A NECESSARY AND SUFFICIENT CONDITION FOR THE EXISTENCE OF A BOUND-STATE CONTINUUM

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In this paper the bound-state spectrum of the radial Schrödinger equation

$$u''(r;K)+\left\{K^2-\frac{l(l+1)}{r^2}-U(r)\right\}u(r;K)=0,\quad u(0;K)=0,$$

is investigated for $K^2<0$. First, it is shown that if the wave function describes bound-states for a continuum of energies, then its derivative becomes unbounded at the origin. This is possible only if both the linearly independent solutions vanish at the origin and conversely if they both vanish at the origin, a continuum of bound-states exists. Finally, a necessary and sufficient condition for the existence of a bound-state continuum is that either (a) both the linearly independent solutions should vanish at the origin or, (b) the derivative of the solution which vanishes at the origin must be unbounded there.

1. Introduction

We start with the Radial Schrödinger equation [1]

$$u''(r;K)+\left\{K^2-\frac{l(l+1)}{r^2}-U(r)\right\}u(r;K)=0, \tag{1}$$

where the primes denote differentiation with respect to r. We assume that $U(r)$ is (*i*) continuous in $0<r<\infty$, (*ii*) $\to 0$ as $r\to\infty$ and (*iii*) has no zeros in $0<r<\varepsilon$ for some ε. Bound state solutions, that is, for which $\int_0^\infty u^2dr<M<\infty$ exist in general only for discrete values of $K^2<0$. But in special cases, a K^2-continuum of bound states exists for $K^2<0$ for example when $|r^nU(r)|\to\infty$ as $r\to 0$, for same $n>2$.

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2. *Problem*

We will show a necessary and sufficient condition for the existence of a bound-state continuum in the following two forms:

A necessary and sufficient condition for a K^2-continuum of bound-state solutions of (1) to exist for $0 > K^2 \in D$ is that, (*i*) $u_1(0; K) = 0 = u_2(0; K)$ for all such K^2, where $u_1(r; K)$ and $u_2(r; K)$ are any two linearly independent solutions of (1). Or, alternatively, (*ii*) $u'(r; K)$ should be unbounded as $r \to 0$ where $u(r; K)$ is any solution of (1) for which $u(0; K) = 0$.

From here we will deduce that for $U(r)$ such that $r^n U(r) \to 0$ as $r \to 0$ for some $n < 2$ only discrete bound states can exist.

We observe that a solution $u(r; K)$ of (1) for which $u(0; K) = 0$, is by Poincaré's Theorem, for fixed r, an entire function of K. Moreover, as $U(r)$ is continuous in $0 < r < \infty$, $u(r; K)$ for fixed K, is continuous in r and in fact, so is $u''(r; K)$. Hence, by Hartog's Theorem, $u(r; K)$ is regular in both r and K. As such, it is uniformly continuous with respect to r and K [2].

In the sequel we will require the following:

Lemma 1

If u and v are two solutions of (1) such that $|u| \to \infty$ and $v \to 0$ as $r \to \infty$, then there exist b and c, both > 0, for which $|\exp(-br)u| \to \infty$ and $\exp(cr)v \to 0$ as $r \to \infty$. (In fact, we can see from (1) that $u, v \to \exp(\pm |K| r)$ as $r \to \infty$.)

Lemma 2

If $u(r; K)$ describes a K^2-continuum of bound state solutions for $K^2 \in G \subset D$, then as $r \to 0$, $u'(r:K)$ is unbounded.

For, let $|u'(r;K)| < M$ for all $r \to 0$. Now,

$$u''(r; K) + \left\{K^2 - \frac{l(l+1)}{r^2} - U(r)\right\} u(r; K) = 0,$$

$$u''(r; K+h) + \left\{(K+h)^2 - \frac{l(l+1)}{r^2} - U(r)\right\} u(r; K+h) = 0,$$

where $(K+h)^2 \in G$. Multiplying the first equation by $u(r;K+h)$ and the second by $u(r;K)$ subtracting and integrating, we get

$$[u'(r; K)u(r; K+h) - u'(r; K+h)u(r; K)]_\varepsilon^R$$

$$= 2Kh \int_\varepsilon^R u(r; K)u(r; K+h)dr + O(h^2). \tag{2}$$

By Lemma 1, as $|u(r;K)|$ and $|u(r;K+h)| < \exp(-cr)$, $c > 0$, as $r \to \infty$, so,

$$u(R; K)u'(R; K+h) - u'(R; K)u(R; K+h) \to 0,$$

and $\int_{r_0}^{R} u(r;K)\,u\,(r;K+h)\,dr$ is uniformly convergent as $R \to \infty$, with respect to h. Moreover, $u(r;K)$ being uniformly continuous in r and K, as $u(0;K) = 0 = u(0;K+h)$, $|u(r;K)| < \eta$ and $|u(r;K+h)| < \eta$, η being arbitrary, for $|r| < \delta$ where δ is independent of h. Also, as we have supposed that $|u'(r;K)|$ and $|u'(r;K+h)| < M$; we have $|u'(r;K)\,u\,(r;K+h) - u'(r;K+h)\,u\,(r;K)| < 2M\eta \equiv \zeta$, for $|r| < \delta$ where ζ is arbitrarily small. Hence, as $R \to \infty$ and $\varepsilon \to 0$,

$$2Kh \int_0^\infty u(r;K)u(r;K+h)dr + O(h^2) = 0,$$

or,

$$\int_0^\infty u(r;K)u(r;K+h)dr + O(h) = 0.$$

As the integral is uniformly convergent and $u(r;K+h)$ is uniformly continuous with respect to r and h, hence [3],

$$0 = \operatorname*{Lt}_{h\to 0} \int_0^\infty u(r;K)u(r;K+h)dr = \int_0^\infty \operatorname*{Lt}_{h\to 0} u(r;K)u(r;K+h)dr$$

i. e.,

$$\int_0^\infty [u(r;K)]^2\,dr = 0,$$

which is impossible. Hence there does not exist a number M such that $|u'(r;K)| < M$ for all $r \to 0$ when $K^2 \in G$. This establishes the Lemma.

Lemma 3

If $u_1'(r;K)$ is unbounded as $r \to 0$, where $u_1(0;K) = 0$, then $u_2(0;K) = 0$ where u_2 is any other linearly independent solution of (1).

We consider two cases:

Case 1. $u_1(r;K)$ has an infinite number of zeroes in $(0, \varepsilon)$ for every $\varepsilon > 0$. (This happens only if $\left[K^2 - \frac{l(l+1)}{r^2} - U(r)\right] \geqslant 1/(4r^2)$ as $r \to 0$.) Then $u_2(r;K)$ also has an infinite number of zeroes in $(0, \varepsilon)$. For, as is well known, between two successive zeroes of u_1 there lies at least one zero of u_2. We observe that because u_1' becomes unbounded as $r \to 0$ so does u_2'. For, let $|u_2'| < M$. Then the Wronskian $u_1u_2' - u_2u_1' = u_1u_2'$ wherever $u_2 = 0$ and as such $\to 0$ as $r \to 0$ because $u_1(r;K) \to 0$, which is impossible. Next we observe that at a zero of u_2, r_1 say, $|u_2'|$ has a local maximum, for $u_2'' = \left[U(r) + \frac{l(l+1)}{r^2} - K^2\right]u_2$ has opposite signs to the left and right of r_1 and as such u_2' is increasing on one side of r_1 and decreasing on the other side. Further, we observe that where $u_1 = 0$ and therefore $|u_1'|$ is large, u_2 is small so that if u_2 does not $\to 0$ as $r \to 0$, then the successive zeroes of u_2 tend to those of u_1. In fact, using the Mean Value Theorem in the interval between successive zeroes, r_1 and r_2 of u_1, we can deduce the stronger result that $|h/(r_2 - r_1)| \to 0$

as $(r_2-r_1) \to 0$ where r_2+h is the intermediate zero of u_2. Now, the Wronskian of u_1 and u_2, $u_1u_2'-u_2u_1' =$ a constant $\neq 0$. Hence whenever $u_2' = 0$, corresponding to a local maximum of $|u_2|$, $|u_1'| < M$, where M is a fixed number.

Let us consider a solution of (1), $w_i = u_1+A_iu_2$ where A_i is chosen such that $w_i(r_i) = 0$, r_i being a point where $u_2'(r_i) = 0$. Remembering that $u_1 \to 0$ but u_2 does not, as $r \to 0$, we have, as $r_i \to 0$, $A_i \to 0$. Moreover, $|w_i'(r_i)| = |u_1'(r_i)| < M$ as seen above. That is, as $r \to 0$, $w_i(r) \to u$ where $u(r)$ is a solution such that $|u'(r)|$ is bounded wherever it has a local maximum and hence everywhere. This is not possible. Hence, both u_1 and $u_2 \to 0$ as $r \to 0$.

Case II. u_1 and therefore u_2 does not have any zero in $0 < r < \varepsilon$, ε suitably small. $\Bigg($Remembering that u_1' is unbounded as $r \to 0$, this is possible only when $0 < \left[K^2-\dfrac{l(l+1)}{r^2}-U(r)\right] < 1/(4r^2).\Bigg)$ Suppose $u_2 \nrightarrow 0$ as $r \to 0$. We observe that $u_1'' = \left[U(r)+\dfrac{l(l+1)}{r_2}-K^2\right]u_1 < 0$ if we take, without loss of generality, u_1 to be > 0 for $0 < r < \varepsilon$. As such u_1' is monotone decreasing and being unbounded, $u_1' \to \infty$ as $r \to 0$ remembering that u_1' must be > 0 as $r \to 0$. Otherwise u_1 cannot $\to 0$. As $u_2 \nrightarrow 0$, $|u_2'|$ must be unbounded as $r \to 0$. For, if $|u_2'| < M$, then $u_2'u_1 \to 0$ as $r \to 0$ and the Wronskian $|u_1u_2'-u_2u_1'| \to \infty$ as $r \to 0$ which is impossible. So $|u_2'| \to \infty$ as $u_2'' = \left[U(r)+\dfrac{l(l+1)}{r^2}-K^2\right]u_2$ is < 0 only or > 0 only and as such u_2' is also monotone. Moreover, if we choose $u_2 > 0$ then we must have $u_2' > 0$ for small r. If $u_2' < 0$, then $u_1u_2' < 0$ so that $\alpha \equiv u_1u_2'-u_2u_1' \to -\infty$ because $u_2u_1' \to +\infty$ as $r \to 0$, which is impossible.

Now, as $u_2' > 0$, u_2 is a monotone increasing function and as such u_2 cannot $\to \infty$ as $r \to 0$. That is, $u_2 \to$ a constant > 0. So, $(u_1/u_2)' = -\alpha/u_2^2 \to$ a constant $\neq 0$, as $r \to 0$. This implies that $u_1' \to$ a constant as $u_2 \to$ a constant $\neq 0$. This is impossible. Hence $u_2 \to 0$ as $r \to 0$ in this case also.

We have proved in Lemma 2 that if a continuum of bound states exists then u_1' is unbounded as $r \to 0$. In Lemma 3 we have shown that if u_1' is unbounded then $u_2 \to 0$ as $r \to 0$. Combining both of these results we have: If a continuum of bound states exists then u_1 and u_2 both $\to 0$ as $r \to 0$.

We now show that if $u_1(0; K) = 0 = u_2(0; K)$ where u_1 and u_2 are any two linearly independent solutions of (1), then a continuum of bound states exists for $K^2 \in D$. If, for all such K^2, either of $u_1(r; K)$ and $u_2(r; K) \to 0$ as $r \to \infty$, then a continuum of bound states exists. Otherwise, let us take, without loss of generality, $u_1(r; K)$ and $u_2(r; K)$ both $\to +\infty$ as $r \to \infty$, for some K^2. Also $u_1(r; K)u_2'(r; K)-u_1'(r; K)u_2(r; K) = \alpha$, where α is a positive constant, suppose. So $(u_2/u_1)' = \alpha/u_1^2$. As $u_1(r; K) \exp(-ar) \to \infty$, when $r \to \infty$, where $a > 0$, so, integrating, we have $0 < [u_2/u_1]_{r_1}^{r_2} = \alpha \int_{r_1}^{r_2} dr/u_1^2 < \varepsilon$, where ε is arbitrarily small, for r_1 and $r_2 >$ a suitably large R. That is, as $r \to \infty$, $(u_2/u_1) \to \beta$, a constant > 0, because, similarly, $(u_1/u_2) \to$ a constant and so $\beta \neq 0$. Now the solution of (1), $u = u_2 - \beta u_1 \to 0$ as $r \to \infty$. Moreover, $u(0; K) = 0$. So $u(r; K)$ describes a bound state. Thus if $u_1(0; K) = 0 = u_2(0; K)$, for all K^2 there exists a bound state solution. Hence the required result in the first form.

Now if both $u_1(r; K)$ and $u_2(r; K)$ vanish at $r = 0$, then we can see that u_1' and u_2' are unbounded when $r \to 0$. Firstly, let $|u_1'| < M$ and $|u_2'| < M$ when $r \to 0$. Then, the Wronskian $|u_2'u_1 - u_1'u_2| < M\,|u_1 + u_2| \to 0$ as $r \to 0$, which is impossible. So, at least one of u_1' and u_2' must be unbounded as $r \to 0$. Suppose u_1' is unbounded. Then, we have seen that in the Case I where u_1 and u_2 have an infinite number of zeroes in any neighbourhood, $0 < r < \varepsilon$, of 0, u_2' also is unbounded.

Suppose u_1 and u_2 have no zeroes in $0 < r < \varepsilon$, corresponding to Case II above. As before, we take $u_1 > 0$ and $u_2 > 0$ for $0 < r < \varepsilon$. We have seen that $u_1' \to +\infty$, as $r \to 0$, and u_2' is monotonic. Let $|u_2'| < M$. So $\mathrm{Lt}_{r\to 0}(u_2'/u_1') = 0 = \mathrm{Lt}_{r\to 0}(u_2/u_1)$ by L'Hospital's rule. Moreover as $u_1u_2' - u_2u_1' = \alpha$, a constant, $(u_2/u_1)' = \alpha/u_1^2$ and so preserves the same sign. As $(u_2/u_1) > 0$ for sufficiently small $r > 0$, and remembering that $u_2/u_1 \to 0$ as $r \to 0$, we have $(u_2/u_1)' = \alpha/u_1^2 > 0$. Otherwise u_2/u_1 cannot $\to 0$ as $r \to 0$. That is $\alpha > 0$. Then, as $u_1u_2' \to 0$ as $r \to 0$, because $|u_2'| < M$, we have $\alpha = u_1u_2' - u_2u_1' \to -u_2u_1' \leqslant 0$ as $r \to 0$, because $u_1' > 0$ and $u_2 > 0$. This is impossible. That is, we have proved that if $u_1(0; K) = 0$ and u_1' is unbounded as $r \to 0$, then u_2' is also unbounded where u_2 is any linearly independent solution for which $u_2(0; K) = 0$.

Finally, if a continuum of bound states exists, then from Lemma I as $r \to 0$, $u'(r; K)$ is unbounded where $u(r; K)$ describes the bound state solution so that $u(0; K) = 0$. So, u_1' is also unbounded where u_1 is any solution of (1) for which $u_1(0; K) = 0$.

Conversely, if $u_1(0; K) = 0$ and u_1' is, as $r \to 0$, unbounded, where u_1 is any solution of (1), then we showed that $u_2(0; K) = 0$, u_2 being any other linearly dependent solution. From here it follows, as shown above, that a continuum of bound states exists. Hence the result in the second form. For potentials $U(r)$ such that $-U(r) \to \lambda/r^2$ as $r \to 0$, $\lambda > l(l+1)$ and for singular attractive potentials, that is, for which $|r^n U(r)| \to \infty$ for some $n > 2$, as $r \to 0$, both the linearly independent solutions of (1), u_1 and u_2 vanish at $r = 0$ and, as is known, a continuum of bound states exists for all $K^2 < 0$ [4]. But if $r^n U(r) \to 0$ as $r \to 0$ for some $n < 2$ it can be shown that one of the two solutions of (1) does not vanish at $r = 0$. Thus a continuum of bound states cannot exist in this case.

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