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Ground-state stability diagrams for two identical particles in an external potential

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Abstract

We study the stability of the ground state of a two-identical-particles system in an attractive external potential. We consider a repulsive interaction between the particles. The existence of a bounded ground state as a function of the strength of Hamiltonian parameters is studied for long- and short-range potentials. The possible scenarios of ionization are discussed. Criteria for the existence of a threshold-energy bound state and the energy critical exponent are given. In particular, we show that for the case of an attractive long-range external potential with short-range repulsive inter-particle interaction, a bound system can become unstable increasing the strength of the attractive potential.

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(Some figures in this article are in colour only in the electronic version)

1. Introduction and definitions

Conditions for the existence of bound states in quantum few-body systems have been the subject of research for many decades. Nowadays, the existence of a bound state and near-threshold behavior for one-body systems in external potentials is well known. Upper and lower bounds on the number of bound states for one-body systems were given in the pioneer works of Jost and Pais [1] and Bargmann [2]. The critical behavior for eigenstates of one-body spherical attractive potentials was studied as a function of the spatial dimension by Klaus and Simon [3] and as a function of the angular momentum, considered as a continuous parameter, by Lassaut *et al* [4]. A considerable amount of work had been done to obtain lower and upper bounds on the energies of few and N -body systems ([5–7], and references therein). Numerical methods to evaluate critical parameters were developed for one- [8] and few-body systems [9, 10], including non-central interactions [11, 12].

In this work, we study the existence of the ground state for two-body systems as a function of the Hamiltonian parameters. Systems under consideration are formed by two identical particles in an external radial potential (which can be a nucleus attraction). We consider spin-independent Hamiltonians, so the spin variables are taken into account via symmetrization of the spatial ground-state wavefunction. We study two-parameter Hamiltonians of the form (atomic units are used throughout this paper)

$$\mathcal{H}(\lambda_1, \lambda_2) = \mathcal{H}_0(\lambda_1; 1, 2) + \lambda_2 W(1, 2), \quad (1)$$

where $\mathcal{H}_0(\lambda_1; 1, 2)$ is a Hamiltonian for two identical non-interacting particles, $W(1, 2) = W(r_{12})$ is the repulsive interaction between the particles, which depends on the interparticle distance r_{12} , and λ_1, λ_2 are positive parameters. The Hamiltonian \mathcal{H}_0 has the form

$$\mathcal{H}_0(\lambda_1; 1, 2) = h(\lambda_1)(1) + h(\lambda_1)(2), \quad (2)$$

where h represents the one-particle Hamiltonian:

$$h(\lambda_1) = -\frac{1}{2}\nabla^2 + \lambda_1 v(r). \quad (3)$$

We consider more attractive than repulsive external interaction $v(r)$. Then, it exists $\lambda_1^{(c)} \geq 0$ such that for $\lambda_1 > \lambda_1^{(c)}$, $h(\lambda_1)$ supports at least one bound state and it does not have bound states for $\lambda_1 < \lambda_1^{(c)}$. We are interested in the existence of a two-particle bounded ground state when a repulsive interaction between the particles is present. We consider purely repulsive potentials $W(r_{12})$ strong enough such that for fixed λ_1 , the two-body Hamiltonian does not support a bound state for large values of λ_2 .

The stability of the ground state and near-threshold behavior of the ground-state energy of one-body radial potentials had been completely studied. Conditions for the existence of a one-body bound state at the threshold and asymptotics of the energy near $\lambda_1^{(c)}$ are known [3, 4, 10].

For the one- and two-body potentials, we assume the following conditions.

- (i) $h(\lambda_1)$ is self-adjoint for $\lambda_1 \geq 0$ and $\mathcal{H}(\lambda_1, \lambda_2)$ is self-adjoint in the region ($\lambda_1 \geq 0, \lambda_2 \geq 0$).
- (ii) $v(r)$ and $W(r_{12})$ have no free parameters; then the Hamiltonian (1) depends only on λ_1 and λ_2 .
- (iii) Both the one-body and the two-body potentials are radial, that is $v = v(r)$ and $W(1, 2) = W(r_{12})$.
- (iv) The potentials decay at infinity, that is $\lim_{r \rightarrow \infty} v(r) = 0$ and $\lim_{r_{12} \rightarrow \infty} W(r_{12}) = 0$.
- (v) $v(r)$ is attractive enough so that $\exists 0 \leq \lambda_1^{(c)} < \infty$ such that the eigenvalue equation for the ground state of the one-particle system, given by

$$h(\lambda_1)\psi_0(\lambda_1; r) = \mathcal{E}_0(\lambda_1)\psi_0(\lambda_1; r), \quad (4)$$

has a bounded solution, $\mathcal{E}_0(\lambda_1) < 0$ and $\|\psi_0(\lambda_1)\| = 1 \forall \lambda_1 > \lambda_1^{(c)}$. $\mathcal{E}_0(\lambda_1^{(c)}) = 0$ could be an eigenvalue.

- (vi) W is completely repulsive $W(r_{12}) > 0 \forall r_{12} \geq 0$.
- (vii) $\exists \hat{\lambda}_1 > \lambda_1^{(c)}$ such that for $\lambda_1^{(c)} < \lambda_1 < \hat{\lambda}_1$ we have $2\mathcal{E}_1(\lambda_1) \geq \mathcal{E}_0(\lambda_1)$, where $\mathcal{E}_1(\lambda_1)$ is the energy of the first excited state of $h(\lambda_1)$ ($\mathcal{E}_1(\lambda_1) = 0$ if $h(\lambda_1)$ supports just one bound state).
- (viii) The interparticle potential W obeys

$$\langle \psi_0(1), \psi_0(2) | W^{-1}(1, 2) | \psi_0(1), \psi_0(2) \rangle > 0, \quad (5)$$

where $|\psi_0(1), \psi_0(2)\rangle$ is the ground state of \mathcal{H}_0 .

As we will show below, conditions (vii) and (viii) give us a sufficient condition for the non-existence of bound states for large values of λ_2 . These conditions are not too restrictive. Condition (vii) holds for attractive short-range potentials, which satisfies $r^2v(r) \rightarrow 0$ for $r \rightarrow \infty$, because the critical values of λ_1 for excited states are strictly greater than the critical value $\lambda_1^{(c)}$ for the ground state. In the case of long-range potential, we note that for the Coulomb potential, condition (vii) is fulfilled: $\forall \lambda_1 > 0$; then, in this case, $\hat{\lambda}_1 = \infty$. Condition (viii) excludes a potential W which vanishes outside some sphere, as the simple step potential. For this potential, the limit $\lambda_2 \rightarrow \infty$ represents finite-size particles that, for example, will have bound states if $v(r)$ is a Coulomb potential.

The eigenvalue equation for the ground state of the two-body system is given by

$$\mathcal{H}(\lambda_1, \lambda_2)\Psi_0(\lambda_1, \lambda_2; r_1, r_2, r_{12}) = E_0(\lambda_1, \lambda_2)\Psi_0(\lambda_1, \lambda_2; r_1, r_2, r_{12}). \quad (6)$$

The main subject of this work is to characterize the ground-state stability diagram as a function of the parameters (λ_1, λ_2) . This means to find the region where a bounded ground state, with $E_0(\lambda_1, \lambda_2) \leq \mathcal{E}_0(\lambda_1)$ and $\|\Psi_0(\lambda_1, \lambda_2)\| = 1$, exists.

The critical line $\lambda_2^{(c)}(\lambda_1)$ is defined by the threshold condition

$$E_0(\lambda_1, \lambda_2^{(c)}(\lambda_1)) = \mathcal{E}_0(\lambda_1). \quad (7)$$

The asymptotic form of the ionization energy at the threshold defines the critical exponent α [10]. We can define a critical exponent α_h for the one-particle ground state energy:

$$\mathcal{E}(\lambda_1) \sim -e(\lambda_1 - \lambda_1^{(c)})^{\alpha_h}, \quad \text{for } \lambda_1 \rightarrow \lambda_1^{(c)+}, \quad (8)$$

where e is a positive constant. Expressions for the critical exponent α_h for a class of attractive spherical potentials are given in [3, 4, 10]. For the two-body case, the energy depends on two parameters and the threshold energy is the one-body ground-state energy. The critical exponent $\alpha_{\mathcal{H}}$ is defined by the asymptotic behavior of the ionization energy near a critical point $(\lambda_1^0, \lambda_2^0)$. This asymptotic behavior can be obtained in an arbitrary direction except the one tangent to the critical line (along this line, the exponent is always greater than $\alpha_{\mathcal{H}}$). For convenience, we always use the direction of the λ_1 -axis

$$E_0(\lambda_1, \lambda_2^0) - \mathcal{E}_0(\lambda_1) \sim -a|\lambda_1^0 - \lambda_1|^{\alpha_{\mathcal{H}}}, \quad \text{for } \lambda_1 \rightarrow \lambda_1^{0b}, \quad (9)$$

where a is a positive constant. Here, the meaning of $\lambda_1 \rightarrow \lambda_1^{0b}$ is that the line must always approach the critical point from the region where a bounded two-body ground state exists. If the line $\lambda_2 = \lambda_2^0$ is tangent to the critical line, we change λ_1 by λ_2 in the definition of $\alpha_{\mathcal{H}}$.

Simon [13] proved that $\alpha = 1$ iff the threshold energy is the eigenvalue of a bounded solution for a given Hamiltonian. Then, in our context, the importance of the critical exponent $\alpha_{\mathcal{H}}$ is that its value determines if the critical line belongs to the bounded region ($\alpha_{\mathcal{H}} = 1$) or not ($\alpha_{\mathcal{H}} > 1$).

2. General results

In this section, we present the possible scenarios for the stability diagram for different potentials and some general results that are valid for a large class of one- and two-body interactions. We assume that the Hamiltonians satisfy conditions (i)–(viii).

Since W is a positive definite operator, $\mathcal{H}(\lambda_1, \lambda_2)$ does not have bound states for $\lambda_1 < \lambda_1^{(c)}$. We also know that if the Hamiltonian $\mathcal{H}(\lambda_1, \lambda_2)$ supports bound states, the eigenenergies are concave increasing functions of λ_2 [14].

Following Thirring [14], we can get lower bounds for the energy of the system for $\lambda_2 \leq \tilde{\lambda}_2(\lambda_1)$ applying the inequality

$$2\mathcal{E}_0(\lambda_1) + \lambda_2 \langle \psi_0(1)\psi_0(2) | \frac{1}{W} | \psi_0(1)\psi_0(2) \rangle^{-1}(\lambda_1) \leq E_0(\lambda_1, \lambda_2), \quad (10)$$

where

$$\tilde{\lambda}_2(\lambda_1) = 2(\mathcal{E}_1(\lambda_1) - \mathcal{E}_0(\lambda_1)) \left\langle \frac{1}{W} \right\rangle_0, \quad (11)$$

and $\mathcal{E}_1(\lambda_1)$ is the first excited state of the one-body Hamiltonian $h(\lambda_1)$. Replacing λ_2 by its limiting value $\tilde{\lambda}_2(\lambda_1)$, and using condition (vii), we get

$$\mathcal{E}_0(\lambda_1) \leq 2\mathcal{E}_1(\lambda_1) \leq E_0(\lambda_1, \tilde{\lambda}_2), \quad (12)$$

which shows that $\tilde{\lambda}_2(\lambda_1)$ is an upper bound for the critical curve $\lambda_2^{(c)}(\lambda_1)$. A lower bound for $\lambda_2^{(c)}(\lambda_1)$ is provided by the following lemma.

Lemma 1. $\forall \lambda_1 > \lambda_1^{(c)}, \exists \lambda_2^* > 0$ such that if $0 \leq \lambda_2 < \lambda_2^*$, then $\mathcal{H}(\lambda_1, \lambda_2)$ supports at least one bound state.

Proof. Using the variational principle with the trial function $\Phi_0(\lambda_1; 1, 2) = \psi_0(\lambda_1; r_1)\psi_0(\lambda_1; r_2)$, we have

$$E_0(\lambda_1, \lambda_2) \leq \langle \mathcal{H}(\lambda_1, \lambda_2) \rangle_0 = 2\mathcal{E}_0(\lambda_1) + \lambda_2 \langle W \rangle_0(\lambda_1). \quad (13)$$

According to the variational principle, the existence of a bound state is assured if we find a trial function such that the expectation value of $\mathcal{H}(\lambda_1, \lambda_2)$ is below the threshold energy $\mathcal{E}_0(\lambda_1)$. This condition on (13) gives

$$\mathcal{E}_0(\lambda_1) + \lambda_2 \langle W \rangle_0(\lambda_1) < 0 \quad (14)$$

from which we define λ_2^* as

$$\lambda_2^*(\lambda_1) = \frac{|\mathcal{E}_0(\lambda_1)|}{\langle W \rangle_0(\lambda_1)} > 0. \quad (15) \quad \square$$

From the above results, it follows that the critical curve lies between the bounds:

$$\lambda_2^*(\lambda_1) \leq \lambda_2^{(c)}(\lambda_1) \leq \tilde{\lambda}_2(\lambda_1). \quad (16)$$

Now, we can describe the possible scenarios for the ground-state stability diagram. Three different regions can exist in which $\mathcal{H}(\lambda_1, \lambda_2)$ supports states with 0, 1 or 2 particles bounded. The first case occurs when $h(\lambda_1)$ does not have bound states. In the second case, $h(\lambda_1)$ has at least one bound state and $\mathcal{H}(\lambda_1, \lambda_2)$ does not have any. Finally, both particles are bounded if \mathcal{H} has a bound state. The critical lines between these regions will be denoted as 1–0 line, 2–1 line and 2–0 line. The stability diagrams can be classified into three cases, which are qualitatively shown in figure 1.

Case 1. No 2–0 line. This case is shown in figure 1(a). For $\lambda_2 > 0$, ionization is always from $2 \rightarrow 1 \rightarrow 0$ particles; no double ionization then exists for $\lambda_2 > 0$.

Case 2. Finite 2–0 line. $\exists \lambda_2^{(mc)} > 0$ such that for $\lambda_2 < \lambda_2^{(mc)}$ the two-body system has at least one bound state for $\lambda_1 > \lambda_1^{(c)}$, but there is no bound states near $\lambda_1^{(c)}$ for $\lambda_2 > \lambda_2^{(mc)}$. Then the line $\lambda_1 = \lambda_1^{(c)}$ is a 2–0 line for $\lambda_2 < \lambda_2^{(mc)}$. This case is shown in figure 1(b).

Case 3. Infinite 2–0 line. This case is obtained from case 2 when $\lambda_2^{(mc)} \rightarrow \infty$. The line $\lambda_1 = \lambda_1^{(c)}$ is a 2–0 line, as is shown in figure 1(c). Note that in this case, the system can lose a two-body bound state increasing the strength of the attractive potential.

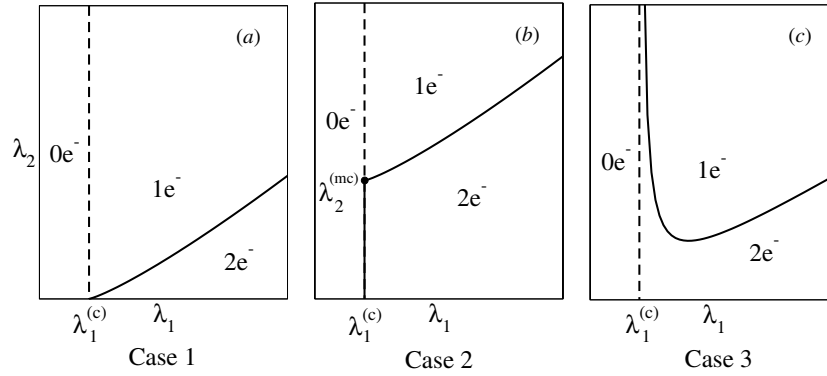


Figure 1. Qualitative stability diagrams. They show the three possible scenarios for the stability diagram. Two of them have the double ionization line $2-0$.

2.1. Existence of the $2-0$ line

The existence of the $2-0$ line is determined by the properties of the involved potentials $v(r)$ and $W(r_{12})$. From (15) it can be seen that as $\lambda_1 \rightarrow \lambda_1^{(c)+}$, the lower bound on the critical line can be finite, infinite or zero, depending on the asymptotic behavior of the energy $\mathcal{E}_0(\lambda_1)$ and $\langle W \rangle_0(\lambda_1)$. Suppose the asymptotic expansion

$$\langle W \rangle_0(\lambda_1) \sim w(\lambda_1 - \lambda_1^{(c)})^\omega \quad \text{for } \lambda_1 \rightarrow \lambda_1^{(c)+}, \tag{17}$$

with $w > 0$. If $\omega > \alpha_h$ then, according to (15), the lower bound goes to infinity indicating that the diagram is of type 3. For $\omega = \alpha_h$, the lower bound is finite; then the diagram is of type 2 or 3. If $\omega < \alpha_h$ the lower bound goes to zero. In this case, we can obtain a first-order perturbative expansion of the two-body system energy in λ_2 :

$$E_0(\lambda_1, \lambda_2) - \mathcal{E}_0(\lambda_1) \sim \mathcal{E}_0(\lambda_1) + \lambda_2 \langle W \rangle_0(\lambda_1) + O(\lambda_2^2). \tag{18}$$

For $\lambda_2 \sim 0$, and $\lambda_1 \rightarrow \lambda_1^{(c)}$, $E_0(\lambda_1, \lambda_2) - \mathcal{E}_0(\lambda_1) > 0$ since $\mathcal{E}_0(\lambda_1)$ decays faster than $\langle W \rangle_0(\lambda_1)$. Then, the diagram is of type 1.

We summarize these results in the following lemma.

Lemma 2. *If the near-threshold behavior of $\langle W(r_{12}) \rangle_0$ is given by (17), then the stability diagram for the ground-state energy of $\mathcal{H}(\lambda_1, \lambda_2)$ corresponds to*

- (i) case 1 if $\omega < \alpha_h$,
- (ii) case 2 or 3 if $\omega = \alpha_h$,
- (iii) case 3 if $\omega > \alpha_h$.

When the one-body potential is of short range, we can prove that the stability diagram can be of type 1, 2 or 3, that is, all cases are possible. A potential $v(r)$ is defined as of short range if $\lim_{r \rightarrow \infty} r^2 v(r) = 0$. Furthermore, in this case, the threshold energy $\mathcal{E}_0 = 0$ is not an eigenvalue and the energy critical exponent is $\alpha_h = 2$ [3, 10].

Theorem 1. *For short-range one-body potentials, the stability diagram is of type 1, 2 or 3.*

Proof. From the near-threshold properties of short-range potentials, we know that the single-particle wavefunction has the form $\psi_0(\lambda_1^{(c)} + \epsilon; r) \sim \epsilon^{1/2} \psi(\epsilon; r)$ with $\psi(0; r) >$

$0 \forall r > 0$. On the other hand, from (vi) $\exists [a, b]$ such that $W(r_{12}) > 0$ in $[a, b]$. Let $W_{\min} = \min_{r_{12} \in [a, b]} W(r_{12})$; then

$$\langle W \rangle_0 \geq \epsilon^2 W_{\min} \int_{r_{12} \in [a, b]} \psi_0^2(r_1) \psi_0^2(r_2) d^3x_1 d^3x_2 > a\epsilon^2, \quad a > 0. \quad (19)$$

So as $\lambda_1 \rightarrow \lambda_1^{(c)+}$, $\langle W \rangle_0 \sim w(\lambda_1 - \lambda_1^{(c)})^\omega$ with $\omega \leq 2$. According to lemma 2, this implies that the stability diagram could be of type 1, 2 or 3. \square

2.2. Exponent $\alpha_{\mathcal{H}}$

The existence of the 2–0 line is determined, as we saw in the previous subsection, by the relative asymptotics of the external potential and the repulsive inter-particle interaction. In this subsection, we study the critical exponent $\alpha_{\mathcal{H}}$ at the 2–0 line.

Lemma 3. *If the 2–0 line exists, then $\alpha_{\mathcal{H}} = \alpha_h$ over this line.*

Proof. The 2–0 line is defined by $(\lambda_1 = \lambda_1^{(c)}, \lambda_2)$ with $\lambda_2 < \lambda_2^{(mc)}$ and $E_0(\lambda_1^{(c)}, \lambda_2) = \mathcal{E}_0(\lambda_1^{(c)}) = 0$. Since $E_0(\lambda_1, \lambda_2)$ is an increasing function of λ_2 ,

$$E_0(\lambda_1, \lambda_2) > E_0(\lambda_1, 0) = 2\mathcal{E}_0(\lambda_1). \quad (20)$$

From (8), for $\lambda_1 \rightarrow \lambda_1^{(c)+}$, we get

$$E_0(\lambda_1, \lambda_2) > -2e(\lambda_1 - \lambda_1^{(c)})^{\alpha_h}; \quad (21)$$

using (8), it follows that

$$\alpha_{\mathcal{H}} \geq \alpha_h. \quad (22)$$

Then, given that the 2–0 line exists,

$$E_0(\lambda_1, \lambda_2) < \mathcal{E}_0(\lambda_1), \quad (23)$$

and in the region $\lambda_1 \uparrow \lambda_1^{(c)}$ this equation becomes

$$E_0(\lambda_1, \lambda_2) < -e(\lambda_1 - \lambda_1^{(c)})^{\alpha_h} \Rightarrow \alpha_{\mathcal{H}} \leq \alpha_h. \quad (24)$$

From (22) and (24), we conclude that

$$\alpha_{\mathcal{H}} = \alpha_h \quad (25)$$

\square

In the next lemma, we prove that the existence of a one-body bound state at the threshold $\lambda_1^{(c)}$ forbids the existence of a 2–0 critical line.

Lemma 4. *If $\alpha_h = 1$, then a 2–0 line does not exist.*

Proof. $\alpha_h = 1 \Rightarrow \|\psi_0(\lambda_1^{(c)})\| = 1$ is an eigenfunction of $h(\lambda_1^{(c)})$ with a vanishing eigenvalue; then $\langle W \rangle_0(\lambda_1^{(c)}) > 0$. A first-order perturbative expansion gives

$$E_0(\lambda_1, \lambda_2) - \mathcal{E}_0(\lambda_1) \sim \mathcal{E}_0(\lambda_1) + \lambda_2 \langle W \rangle_0(\lambda_1), \quad (26)$$

for $\lambda_1 \sim \lambda_1^{(c)}$ and $\lambda_2 \sim 0$. The fact that $\mathcal{E}_0 \rightarrow 0$ for $\lambda_1 \rightarrow \lambda_1^{(c)}$ and $\langle W \rangle_0(\lambda_1^{(c)}) > 0$ implies that $\lambda_2^{(c)} \rightarrow 0$, because otherwise $E_0(\lambda_1^{(c)}, \lambda_2 \sim 0) - \mathcal{E}_0(\lambda_1^{(c)})$ would be positive.

Furthermore, $\frac{\partial E_0}{\partial \lambda_2} = \langle W \rangle_0(\lambda_1^{(c)}) > 0$ at $(\lambda_1^{(c)}, \lambda_2 = 0)$; then applying the implicit function theorem to $E_0(\lambda_1, \lambda_2) - \mathcal{E}_0 = 0$, we get the value of $\frac{\partial \lambda_2^{(c)}(\lambda_1^{(c)})}{\partial \lambda_1}$ at $\lambda_2 = 0$,

$$\frac{\partial \lambda_2^{(c)}(\lambda_1^{(c)})}{\partial \lambda_1} = \frac{\partial(\mathcal{E}_0 - E_0)}{\partial \lambda_1} \frac{1}{\frac{\partial E_0}{\partial \lambda_2}} \tag{27}$$

$$= -\frac{\langle v \rangle_0}{\langle W \rangle_0} \geq 0. \tag{28}$$

Then $0 \leq \frac{\partial \lambda_2^{(c)}(\lambda_1^{(c)})}{\partial \lambda_1} < \infty$ at $(\lambda_1^{(c)}, \lambda_2 = 0)$. □

From lemmas 3 and 4 we obtain an extra conclusion, that is

Theorem 2. *If a 2-0 line exists, then $\alpha_{\mathcal{H}} = \alpha_h > 1$ over this line.*

In the following section, we show how the different scenarios for the stability diagrams are possible if the relative properties between repulsion and attraction are appropriate. Section 4 will be focused entirely on Coulomb one-body attractive potentials.

3. Examples of the three cases of stability diagram

In what follows, we give a simple example and then a theorem for a certain class of external potentials. With a short-range one-body potential $v(r)$ the three behaviors are possible, depending on the repulsion $W(r_{12})$. For the single one-body potential, we use the Hulthén potential [15]:

$$v(r) = -\frac{e^{-r}}{1 - e^{-r}}. \tag{29}$$

This potential is exactly solvable for s-waves; their energies and eigenfunctions have analytic expressions. For the energies, we have

$$\mathcal{E}_n(\lambda_1) = -\frac{(2\lambda_1 - (n + 1))^2}{8(n + 1)}, \quad n = 0, \dots, \sqrt{2\lambda_1} - 1, \tag{30}$$

and particularly, for the ground state,

$$\mathcal{E}_0(\lambda_1) = -\frac{(2\lambda_1 - 1)^2}{8}, \quad \lambda_1^{(c)} = \frac{1}{2}. \tag{31}$$

Since we are interested in regions where $\lambda_1 \sim \lambda_1^{(c)}$, we can write $\lambda_1 = \lambda_1^{(c)} + \epsilon/2 = (1 + \epsilon)/2$. Using this notation, the ground-state function has the form

$$\psi_0(\epsilon; r) = \frac{1}{4\pi} C(\epsilon) e^{-\epsilon r/2} \frac{(1 - e^{-r})}{r}, \quad C(\epsilon) = \sqrt{\frac{\epsilon}{2}(1 + \epsilon)(2 + \epsilon)}. \tag{32}$$

The three different critical pictures can be achieved changing the range of W .

Short-range interaction. For the repulsion between particles, we use a δ -like potential (note that this potential does not fulfill all conditions (i)–(viii), but they are sufficient conditions),

$$W(\vec{x}_1, \vec{x}_2) = \delta(\vec{x}_1 - \vec{x}_2) = \frac{1}{r_1^2} \delta(r_1 - r_2) \delta(\cos \theta_1 - \cos \theta_2) \delta(\varphi_1 - \varphi_2). \tag{33}$$

For this kind of repulsion, the mean value of the potential is easily calculated:

$$\begin{aligned} \langle W \rangle_0(\lambda) &= \int d^3x_1 \int d^3x_2 \psi_0^2(\epsilon; r_1) \psi_0^2(\epsilon; r_2) \delta(\vec{x}_1 - \vec{x}_2) \\ &= 4\pi(5 \ln 2 - 3 \ln 3)\epsilon^2 + O(\epsilon^3). \end{aligned} \tag{34}$$

From this result and (16), we obtain a lower bound λ_2^* for the critical line $\lambda_2^{(c)}(\lambda_1)$:

$$\lambda_2^{(c)}(\lambda_1) \geq \lambda_2^* = 1/8\pi(5 \ln 2 - 3 \ln 3). \tag{35}$$

According to lemma 2, this means that the diagram is in case 2 or 3.

Long-range interaction. As a typical example of a long-range potential, we choose a Coulomb repulsion:

$$W(r_{12}) = \frac{1}{r_{12}}. \tag{36}$$

With this potential, we obtain

$$\langle W \rangle_0(\lambda_1) = \epsilon \ln 4; \tag{37}$$

then the diagram is of type 1, as expected from lemma 2.

The reason for the non-existence of the 2–0 line in the example above is related to the long range of the repulsive interaction, and not to other characteristics of the potentials. Indeed, we can understand this in the following qualitative way. It is known that the one-particle wavefunction spreads when $\lambda_1 \rightarrow \lambda_1^{(c)}$. Now, when the repulsive coupling λ_2 is turned on, if W is of short range the particles are so apart that they actually do not see each other, and the system can have a bound state for $\lambda_2 > 0$ near $\lambda_1 \sim \lambda_1^{(c)}$. In the long-range case, the situation is the opposite one. The repulsive interaction is long enough to tear apart the system for all $\lambda_2 > 0$ near $\lambda_1 \sim \lambda_1^{(c)}$. These considerations are actually valid even when the attraction is of long range, as is shown in the following section.

Theorem 3. *If $v(r)$ is of short range, $\alpha_h = 2$ and W is a Coulomb repulsion potential, then the diagram corresponds to case 1.*

Proof. For short-range potentials, we can define a constant R such that $v(r) \sim 0$ for $r > R$. Then the asymptotic form of the wavefunction is

$$\psi_0(\lambda_1; r)_{r \rightarrow \infty} \sim \frac{\exp(-\sqrt{2\mathcal{E}_0}r)}{r}, \tag{38}$$

which is exact for v of compact support. This expression is valid for $r > R$, so we can write

$$\psi_0(\lambda_1; r) = \begin{cases} \mathcal{N}\psi_{<}(\lambda_1; r) & \text{if } r < R \\ \mathcal{N}\psi_{<}(\lambda_1; R) \frac{R}{r} \exp(-\sqrt{2\mathcal{E}_0}(r - R)) & \text{if } r > R, \end{cases} \tag{39}$$

where \mathcal{N} is a normalization constant given by $\|\psi_0\| = 1$. Since $\psi_{<}$ is a well-behaved function in $\lambda_1 = \lambda_1^{(c)}$, we exclude it from the critical behavior. The norm of $\psi_{<}$ can be arbitrarily chosen; we then use

$$4\pi \int_0^R \psi_{<}^2(\lambda_1; r)r^2 dr = 1, \tag{40}$$

from which we obtain

$$\mathcal{N}(\epsilon) = \left[\frac{\sqrt{\mathcal{E}_0}}{\sqrt{2}(2\pi\sqrt{2\mathcal{E}_0} + R^2\psi_{<}^2(\lambda_1; R))} \right]^{1/2} \sim A\epsilon^{\alpha_h/4} \quad \text{for } \lambda_1 \rightarrow \lambda_1^{(c)}, \tag{41}$$

where $A > 0$ is a constant, $\epsilon = \lambda_1 - \lambda_1^{(c)}$ and $\psi_{<}^2(\lambda_1; R)$ is strictly positive and finite even for $\lambda_1 = \lambda_1^{(c)}$. Since we do not know the explicit behavior of the potential near the origin, $\psi_{<}(\lambda_1; R)$ is undetermined.

We are interested in the asymptotic condition for $\epsilon \rightarrow 0$. Since $\psi_{<}(\lambda_1; R)$ does not vanish and the coefficient in the expression for $r > R$ is positive and non-zero for $r = R$, then

$$\psi_0(\lambda_1; r) = \mathcal{N}(\epsilon)C(\epsilon)\frac{\exp(-\sqrt{2\mathcal{E}_0}r)}{r}, \tag{42}$$

where $C(\epsilon = 0) = C_0 > 0$. Now we study the asymptotic behavior of $\langle W \rangle_0(\lambda_1)$:

$$\langle W \rangle_0(\lambda_1) = 4\pi^2 \int_0^\infty dr_1 r_1 \psi_0^2(\lambda_1; r_1) \int_0^\infty dr_2 r_2 \psi_0^2(\lambda_1; r_2) \int_{|r_1-r_2|}^{r_1+r_2} dr_{12} r_{12} W(r_{12}). \tag{43}$$

Up to here, we have not used the fact that W is a Coulomb potential. We now introduce $W(r_{12}) = 1/r_{12}$ and solve the last integral, which results from straightforward calculations

$$\begin{aligned} \langle W \rangle_0(\lambda_1) &= (4\pi)^2 \int_0^\infty dr_{>} r_{>} \psi_0^2(\lambda_1; r_{>}) \int_0^{r_{>}} dr_{<} r_{<}^2 \psi_0^2(\lambda_1; r_{<}) \\ &= (4\pi)^2 \mathcal{N}^4 \left\{ \int_0^R dr_{>} r_{>} \psi_{<}^2(r_{>}) \int_0^{r_{>}} dr_{<} r_{<}^2 \psi_{<}^2(r_{<}) \right. \\ &\quad \left. + C(\epsilon)^2 \int_R^\infty dr_{>} \frac{\exp(-2\sqrt{2\mathcal{E}_0}r_{>})}{r_{>}} \left[\int_0^R dr_{<} r_{<}^2 \psi_{<}^2(r_{<}) \right. \right. \\ &\quad \left. \left. + C(\epsilon)^2 \int_R^{r_{>}} dr_{<} \exp(-2\sqrt{2\mathcal{E}_0}r_{>}) \right] \right\}. \tag{44} \end{aligned}$$

We are concerned with the dominant behavior of the integral for $\epsilon \rightarrow 0$. The first integral in (44) is in the region $r < R$ and is therefore a positive constant in $\epsilon = 0$. From the integrals between square brackets, it follows that the first equals 1 and the second is of order $\epsilon^{-\alpha_h/2}$. Then the second integral is the dominant term. Let us define β and Δ by the relations $2\sqrt{3\mathcal{E}_0} \sim \beta\epsilon^{\alpha_h/2}$ and $\Delta = (4\pi)^2 A^4 C_0^4 / \beta > 0$, respectively. Replacing in the integral, we obtain

$$\begin{aligned} \langle W \rangle_0(\lambda_1) &\sim \Delta \epsilon^{\alpha_h} \int_R^\infty dr_{>} \frac{\exp(-\beta\epsilon^{\alpha_h/2}r_{>})}{r_{>}} \left(\frac{\exp(-\beta\epsilon^{\alpha_h/2}R) - \exp(-\beta\epsilon^{\alpha_h/2}\epsilon r_{>})}{\epsilon^{\alpha_h/2}} \right) \\ &= \Delta [\exp(-\beta\epsilon^{\alpha_h/2}R)E_1(\beta\epsilon^{\alpha_h/2}R) - E_1(2\beta\epsilon^{\alpha_h/2}R)]\epsilon^{\alpha_h/2}, \tag{45} \end{aligned}$$

where $E_1(x)$ is the exponential integral [16], which diverges at $x = 0$, but the divergences cancel out each other in the expression, resulting in

$$\lim_{\epsilon \rightarrow 0} [\exp(-\beta\epsilon^{\alpha_h/2}R)E_1(\beta\epsilon^{\alpha_h/2}R) - E_1(2\beta\epsilon^{\alpha_h/2}R)] = \ln 2. \tag{46}$$

Then,

$$\langle W(1, 2) \rangle_0(\lambda_1) \sim \epsilon^{\alpha_h/2} \quad \text{for } \epsilon \rightarrow 0; \tag{47}$$

therefore, according to lemma 2, the diagram is of type 1

□

4. Long-range, Coulomb one-body potential

In this section, we show examples with $v(r)$ as a Coulomb attraction and give the stability diagram for different repulsion potentials. The results are expected to be valid for general long-range potentials $v(r)$ such that $v(r) \rightarrow 0$ for $r \rightarrow \infty$ and $\lim_{r \rightarrow \infty} v(r)r^2 \rightarrow \infty$. Long-range potentials have a one-body critical strength $\lambda_1^{(c)} = 0$.

The complete solution for the one-body Hamiltonian with the potential $v(r) = -1/r$ is presented in any textbook of quantum mechanics. The ground-state function and energy of $h(1) + h(2)$ are

$$\psi_0(\lambda_1; r_1)\psi_0(\lambda_1; r_2) = \frac{1}{\pi} \sqrt{2}\lambda_1^3 e^{-\lambda_1(r_1+r_2)}; \quad E_0(\lambda_1, \lambda_2 = 0) = -\lambda_1^2. \tag{48}$$

We choose a short-range Yukawa potential for the interaction between particles:

$$W(r_{12}) = \frac{\exp(-r_{12})}{r_{12}}; \tag{49}$$

then, from equation (43), we obtain

$$\langle W \rangle_0 = \frac{(1 + 8\lambda_1 + 20\lambda_1^2)}{(1 + 2\lambda_1)^4} \lambda_1^3. \tag{50}$$

The energy can be expanded to first order in λ_2 as

$$E_0(\lambda_1, \lambda_2) = -\lambda_1^2 + \frac{(1 + 8\lambda_1 + 20\lambda_1^2)}{(1 + 2\lambda_1)^4} \lambda_1^3 \lambda_2 + O(\lambda_2^2). \tag{51}$$

From lemma 2 and taking into account that $\alpha_n = 2$, the diagram is of type 3. The lower bound $\lambda_2^*(\lambda_1)$ of (16) can be written as

$$\lambda_2^{(c)}(\lambda_1) \geq \lambda_2^*(\lambda_1) = \frac{(1 + 2\lambda_1)^4}{2(1 + 8\lambda_1 + 20\lambda_1^2)} \frac{1}{\lambda_1} \sim \frac{1}{\lambda_1} \quad \text{for } \lambda_1 \rightarrow 0, \tag{52}$$

and we obtain $\lambda_2 = \infty$ as a lower bound, which means that $\lambda_2^{(c)} \rightarrow \infty$ for $\lambda_1 \rightarrow 0$.

The upper bound $\tilde{\lambda}_2(\lambda_1)$ of (16) assures the existence of the critical line. First, we must check that $2\mathcal{E}_1(\lambda_1) \geq \mathcal{E}_0(\lambda_1)$ in order to fulfill condition (vii); indeed

$$2\mathcal{E}_n(\lambda_1) = -2 \frac{\lambda_1^2}{2(n+1)^2}, \tag{53}$$

for $n = 1$, $2\mathcal{E}_1 = -\lambda_1^2/4 > -\lambda_1^2/2$. Since the Yukawa potential fulfills condition (viii), we calculate $\tilde{\lambda}_2(\lambda_1)$,

$$\tilde{\lambda}_2 = \lambda_1^2 \frac{3}{4} \langle r e^r \rangle_0 = \lambda_1^5 \frac{3(3 - 36\lambda_1 + 140\lambda_1^2)}{2(1 - 2\lambda_1)^6}. \tag{54}$$

Note that the upper bound tends to infinity for $\lambda_1 \rightarrow 1/2$, and the lower bound tends to infinity but for $\lambda_1 \rightarrow 0$. Figure 2 shows the variational lower and upper bounds.

Sharper lower bounds can be obtained using a simple variational function that includes correlation between particles:

$$\psi_v(r_1, r_2, r_{12}) = \frac{\sqrt{16\lambda_1^4}}{\pi \sqrt{8\lambda_1^2 + 35\lambda_1 c + 48c^2}} e^{-\lambda_1(r_1+r_2)} (1 + cr_{12}), \tag{55}$$

where c is a free parameter. We plot the critical line for different values of $c \in (0, \infty)$ in figure 2.

From the stability diagram of figure 2, and its bounds, we obtain some conclusions about the exact critical line. For example, all systems with $\lambda_2 < \min_{\lambda_1} \lambda_2^*(\lambda_1)$ have at least one bound state below the threshold. The exact critical line must have a minimum $\lambda_2^{(\min)}$ at some point between λ_1^m and λ_1^M , defined as

$$\lambda_1^m = \{\min_{\lambda_1} \lambda_1 : \lambda_2^*(\lambda_1) = \min_{\lambda_1} \tilde{\lambda}_2(\lambda_1)\} \tag{56}$$

and

$$\lambda_1^M = \{\max_{\lambda_1} \lambda_1 : \lambda_2^*(\lambda_1) = \min_{\lambda_1} \tilde{\lambda}_2(\lambda_1)\}. \tag{57}$$

These bounds for the minimum of the critical line are shown in figure 2. The fact that the critical line presents a minimum has interesting physical consequences. For a given value of $\lambda_2 > \lambda_2^{(\min)}$, decreasing λ_1 from $\lambda_1 = \infty$ the system crosses the bounds in an ordered sequence

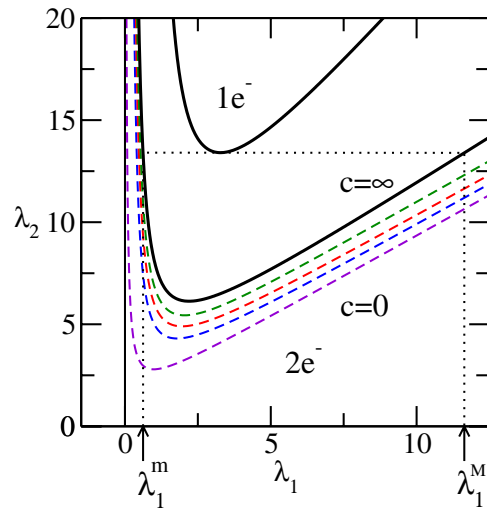


Figure 2. Upper and lower bounds for the stability line when h is a hydrogen-like Hamiltonian and W is a Yukawa potential. The trial wavefunction is given by equation (55), for several values of c . The exact critical curve lies between the full lines, the upper bound and the better lower bound ($c = \infty$). λ_1^m and λ_1^M are also shown.

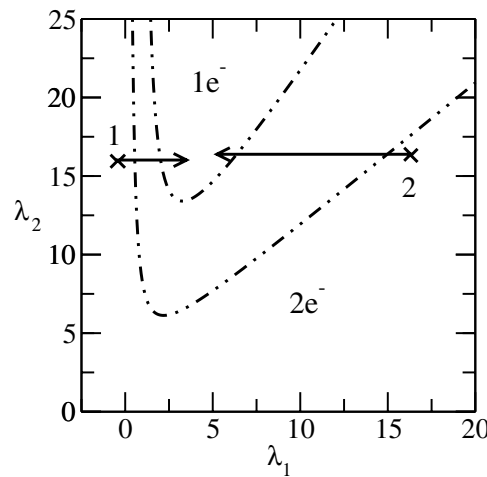


Figure 3. Sketch of the behavior in case 3. The dash-dotted curves are the upper and lower bounds to the exact critical curve. Points 1 and 2 represent systems with a bounded ground state that unbinds when λ_1 increases or decreases, respectively.

lower–upper. As the exact critical line is in the region between lower and upper bounds, we see that by decreasing λ_1 the system unbinds as expected. If we now *increase* λ_1 from $\lambda_1^{(c)}$, the system crosses the bounds in the same order lower–upper. Then, it loses the bound state *increasing the attractive strength of the one-body potential* λ_1 . A schematic sketch of this process is shown in figure 3. From point 2 by decreasing λ_1 the system unbinds, and from point 1 by *increasing* λ_1 the system also unbinds.

A physical explanation of this behavior can be made in terms of the ranges of the potentials. For a fixed value of λ_2 and λ_1 large enough the system binds two particles, no matter how repulsive W is. For a less attractive coupling λ_1 , the system loses the bound states because the repulsion W is too strong against the attraction. But, near $\lambda_1^{(c)}$, as is well known from the critical behavior of weakly bound systems, the wavefunction spreads and the distance between the particles diverges. Indeed, $\langle r_{12} \rangle_0 \sim 1/\lambda_1$, then the short-range repulsion W becomes unimportant and can be ignored because the distance between particles is larger than the range of the repulsion potential. Then, the system is again bounded by the long-range Coulomb attraction. If W is of long range, this argument is not valid. In fact, if $W(r_{12}) \geq 1/r_{12} \forall r_{12} > 0$, the upper bound for the critical line forbids this behavior (see remark (ii)).

- (i) For $W = 1/r_{12}$, the homogeneity of the potential allows us to obtain the functional form of the critical line [18] $\lambda_2^{(c)} = C\lambda_1 \sim 1.1\lambda_1$. There is no 2–0 line; the stability diagram is then of type 1. Since the ground state is bounded at $\lambda_2 = \lambda_2^{(c)}(\lambda_1)$ [18], the exponent is $\alpha_{\mathcal{H}} = 1$.
- (ii) Suppose two potentials W_a and W_b such that $W_b > W_a$. The corresponding Hamiltonians are $\mathcal{H}_\gamma = h(1) + h(2) + \lambda_2 W_\gamma$, $\gamma = a, b$, then

$$\begin{aligned} E_a(\lambda_1, \lambda_2) &\leq \langle b | \mathcal{H}_a | b \rangle \\ &= E_b(\lambda_1, \lambda_2) + \lambda_2 \langle b | W_a - W_b | b \rangle \\ &\leq E_b(\lambda_1, \lambda_2), \end{aligned} \tag{58}$$

where $| \gamma \rangle$ is the ground state of \mathcal{H}_γ . This relation for the energies implies that $\lambda_2^{(c)}(a) > \lambda_2^{(c)}(b)$, meaning that if an upper (lower) bound for $\lambda_2^{(c)}(a)$ ($\lambda_2^{(c)}(b)$) exists, then it is an upper (lower) bound for $\lambda_2^{(c)}(b)$ ($\lambda_2^{(c)}(a)$) too. So, from the previous remark, if $W > 1/r \forall r$, there is no 2–0 line, and the diagram is of type 3 (this does not include $1/r^n$ potentials with $n > 1$, unless the tail is changed for $1/r$).

- (iii) For $W = 1/r^\beta$ and $2 \leq \beta < 3$, it follows that $\langle W \rangle_0 \sim \lambda_1^\beta$. The diagram is of type 3 for $\beta > 2$ and of type 2 or 3 for $\beta = 2$. For $\beta \rightarrow 3$, $\langle W \rangle_0 \rightarrow \infty$ for all λ_1 .
- (iv) If W has a short-range repulsive tail and a $1/r^2$ behavior at the origin, $\langle W \rangle_0 \sim \lambda_1^3$, then the diagram is of type 3.

The last remark shows that the behavior at $r = 0$ of the repulsion is also important for the behavior of $\langle W \rangle_0$ at $\lambda_1 \rightarrow 0$.

Finally, we search a potential that has the two bounds finite for all λ_1 ; the diagram is then of type 2. We search a bounded potential that fulfills $W < 1/r$, so the critical line is above that for $W = 1/r$. A possible choice is

$$W = \left(-\frac{r^2}{2} + \frac{3}{2} \right) \Theta(1 - r) + \frac{1}{r^2} \Theta(r - 1). \tag{59}$$

This potential fulfills condition (viii), so we calculate the upper and lower bounds which are shown in figure 4. The limiting values for the bounds are

$$\lim_{\lambda_1 \rightarrow 0} \lambda_2^*(\lambda_1) = \lim_{\lambda_1 \rightarrow 0} \frac{|\mathcal{E}_0(\lambda_1)|}{\langle W \rangle_0} = \frac{3}{8} \tag{60}$$

$$\lim_{\lambda_1 \rightarrow 0} \tilde{\lambda}_2(\lambda_1) = \lim_{\lambda_1 \rightarrow 0} 2(\mathcal{E}_1(\lambda_1) - \mathcal{E}_0(\lambda_1)) \left\langle \frac{1}{W} \right\rangle_0 = 9; \tag{61}$$

then $3/8 \leq \lambda_2^{(mc)} \leq 9$ (see figure 1).

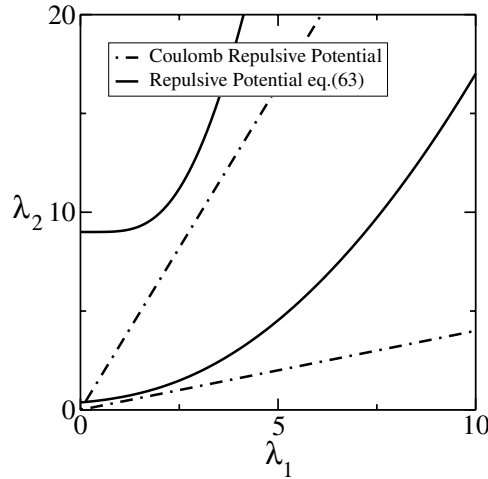


Figure 4. Upper and lower bounds for the repulsive potential W of (59). For comparison we also show the bounds for $W = 1/r$, calculated from equations (11) and (15).

4.1. Existence of critical lines for a large class of potentials W

The upper and lower bounds for the Yukawa repulsion can be used to prove, using a variational argument, that the critical line exists for other repulsive potentials with the same attractive interaction. As proved above, for $W = e^{-r}/r$ there exists a critical line at least for $\lambda_1 > 1/2$. Note that if we make a dilation $r \rightarrow \tau r$ on the Hamiltonian and rescale the energy $\mathcal{H} \rightarrow \mathcal{H}\tau^2$, we obtain

$$\mathcal{H}(\lambda_1, \lambda_2) \rightarrow \mathcal{H}(\lambda_1/\tau, \lambda_2/\tau). \tag{62}$$

Then the upper bound obtained for the Yukawa potential now turns into

$$\lambda_1^{(c)}(\tau) = \lambda_1^{(c)}(1)\tau \quad \lambda_2^{(c)}(\tau) = \lambda_2^{(c)}(1)\tau, \tag{63}$$

which is an upper bound for $e^{-\tau r}/r$. Making $\tau \rightarrow 0$, we see that the upper bound (54) tends to $105\lambda_1/32$. This is the bound $\tilde{\lambda}_2(\lambda_1)$ for $W = 1/r$, which can be easily calculated from equation (11) as we did for the Yukawa potential. The bound keeps the divergence at $\lambda_1 = \tau/2 \forall \tau > 0$, and vanishes for $\tau = 0$.

With this family of upper bounds, we are able to prove the existence of the critical line for several potentials. For example, potentials of the form $1/r^n$ with $n > 1$ satisfy the condition $1/r^n > e^{-\tau(n)r}/r$, with $\tau(n) \geq (n-1)/e$, so the critical lines for these potentials exist. In fact, for $\lambda_2 = 0$ there is always at least one bound state with energy $2\mathcal{E}_0(\lambda_1)$. Since the threshold is $\mathcal{E}_0(\lambda_1)$, from the continuity of the energy in λ_2 we conclude that there exists a region below the upper bound with $\lambda_2 > 0$ where the system has a bounded ground state.

It is also possible to prove the existence of the 2-1 critical line for short-range one-body potentials that are finite at the origin. For this purpose, we use an exponential potential e^{-r} , which has an upper bound

$$\tilde{\lambda}_2 = \lambda_1^2 \frac{3}{4} (e^r)_0 = \lambda_1^5 \frac{3(1 - 10\lambda_1 + 32\lambda_1^2)}{2(2\lambda_1 - 1)^5}. \tag{64}$$

As in the Yukawa case, we use this bound to obtain a bound for $e^{-\tau r}$,

$$\lambda_1^{(c)}(\tau) = \lambda_1^{(c)}(1)\tau \quad \lambda_2^{(c)}(\tau) = \lambda_2^{(c)}(1)\tau^2. \tag{65}$$

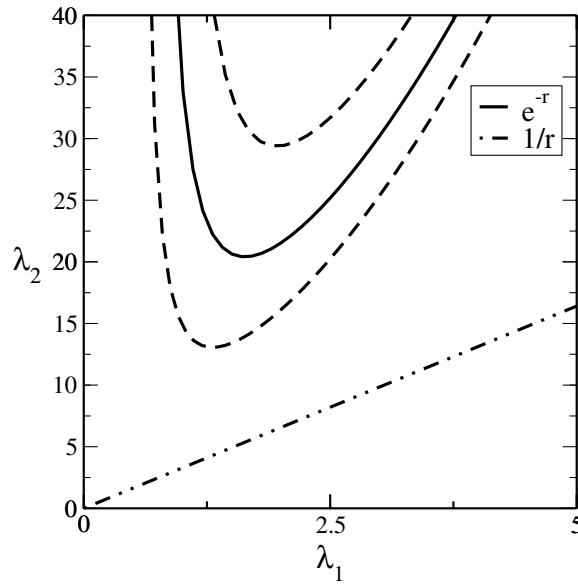


Figure 5. The graphic shows the upper bounds given by (54) and (64) for the exponential potential and for the Coulomb potential (slash-dotted). Also the bounds for two exponentials are shown (slashed): $e^{-\tau r}$ with $\tau = 0.8, 1.2$ obtained from (65).

These bounds are shown in figure 5. Note that this bound actually proves the existence of the critical line for every potential that fulfills

$$\begin{aligned}
 W(0) &\geq 1, & W'(0) &\geq -\tau \\
 W(r) &> e^{-\tau r} \quad \forall r > 0 & \text{for some } \tau > 0.
 \end{aligned}
 \tag{66}$$

5. Conclusions

In this work, we presented the possible stability diagrams for the ground-state energy for two identical particles in an external attractive potential. The critical exponent that characterizes the asymptotic form of the energy near a critical point was also discussed.

The main result of this work is that a *rebinding* phenomenon may occur for some two-body systems when the attractive coupling is decreased. As we have showed, this effect is a consequence of a competition between the attractive long-range external potential and the short-range inter-particle repulsion of these systems.

Remarkably, for one-body Coulomb attractive potentials the three types of diagrams discussed in this work are possible.

We also showed that $\alpha_{\mathcal{H}} > 1$ over a 2–0 line, and hence the wavefunction spreads when $\lambda_1 \rightarrow \lambda_1^{(c)-}$ for $\lambda_2 < \lambda_2^{(mc)}$ fixed. However, some questions are still unanswered. One of them is the value of the critical exponent over the 2–1 line. We were unable to obtain this value in a rigorous mathematical way, but we can argue that $\alpha_{\mathcal{H}} = 1$, and then a bounded two-particle solution exists over this line. Over a 2–1 line, the one-particle Hamiltonian has a well-defined bounded ground state with negative energy. Two identical particles in the ground state have the same spatial quantum numbers. Then the ground-state function of a two-identical particle

system cannot spread continuously to a state corresponding to one particle bounded and one particle unbounded, and therefore the critical exponent $\alpha_{\mathcal{H}}$ has to be equal to 1 over a 2–1 line. This assumption was proved for the two-electron atom [18].

Another open question is the value of the critical exponent at the point $(\lambda_1^{(c)}, \lambda_2^{(mc)})$ when the stability diagram corresponds to case 2.

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