in I$.*

Proof. Since

$$\frac{d[F_\lambda(v)/G_\lambda(v)]}{dv} = -\frac{1}{G_\lambda^2(v)} < 0 \text{ for } G_\lambda(v) \neq 0, \quad (4)$$

we have

$$\left| \frac{F_\lambda(v_2)}{G_\lambda(v_2)} - \frac{F_\lambda(v_1)}{G_\lambda(v_1)} \right| \leq 4 \left(\frac{1}{v_1 - v_0} - \frac{1}{v_2 - v_0} \right)$$

for all $\lambda \in I$ and $v_2 > v_1 > v_0$. Thus $\frac{F_\lambda(v)}{G_\lambda(v)}$ converges uniformly with respect to λ as $v \rightarrow \infty$. Since $\frac{F_\lambda(v)}{G_\lambda(v)}$ is a continuous function of λ for every fixed $v > v_0$ [7, p. 94, Theorem 2.1], it then follows that $\lim_{v \rightarrow \infty} \frac{F_\lambda(v)}{G_\lambda(v)}$ is a continuous function of λ . \square

The following lemma shows a kind of stability for unbounded solutions of (3).

Lemma 3.5. *Let Q satisfy A1 and A3, and $R_\lambda(v, x, y)$ denote the solution to (3) satisfying $R_\lambda(a) = x$ and $R'_\lambda(a) = y$, where a is a constant. If $|R_\lambda(v, x, y)| \rightarrow \infty$ as $v \rightarrow \infty$ at a certain point $(\lambda, x, y) = (\lambda_0, x_0, y_0)$, then there exist a number v_1 and a neighborhood O of (λ_0, x_0, y_0) in \mathbb{R}^3 such that $R_\lambda(v, x, y) \neq 0$ for all $v \geq v_1$ and $|R_\lambda(v, x, y)| \rightarrow \infty$ as $v \rightarrow \infty$, when $(\lambda, x, y) \in O$. Symmetrically, if $|R_\lambda(v, x, y)| \rightarrow \infty$ as $v \rightarrow -\infty$ at a certain point $(\lambda, x, y) = (\lambda_0, x_0, y_0)$, then there exist a number v_1 and a neighborhood O of (λ_0, x_0, y_0) in \mathbb{R}^3 such that $R_\lambda(v, x, y) \neq 0$ for all $v \leq v_1$ and $|R_\lambda(v, x, y)| \rightarrow \infty$ as $v \rightarrow -\infty$, when $(\lambda, x, y) \in O$.*

Proof. Without loss of generality, we suppose $R_{\lambda_0}(v, x_0, y_0) \rightarrow \infty$ as $v \rightarrow \infty$. Choose $v_1 > 0$ such that $R_{\lambda_0}(v, x_0, y_0) > 0$ for all $v \geq v_1$ and $\int_{v_1}^{\infty} v Q_-(v, b) dv < 1/2$. Let $P_\lambda(v)$ and $S_\lambda(v)$ be the solutions to (3) with the initial conditions $P_\lambda(v_1) = 1$, $P'_\lambda(v_1) = 0$ and $S_\lambda(v_1) = 0$, $S'_\lambda(v_1) = 1$, respectively. Obviously, P_λ and S_λ have the same properties as we described before for F_λ and G_λ . Observe that

$$\frac{R_\lambda(v, x, y)}{S_\lambda(v)} = R_\lambda(v_1, x, y) \frac{P_\lambda(v)}{S_\lambda(v)} + R'_\lambda(v_1, x, y),$$

where $R_\lambda(v_1, x, y)$ and $R'_\lambda(v_1, x, y)$ are continuous functions of (λ, x, y) .

According to Lemma 3.4, $\lim_{v \rightarrow \infty} \frac{P_\lambda(v)}{S_\lambda(v)}$ is a continuous function of λ .

So $\lim_{v \rightarrow \infty} \frac{R_\lambda(v, x, y)}{S_\lambda(v)}$ is a continuous function of (λ, x, y) . By Lemma 3.3, $\lim_{v \rightarrow \infty} \frac{R_{\lambda_0}(v, x_0, y_0)}{S_{\lambda_0}(v)} > 0$. Thus there exists a neighborhood O of (λ_0, x_0, y_0) in which

$$\lim_{v \rightarrow \infty} \frac{R_\lambda(v, x, y)}{S_\lambda(v)} > 0 \text{ and } R_\lambda(v_1, x, y) > 0.$$

So $R_\lambda(v, x, y) \rightarrow \infty$ as $v \rightarrow \infty$ when $(\lambda, x, y) \in O$. And according to formula (4), $P_\lambda(v)/S_\lambda(v)$ is a decreasing function of $v > v_1$. Since

$R_\lambda(v_1, x, y) > 0$ for $(\lambda, x, y) \in O$, $R_\lambda(v, x, y)/S_\lambda(v)$ is also a decreasing function of $v > v_1$ when $(\lambda, x, y) \in O$. So

$$\frac{R_\lambda(v, x, y)}{S_\lambda(v)} > \lim_{v \rightarrow \infty} \frac{R_\lambda(v, x, y)}{S_\lambda(v)} > 0 \text{ for all } v > v_1 \text{ and } (\lambda, x, y) \in O.$$

Thus $R_\lambda(v, x, y) \neq 0$ for all $v \geq v_1$ when $(\lambda, x, y) \in O$. \square

Now we can prove Theorem 2.2.

Proof of Theorem 2.2. It suffices to prove that no λ for which T_λ is unbounded can belong to $D(Z)$, the set of discontinuities of function Z . Let T_{λ_0} be unbounded. By Lemma 3.3, $|T_\lambda(v)| \rightarrow \infty$ as $v \rightarrow -\infty$. Since $T_\lambda(v_0) = 1$ and $T'_\lambda(v_0) = -\lim_{v \rightarrow \infty} \frac{F_\lambda(v)}{G_\lambda(v)}$, where the latter is continuous with respect to λ , by Lemma 3.5, there must be a neighborhood O_1 of λ_0 and a number v_1 such that $T_\lambda(v) \neq 0$ for all $\lambda \in O_1$ and $v \leq v_1$. According to formula (4), $T_\lambda(v) > 0$ if $v > v_0$. Thus all the zeros of T_λ must lie in $[v_1, v_0]$ when $\lambda \in O_1$. According to the continuity of $T_\lambda(v)$ as a function of $(\lambda, v) \in I \times [v_1, v_0]$, there is a neighborhood O_2 of λ_0 in which all the T_λ have the same number of zeros on $[v_1, v_2]$ as $\lambda \in O_2$. Therefore, all the T_λ , for $\lambda \in O_1 \cap O_2$, have the same number of zeros, so $Z(\lambda)$ is continuous at λ_0 . \square

The shooting method produces all the eigenvalues and eigenfunctions of (3) only if the converse of Theorem 2.2 holds. The converse, however, is not necessarily true if no additional conditions are imposed on Q other than A1 and A3. A counterexample can be simply constructed by letting

$$Q(v, \lambda) = 4v^2 - 2, \quad v \in (-\infty, \infty) \text{ and } \lambda \in [-1, 1].$$

Obviously, Q satisfies A1 and A3, and it is easy to check that $T_\lambda(v) = e^{-v^2}$ are bounded solutions of (3) for all $\lambda \in [-1, 1]$, but $Z = 0$ has no discontinuities. Nevertheless, we can prove the converse if A2 is added, which is Theorem 2.3.

The next lemma follows immediately from Theorem 2.1 and Lemma 3.3.

Lemma 3.6. *Let Q satisfy A3 and F_λ , G_λ and T_λ be defined as above.*

Then T_λ is bounded if and only if $\lim_{v \rightarrow -\infty} \frac{F_\lambda(v)}{G_\lambda(v)} = \lim_{v \rightarrow \infty} \frac{F_\lambda(v)}{G_\lambda(v)}$.

The following equality is extremely important, since it reveals some essential properties of the system (3).

Lemma 3.7. *Suppose Q satisfies A1 and A3, and v_0 , F_λ and G_λ are chosen and defined as above; then for $G_\lambda(v) \neq 0$, $\frac{\partial[F_\lambda(v)/G_\lambda(v)]}{\partial\lambda}$ exists and has the value*

$$\frac{\partial[F_\lambda(v)/G_\lambda(v)]}{\partial\lambda} = \int_{v_0}^v \frac{\partial Q(s, \lambda)}{\partial\lambda} \left[F_\lambda(s) - G_\lambda(s) \frac{F_\lambda(v)}{G_\lambda(v)} \right]^2 ds. \quad (5)$$

Proof. Since $\partial Q(s, \lambda)/\partial\lambda$ is continuous, $z(v) = \partial F_\lambda(v)/\partial\lambda$ exists and is the solution to

$$\frac{d^2 z}{dv^2} - Q(v, \lambda)z = \frac{\partial Q(v, \lambda)}{\partial\lambda} F_\lambda(v)$$

satisfying the initial conditions $z(v_0) = z'(v_0) = 0$ [7, p. 95]; thus

$$\frac{\partial F_\lambda(v)}{\partial\lambda} = \int_{v_0}^v \frac{\partial Q(s, \lambda)}{\partial\lambda} F_\lambda(s) [F_\lambda(s)G_\lambda(v) - F_\lambda(v)G_\lambda(s)] ds.$$

Similarly,

$$\frac{\partial G_\lambda(v)}{\partial\lambda} = \int_{v_0}^v \frac{\partial Q(s, \lambda)}{\partial\lambda} G_\lambda(s) [F_\lambda(s)G_\lambda(v) - F_\lambda(v)G_\lambda(s)] ds.$$

By a straightforward calculation, we get (5). \square

Lemma 3.8. *If Q satisfies A1 and A3 and λ_0 is an eigenvalue of (3) under the boundedness condition then,*

- (i) *there exists a neighborhood O of λ_0 in which $Z(\lambda) = Z(\lambda_0)$ if $\lambda < \lambda_0$ and $Z(\lambda) \geq Z(\lambda_0)$ if $\lambda > \lambda_0$;*
- (ii) *in addition, if Q satisfies A2, O can be chosen such that $Z(\lambda) = Z(\lambda_0) + 1$ if $\lambda > \lambda_0$ and $\lambda \in O$.*

Proof. First, observe that λ_0 is an eigenvalue of (3) under the boundedness condition if and only if T_{λ_0} is bounded. Theorem 2.1 and Lemma 3.3 imply that $|G_{\lambda_0}(v)| \rightarrow \infty$ as $v \rightarrow -\infty$. Without loss of generality, suppose $G_{\lambda_0}(v) \rightarrow \infty$ as $v \rightarrow -\infty$. Then according to Lemma 3.5, there exist a number $v_1 < v_0$ and a neighborhood O_1 of λ_0 in which $G_\lambda(v) \rightarrow \infty$ as $v \rightarrow -\infty$ and $G_\lambda(v) > 0$ for all $v \leq v_1$.

Formula (5) shows that as a function of λ , $F_\lambda(v)/G_\lambda(v)$ is nondecreasing for a fixed $v \leq v_1$ and nonincreasing for a fixed $v > v_0$. Therefore,

$$\lim_{v \rightarrow -\infty} \frac{F_\lambda(v)}{G_\lambda(v)} \leq \lim_{v \rightarrow -\infty} \frac{F_{\lambda_0}(v)}{G_{\lambda_0}(v)}, \quad \text{and} \quad \lim_{v \rightarrow \infty} \frac{F_\lambda(v)}{G_\lambda(v)} \geq \lim_{v \rightarrow \infty} \frac{F_{\lambda_0}(v)}{G_{\lambda_0}(v)}$$

for all $\lambda \leq \lambda_0$ and $\lambda \in O_1$. And by Lemma 3.6,

$$\lim_{v \rightarrow -\infty} \frac{F_{\lambda_0}(v)}{G_{\lambda_0}(v)} - \lim_{v \rightarrow \infty} \frac{F_{\lambda_0}(v)}{G_{\lambda_0}(v)} = 0.$$

Thus,

$$\lim_{v \rightarrow -\infty} \frac{F_\lambda(v)}{G_\lambda(v)} - \lim_{v \rightarrow \infty} \frac{F_\lambda(v)}{G_\lambda(v)} \leq 0 \text{ for all } \lambda \leq \lambda_0 \text{ and } \lambda \in O_1.$$

According to (4),

$$\begin{aligned} T_\lambda(v) &= G_\lambda(v) \left[\frac{F_\lambda(v)}{G_\lambda(v)} - \lim_{v \rightarrow \infty} \frac{F_\lambda(v)}{G_\lambda(v)} \right] \\ &< G_\lambda(v) \left[\lim_{v \rightarrow -\infty} \frac{F_\lambda(v)}{G_\lambda(v)} - \lim_{v \rightarrow \infty} \frac{F_\lambda(v)}{G_\lambda(v)} \right] \\ &\leq 0 \text{ for all } v \leq v_1, \lambda \in O_1, \lambda \leq \lambda_0. \end{aligned}$$

And since $T_\lambda(v) > 0$ for $v > v_0$, all zeros of T_λ lie in $[v_1, v_0]$ when $\lambda \in O_1$ and $\lambda \leq \lambda_0$. By the continuity of $T_\lambda(v)$ at $(\lambda, v) \in I \times [v_1, v_0]$, there is a neighborhood $O \subset O_1$ of λ_0 such that $T_\lambda(v)$ has the same number of zeros in $[v_1, v_0]$ and $T_\lambda(v_1) < 0$ for all $\lambda \in O$. Then part (i) is obvious.

For $\lambda \in O$ and $\lambda > \lambda_0$, with (5) we have

$$\begin{aligned} &\lim_{v \rightarrow -\infty} \frac{F_\lambda(v)}{G_\lambda(v)} - \lim_{v \rightarrow -\infty} \frac{F_{\lambda_0}(v)}{G_{\lambda_0}(v)} \\ &= \lim_{v \rightarrow -\infty} \int_{\lambda_0}^\lambda \int_v^{v_0} -\frac{\partial Q(s, t)}{\partial t} \left[F_t(s) - G_t(s) \frac{F_t(v)}{G_t(v)} \right]^2 ds dt. \end{aligned}$$

Since $-\frac{\partial Q(s, t)}{\partial t} \left[F_t(s) - G_t(s) \frac{F_t(v)}{G_t(v)} \right]^2 \geq 0$ when $t \in O$ and $v \leq v_1$, according to Fatou's Lemma [1, p. 131],

$$\begin{aligned} &\lim_{v \rightarrow -\infty} \frac{F_\lambda(v)}{G_\lambda(v)} - \lim_{v \rightarrow -\infty} \frac{F_{\lambda_0}(v)}{G_{\lambda_0}(v)} \\ &\geq \int_{\lambda_0}^\lambda \left\{ \lim_{v \rightarrow -\infty} \int_v^{v_0} -\frac{\partial Q(s, t)}{\partial t} \left[F_t(s) - G_t(s) \frac{F_t(v)}{G_t(v)} \right]^2 ds \right\} dt \\ &\geq \int_{\lambda_0}^\lambda \int_{-\infty}^{v_0} -\frac{\partial Q(s, t)}{\partial t} \left[F_t(s) - G_t(s) \lim_{v \rightarrow -\infty} \frac{F_t(v)}{G_t(v)} \right]^2 ds dt \end{aligned}$$

when $\lambda \in O$ and $\lambda > \lambda_0$. Similarly, we can prove

$$\begin{aligned} &\lim_{v \rightarrow \infty} \frac{F_\lambda(v)}{G_\lambda(v)} - \lim_{v \rightarrow \infty} \frac{F_{\lambda_0}(v)}{G_{\lambda_0}(v)} \\ &\leq \int_{\lambda_0}^\lambda \int_{v_0}^\infty \frac{\partial Q(s, t)}{\partial t} \left[F_t(s) - G_t(s) \lim_{v \rightarrow \infty} \frac{F_t(v)}{G_t(v)} \right]^2 ds dt \end{aligned}$$

when $\lambda \in O$ and $\lambda > \lambda_0$. Therefore,

$$\begin{aligned} & \lim_{v \rightarrow -\infty} \frac{F_\lambda(v)}{G_\lambda(v)} - \lim_{v \rightarrow \infty} \frac{F_\lambda(v)}{G_\lambda(v)} \\ & \geq \int_{\lambda_0}^\lambda \left\{ \int_{-\infty}^{v_0} -\frac{\partial Q(s,t)}{\partial t} \left[F_t(s) - G_t(s) \lim_{v \rightarrow -\infty} \frac{F_t(v)}{G_t(v)} \right]^2 ds \right. \\ & \quad \left. - \int_{v_0}^\infty \frac{\partial Q(s,t)}{\partial t} \left[F_t(s) - G_t(s) \lim_{v \rightarrow \infty} \frac{F_t(v)}{G_t(v)} \right]^2 ds \right\} dt \geq 0 \end{aligned}$$

when $\lambda \in O$ and $\lambda > \lambda_0$. If $Q(v, \lambda)$ satisfies A2, the equality can never hold, that is,

$$\lim_{v \rightarrow -\infty} \frac{F_\lambda(v)}{G_\lambda(v)} - \lim_{v \rightarrow \infty} \frac{F_\lambda(v)}{G_\lambda(v)} > 0$$

when $\lambda \in O$ and $\lambda > \lambda_0$. Thus $T_\lambda(v) \rightarrow \infty$ as $v \rightarrow -\infty$ when $\lambda \in O$ and $\lambda > \lambda_0$. Since $T_\lambda(v_1) < 0$ and $\frac{F_\lambda(v)}{G_\lambda(v)} - \lim_{v \rightarrow \infty} \frac{F_\lambda(v)}{G_\lambda(v)}$ is decreasing in v for a fixed $\lambda \in O$ by formula (4), T_λ must have exactly one zero in (∞, v_1) when $\lambda \in O$ and $\lambda > \lambda_0$. Part (ii) follows immediately. \square

Lemma 3.8 directly implies Theorem 2.3; and it further implies Theorem 2.4, as follows.

Proof of Theorem 2.4. If Z is not a nondecreasing function then, since Z is integer-valued, there is some $\lambda_0 \in \mathbb{R}$ at which Z is discontinuous. So T_{λ_0} is bounded (see Theorem 2.2). But this contradicts (i) of Lemma 3.8. \square

Theorem 2.4 reveals the structure of $D(Z)$, or equivalently, the eigenvalues of (3) under the boundedness condition, when Q satisfies A1, A2, and A3; $D(Z)$ must be composed of $\lambda_n = \sup\{\lambda : T_\lambda \text{ has } n - 1 \text{ zeros}\}$, where $Z(a) < n \leq Z(b)$. Therefore Z has only a finite number of discontinuities in $I = [a, b]$.

4. APPLICATIONS TO THE SCHRÖDINGER EQUATION

In this section, we apply the shooting method to the radial equation associated with the n -dimensional Schrödinger equation with spherically symmetric potential function

$$\frac{d^2 R_0}{dr^2} + \left(\frac{n-1}{r} \right) \frac{dR_0}{dr} + \left(c[\lambda - V(r)] + \frac{k_n(l)}{r^2} \right) R_0 = 0 \quad (6)$$

subject to

$$\int_0^\infty |R_0(r)|^2 r^{n-1} dr < \infty. \quad (7)$$

(In the above, l is the angular number, $k_n(l)$ denotes the l th eigenvalue of the Laplace-Beltrami operator corresponding to the sphere in n -dimensional space, and $c > 0$ is a constant; see [9, Vol. 2, pp. 160-161].) Setting $r = e^{v/n}$ and $R_0(e^{v/n}) = e^{(1/n-1/2)v} R(v)$ in (6) and (7), yields

$$\frac{d^2 R}{dv^2} = \left(\frac{c}{n^2} [V(e^{v/n}) - \lambda] e^{2v/n} - \frac{k_n(l)}{n^2} + \left(\frac{1}{2} - \frac{1}{n} \right)^2 \right) R \quad (8)$$

and

$$\int_{-\infty}^\infty |R(v)|^2 e^{2v/n} dv < \infty. \quad (9)$$

We pause the general discussion to give three typical examples. (Positive physical coefficients in the potential functions are ignored).

Example 4.1. Setting $n = 2$ and $V(r) = \log r$ gives the equation of the two-dimensional hydrogen atom with logarithmic potential function mentioned at the beginning

$$\frac{d^2 R}{dv^2} = \left[\frac{l^2}{4} + c \left(\frac{v}{2} - \lambda \right) e^v \right] R \quad (10)$$

subject to

$$\int_{-\infty}^\infty |R(v)|^2 e^v dv < \infty. \quad (11)$$

To see that the system (10)-(11) is equivalent to (1)-(2), it suffices to make the substitution $v = u + 2\lambda$ and set $\sigma = ce^{2\lambda}/2$.

Example 4.2. The familiar three-dimensional hydrogen atom with the Coulomb potential, i.e. $n = 3$ and $V(r) = -1/r$, was discussed via the shooting method in [4],

$$\frac{d^2 R}{dv^2} = \left(\frac{c}{9} (-e^{-v/3} - \lambda) e^{2v/3} + \frac{l(l+1)}{9} + \frac{1}{36} \right) R \quad (12)$$

subject to $\int_{-\infty}^\infty |R(v)|^2 e^{2v/3} dv < \infty$.

Example 4.3. Again in [4], the shooting method was used to study the three-dimensional Schrödinger equation with isotropic harmonic

oscillator potential function. In this case ($n = 3$ and $V(r) = r^2$), the system is

$$\frac{d^2R}{dv^2} = \left(\frac{c}{9}(e^{2v/3} - \lambda)e^{2v/3} + \frac{l(l+1)}{9} + \frac{1}{36} \right) R \quad (13)$$

subject to $\int_{-\infty}^{\infty} |R(v)|^2 e^{2v/3} dv < \infty$.

Let us return now to the general case. Note that if $V(r)$ is continuous on $r \in (0, \infty)$, then

$$Q(v, \lambda) = \frac{c}{n^2} [V(e^{v/n}) - \lambda] e^{2v/n} - \frac{k_n(l)}{n^2} + \left(\frac{1}{2} - \frac{1}{n} \right)^2$$

satisfies both A1 and A2. To ensure that A3 holds, we will consider continuous potential functions satisfying the following conditions.

A4. $\lim_{v \rightarrow \infty} V(e^{v/n}) = \sup V(e^{v/n}) = M$, where M may be ∞ . If M is finite, then for all $\lambda \geq M$, there exists v_0 such that $Q(v, \lambda)$ is negative and has a negative partial derivative with respect to v when $v > v_0$.

A5. $\int_{-\infty}^0 |vQ_-(v, 0)| dv < \infty$.

Obviously, both A4 and A5 are satisfied in Examples 4.1, 4.2 and 4.3.

The next theorem implies the well-known fact that all eigenvalues in Example 4.2 are negative [11].

Theorem 4.1. *If $V(r)$ is continuous for $r \in (0, \infty)$ and satisfies A4, then all eigenvalues of the system (8) and (9) lie in the interval $(-\infty, M)$.*

Proof. It is trivial for $M = \infty$. Suppose that M is finite. If there is an eigenvalue $\lambda \geq M$ of (8) and (9), let R be a corresponding eigen-solution. Since $-Q(v, \lambda)$ is positive and increasing when $v > v_0$, by Sturm's Separation Theorem [3, p. 223], it is easy to see that R has a sequence of zeroes, say v_n , which approaches ∞ .

Since

$$\frac{d\{-Q(v, \lambda)R^2(v) + [R'(v)]^2\}}{dv} = -\frac{\partial Q(v, \lambda)}{\partial v} R^2(v)$$

and $\partial Q(v, \lambda)/\partial \lambda < 0$ when $v > v_0$, it is easy to show that

$$\int_0^{\infty} [R'(v)]^2 dv - \int_0^{\infty} Q(v, \lambda) R^2(v) dv = \infty.$$

On the other hand,

$$\begin{aligned} \int_0^{v_n} Q(v, \lambda) R^2(v) dv &= \int_0^{v_n} R(v) R''(v) dv \\ &= - \int_0^{v_n} [R'(v)]^2 dv - R(0) R'(0). \end{aligned}$$

Since $v_n \rightarrow \infty$ as $n \rightarrow \infty$, it is easy to deduce $\int_0^\infty -Q(v, \lambda) R^2(v) dv = \infty$. Clearly, there exists a constant $k > 0$ such that $-Q(v, \lambda) < k e^{2v/n}$ when v is large enough, and therefore $\int_0^\infty R^2(v) e^{2v/n} dv = \infty$, a contradiction. \square

It is not difficult to obtain the following theorem.

Theorem 4.2. *If V is continuous and satisfies both A4 and A5, then the corresponding $Q(v, \lambda)$ satisfies A3 on every closed interval $\lambda \in I \subset (-\infty, M)$.*

If $V(r)$ satisfies both A4 and A5, then the shooting method can be applied to find all the eigenvalues and eigensolutions of the system consisting of (8) and the boundedness condition that $R_\lambda(v)$ is bounded on $(-\infty, \infty)$. The next result shows the relationship between this eigenvalue problem and the one consisting of (8) and (9).

Theorem 4.3. *Let V be continuous and satisfy both A4 and A5; then every bounded solution of (8) also satisfies (9).*

Proof. Let T_λ be any nontrivial bounded solution of (8). Obviously,

$$\int_{-\infty}^0 |T_\lambda(v)|^2 e^{2v/n} dv < \infty.$$

Since $\lambda < M$, $Q(v, \lambda) \rightarrow \infty$ as $v \rightarrow \infty$. So there exists a number v_0 such that $Q(v, \lambda) > 4$ for all $v > v_0$. Let F_λ be the solution of (8) satisfying the initial conditions $F_\lambda(v_0) = 1$ and $F'_\lambda(v_0) = 0$. Clearly, $F_\lambda(v) > 0$ and $F'_\lambda(v) > 0$ for all $v > v_0$. Applying Lemma 3.1 by comparing (8) with $R'' = 4R$, we get

$$\begin{aligned} F_\lambda(s) &\geq F_\lambda(v) \frac{e^{2(s-v_0)} + e^{-2(s-v_0)}}{e^{2(v-v_0)} + e^{-2(v-v_0)}} \\ &> F_\lambda(v) \frac{e^{2(s-v)}}{2} \text{ for all } s > v \geq v_0. \end{aligned}$$

Without loss of generality, we may suppose $T_\lambda(v_0) = \int_{v_0}^\infty F_\lambda^{-2}(v) dv$. It is not difficult to see that $T_\lambda(v) = F_\lambda(v) \int_v^\infty F_\lambda^{-2}(s) ds$ for all $v \geq v_0$. Therefore, $T_\lambda(v) < 1/F_\lambda(v) < 2e^{2(v_0-v)}$ for all $v \geq v_0$. So (9) must hold for $R(v) = T_\lambda(v)$. \square

The shooting method can only be used to find the bounded solutions of (8), and although we have seen in Theorem 4.3 that bounded solutions must be eigensolutions of (8) and (9), the converse is not always true. In the ground state, that is, when $l = 0$, Examples 4.1 and 4.3 have all $\lambda \in \mathbb{R}$ as their eigenvalues of (8) and (9), while Example 4.2 has all the negative numbers as its eigenvalues of (8) and (9) [2]. In these cases, the shooting method only produces a part of all the eigenvalues and eigensolutions. In fact, the eigensolutions to (8) largely depend on the domain of Schrödinger operator. It is not surprising at all that we get different eigenvalues and eigensolutions if we change condition (9). But it is also easy to see in our three examples, when $l \neq 0$, the eigensolutions of (8) and (9) must be bounded. Even in the ground state, the bounded solutions are still the most interesting ones in a physical sense [10, p. 32]. The shooting method is sufficiently general to solve a wide class of Schrödinger equations.

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