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Rigorous conditions for the existence of bound states at the threshold in the two-particle case*

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Abstract
In the framework of non-relativistic quantum mechanics and with the help of Green's functions formalism, we study the behaviour of weakly bound states in a non-central two-particle potential as they approach the continuum threshold. Through estimating Green's function for positive potentials we derive rigorously the upper bound on the wavefunction, which helps us to control its falloff. In particular, we prove that for potentials whose repulsive part decays slower than $1/r^2$ the bound states approaching the threshold do not spread and eventually become bound states at the threshold. This means that such systems never reach supersizes, which would extend far beyond the effective range of attraction. The method presented here is applicable in the many-body case.

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1. Introduction

In many problems of quantum mechanics, it is important to know what happens to the wavefunction of a system as the bound state approaches the dissociation (decay) threshold. In particular, how does the size of the system in the ground-state change as the system becomes loosely bound. Among multiple examples of loosely bound systems in physics, one could mention negative atomic and molecular ions [1], Efimov states [2] and halo nuclei [3, 5].

For a bound state of the system as it approaches the threshold, there could be two possibilities. The first one is that the probability distribution given by this bound-state spreads, meaning that the probability to find all particles together in the fixed bounded region of space goes to zero (the size of the system goes to infinity). One observes such spreading in helium dimer [4] or in halo nuclei like ^{6}He or ^{11}Li, which are so loosely bound that two neutrons are about to leave the system and form dilute nuclear matter around the core nucleus (^{4}He and ^{9}Li

* Dedicated to Walter Greiner on his seventieth anniversary.

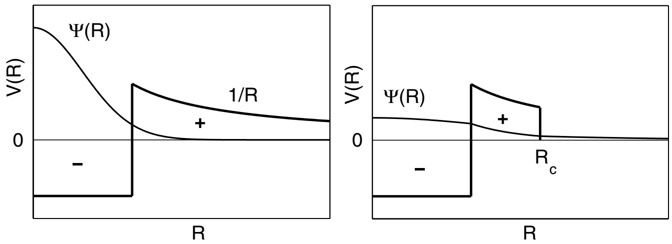

Figure 1. Sketched behaviour of the ground-state wavefunctions approaching the threshold in two potentials. Left: the potential has a positive Coulomb tail. Right: the same potential is cut off at some distance R_c.

respectively) [3]. The second possibility is that the bound state does not spread and in this case it eventually becomes a *bound state at the threshold* (the size of the system remains finite). This phenomenon is called the eigenvalue absorption. This is the case for doubly negative ions and proton halos [1, 5].

Recall, that for two particles interacting through spherically symmetric potentials with finite range S-states always spread, while all states with nonzero angular momentum become bound [6]. Incidentally, it is natural to conjecture that the ground state of a multi-particle system with pair interactions of finite range ($V_{ij}(x) = 0$ for $|x| \geqslant R$) cannot be bound at the threshold given that the particles are either bosons or distinguishable. For fermions with short-range interactions, it is hard to say from general principles whether the ground state would spread or not. The physical approach in this case is to use some kind of shell model and to figure out if there is a centrifugal barrier, which prevents the wavefunction from spreading.

On the other hand, there are potentials, for which bound states do not spread at all and when approaching the continuum they give rise to bound states exactly at the threshold [7, 8]. In particular, the physically important case of repulsive Coulomb tail case belongs to this type (see the discussion in [9]). Let us illustrate this situation by a simple example. Consider the square well potential plus a repulsive Coulomb tail, as in figure 1 (left), and imagine the ground state in this potential as it approaches the threshold. The probability distribution for this state would remain a confined wave packet regardless of how small is the binding energy. For zero binding energy there would be a bound state, which would have a falloff of the type $\sim \exp(-\sqrt{r})$. In contrast, if we cut off the positive tail at some arbitrary distance R_c, the ground state approaching the threshold would eventually spread when the binding energy is sufficiently small, i.e. the probability to find the particle in some bounded region of space goes to zero with the binding energy. The state 'tunnels' through the barrier. Note that this change in the behaviour does not depend on the value of R_c, which can be made as large as we please, so this effect is solely due to the repulsive Coulomb tail.

A rigorous proof of the eigenvalue absorption in the case of a general short-range potential plus a repulsive Coulomb tail was given by Bolle, Gesztesy and Schweiger in [8]. The main idea in [8] is to derive upper bound on the resolvent of the operator $H = p^2 + 1/r$. This upper bound helps then to control the falloff of wavefunctions. However, the approach in [8], based on Green's function expansion, is aimed specifically at the Coulomb long-range part and does not allow for generalizations, for example, to potentials having long-range parts of the form $r^{-1} + Ar^{-2}$, which may arise in multipole expansions. In this paper, we show how one can easily derive upper and lower bounds on such resolvents (Green's functions) and this allows us to derive more general results on the eigenvalue absorption. In [8] the zero energy bound state is first constructed as a solution in the sense of distributions and then using the upper bound on the resolvent one shows that this solution is a true L^2 bound state belonging to the domain of the Hamiltonian. Here, we rather use the coupling constant of the interaction to propagate true bound states to the zero energy level and by controlling their falloff we can tell whether they become zero energy bound states or only resonances. This treatment of zero energy states is more physical in the sense that one can follow the behaviour of wavefunctions as they approach the continuum.

The analysis in [7] illuminates the possibilities for various radially dependent long-range parts. However, the arguments given there are not rigorous. Finally, we should mention, that the phenomenon of the ground-state absorption was proved rigorously in [10] for a 3-body system with pure Coulomb interactions and the infinitely massive core. This makes one conjecture that at the point of critical charge negative ions have bound states at the threshold, see the discussion in [1]. In a forthcoming article, we shall give the rigorous proof of this conjecture for distinguishable particles and bosons [11], see also the discussion concerning many-body systems in the last section.

The paper is organized as follows. In section 2, we set the criterion for the eigenvalue absorption. In section 3, we derive useful upper bounds for Green's function. These bounds can also be used to control numerical solutions. In section 4, we prove our main result saying that potentials decaying slower than $1/r^2$ give rise to bound states at the threshold. The last section presents conclusions and a short discussion concerning many-body systems. Finally, the appendix contains technical details necessary for the proof in section 2.

2. Bound states near threshold

In nature, we can make the bound state of the system approach the threshold by changing the number and the type of particles. In theory, we reproduce this behaviour changing continuously some parameters in the system. For example, in the case of ions diminishing the atomic charge Z down to the critical value $Z = Z_{\mathrm{cr}}$ makes the ground state approach the threshold [1]. Here, as the parameter whose change forces the states to approach the threshold, we take the coupling constant of the interaction.

In our analysis, we shall consider the Hamiltonian of two particles $H = H_0 + \lambda W$, where $H_0 = p^2$ is the free Hamiltonian (we use the units where $\hbar = 1$ and $m = 1/2$), W is the interaction and λ is a coupling constant. By decreasing λ we can lift any bound state to the continuum. For convenience we shall consider only $W \in L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ [12]. This is a large class of interactions, which allows singularities not worse than $r^{-\alpha}$ for $\alpha < 3/2$. In this case H is self-adjoint on the domain $D(H_0) = D(-\Delta)$ [12]. However, one could extend our results to potentials having singularities of the type $r^{-\alpha}$ for $\alpha < 2$.

Let us assume that there is a bound state having the energy $E(\lambda) < 0$ for some value of the coupling constant λ. $E(\lambda)$ increases monotonously when λ decreases and eventually $E(\lambda)$ becomes zero for $\lambda = \lambda_{\mathrm{cr}}$, where λ_{cr} is called the critical coupling constant [6]. In the following, we show, using a simple example, how the wavefunction spreads in the case of exponentially decaying potentials. In this simple case, the analyticity of the energy as a function of λ helps us to establish an upper bound on the wavefunction

Theorem 1. *If there exist $A, a > 0$ such that $|W| \leqslant A\,\mathrm{e}^{-a|x|}$ and at $\lambda = \lambda_{\mathrm{cr}}$ there is no zero-energy bound state then the following upper bound holds for the normalized bound state ψ having the energy $E(\lambda)$ in the neighbourhood of $E(\lambda_{\mathrm{cr}}) = 0$*

$$|\psi| \leqslant \frac{C|E|^{1/4}\,\mathrm{e}^{-\sqrt{|E|}r}}{r}, \tag{1}$$

where $C > 0$ is some constant independent of E.

Proof. ψ satisfies the integral equation $\psi = -\lambda[H_0 - E]^{-1}W\psi$, which could be rewritten as

$$\psi(x) = -\lambda \int \mathrm{d}y \frac{\mathrm{e}^{-\sqrt{|E|}|x-y|}W(y)\psi(y)}{4\pi|x-y|}. \tag{2}$$

Using $|W| \leqslant A\,\mathrm{e}^{-a|x|}$ and applying the Schwarz inequality to equation (2) gives us

$$|\psi| \leqslant \lambda\langle\psi||W||\psi\rangle^{1/2}\left[\int \mathrm{d}y \frac{A\,\mathrm{e}^{-a|y|}\,\mathrm{e}^{-2\sqrt{|E|}|x-y|}}{|x-y|^2}\right]^{1/2} \leqslant \lambda\langle\psi||W||\psi\rangle^{1/2}\frac{C'\,\mathrm{e}^{-\sqrt{|E|}r}}{r} \tag{3}$$

where C' is some constant and $r = |x|$. On the other hand, recall [6] that at $\lambda = \lambda_{\mathrm{cr}}$ the energy $E(\lambda)$ is analytic and can be expanded into convergent power series $E(\lambda) = \sum_{k=2}^{\infty} a_k(\lambda-\lambda_{\mathrm{cr}})^k$, where $a_2 < 0$ ($a_1 = 0$ because by condition there is no zero-energy bound state at $\lambda = \lambda_{\mathrm{cr}}$). Applying the Hellman–Feynman theorem $\langle\psi|H_0|\psi\rangle = E(\lambda) - \lambda\,\mathrm{d}E/\mathrm{d}\lambda$ gives us $\langle\psi|H_0|\psi\rangle/|E|^{1/2} = O(1)$. Because $|W| \leqslant A\,\mathrm{e}^{-a|x|}$ there must exist such constant L that $|W| \leqslant L(2r)^{-2}$ and thus by the uncertainty principle [12, 13] $\langle\phi||W||\phi\rangle \leqslant L\langle\phi|H_0|\phi\rangle$ for any $\phi \in D(H_0)$. Thus $\langle\psi||W||\psi\rangle/|E|^{1/2} = O(1)$, which together with equation (3) proves the statement. □

As one can easily see, the function on the right-hand side of equation (1) dominates the wavefunction and spreads as $E \to 0$ maintaining the constant norm independent of E. The probability to find the particle in some fixed region of space goes to zero.

Now, let us consider potentials with positive tails. Throughout the paper, we shall assume for such potentials that $W(x) \geqslant 0$ for $|x| \geqslant R_0$, i.e., that outside some sphere the positive part dominates. Below we present a simple criterion, which tells us when bound states become bound states at the threshold. From the discussion above and from theorem 1 it is clear that the strategy could be proving that as $\lambda \searrow \lambda_{\mathrm{cr}}$ bound states remain confined in some region of space, i.e. do not spread. One way to achieve this is to show that bound states are dominated by some fixed function $g \in L^2$.

Theorem 2. *Let λ_n be a sequence of coupling constants and $\lambda_n \searrow \lambda_{\mathrm{cr}}$. The following is true (a) if for each λ_n there is a bound state ϕ_n with the energy E_n such that $|\phi_n| \leqslant g$, where $g \in L^2$ and $E_n \to 0$ then there exists a normalized bound state at the threshold, that is $\phi_0 \in D(H)$ and $H(\lambda_{\mathrm{cr}})\phi_0 = 0$. (b) If for each λ_n there are m orthogonal bound states $\phi_n^{(m)}$ with the energies $E_n^{(m)}$ such that $|\phi_n^{(m)}| \leqslant g$, where $g \in L^2$ and $\lim_{n\to\infty} E_n^{(m)} = 0$ then there exist m orthonormal bound states at the threshold.*

The proof of this theorem, which follows the method in [14], is given in the appendix. Intuitively, this proposition is obvious. If the states do not spread they should finally form some bound state at the threshold. A similar theorem concerning many-body systems appeared in Zhislin and Zhizhenkova [15]. There the authors proved that if a minimizing sequence for the energy functionals does not spread, then there exists a minimizer in L^2. Their result could be explained from the practitioner's point of view. Imagine that the system has no bound states with negative energy. Then, if the function minimizing the energy functional does not go to zero as the number of basis functions increases, then there must exist a zero-energy bound state.

Now let us see how the criterion in theorem 2 works. First, we separate positive and negative parts of the potential $W = W_+ - W_-$, where $W_+ = \max(0, W)$ and $W_- = \max(0, -W)$ and $W_\pm \geqslant 0$. The equation for the bound states reads $H(\lambda)\phi = -k^2\phi$, where $k \to 0$ as $\lambda \to \lambda_{\mathrm{cr}}$. This can be rewritten as

$$(H_0 + k^2 + \lambda W_+)\phi = \lambda W_-\phi \tag{4}$$

or equivalently

$$\phi = \lambda(H_0 + k^2 + \lambda W_+)^{-1} W_- \phi. \tag{5}$$

The operator $(H_0 + k^2 + \lambda W_+)^{-1}$ is an integral operator, whose kernel is positive and real [17]. Thus we can rewrite equation (5) as

$$|\phi| \leqslant 2\lambda_{\mathrm{cr}}(H_0 + k^2 + \lambda W_+)^{-1} W_- |\phi|, \tag{6}$$

where because $\lambda \searrow \lambda_{\mathrm{cr}}$ we have taken $\lambda \leqslant 2\lambda_{\mathrm{cr}}$ without loss of generality. If we show that the right-hand side of equation (6) is bounded by some fixed square integrable function, then according to theorem 2 we would have bound states at the threshold. The operator $(H_0 + k^2 + \lambda W_+)^{-1}$ is an integral operator, and its kernel is Green's function having two arguments. Because the function $W_-|\phi|$ vanishes outside some sphere, the behaviour of $|\phi|$ at infinity is determined by the asymptotic of Green's function when the integration argument is fixed within the sphere. Thus to find the asymptotic we need to derive upper and lower bounds on Green's function.

3. Bounds on Green's functions

3.1. Potential tails decaying as $1/r^2$

3.1.1. Upper bound. We introduce the function which would play the role of potential's tail:

$$\eta(A, R_0; x) = \begin{cases} 0 & \text{if } r < R_0 \\ Ar^{-2} & \text{if } r \geqslant R_0, \end{cases}. \tag{7}$$

We are interested in the kernel of the integral operator $[H_0 + k^2 + \eta(A, R_0; x)]^{-1}$ for k real, which we denote as $G_k(A, R_0; x, y)$. Note that the kernel of such an operator is a positive function, continuous away from $x = y$ [17]. Our aim in this section is to find an upper bound on $G_k(A, R_0; x, y)$. For that we need the following lemma.

Lemma 1. *Let $G_{1,2}(x, y)$ denote the integral kernels of $[H_0 + k^2 + V_{1,2}]^{-1}$ and suppose $V_1(x) \leqslant V_2(x)$. Then $G_2(x, y) \leqslant G_1(x, y)$.*

Proof. Through the integral representation we get

$$G_2(x, y) = G_1(x, y) - \int \mathrm{d}y' G_1(x, y')[V_2(y') - V_1(y')]G_2(y', y). \tag{8}$$

Equation (8) is the kernel representation of the equation $(A+B)^{-1} = A^{-1} - A^{-1}B(A+B)^{-1}$, where $A = H_0 + k^2 + V_1$ and $B = V_2 - V_1$. Now, because $G_{1,2}(x, y)$ are positive [17] and the potential difference $V_2 - V_1$ is non-negative, the integral in equation (8) must be non-negative and the statement is proved. □

There is another elucidating and more direct way to prove lemma 1. The proposition of the Lemma follows from the Laplace transform and the Trotter product formula, which lie at the heart of path-integrals [12]:

$$(H_0 + k^2 + V_1)^{-1} = \int_0^\infty \mathrm{e}^{-k^2 t}\, \mathrm{e}^{-t(H_0+V_1)}\, \mathrm{d}t \tag{9}$$

$$\mathrm{e}^{-t(H_0+V_1)} = \text{s-}\lim_{m\to\infty} [\mathrm{e}^{-tH_0/m}\, \mathrm{e}^{-tV_1/m}]^m. \tag{10}$$

Because e^{-tH_0} in equation (10) has a positive kernel, namely $(4\pi t)^{-3/2}\, \mathrm{e}^{-|x-y|^2/4t}$, the kernel of the operator on the left in equation (10) becomes smaller when V_1 is replaced by V_2.

The idea behind the upper bound on Green's function is rather simple. Suppose we have found such a function $F(A, R_0, x)$, independent of k, so that $G_k(A, R_0; x, 0) \leqslant F(A, R_0; x)$ holds for all k and x. First, we shall derive the upper bound in terms of the function F, and then we shall determine F explicitly.

Let us fix the functions $\tilde{A}(s)$, $\tilde{R}_0(s)$ so that the following inequality holds

$$\eta(A, R_0; x) \geqslant \eta(\tilde{A}, \tilde{R}_0; x - s), \tag{11}$$

where s is some fixed three-dimensional vector. From simple geometric arguments it follows that equation (11) would be satisfied if $\tilde{A}(s)$, $\tilde{R}_0(s)$ satisfy the inequalities:

$$\tilde{R}_0(s) \geqslant R_0 + |s| \tag{12}$$

$$\tilde{A}(s) \leqslant A \frac{\tilde{R}_0^2}{(\tilde{R}_0 + |s|)^2}. \tag{13}$$

Let us mention that the closer $\tilde{A}$ is to A the better is the asymptotic behaviour of the bound; hence, it is reasonable to take $\tilde{R}_0$ large.

Translating the arguments one finds that $G_k(\tilde{A}, \tilde{R}_0; x - s, y - s)$ is the integral kernel of the operator $[H_0 + k^2 + \eta(\tilde{A}, \tilde{R}_0; x - s)]^{-1}$. Now, using equation (11) and lemma 1 we obtain the upper bound

$$G_k(A, R_0; x, y) \leqslant G_k(\tilde{A}, \tilde{R}_0; x - s, y - s). \tag{14}$$

Equation (14) is valid for all s, so we can put $s = y$, which gives us

$$G_k(A, R_0; x, y) \leqslant F(\tilde{A}(y), \tilde{R}_0(y); x - y). \tag{15}$$

It remains to find F, which is the upper bound on $G_k(A, R_0; x, 0)$. This is easy because $G_k(A, R_0; x, 0)$ is spherically symmetric in x. From now on for simplicity of notation we shall drop A, R_0 in the arguments, writing, for example, $F(x)$ instead of $F(A, R_0; x)$. First, we shall give a formal solution, then we shall prove that this solution is indeed correct. By lemma 1 $G_k(x, 0) \leqslant G_{k'}(x, 0)$ if $k' \leqslant k$, so we can take $F(x) = \lim_{k\to 0} G_k(x, 0)$. Because $G_k(x, 0)$ is continuous away from $x = 0$ [17] and the functions $G_k(x, 0)$ increase monotonically when $k \to 0$, the pointwise limit makes sense. By lemma 1 $G_k(x, 0) \leqslant G_k^{(0)}(x, 0)$, where $G_k^{(0)}(x, y) = (4\pi|x - y|)^{-1} \exp(-k|x - y|)$ is the free propagator, i.e. the integral kernel of the operator $[H_0 + k^2]^{-1}$. This means $F(x)$ is bounded away from $x = 0$ and $F(x) \leqslant (4\pi r)^{-1}$. Because $G_k(x, y)$, formally satisfies the equation $[H_0 + k^2 + \eta]G_k(x, y) = \delta(x - y)$ one expects that $F(x)$ satisfies the equation

$$[H_0 + \eta]F = \delta(x). \tag{16}$$

To find the solution of equation (16) we set

$$F = \frac{1}{4\pi r} \times \begin{cases} 1 + br & \text{if } r \leqslant R_0 \\ cr^{-a} & \text{if } r \geqslant R_0, \end{cases} \tag{17}$$

where a is the positive root of the equation $a(a + 1) = A$ and the constants b, c are fixed requiring, as usual, that F and its derivative are continuous at $r = R_0$. This gives us

$$F(A, R_0; r) = \frac{1}{4\pi r} \times \begin{cases} 1 - R_0^{-1} a(a+1)^{-1} r & \text{if } r \leqslant R_0 \\ R_0^a (1 + a)^{-1} r^{-a} & \text{if } r \geqslant R_0. \end{cases} \tag{18}$$

One can check that $F(x)$ defined by equation (18) indeed satisfies equation (16).

For completeness we give the accurate proof, which justifies equation (18).

Lemma 2. *$F(x)$ defined as $F(x) = \lim_{k\to 0} G_k(x, 0)$ equals a.e. the expression given by equation (18).*

Proof. The integral equation for the resolvent reads [12]

$$G_k(x, y) = G_k^{(0)}(x, y) - \int \mathrm{d}y' G_k^{(0)}(x, y')\eta(y')G_k(y', y). \tag{19}$$

Substituting the expression for $G_k^{(0)}(x, y)$ and setting $y = 0$ we obtain

$$G_k(x, 0) = \frac{\mathrm{e}^{-kr}}{4\pi r} - \frac{1}{4\pi}\int \mathrm{d}y' \frac{\mathrm{e}^{-k|x-y'|}}{|x - y'|}\eta(y')G_k(y', 0). \tag{20}$$

Applying $\lim_{k\to 0}$ to both sides of equation (20) gives us the integral equation

$$F(x) = \frac{1}{4\pi r} - \frac{1}{4\pi}\int \mathrm{d}y' \frac{\eta(y')}{|x - y'|}F(y'). \tag{21}$$

By simple substitution and calculating the integrals one can check that F given by equation (18) indeed solves the integral equation equation (21). It remains to prove that no other solution exists. Suppose there are two solutions and denote their difference $Z = F_1 - F_2$. Then Z satisfies the integral equation:

$$Z(x) = -\frac{1}{4\pi}\int \mathrm{d}y' \frac{1}{|x - y'|}\eta(y')Z(y'). \tag{22}$$

We need to show that $Z = 0$ a.e. Let $\tilde{Z} = \eta^{1/2}Z$, then $\tilde{Z} \in L^2$ by the dominated convergence theorem and $\|\tilde{Z}\| \neq 0$, because otherwise from equation (22) it follows $Z = 0$ and we are done. From equation (22) we obtain

$$\int \mathrm{d}x\, \mathrm{d}y \frac{\eta^{1/2}(x)\tilde{Z}(x)\eta^{1/2}(y)\tilde{Z}(y)}{|x - y|} = -\|\tilde{Z}\|^2 < 0. \tag{23}$$

But equation (23) cannot hold because $|x - y|^{-1}$ is the kernel of a strictly positive operator (this could be easily checked in the Fourier-transformed space). This means equation (22) holds only if $Z = 0$. $\square$

Now let us formulate the bound in the form required in section 4.

Corollary 1. *Let $A > 3/4$, then there exist $C > 0, \delta > 0$ and R such that for $|y| \leqslant R_0$ and $|x| \geqslant R$ the inequality holds $G_k(A, R_0; x, y) \leqslant C|x|^{-3/2-\delta}$.*

Proof. For $|y| \leqslant R_0$ we can fix the values $\tilde{R}_0$ and $\tilde{A}$ independently of y. Both inequalities (12) and 13) would be satisfied if $\tilde{R}_0 \geqslant 2R_0$ and $\tilde{A} \leqslant A\tilde{R}_0^2(\tilde{R}_0 + R_0)^{-2}$. When $\tilde{R}_0$ becomes large $\tilde{A}$ gets closer to A, so we can fix the values of $\tilde{R}_0$ and $\tilde{A}$ to ensure that the following inequality holds $3/4 < \tilde{A} < A$. If we set $R = \tilde{R}_0 + R_0$, then for $|y| \leqslant R_0$ and $|x| \geqslant R$ we have $|x - y| \geqslant \tilde{R}_0$ and from equations (15) and (18), we get

$$G_k(A, R_0; x, y) \leqslant (4\pi|x|)^{-1}\tilde{R}_0^{\tilde{a}}(1 + \tilde{a})^{-1}|x - y|^{-\tilde{a}} \leqslant C|x|^{-1-\tilde{a}}, \tag{24}$$

where $\tilde{a}$ is the positive root of the equation $\tilde{a}(\tilde{a} + 1) = \tilde{A}, \tilde{a} > 1/2$. $\square$

3.1.2. Lower bound. Here, we shall briefly discuss how the same method can be applied to the construction of lower bounds. We shall need this in section 4 where we show that the ground state of potentials decaying faster than $(3/4)r^{-2}$ spreads near the point of critical binding. For that we need the following type of potential

$$\xi(A, R_0, ; x) = \begin{cases} V_0 & \text{if } r < R_0 \\ Ar^{-2} & \text{if } r \geqslant R_0, \end{cases} \tag{25}$$

and we need the upper bound for Green's function of the operator $\Xi_k(A, R_0) = [H_0 + \xi + k^2]^{-1}$, which has the integral kernel $\Xi_k(A, R_0; x, y)$. We shall derive the lower bound in terms of the function $f_k(A, R_0; r) = \Xi_k(A, R_0; x, 0)$, which falls off at infinity and solves the following equation

$$[H_0 + \xi + k^2] f_k = \delta(x) \tag{26}$$

where f_k depends only on $r = |x|$ (because the potential is spherically symmetric) and is a continuous function away from $r = 0$. By definition of f_k we have $0 < f_k \leqslant 1/(4\pi r)$. Setting $f_k = (4\pi r)^{-1} \hat{f}_k$ from equation (26) we obtain the equation on $\hat{f}_k$

$$-\hat{f}_k'' + \xi \hat{f}_k + k^2 \hat{f}_k = 0 \tag{27}$$

with the boundary conditions $\hat{f}_k(0) = 1$ and $\hat{f}_k(\infty) = 0$. The function $0 < \hat{f}_k(r) \leqslant 1$ comes out as a solution of a simple radial equation and thus can easily be calculated. As usual, one calculates the solutions $\hat{f}_k\,(r < R_0)$ and $\hat{f}_k\,(r > R_0)$ and determines the constants so that $\hat{f}_k$ and its derivative are continuous at R_0. The following lemma is useful for the lower bound.

Lemma 3. *For $r \geqslant R_0$ there exists C_0 independent of k such that*

$$\hat{f}_k(r) \geqslant C_0\, \mathrm{e}^{-kr} r^{-a}. \tag{28}$$

Proof. According to equation (27) on the interval $[R_0, \infty]$ the function $\hat{f}_k$ satisfies the equation:

$$-\hat{f}_k'' + Ar^{-2} \hat{f}_k + k^2 \hat{f}_k = 0. \tag{29}$$

Let us set $\hat{f}_k(r) = g_k(r)\, \mathrm{e}^{-kr} r^{-a}$. Then for $g_k(r)$ on the interval $[R_0, \infty]$ the equation becomes

$$-g_k'' + 2(ar^{-1} + k) g_k' = 2akr^{-1} g_k. \tag{30}$$

Because f_k is positive, g_k should be also positive. Hence from equation (30) we get

$$g_k'' \leqslant 2(ar^{-1} + k) g_k'. \tag{31}$$

We want to show that $g_k' \geqslant 0$. Indeed, if in contrast $g_k'(y) < 0$ at some point y, then at this point due to equation (31) $g_k''(y) < 0$. Hence g' is a monotonically decreasing function for $r \geqslant y$. Thus from equation (31) we conclude that $g_k'' \leqslant 2k g_k'(y)$ for all $r > y$, i.e. the second derivative is less than a fixed negative value, which means that at some point g_k becomes negative. Hence the assumption was false and $g_k' \geqslant 0$ holds. On the other hand, $f_k > 0$ and as $k \to 0$ the function f_k monotonically increases at all points. Hence, there must exist $C_0 > 0$ such that $g_k(R_0) \geqslant C_0$. Together with $g_k' \geqslant 0$ this means that g_k stays above C_0 and equation (28) holds. □

Now we follow the above procedure and define $\tilde{A}$, $\tilde{R}_0$ as satisfying the inequality

$$\xi(\tilde{A}, \tilde{R}_0, ; x - s) \geqslant \xi(A, R_0, ; x). \tag{32}$$

By geometrical arguments $\tilde{A}$, $\tilde{R}_0$ must satisfy

$$\tilde{R}_0(s) \geqslant R_0 + |s| \tag{33}$$

$$\tilde{A}(s) \geqslant A \frac{\tilde{R}_0^2}{(\tilde{R}_0 + |s|)^2}. \tag{34}$$

Just as in the previous subsection through equation (32) we obtain the desired lower bound

$$\Xi_k(A, R_0; x, y) \geqslant \Xi_k(\tilde{A}, \tilde{R}_0; x - y, 0) = f_k(\tilde{A}, \tilde{R}_0; |x - y|). \tag{35}$$

Now suppose $A < 3/4$. Looking at equations (33)–(34) one can see that we can fix $\tilde{R}_0$ and $\tilde{A}$ so that $\tilde{A} < 3/4$ and equations (33)–(34) are valid. Then from equation (35) and lemma 3 it is clear that there exists a constant $C > 0$ such that for $|x| \geqslant 2\tilde{R}_0$ and for $|y| \leqslant R_0$ the following inequality holds

$$\Xi_k(A, R_0; x, y) \geqslant f_k(\tilde{A}, \tilde{R}_0; |x - y|) \geqslant C\, \mathrm{e}^{-k|x|}|x|^{-3/2}. \tag{36}$$

We would need inequality equation (36) in section 4.

3.2. Potential tails decaying as $1/r$

Here, we would like to apply the results of the previous section to potentials with positive Coulomb tails. This helps us to establish the decay properties of eigenfunctions lying at the threshold. We shall not present a detailed exposition, because everything is similar to the previous section. One can follow the steps of the previous section and derive the bound in terms of the solution of the equation $[H_0 + \eta']F = \delta(r)$, where η' is the Coulomb tail. This however could not be expressed through elementary functions, so we shall make a couple of simplifying approximations. We shall consider the following potential tail:

$$\zeta(a, R_0; x) = \begin{cases} 0 & \text{if } r < R_0 \\ (a^2/4)r^{-1} + (a/4)r^{-3/2} & \text{if } r \geqslant R_0. \end{cases} \tag{37}$$

The repulsive Coulomb tail dominates in the potential of equation (37) and one can choose the constants so that the actual Coulomb tail is greater than the function in equation (37). Let $G_k^c(a, R_0; x, y)$ be the integral kernel of the operator $[H_0 + k^2 + \zeta(a, R_0; x)]^{-1}$, where c stands for Coulomb. The rest follows as above.

Let us fix the functions $\tilde{a}(s)$, $\tilde{R}_0(s)$ so that the following inequality holds

$$\zeta(a, R_0; x) \geqslant \zeta(\tilde{a}, \tilde{R}_0; x - s). \tag{38}$$

Again from geometric arguments it follows that equation (38) would be satisfied if $\tilde{a}(s)$, $\tilde{R}_0(s)$ satisfy the inequalities

$$\tilde{R}_0(s) \geqslant R_0 + |s| \tag{39}$$

$$\tilde{a}(s) \leqslant a \left(\frac{\tilde{R}_0}{\tilde{R}_0 + |s|} \right)^{3/2}. \tag{40}$$

Again let us define $F^c(x) = \lim_{k\to 0} G_k^c(x, 0)$, which makes $F^c(x)$ satisfy the equation

$$[H_0 + \zeta]F^c = \delta(x). \tag{41}$$

As one can easily check, the solution of equation (41) is given by

$$F^c(A, R_0; r) = \frac{1}{4\pi r} \times \begin{cases} 1 - \dfrac{1}{R_0 + 2\sqrt{R_0/a}} r & \text{if } r \leqslant R_0 \\ \dfrac{\mathrm{e}^{a\sqrt{R_0}}}{1 + (a/2)\sqrt{R_0}}\, \mathrm{e}^{-a\sqrt{r}} & \text{if } r \geqslant R_0. \end{cases} \tag{42}$$

Finally, the upper bound reads

$$G_k^c(a, R_0; x, y) \leqslant F^c(\tilde{a}(y), \tilde{R}_0(y); x - y), \tag{43}$$

where $\tilde{a}$ and $\tilde{R}_0$ satisfy equations (39)–(40). As in corollary 1 from equation (43), we find that there exists such $R > 0$ and $C > 0$ that

$$G_k^c(a, R_0; x, y) \leqslant C\,\mathrm{e}^{-a\sqrt{|x|}} \qquad \text{if} \quad |y| \leqslant R_0 \quad \text{and} \quad |x| \geqslant R. \tag{44}$$

As we have mentioned for potentials with positive tails the asymptotic of Green's function determines the fall-off behaviour of bound-state wavefunctions. Hence the bound-state wavefunctions fall off at least as fast as $\mathrm{e}^{-a\sqrt{r}}$. Calculating in the same way the lower bound one finds that this is the actual fall-off.

4. Main result

Now we state the main result of this paper.

Theorem 3. *If there are R_0 and $A > 3/4$ such that $\lambda W_+ \geqslant \eta(A, R_0; x)$ then at $\lambda = \lambda_{\mathrm{cr}}$ all states that hit the threshold at $\lambda = \lambda_{\mathrm{cr}}$ become zero energy bound states.*

Proof. Let us define $G_k(A, R_0; x, y)$ the positive integral kernel of the operator $[H_0 + k^2 + \eta]^{-1}$. Then from equation (6) and by lemma 1 we get the bound

$$|\phi|(x) \leqslant 2\lambda_{\mathrm{cr}} \int_{|y|\leqslant R_0} \mathrm{d}y G_k(A, R_0; x, y) W_-(y)|\phi|(y), \tag{45}$$

where we have used that $W_-(y) = 0$ for $|y| \leqslant R_0$. Now we shall use the upper bounds on Green's function $G_k(A, R_0; x, y)$ derived in section 3. For $|x| \geqslant R$ we can use corollary 1 to obtain from equation (45):

$$|\phi|(x) \leqslant 2\lambda_{\mathrm{cr}} C|x|^{-3/2-\delta} \int_{|y|\leqslant R_0} \mathrm{d}y W_-(y)|\phi|(y) \leqslant C_1|x|^{-3/2-\delta} \equiv g_>(x), \tag{46}$$

where we have applied the Schwarz inequality and used $W \in L^2 + L^\infty$. For $|x| \leqslant R$ we can use $G_k(A, R_0; x, y) \leqslant (4\pi)^{-1}|x - y|^{-1}$ to obtain from equation (45):

$$\begin{aligned} |\phi|(x) &\leqslant 2\lambda_{\mathrm{cr}}(4\pi)^{-1} \int_{|y|\leqslant R_0} \mathrm{d}y|x - y|^{-1} W_-(y)|\phi|(y) \\ &\leqslant C_2 \left[\int_{|y|\leqslant R_0} \mathrm{d}y|x - y|^{-2} W_-^2(y) \right]^{1/2} \equiv g_<(x). \end{aligned} \tag{47}$$

Thus, we get $|\phi|(x) \leqslant g(x)$, where $g(x) = g_<(x)$ for $|x| \leqslant R$ and $g(x) = g_>(x)$ for $|x| > R$. Because $g(x) \in L^2$ theorem 2 applies and the theorem is proved. □

Theorem 3 shows that *all* states in potentials whose repulsive part decays slower than $(3/4)r^{-2}$ become zero energy bound states at critical coupling. The following theorem is also true.

Theorem 4. *If there exists R_0 such that*

$$W(x) \leqslant (3/4)|x|^{-2} \text{ for } |x| \geqslant R_0 \tag{48}$$

then the ground state cannot be a zero energy bound state.

Proof. For simplicity we shall assume that there exists a constant V_0 such that $W_+ \leqslant V_0$. A proof by contradiction. Suppose that the ground state ψ_0 exists. Then the equation for the bound state at the threshold can be written as $[H_0 + W_+]\psi_0 = W_-\psi_0$. This is equivalent to the equation $[H_0 + W_+ + k^2]\psi_0 = W_-\psi + k^2\psi_0$, which in turn can be transformed into the integral equation:

$$\psi_0 = [H_0 + W_+ + k^2]^{-1} W_-\psi_0 + k^2[H_0 + W_+ + k^2]^{-1}\psi_0. \tag{49}$$

The ground-state wavefunction is always nonnegative $\psi_0 \geqslant 0$ [12]. Because $W_- \geqslant 0$, $\psi_0 \geqslant 0$ in equation (49) on the right-hand side we have a sum of two positive terms (the operator $[H_0 + W_+ + k^2]^{-1}$ has a positive integral kernel). Hence, we must have

$$\|[H_0 + W_+ + k^2]^{-1} W_-\psi_0\| \leqslant 1 \tag{50}$$

for all k. Because the positive part of W is bounded we have $W_+ \leqslant \xi(A, R_0; x)$, where ξ is defined by equation (25).

From equation (50) and using lemma 1, we conclude $\|\Xi_k(A, R_0)W_-\psi_0\| \leqslant 1$ for all k, where $\Xi_k(A, R_0) = [H_0 + \xi + k^2]^{-1}$. Our aim is to prove $\lim_{k\to 0} \|\Xi_k(A, R_0)W_-\psi_0\| = \infty$ thus obtaining the desired contradiction. We shall use the lower bound on $\Xi_k(A, R_0; x, y)$ from section 3.1.2. Let us fix $\tilde{R}_0$ as in the last part of section 3.1.2. Then using the bound equation (36) we obtain for the square of the norm

$$\|\Xi_k W_-\psi_0\|^2 \geqslant \int_{|y_1|\leqslant R_0} \int_{|y_2|\leqslant R_0} \mathrm{d}y_1\, \mathrm{d}y_2\, W_-(y_1)\psi_0(y_1)W_-(y_2)\psi_0(y_2) \tag{51}$$

$$\times \int_{|x|\geqslant 2\tilde{R}_0} \mathrm{d}x\, \Xi_k(A, R_0; x, y_1)\Xi_k(A, R_0; x, y_2) \tag{52}$$

$$\geqslant M^2C^2 \int_{|x|\geqslant 2\tilde{R}_0} \mathrm{d}x |x|^{-3}\, \mathrm{e}^{-2k|x|} \tag{53}$$

where $M = \int_{|y|\leqslant R_0} \mathrm{d}y\, W_-(y)\psi_0(y)$ is some fixed constant. Note that $M \neq 0$ because that would mean $\psi_0 = 0$. It is clear that the right-hand side in equation (53) becomes infinitely large as $k \to 0$ and thus $\|\Xi_k(A, R_0)W_-\psi_0\| \leqslant 1$ cannot hold for small k. □

Finally, let us mention how the method can be generalized to potentials in the class $W_+ \in \mathcal{R} + L^\infty$ and $W_- \in \mathcal{R} \cap L^1$, where $\mathcal{R}$ denotes the Rollnik class [12, 18]. In this case the Hamiltonian is defined as a quadratic form and the singularities of the type $r^{-\alpha}$, where $\alpha < 2$, are allowed. The statements of theorems 3 and 2 remain unchanged in this case. Only the proof of theorem 3 has to be slightly modified. Namely, in equations (46) and (47), one uses the fact that $\langle\phi|W_-|\phi\rangle$ is uniformly bounded (this is the consequence of W_- being form-bounded with respect to the kinetic energy with a relative bound zero).

5. Conclusions

We have proposed the method to derive lower and upper bounds on Green's functions, which helps us to determine the fall-off of bound states. Using these bounds we have proved that potentials, whose tails decay as $(2\mu/\hbar^2)V > (3/4)r^{-2}$, where μ is the reduced mass, absorb the eigenvalues, meaning that their bound states do not spread and become bound states at the threshold. We have also found that ground states in potentials, whose tails decay as $(2\mu/\hbar^2)V < (3/4)r^{-2}$, always spread as they approach the continuum.

These methods can be applied to the many-particle case, where it is still not known, for which pair interactions between decaying particles or clusters the bound state would become absorbed. The difficulty is that it is hard to control the asymptotic of the many-body bound-state wavefunction. Using bounds on Green's functions derived here one can demonstrate [11]

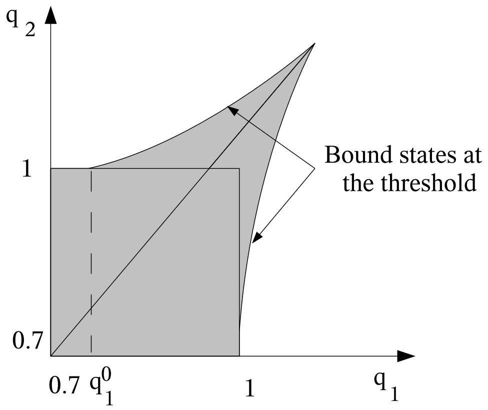

Figure 2. Typical stability diagram (sketch) for three Coulomb charges $\{-1, q_1, q_2\}$, the shaded area representing stable systems. On the arcs of stability curve where either $q_1 > 1$ or $q_2 > 1$ there are bound states at the threshold.

that when there is a long-range Coulomb repulsion between decaying components (particles or clusters), then the bound state must get absorbed.

Two types of behaviour, namely spreading and eigenvalue absorption can be perfectly illustrated by a stability diagram for three Coulomb charges, see [19]. When masses are fixed the diagram has the form as in figure 2. If we consider, for example, the upper arc, which is the stability border, it has the following property [19]. Up to some nonzero value of q_1^0 the stability border is given by the equation $q_2 = 1$. Then at the point $\{q_1^0, 1\}$ the arc goes up. With the same method as here it can be proved [11] that if one approaches the stability border from the side where $q_2 = 1$ then the ground state spreads and there is no bound state at the threshold. In contrast, for the points on the arc the ground state becomes absorbed, i.e. it does not spread and becomes a bound state at the threshold. The reason is that on the stability border, where $q_2 = 1$ the system decays into a neutral cluster and one charged particle, and for $q_2 > 1$ both cluster and the particle are charged positively. The resulting Coulomb repulsion between these objects hinders the spreading of the wavefunction and the ground state becomes absorbed. Note that it has already been proved rigorously [10], that in the case of an infinite core and two other masses being equal, the sharp point on the diagram, see figure 2, has a bound state at the threshold. Our method helps to extend this result to many particles.

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Appendix. Proof of theorem 2

Proof. Let us prove part (a). We follow the argument from [14]. Because $\|\phi_n\| = 1$ we can extract a weakly converging subsequence (for which we reserve the same index n) such that $\phi_n \xrightarrow{w} \phi_0$, where $\phi_0 \in L^2$. Because H is self-adjoint in order to prove that $\phi_0 \in D(H)$ and $H(\lambda_{cr})\phi_0 = 0$ it is enough to show that for every $f \in D(H)$ we have $\langle H(\lambda_{cr}) f|\phi_0\rangle = 0$. The latter we obtain as follows:

$$\langle H(\lambda_{\rm cr})f|\phi_0\rangle = \lim_{n\to\infty}\langle H(\lambda_{\rm cr})f|\phi_n\rangle = \lim_{n\to\infty}[\langle H(\lambda_n)f|\phi_n\rangle - (\lambda_n-\lambda_{\rm cr})\langle Wf|\phi_n\rangle] \tag{A.1}$$

$$= \lim_{n\to\infty}\langle f|H(\lambda_n)\phi_n\rangle = \lim_{n\to\infty} E_n\langle f|\phi_n\rangle = 0. \tag{A.2}$$

The only thing that remains to show is that $\phi_0 \neq 0$. We shall prove this by contradiction assuming that $\phi_n \stackrel{w}{\to} 0$. Let us introduce χ_R, the characteristic function of the interval $[0, R]$ (i.e. $\chi_R(x) = 1$ when $|x| \in [0, R]$ and $\chi_R(x) = 0$ otherwise). Because $|\phi_n| \leqslant g$ and $g \in L^2$ we can fix R so that $\langle\phi_n|\chi_R|\phi_n\rangle > 1/2$. We would like to show that for $\phi_n \stackrel{w}{\to} 0$ the condition $\langle\phi_n|\chi_R|\phi_n\rangle > 1/2$ cannot hold for large n. One way to do this is to use that $\int|\nabla\phi_n|^2\,\mathrm{d}x \leqslant$ const and apply the Rellich–Kondrashov lemma [16] giving $\chi_R\phi_n \to 0$ strongly, or we can use the argument similar to the one in [14]. Using the equation $(H_0+1)\phi_n = (E_n+1)\phi_n - \lambda_n W\phi_n$ we get $\phi_n = (E_n+1)(H_0+1)^{-1}\phi_n - \lambda_n(H_0+1)^{-1}W\phi_n$. Substituting this into $\langle\phi_n|\chi_R|\phi_n\rangle > 1/2$ we obtain

$$(E_n+1)\langle\phi_n|\chi_R(H_0+1)^{-1}\phi_n\rangle - \lambda_n\langle\phi_n|\chi_R(H_0+1)^{-1}W\phi_n\rangle > 1/2. \tag{A.3}$$

The operators $\chi_R(H_0+1)^{-1}$ and $\chi_R(H_0+1)^{-1}W$ have square integrable kernels and are therefore compact. Acting on weakly convergent sequences they make them converge strongly and hence both terms on the left-hand side of equation (A.3) go to zero. Thus equation (A.3) cannot hold for large n, which proves (a).

Part (b) easily follows if we prove that from $\phi_n \stackrel{w}{\to} \phi_0$ follows $\phi_n \to \phi_0$ in norm. Indeed, for each λ_n there are bound states $\phi_n^{(i)}$ $(i = 1,\ldots,m)$ satisfying $H(\lambda_n)\phi_n^{(i)} = E_n^{(i)}\phi_n^{(i)}$. Moreover $\langle\phi_n^{(i)}|\phi_n^{(k)}\rangle = \delta_{ik}$ and as $\lambda_n \searrow \lambda_{\rm cr}$ the energies go to zero $E_n^{(i)} \to 0$. In this case since $|\phi_n^{(i)}| < g \in L^2$ there are m bound states at the threshold, $\phi_n^{(i)} \stackrel{w}{\to} \phi_0^{(i)}$. Because this convergence is in norm $\langle\phi_0^{(i)}|\phi_0^{(k)}\rangle = \delta_{ik}$ holds.

To prove that from $\phi_n \stackrel{w}{\to} \phi_0$ follows $\phi_n \to \phi_0$ in norm let us define $\xi_n = \phi_n - \phi_0$, then $\xi_n \stackrel{w}{\to} 0$ and we would like to show that $\|\xi_n\| \to 0$. A proof by contradiction. If not then there must exist a constant $a > 0$ and a subsequence (for which we again reserve the same index n) such that $\|\xi_n\|^2 > a$. Again because $|\phi_n| \leqslant g$ and $\phi_0 \in L^2$ we can fix R so that $\langle\xi_n|\chi_R|\xi_n\rangle > a/2$. We have $\xi_n \in D(H)$ and $(H_0+\lambda_n W)\xi_n = E_n\phi_n + (\lambda_{\rm cr}-\lambda_n)W\phi_0$. From this equation we easily get

$$\xi_n = (H_0+1)^{-1}\xi_n - \lambda_n(H_0+1)^{-1}W\xi_n + E_n(H_0+1)^{-1}\phi_n + (\lambda_{\rm cr}-\lambda_n)(H_0+1)^{-1}W\phi_0. \tag{A.4}$$

Substituting one ξ_n from equation (A.4) into $(\xi_n, \chi_R\xi_n)$ and using that $\chi_R(H_0+1)^{-1}$ and $\chi_R(H_0+1)^{-1}W$ are compact and $\xi_n \stackrel{w}{\to} 0$ we obtain $\langle\xi_n|\chi_R|\xi_n\rangle \to 0$. This is a contradiction. □

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