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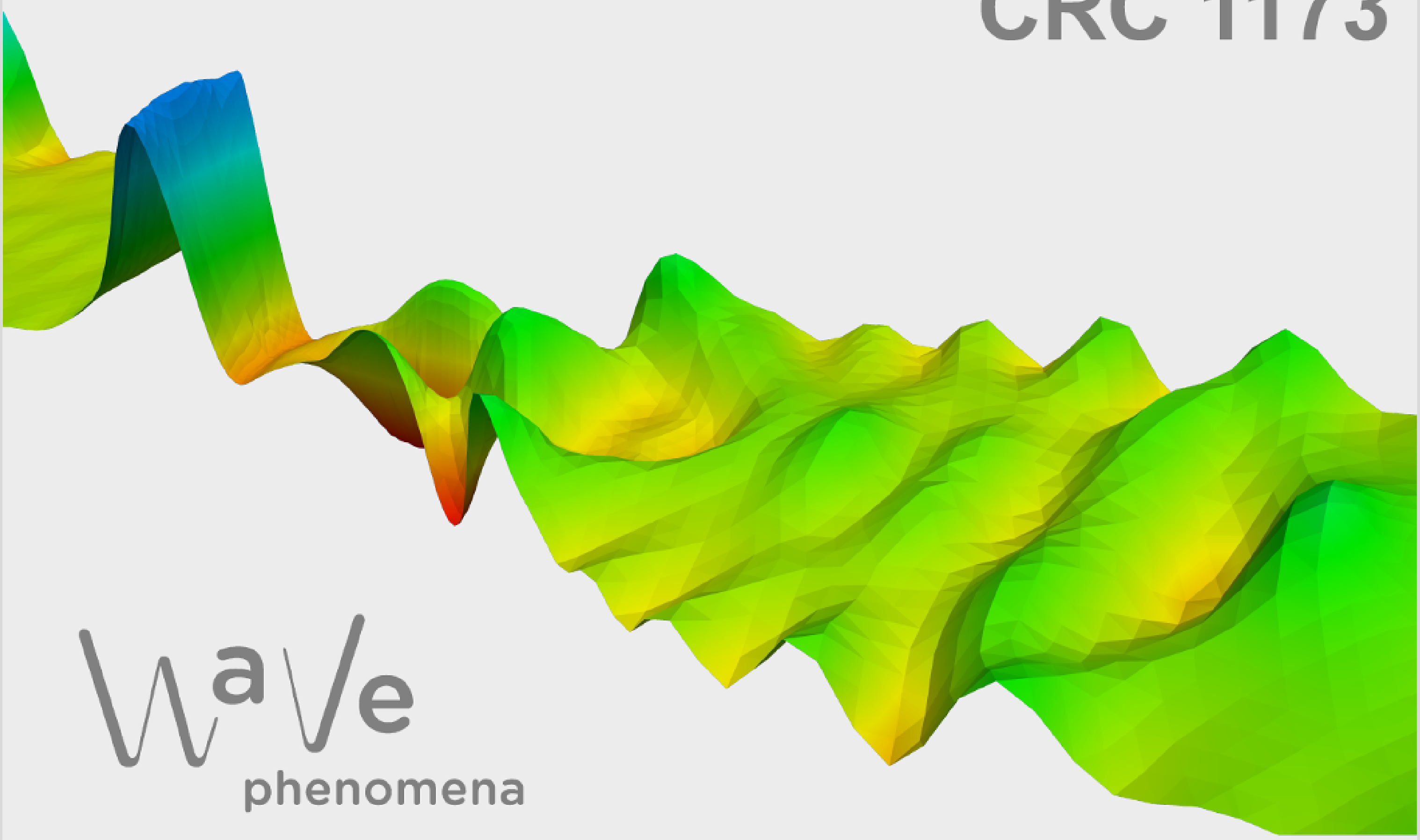

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QUANTUM SYSTEMS AT THE BRINK: HELIUM–TYPE SYSTEMS

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Abstract. In the present paper we study two challenging problems for helium–type systems. Existence of eigenvalues at thresholds and the asymptotic behavior of the corresponding eigenfunctions. Since the usual methods for addressing these problems need a safety distance to the essential spectrum, they cannot be applied in critical cases, when an eigenvalue enters the continuum.

We develop a method to address both problems and derive *sharp upper and lower bounds* for the asymptotic behavior of the ground state of critical helium–type systems at the threshold of the essential spectrum. This is the first proof of the precise asymptotic behavior of the ground state for this benchmark problem in quantum chemistry. Moreover, our bounds describe precisely how the asymptotic decay of the ground state changes, when the system becomes critical. In addition, we show the existence of a ground state of this quantum critical system with a finite nuclear mass. Previously this had been known only in the Born–Oppenheimer approximation of infinite nuclear mass.

Contents

1. Introduction

From the beginning of quantum mechanics, many important questions about a quantum system are related to the existence and behavior of its bound states. These states are given

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by the square integrable eigenvectors of the operator describing the quantum system. In this paper we consider two particle operators of the form

$$H_U = P_1^2 + P_2^2 - \frac{1}{|x_1|} - \frac{1}{|x_2|} + \frac{U}{|x_1 - x_2|} \,. \tag{1.1}$$

Here $x_j \in \mathbb{R}^3$ are the positions of the two particles, and P_j^2 their kinetic energy, where $P_j = -i\nabla_{x_j}$ is the momentum operator of the particle and $j = 1, 2$. The Hamiltonian H_U is well-defined and self-adjoint on $\mathcal{D}(H_U) = H^2(\mathbb{R}^6)$, where $H^2(\mathbb{R}^6)$ is the usual Sobolev space of weakly differentiable functions in $L^2(\mathbb{R}^6)$ with square integrable weak derivatives up to second order.

The operator H_U arises from scaling two–particle helium–type systems described by the operator

$$H = \sum_{j=1}^{2} \left(\frac{1}{2m} P_j^2 - \frac{Ze^2}{|x_j|} \right) + \frac{e^2}{|x_1 - x_2|}$$

where Z is the nuclear charge and e the unit for the elementary electric charge. Here we use units, where other physical constants such as Planck's constant $\hbar$ are set equal to one. Using scaling, i.e., a change of length–scale, given by $U_s\psi(x) = s^3\psi(sx)$, $x \in \mathbb{R}^6$, which is unitary on $L^2(\mathbb{R}^6)$, one gets with $s = 2mZe^2$ and $U = 1/Z$

$$U_s^* H U_s = 2mZ^2e^4 H_U \,.$$

Thus H_U with $U = 1/Z$ is the operator describing helium-type systems such as Li^+ for $Z = 3$, He for $Z = 2$, and H^- for $Z = 1$.

We denote the ground state energy of H_U by E_U. More precisely, $E_U = \inf_{\|\psi\|=1}\langle \psi, H_U\psi\rangle$, which is concave and increasing in $U \geq 0$, since H_U is linear in U and the two particle Coulomb repulsion is positive. Hence the ground state energy E_U is continuous in $U \geq 0$. Of course, one should also include the spin of the particles, e.g., electrons, in which case one should consider H_U on $L^2((\mathbb{R}^3 \times \mathbb{C}^2)^2)$, or the antisymmetric subspace of functions which are antisymmetric when permuting the particles. Since the potential does not couple different spins, all bound states of H_U on $L^2((\mathbb{R}^3 \times \mathbb{C}^2)^2)$ can be classified as two particle bound states with parallel or antiparallel spins. In the first case the wave functions is anti-symmetric, in the second case it is symmetric under permutation of the particle *positions*. The ground state of H_U on $L^2((\mathbb{R}^3 \times \mathbb{C}^2)^2)$ lies in the latter, so it is enough to consider H_U on the subspace of $L^2(\mathbb{R}^3 \times \mathbb{R}^3)$ which is symmetric under permutation of the particle positions, see the discussion in [41, Chapter 4.3].

The HVZ Theorem [43], [32, Theorem XIII.17], shows that the essential spectrum of H_U is a half–line whose bottom is given by the ground state energy of the system with one less electron, i.e., hydrogen whose ground state energy is $-1/4$. Thus

$$\sigma_{\mathrm{ess}}(H_U) = \big[-\frac{1}{4}, \infty \big)$$

for any $U \geq 0$. Since usual perturbation theory applies when $E_U < \inf \sigma_{\mathrm{ess}}(H_U) = -1/4$, the regular first order perturbation theory [32], also called the Feynman-Hellmann formula, gives

$$\frac{d}{dU} E_U = \langle \psi_U, (\partial_U H_U)\psi_U \rangle = \langle \psi_U, \frac{1}{|x_1 - x_2|}\psi_U \rangle > 0 \tag{1.2}$$

for all $U \geq 0$ with $E_U < -1/4$.

Since the work of Stillinger [40], see also [39], these Helium–type atoms at critical coupling are an intensely studied benchmark problem in quantum chemistry. For a review see, e.g., [15] and the references therein. In particular, there has been interest in the precise value of the critical U_c, for which the ground state energy of H_U enters the edge of the essential spectrum, that is, U_c is the smallest coupling for which $E_U = -1/4$. Numerically one finds $U_c \simeq 1.1$ [40]. The calculation of U_c and the bound state at critical coupling $U = U_c$ continues to serve as an important benchmark problem in quantum chemistry. E.g., going up to order 401 in perturbation theory, the critical value was calculated in the very nice paper [6] to be approximately $U_c \simeq 1.09766$, which was further pushed in [25]. A variational calculation of U_c was done in [34]. Recently [12] pushed the calculations to $U_c \sim 1,097\,660\,833\,738\,56$. Without the Born–Oppenheimer approximation the critical coupling, which depends on the nuclear mass, was calculated numerically in [26].

It is easy to see rigorously that there is a critical $1 < U_c \leq 2$ such that $E_{U_c} = \inf \sigma_{\text{ess}}(H_U)$. As discussed in Appendix D, $E_U < -1/4$ implies $U < 2$ for this two-particle system. So clearly $U_c \leq 2$. To see that $U_c > 1$ we note that the classical result by Bethe [8], using a test function ansatz due to Hylleras [24], shows that hydrogen can bind two electrons, i.e., H_U has a ground state with energy $< -1/4$ for $U = 1$. Hill showed that this is also true without the Born–Oppenheimer approximation, as long as the mass of the nucleus is not too small compared to the mass of the lighter particles. So by continuity of E_U in U, one knows that E_U is below the ionization threshold even for some $U > 1$, so $U_c > 1$. Moreover, the work of Hill [17] shows that for $1 \leq U < U_c$ the operator H_U has exactly one bound state with energy below the essential spectrum. This also holds for finite nuclear mass [18].

Although the Hamiltonian H_U with $U = U_c$ has been intensely studied with asymptotic and numerical methods, little is known rigorously. The existence of a ground state ψ_c of H_{U_c} at critical coupling was proved in [19] with the help of PDE methods. An alternative existence proof was given in [14]. General features of the behavior of the ground state energy of quantum systems near coupling constant threshold had been discussed, for example, in [27, 28]. Unfortunately, still very little is known so far concerning *precise quantitative properties* of the ground state ψ_c *at critical coupling*.

This is the main motivation for our work. We provide sharp upper and lower bounds on the asymptotic behavior of the ground state of helium-type atoms at critical coupling. Moreover, we prove a family of sharp upper and lower bounds which are uniform in the coupling $0 \leq U \leq U_c$. Our results provide the first rigorous bounds on the asymptotic behavior of bounds states which correspond to eigenvalues *at the edge of the essential spectrum*. In addition, even in the subcritical case our upper and lower bounds improve on previously known results, since our upper and lower bounds have *the same leading order* and differ only in lower order terms. Our main results are

Theorem 1.1 (Global upper bound at critical coupling)**.** *Given parameters $K_1, K_2 > 0$, $1/6 < \kappa_1 < 1/2$, and $(3 - 2\kappa_1)/4 < \kappa_2 < 1$ define*

$$F_+(r_1, r_2) = 2(U_c - 1)^{1/2} r_1^{1/2} - K_1 r_1^{\kappa_1} + \frac{1}{2} r_2 - K_2 r_2^{\kappa_2} \tag{1.3}$$

for $r_1, r_2 \geq 0$. Then at critical coupling $U = U_c$ the helium atom has a ground state ψ_c with energy $-1/4$ and we have the pointwise upper bound

$$\psi_c(x) \leq C \exp\big(-F_+(|x|_\infty, |x|_0)\big) \tag{1.4}$$

for the unique positive ground state.

Here $|x|_0 = \min(|x_1|, |x_2|)$, respectively $|x|_\infty = \max(|x_1|, |x_2|)$, is the distance of the particle closer to, respectively farther from, the nucleus.

Remark 1.2. The constant C in the upper bound (1.4) depends only on κ_1, κ_2, K_1, K_2, an easy a-priori uniform bound on ψ_c, and on local bounds of the form $e^{-F_+(x)} \geq c_K > 0$ for $x \in K$ where K is a suitable compact subset of $\mathbb{R}^d$, see the proof in Section 8.

Since the ground state ψ_c at critical coupling is L^2 and the Coulomb interaction is in the Kato–class, an a-priori bound of the form $\|\psi_c\|_\infty \lesssim \|\psi_c\|_2$ exists, since the semigroup $\exp(-tH_U)$ is bounded from $L^2(\mathbb{R}^6)$ to $L^\infty(\mathbb{R}^6)$, see [36].

The matching *lower bound* is provided by

Theorem 1.3 (Global lower bound at critical coupling)**.** *Given parameters* $1/6 < \kappa_1 < 1/2 < \kappa_2 < 1$*, and* $K_1, K_2 > 0$ *define*

$$F_-(r_1, r_2) = 2(U_c - 1)^{1/2} r_1^{1/2} + K_1 r_1^{\kappa_1} + \frac{1}{2} r_2 + K_2 r_2^{\kappa_2} \,. \tag{1.5}$$

Then we have the pointwise lower bound

$$\psi_c(x) \gtrsim \exp\big(- F_-(|x|_\infty, |x|_0)\big) \tag{1.6}$$

for the unique positive ground state ψ_c *of* H_{U_c} *at critical coupling. Here again* $|x|_0 = \min(|x_1|, |x_2|)$ *and* $|x|_\infty = \max(|x_1|, |x_2|)$*.*

Remark 1.4. Note that, up to the sign of lower order terms $r_1^{\kappa_1}$ and $r_2^{\kappa_2}$, our upper and lower bounds from Theorem 1.1 and Theorem 1.3 perfectly match each other. Thus we get the *precise leading order coefficients* for the asymptotic decay of the ground state for the helium–type systems, unlike previous methods.

The existence of a ground state at critical coupling was shown in [19] by PDE methods. The upper bound from Theorem 1.1, even a much simpler version, see Theorem 4.1, allows for a simple variational proof of *existence* of a ground state of helium–type atoms at critical coupling similar to [14]. We can even avoid the Born–Oppenheimer approximation, see Section 9 .

Of course, while being sharp, the above upper and lower bounds hold only at critical coupling. We also have upper and lower bounds which hold uniformly in the coupling. For $0 \le U \le U_c$ we define a_U and ε_U by

$$a_U := (U - 1)_+^{1/2}, \quad \varepsilon_U := -\frac{1}{4} - E_U \tag{1.7}$$

so ε_U is the ionization energy, the distance of the energy E_U to the edge of the essential spectrum, which is at $-1/4$. By the HVZ theorem, this is the minimal energy needed to move one particle to infinity. Furthermore, we set

$$F_U(r) := \big(\varepsilon_U + \frac{a_U^2}{r}\big)^{1/2} r + \frac{a_U}{\varepsilon_U} \ln\left[\Big(1 + \frac{\varepsilon_U r}{a_U^2}\Big)^{1/2} + \frac{\sqrt{\varepsilon_U r}}{a_U}\right] \tag{1.8}$$

and

$$F_\pm^U(r_1, r_2) := F_U(r_1) + \frac{1}{2} r_2 \mp (K_1 r_1^{\kappa_1} + K_2 r_2^{\kappa_2}) \,. \tag{1.9}$$

Again, we suppress the explicit dependence of $F_\pm^U$ on the parameters κ_1, κ_2 and K_1, K_2, for notational simplicity. We also set $F_\pm^U(x) = F_\pm^U(x_1, x_2) = F_\pm^U(|x|_\infty, |x|_0)$ for $x = (x_1, x_2) \in \mathbb{R}^3 \times \mathbb{R}^3$, with a slight abuse of notation.

Remark 1.5. The precise form of F_U is of no relevance, what is important is that

$$F_U'(r) = \left(\varepsilon_U + \frac{a_U^2}{r}\right)^{1/2} \,. \tag{1.10}$$

Clearly, as long as the ionization energy ε_U is positive, the leading order behavior of F^U is asymptotic to $F^U(r_1) \sim (\varepsilon_U + a_U^2/r_1)^{1/2} r_1 \sim \sqrt{\varepsilon_U} r_1$, but it changes to $2a_U\sqrt{r_1}$ *at critical* *coupling* $U = U_c$, when the ionization energy vanishes. Thus one recovers $F_\pm$ from $F_\pm^U$ in the limit of critical coupling, when the ionization energy vanishes.

However, we want to stress the fact that in order to get the correct asymptotic in the limit $\varepsilon_U \to 0$, one cannot ignore the logarithmic term in (1.8), which for fixed $\varepsilon_U > 0$ is *always of much lower order* compared to the first term. In the limit of vanishing ionization energy the second term gives the *same contribution* as the first term and should not be discarded, see the discussion in Remark 2.7.

Theorem 1.6 (Sharp upper and lower bounds, arbitrary coupling)**.** *For any choice of parameters $K_1, K_2 > 0$, $1/6 < \kappa_1 < 1/2$, and $(3 - 2\kappa_1)/4 < \kappa_2 < 1$ there exist positive constants $C_\pm$ depending only on κ_1, κ_2, K_1, and K_2, such that for the unique positive ground state of the helium-type operator H_U the two–sided pointwise bound*

$$C_- \exp\left(-F_-^U(|x|_\infty, |x|_0)\right) \le \psi_U(x) \le C_+ \exp\left(-F_+^U(|x|_\infty, |x|_0)\right) \tag{1.11}$$

holds uniformly in $0 \le U \le U_c$.

For the subcritical case, where for fixed small $\mu > 0$ the repulsion parameter U is allowed to vary uniformly in $\mu \le U \le U_c - \mu$, assume that $0 < \kappa_1 < 1$ and $1/2 < \kappa_2 < 1$, and $K_1, K_2 > 0$. Then there exist positive constants $\widetilde{C}_\pm$, depending only on $\kappa_1, \kappa_2, K_1, K_2$, and also μ, such that the two–sided bound

$$\widetilde{C}_- \exp\left(-F_-^U(|x|_\infty, |x|_0)\right) \le \psi_U(x) \le \widetilde{C}_+ \exp\left(-F_+^U(|x|_\infty, |x|_0)\right) \tag{1.12}$$

holds for all $\mu \le U \le U_c - \mu$.

We would like to stress the fact that the constants $C_\pm$ depend on the parameters $\kappa_1, \kappa_2, K_1, K_2$ but not on the coupling U in the range $0 \le U \le U_c$, i.e., they are uniform up to the critical coupling U_c.

To put our results into perspective, let us compare them with previously known results which only addressed the subcritical case $U < U_c$. The first precise bounds for the asymptotic behavior of eigenfunction of H_U with energy strictly below the essential spectrum are due to the groundbreaking works of Slaggie and Wichmann for three–body systems [38], Ahlrichs for atoms [3], O'Connor [31], Combes and Thomas [9], Deift, Hunziker, Simon, and Vock [11] for multi–particle systems, culminating in the work of Agmon [1]. The last result provides bounds for asymptotic behavior of bound states for general multi-particle systems, based on energy methods.

For two particle systems in the *subcritical* case, the ionization energy ε_U is positive and Agmon's method yields the upper bound

$$|\psi_U(x)| \le C_\delta \exp\left(-c_1|x|_\infty - c_2|x|_0\right) \tag{1.13}$$

for $c_1 = \sqrt{\varepsilon_U} - \delta$ and $c_2 = 1/2 - \delta$ for any small $\delta > 0$ and some constant C_δ which diverges for $\delta \to 0$. Here $|x|_\infty = \max(|x_1|, |x_2|)$ is the distance to the nucleus of the particle *farther from*, and $|x|_0 = \min(|x_1|, |x_2|)$ is the distance to the nucleus of the particle *closer to*, the nucleus.

Recall that ε_U is the ionization energy of the two–particle system. After one particle is removed one is left with hydrogen, whose ionization energy is $1/4$ in the units we chose. So both constants c_1 and c_2 have a clear physical meaning in the upper bound (1.13). Thus, except for reducing the constants by an arbitrarily small amount, the upper bound (1.13) is exactly what is predicted by WKB–type physical heuristics.

Using subsolution estimates, it was shown in [21] that one can set $\delta = 0$ at the expense of having polynomial prefactors in the upper bound. A matching lower bound for the ground state ψ, where $U = 1/Z = 1/2$, of the two particle system describing helium has been derived by Thomas Hoffmann–Ostenhof in [20],

$$\psi(x) \geq c_\delta \exp\left(-(\sqrt{\varepsilon_1}+\delta)|x|_\infty - \frac{1}{2}|x|_0\right) \tag{1.14}$$

for arbitrary $\delta > 0$ and some constant $c_\delta > 0$, which goes to zero as $\delta \to 0$.

Thus, except for decreasing/increasing the constants, which are the square roots of the successive ionization energies, in the upper/lower bounds by an arbitrary amount, these bounds settle the asymptotic behavior of the ground state wave functions and they can also be extended to subcritical $U < U_c$ where $E_U < -1/4$.

However, these results are *useless at critical coupling*, since then the first ionization energy ε_U is zero, i.e., there is *no energy cost* for removing the first particle. The only known decay property of the ground state $\psi_c = \psi_{U_c}$ of H_{U_c} at critical coupling is the result in [19] where they show that a positive solution of the Schrödinger equation exists and fulfills the upper bound

$$|\psi_c(x)| \leq C_m(1+|x|_\infty + |x|_0^2)^{-m} \tag{1.15}$$

for some constants $C_m < \infty$ for any $m > 0$ and all $x_1, x_2 \in \mathbb{R}^3$. Of course, this implies that $\psi_c \in L^2(\mathbb{R}^6)$, so a ground state for this critical two-particle system exists. Moreover, in the remark in Section 4 of [19], they note that one can use the "Schrödinger inequalities" method of Ahlrichs and M. and T. Hoffmann-Ostenhof [21] to derive sharp upper and lower bounds for the *one-particle density* ρ_c of the ground state ψ_c,

$$\begin{aligned}\sqrt{\rho_c(y)} &\leq C_\delta^+(1+|y|)^{-3/4+\delta}\exp\left(-2(U_c-1)^{1/2}|y|^{1/2}\right),\\ \sqrt{\rho_c(y)} &\geq C_\delta^-(1+|y|)^{-3/4-\delta}\exp\left(-2(U_c-1)^{1/2}|y|^{1/2}\right)\end{aligned} \tag{1.16}$$

for some constants $0 < C_\delta^\pm < \infty$, $\delta > 0$ and all $y \in \mathbb{R}^3$. Here ρ_c is given by

$$\rho_c(y) \coloneqq \int_{\mathbb{R}^3} |\psi_c(y,z)|^2\, dz$$

that is, it is the marginal of the ground state probability density $|\psi_c|^2$ on $\mathbb{R}^6$, which is symmetric under permutations of the particles.

However, all these results says nothing about the asymptotic decay of the *full ground state* ψ_c. We fill this gap by proving sharp anisotropic upper and lower bounds on the asymptotic behavior of the wave function ψ_U of H_U at or below critical coupling and also determine rigorously, how the decay changes in the whole critical range $0 \leq U \leq U_c$.

Organization of the paper. The proof of the upper bound from Theorem 1.1 is via a combination of energy methods and pointwise subsolution type bounds in the spirit of well–known subsolution comparison principles from elliptic PDE. We have to overcome two obstacles, however. We need a low regularity version of these comparison principles which goes back to Agmon [2]. But even having such a low regularity version, we cannot apply it directly. The comparison principle works well for one or two body problems, but not, in general, for multi–particle problems. Even for a restricted three body–body problem such as helium–type atoms in the infinite nuclear mass approximation, the comparison principle is not directly applicable because in order to control the errors, both particle have to be far from the nucleus.

To overcome this, we first prove an anisotropic L^2 upper bound, which is transferred to pointwise bounds by a standard argument. Except for a transition region, this upper bound has *the correct* asymptotic in certain directions. We use this as an input for our proof of the sharp global anisotropic upper bound.

By now, the derivation of L^2–type upper bounds on the asymptotic decay of eigenfunctions is standard. However, we would like to stress that, following the general approach a la Agmon [1], one loses an epsilon in the constants of the leading order terms, which we have to avoid. In addition, the methods of Agmon [1] or [11] and the works before them need a *safety distance* of the ground state energy to the bottom of the essential spectrum. We do not have such a safety distance, since the ground state energy at critical coupling is at the edge of the essential spectrum.

As a warm-up, we explain our main new ideas, which prove why a *long-range repulsive* part of the potential can stabilize bound states at the ionization threshold for a one particle system in Section 2. We derive sharp upper and lower bounds on the asymptotic behavior of zero energy ground state of such quantum systems.

The necessary local energy bounds, needed for the proof of the anisotropic L^2 upper bound for Helium type systems, are derived in Section 3. A main new feature here is that we do not use conical regions to localize the particles, which is the usual approach in the study of many-particle systems. Instead, to be able to get a sharp anisotropic upper bound, it is crucial to use paraboloidal regions.

We derive an isotropic upper bound for the ground state in Section 4 , which is considerably simpler than the proof our sharp anisotropic bounds. The proof of the anisotropic upper bound is done in Sections 5 and 6, see, in particular, the proof of Theorem 6.5.

The proof of the lower bounds is done with a subharmonic comparison principle. As a first step we derive in Section 7 a lower bound in the *tricky region*, where one particle tries to escape to infinity and the other one stays (essentially) close to the nucleus. The global anisotropic lower bound is proven in Section 8. The main difficulty there is to control the singular Coulomb repulsion between the two particles with terms which are only of lower order. See, in particular, the proof of Theorem 8.4.

Lastly we show how one can relax the use of the Born–Oppenheimer approximation, that is, the the assumptions that the nucleus has infinite mass, in Section 9.

Certain technical tools are gathered in the appendix. The main reason for including them is that our exponential weights for the upper bounds and the comparison functions used in the proofs of the lower bounds lack the usually required high enough regularity. Their derivatives have jumps along codimension one Lipshitz surfaces, so standard results cannot, or at least not straightforwardly, be applied.

2. One particle case

To explain the main ideas of our approach, we consider one particle moving in an external potential. This external potential consists of an attractive and a repulsive part with Hamiltonian given by

$$H = -\Delta - V + W \tag{2.1}$$

where we assume $V, W \geq 0$ are infinitesimally (form) bounded with respect to $-\Delta$. For simplicity, we also assume that $\operatorname{supp} V(x)$, the support of V, is compact. However, our proof works even for cases where the support of V is unbounded provided that the repulsion W dominates the attractive part V outside some bounded region. We also assume that W goes to zero at infinity, so the essential spectrum of the system is given by $\sigma_{\mathrm{ess}}(H) = [0, \infty)$, the discrete spectrum of H is below zero.

In the following we assume that the operator $H = -\Delta - V + W$ is defined in the sense of quadratic forms, that is,

$$\langle \varphi, H\psi \rangle = \langle \nabla\varphi, \nabla\psi \rangle + \langle \varphi, (-V + W)\psi \rangle$$

for all φ, ψ in the standard Sobolev space $H^1(\mathbb{R}^d)$. We consider (weak) eigenfunctions ψ of H, by which we mean that

$$\langle \varphi, H\psi \rangle = E\langle \varphi, \psi \rangle \tag{2.2}$$

for all $\varphi \in H^1(\mathbb{R}^d)$. By density of $\mathcal{C}_0^\infty(\mathbb{R}^d)$ in $H^1(\mathbb{R}^d)$ it is enough to require that (2.2) holds for all $\varphi \in \mathcal{C}_0^\infty(\mathbb{R}^d)$. We are interested in the question whether zero, the edge of the essential spectrum, can be an eigenvalue of the system and if so, how does the corresponding eigenfunction decay at infinity? An extreme case is the situation where a parameter, say the repulsion W or the depth of the well V is tuned in such a way that the ground state eigenvalue hits zero. Does the bound state survive or does it dissipate? This is clearly a non-perturbative situation.

Using previous approaches, such as Agmon's method [1], one can easily show that the eigenvectors corresponding to negative eigenvalues decay exponentially. However, these approaches need a safety distance to the essential spectrum and yield nothing for eigenfunctions at the edge of the essential spectrum!

We will first discuss how to get upper bounds on eigenfunctions without having a safety distance of the corresponding eigenvalue to the essential spectrum. Once one has such a type of bound, this also implies existence of eigenvalues at the edge of the essential spectrum, Details of this argument are given in Appendix C and D in a more complicated situation.

2.1. **Taking advantage of long-range repulsion.** In the following we show how to derive upper bounds on the asymptotic behavior of zero energy eigenfunctions. These upper bounds illustrate how the type of asymptotic decay of ψ is directly related to the repulsive potential W.

Lemma 2.1. *Let H be given as in (2.1) and assume that V has compact support. Let $\psi \in L^2(\mathbb{R}^d)$ be a weak eigenfunction of H with energy $E \le 0$. Furthermore, assume that $F \ge 0$ is a locally bounded and differentiable function such that for some $R > 0$*

$$|\nabla F(x)|^2 < W(x) \quad \text{for all } |x| \ge R\,. \tag{2.3}$$

Then

$$\int_{|x|\ge R} e^{2F(x)+\ln\left(W(x)-|\nabla F(x)|^2\right)} |\psi(x)|^2\, dx \le C_{F,R}\|\psi\|^2 \tag{2.4}$$

with

$$C_{F,R} = 8 \sup_{R/2\le|x|\le R} e^{2F(x)}\left(2R^{-2} + R^{-1}|\nabla F(x)|\right)\,. \tag{2.5}$$

Remark 2.2. The point of the bound above is that the right hand side is *uniform* in the eigenvalue $E \le 0$. It *does not need a safety distance* to the essential spectrum. Moreover, the constant $C_{F,R}$ depends on *local* bounds of F, hence it is finite even for unbounded functions F. Of course, as W tends to zero at infinity, so does $|\nabla F|^2$. Nevertheless F can still go to infinity under this condition, and the main question is which of the terms in $2F + \ln\left(W - |\nabla F|^2\right)$ will win this tug–of–war. It is easy to see that the borderline case is a decay of the form $W(x) \sim |x|^{-2}$ at infinity. Any slower decay of W will lead to a growth of F which out–paces the second term $\ln\left(W - |\nabla F|^2\right)$.

Proof of Lemma 2.1: Let ξ be any real-valued bounded and differentiable function and use $\varphi = \xi^2\psi$ in the weak form of the eigenvalue equation. Then $E\|\xi\psi\|^2 = E\langle \xi^2\psi, \psi\rangle = \langle \xi^2\psi, H\psi\rangle$ and since $E\|\xi\psi\|^2$ is real we can use the IMS localization formula, see [10, 16] or Appendix A, to get

$$E\|\xi\psi\|^2 = \mathrm{Re}\langle \xi^2\psi, H\psi\rangle = \langle \nabla(\xi\psi), \nabla(\xi\psi)\rangle + \langle \xi\psi, (-V+W)\xi\psi\rangle - \langle \psi, |\nabla\xi|^2\psi\rangle \tag{2.6}$$

Rearranging and dropping the kinetic energy term, which is positive, gives

$$\langle \xi\psi, (-V + W - E)\xi\psi\rangle \le \langle \psi, |\nabla\xi|^2\psi\rangle \tag{2.7}$$

Take $\chi \in \mathcal{C}^\infty(\mathbb{R}_+)$ with $0 \le \chi \le 1$, $\chi(r) = 0$ if $r \le 1/2$, $\chi(r) = 1$ if $r \ge 1$, and set

$$\chi_R(x) \coloneqq \chi\left(|x|/R\right) \quad \text{for } x \in \mathbb{R}^d\,. \tag{2.8}$$

It is easy to see that a function χ fulfilling the above constraints exists and for which one has $\|\chi'\|_\infty \le 4$. For any such choice we have $\chi_R \in \mathcal{C}^\infty(\mathbb{R}^d)$ and $\|\nabla\chi_R\|_\infty \le 4/R$.

Now assume that F is bounded and differentiable, for the moment, and use $\xi = \xi_R = \chi_R e^F$. Using

$$\nabla\xi = e^F\nabla\chi_R + e^F\chi_R\nabla F\,,$$

in (2.7) and reshuffling the terms a bit we see

$$\langle \xi_R\psi, (-V + W - E - |\nabla F|^2)\xi_R\psi\rangle \le \langle \psi, e^{2F}\left(|\nabla\chi_R|^2 + 2\chi_R\nabla\chi_R\nabla F\right)\psi\rangle\,. \tag{2.9}$$

Moreover, we can use $0 \le \chi_R \le 1$ on the right hand side and $E \le 0$ to drop the term $-E$ on the left hand side in (2.9) to get

$$\langle \xi_R\psi, (W - |\nabla F|^2)\xi_R\psi\rangle \le \langle \psi, e^{2F}\left(|\nabla\chi_R|^2 + 2|\nabla\chi_R||\nabla F|\right)\psi\rangle\,. \tag{2.10}$$

where we also took R so large that χ_R, hence also ξ_R, is zero on the support of V.

In the case that $F \ge 0$ is not bounded, we regularize it by considering

$$F_\delta = \frac{F}{1 + \delta F}\,. \tag{2.11}$$

Then $F_\delta \le F$ and

$$\nabla F_\delta = \frac{\nabla F}{(1 + \delta F)^2}$$

so $|\nabla F_\delta| \le |\nabla F|$. Thus (2.9) yields

$$\langle \chi_R e^{F_\delta}\psi, (W - |\nabla F|^2)\chi_R e^{F_\delta}\psi\rangle \le \langle \psi, e^{2F}\left(|\nabla\chi_R|^2 + 2|\nabla\chi_R||\nabla F|\right)\psi\rangle \le C_{F,R}\|\psi\|^2 \tag{2.12}$$

since the support of $\nabla\chi_R$ is contained in the annulus $R/2 \le |x| \le R$. Since $0 \le \chi_R \le 1$ and $\chi_R(x) = 1$ for $|x| \ge R$ we get

$$\int_{|x|\ge R} e^{2F_\delta(x) + \ln\left(W(x) - |\nabla F(x)|^2\right)}|\psi(x)|^2\,dx \le C_{F,R}\|\psi\|^2 \tag{2.13}$$

and using that F_δ converges pointwise monotonically to F in the limit $\delta \to 0$ we see that (2.4) holds. ∎

Remark 2.3. Of course, one should not always drop the term $-E$ from the left hand side of (2.9). Keeping it we get the bound

$$\int_{|x|\ge R} e^{2F(x) + \ln\left(W(x) - E - |\nabla F(x)|^2\right)}|\psi(x)|^2\,dx \le C_{F,R}\|\psi\|^2 \tag{2.14}$$

under the condition

$$|\nabla F(x)|^2 < W(x) - E \tag{2.15}$$

which allows for a larger class of functions F, which can grow linearly in $|x|$. This leads to exponential L^2-type upper bounds when $E < 0$, i.e., when one has a *safety distance* to the bottom of the essential spectrum. How one can easily choose exponential weights F which fulfill condition (2.3), respectively (2.15), is shown in sections 2.2 and 2.4.

2.2. **An example with a repulsive Coulomb tail.** Assume that V has compact support and $W(x) = \eta/|x|$ outside some compact set. Use

$$F(r) = 2(\eta r)^{1/2} - Kr^{\kappa}/2 \tag{2.16}$$

for some $0 < \kappa < 1/2$ and $K > 0$ and also set $F(x) = F(|x|)$ by a slight abuse of notation. Then $|\nabla F(x)| = |F'(|x|)|$ and for any eigenfunction ψ of H with energy $E \leq 0$, we have

$$W(x) - |\nabla F(x)|^2 = 2\eta^{1/2}|x|^{\kappa-3/2} - (K\kappa)^2|x|^{2(\kappa-1)}/4 \gtrsim |x|^{\kappa-3/2} \geq |x|^{-3/2} \tag{2.17}$$

since $\kappa - 3/2 > 2(\kappa - 1)$ iff $\kappa < 1/2$. In this case, Lemma 2.1 shows that

$$x \mapsto e^{2(\eta|x|)^{1/2} - K|x|^{\kappa}/2 - \frac{3}{2}\ln|x|}\psi(x)$$

is in $L^2(\mathbb{R}^d)$ outside of some large enough ball $|x| \geq R$, uniformly in the energy $E \leq 0$ for normalized eigenfunctions ψ. Since any fractional power r^{κ} bounds logarithmic terms $\ln r$ for large r and ψ is globally L^2 we see that

$$x \mapsto e^{2(\eta|x|)^{1/2} - K|x|^{\kappa}}\psi(x) \in L^2(\mathbb{R}^d) \tag{2.18}$$

for any $K > 0$ and $0 < \kappa < 1/2$.

Using subsolution bounds, or the Harnack inequality for ground states, one can get the pointwise upper bound

$$|\psi(x)| \lesssim \exp(-2(\eta|x|)^{1/2} + K|x|^{\kappa}) \tag{2.19}$$

from this, see the proof of Corollary 5.4.

Moreover, Lemma 2.1 can also be used to show that if the attractive part $V = V_\lambda$ is tuned in the parameter λ in such a way that $H_\lambda = -\Delta - V_\lambda + W$ converges to some limiting operator H_λ and H_λ has a ground state energy $E_\lambda < 0$ which converges to zero as $\lambda \to \lambda_{\mathrm{cr}}$, then the limiting operator $H_c = H_{\lambda_{\mathrm{cr}}}$ has a zero energy eigenvalue embedded at the edge of its essential spectrum. This follows from tightness and weak convergence arguments similarly to the discussion in Appendix C and D.

2.3. **Lower bound for zero energy ground states of systems with a repulsive Coulomb tail.** Assume that $H = -\Delta - V + W$ is as above with $W(x) = \eta/|x|$ outside of a compact, V has compact support, and ψ is a positive zero energy ground state of H. Then the upper bound in (2.19) is sharp in the sense that we have

Lemma 2.4. *In the above situation, we have the lower bound*

$$\psi(x) \gtrsim \exp(-2(\eta|x|)^{1/2} - K|x|^{\kappa}) \tag{2.20}$$

for all $x \in \mathbb{R}^d$, where ψ is the unique positive zero energy ground state of H.

Proof. We will use the subharmonic comparison principle. Since ψ is only a weak eigenfunction of H in the sense of quadratic forms, we use the quadratic form version of the subharmonic comparison principle due to Agmon [2], see also Appendix B.

Define $g = e^{-F}$, which is $\mathcal{C}^2$ on $|x| > R$ for any $R > 0$ and assume that $g \in L^2$, or at least on $|x| > R$. Calculating

$$\nabla g = -g\nabla F \quad \text{and} \quad -\Delta g = g\left(\Delta F - |\nabla F|^2\right) \tag{2.21}$$

we see that if

$$W(x) \leq |\nabla F(x)|^2 - \Delta F(x) \tag{2.22}$$

then $Hg \leq 0$ on $|x| > R$, or, as quadratic forms

$$\langle \varphi, Hg\rangle \leq 0 \quad \text{for all } 0 \leq \varphi \in \mathcal{C}_0^\infty(\Omega_R) \tag{2.23}$$

with $\Omega_R = \{|x| > R\}$. Since $\psi > 0$ is continuous (here we assume that V and W are Kato–class potentials) it is bounded away from zero on $\{|x| \le R\}$, which is compact. Since g is bounded, there exist a constant $C > 0$ such that

$$\psi(x) \ge Cg(x) \quad \text{for all } |x| \le R+1\,. \tag{2.24}$$

Hence on the boundary layer $R < |x| < R+1$, which is a boundary layer for the boundary $\partial\Omega_R$ in the sense of Definition B.2, we have

$$\psi(x) \ge Cg(x) \quad \text{for all } R < |x| < R+1 \tag{2.25}$$

and then subharmonic comparison principle implies

$$\psi(x) \ge Cg(x) = C\exp(-F(x)) \quad \text{for all } |x| \ge R\,. \tag{2.26}$$

By the choice of C this also holds for $|x| \le R$, hence globally.

We apply the above with the radial choice

$$F(r) = 2(\eta r)^{1/2} + Kr^{\kappa}, \quad r = |x| \tag{2.27}$$

for which one calculates $\nabla F(x) = F'(r)\frac{x}{|x|}$ and $\Delta F(x) = F''(r) + F'(r)\frac{d-1}{r}$, hence

$$\begin{aligned}&|\nabla F(x)|^2 - \Delta F(x) - W(x)\\ &\quad = 2\eta^{1/2}K\kappa r^{\kappa-3/2} + (K\kappa)^2 r^{2(\kappa-1)} - \eta^{1/2}(d-\frac{1}{2})r^{-3/2} - K\kappa(\kappa+d-2)r^{\kappa-2} > 0\end{aligned} \tag{2.28}$$

since the first term dominates the negative terms for all large enough r_1 when $\kappa > 0$. This proves (2.20). ∎

Remark 2.5. This lower bound together with the upper bound from (2.19) shows that any zero energy ground state of a one–particle Hamiltonian with a long range Coulomb–type repulsion $W(x) = \lambda|x|^{-1}$ obeys for all $x \in \mathbb{R}^d$ the two sided bound

$$C_- \exp(-2(\eta|x|)^{1/2} - K|x|^{\kappa}) \le \psi(x) \le C_+ \exp(-2(\eta|x|)^{1/2} + K|x|^{\kappa}) \tag{2.29}$$

for any $0 < \kappa < 1/2$ and $K > 0$ and some $0 < C_- \le C_+ < \infty$. In particular, the leading order terms in these bounds are sharp.

Similar sharp lower and upper bounds can be proven for long range repulsive tails of the form $W(x) = \eta|x|^{-2\rho}$ for any $0 < \rho < 1$. In this case F needs to fulfill $F'(r) \sim r^{-\rho}$, hence $F(r) \sim r^{1-\rho}$ and thus any zero energy ground state will have an asymptotic decay of the form

$$\psi(x) \sim \exp\left(-\frac{\sqrt{\eta}}{1-\rho}|x|^{1-\rho}\right) \quad \text{for } |x| \gg 1\,. \tag{2.30}$$

We leave the details to the interested reader. A detailed study of the one–particle case can be found in [22], where for short range repulsive tails a phase transition for the non-existence versus existence of zero energy ground states was proved, depending on the dimension $d \le 3, d = 4$, and $d \ge 5$.

2.4. **Repulsive Coulomb-tail: Interpolating between the subcritical and critical cases.** We can also consider a subcritical situation

$$H_\lambda = -\Delta - V_\lambda(x) + \frac{\eta}{|x|} \tag{2.31}$$

with ground state eigenvalue $E_\lambda < 0$ for $0 \le \lambda < \lambda_{\mathrm{cr}}$ and $E_\lambda = 0$ for $\lambda = \lambda_{\mathrm{cr}}$. The a–priori bounds above and the discussion in Appendix C and D show that then $H_c = H_{\lambda_{\mathrm{cr}}}$ has a zero energy bound state. Again, let us assume, for simplicity, that V_λ has a compact support. For $\lambda < \lambda_{\mathrm{cr}}$ the ground states clearly have exponential decay and at critical coupling this exponential decay switches over to the stretched exponential decay with $\lambda = \lambda_{\mathrm{cr}}$ as discussed above.

The question is how the decay rate changes precisely from exponential to subexponential as the gap between the essential spectrum and the ground state closes for $\lambda \nearrow \lambda_{\mathrm{cr}}$. In such a case, one should also take advantage of the fact that we can allow $|\nabla F|^2 < \eta/|x| - E_\lambda$, see Remark 2.3. With $\varepsilon = -E_\lambda$, the ionization energy, and choosing F to be radial, one sees that one needs to find a function $F = F_{\varepsilon,\eta}$ such that

$$|F'_{\varepsilon,\eta}(r)|^2 = \varepsilon + \frac{\eta}{r} \tag{2.32}$$

for large enough r. It is straightforward to check that

$$F_{\varepsilon,\eta}(r) = \int \sqrt{\varepsilon + \frac{\eta}{r}}\mathrm{d}r = \left(\varepsilon + \frac{\eta}{r}\right)^{1/2} r + \frac{\eta}{\sqrt{\varepsilon}} \ln\left(\left(1 + \frac{\varepsilon r}{\eta}\right)^{1/2} + \sqrt{\frac{\varepsilon r}{\eta}}\right). \tag{2.33}$$

It is easy to see that the second term in $F_{\varepsilon,\eta}(r)$ is positive and only logarithmically growing in r for fixed $\varepsilon > 0$. Thus $F_{\varepsilon,\eta}(r)$ is linearly growing in r and asymptotic to $\sqrt{\varepsilon}r$, which is the decay rate predicted by WKB methods when the ionization energy is positive.

Using Lemma 2.1, we again conclude that the ground state corresponding to a negative eigenvalue $E < 0$ behaves as

$$\psi(x) \le C_+ \exp\left(-F_{\varepsilon,\eta}(|x|) + K|x|^\kappa\right) \tag{2.34}$$

for some constant $C_+ < \infty$ and any $0 < \kappa < 1/2$, $K > 0$.

One first uses Lemma 2.1 to get an L^2 upper bound and then transfers this into a pointwise upper bound via subsolution bounds of Trudinger, see [36, Theorem C.1.3], or the Harnack inequality for the ground state, similar as in the proof of Corollary 5.4 below.

To derive a lower bound on the ground state ψ, we use the variant

$$g = \exp(-F_{\varepsilon,\eta}(|x|) - K|x|^\kappa)$$

of the function used in Section 2.3. A straightforward but slightly tedious calculation shows that g is also a classical subsolution of $H_\lambda = -\Delta - V_\lambda + \eta/|x|$ at energy $E_\lambda = -\varepsilon$ outside a large enough ball in $\mathbb{R}^d$, i.e., $(H_\lambda - E_\lambda)g(x) \le 0$ for $|x|$ large enough. We leave the details of these calculations to the interested reader.

Exactly as in the proof of Lemma 2.4 one then concludes that the lower bound

$$\psi(x) \ge C_- \exp\left(-F_{\varepsilon,\eta}(|x|) - K|x|^\kappa\right) \tag{2.35}$$

holds for some constant $C_- > 0$ and any $0 < \kappa < 1/2$, $K > 0$.

Collecting the upper and lower bounds one sees that they yield sharp upper and lower bounds for one–particle quantum systems with a long range Coulomb repulsion.

Theorem 2.6. *Let ψ_λ be a ground state of the one–particle Hamiltonian H_λ corresponding to the energy $E_\lambda \le 0$. Then we have the two–sided bound*

$$C_1 \exp\left(F_{|E_\lambda|,\eta}(|x|) - K|x|^\kappa\right) \le \psi_\lambda \le C_2 \exp\left(F_{|E_\lambda|,\eta}(|x|) + K|x|^\kappa\right) \tag{2.36}$$

for some constants $0 < C_1 \le C_2 < \infty$ and all $0 < \kappa < 1/2$, $K > 1$.

The constants C_1, C_2 may be dependent on the parameter λ, in general, but will be independent of it for most physically relevant cases, see the end of Remark 2.7 below.

Remark 2.7. The logarithmic term in (2.33) is positive and, for fixed ionization energy $\varepsilon > 0$ only logarithmically growing in r. In this case, the leading order behavior of $F_{\varepsilon,\eta}$ is dominated by the first term and is given by

$$F_{\varepsilon,\eta}(r) \sim \left(\varepsilon + \frac{\eta}{r}\right)^{1/2} r \sim \varepsilon^{1/2} r \tag{2.37}$$

for large r.

Clearly, $(\varepsilon+\eta/r)^{1/2}r \to (\eta r)^{1/2}$ in the limit of vanishing ionization energy, $\varepsilon = -E \to 0$, which is exactly half of the leading order term in the estimate (2.29) for the ground state. It is easy to see directly from the definition of $F_{\varepsilon,\eta}$ as an integral in (2.33), that

$$F_{0,\eta}(r) = \lim_{\varepsilon\to 0} F_{\varepsilon,\eta}(r) = 2(\eta r)^{1/2} \tag{2.38}$$

which is *twice* of the limit of the *leading order term* in the expression of $F_{\varepsilon,\eta}$ on the right hand side of (2.33). Alternatively, we note that the second term in the right–hand–side of (2.33) can be written as

$$\frac{\eta}{\sqrt{\varepsilon}} \ln\left(\left(1+\frac{\varepsilon r}{\eta}\right)^{1/2} + \sqrt{\frac{\varepsilon r}{\eta}}\right) = \frac{\sqrt{\eta r}}{t} \ln\left((1+t^2)^{1/2}+t\right)$$

with $t = \sqrt{\varepsilon r/\eta}$. Since

$$\frac{1}{t}\ln\left((1+t^2)^{1/2}+t\right) = \ln\left(\left((1+t+O(t^2)\right)^{1/t}\right) \to \ln e = 1$$

in the limit $t = \sqrt{\varepsilon r/\eta} \to 0$, we see that the logarithmic term in (2.33), which for fixed $\varepsilon > 0$ is *always of much lower order* than the first term, gives the *same contribution as the first term* in the limit of vanishing ionization energy $\varepsilon \to 0$ and should not be discarded.

Because of (2.38) the upper and lower bounds (2.34) and (2.35) also hold in the limit of vanishing ionization energy and one recovers our previous subexponential upper and lower bounds for zero energy ground states. Thus the function $F_{\varepsilon,\eta}$ describes precisely the phase transition between exponential and subexponential decay of the ground states of H_λ in the critical limit of vanishing ionization energy.

If the potentials W and V_λ are in the so-called Kato–class, for definitions see [4, 10, 36], and V_λ is continuous in the Kato–norm, one can show that the constants C_1, C_2 in (2.36) can be chosen to be *independent of λ up to the critical coupling* by an argument which parallels the one we give for helium–type systems, using a one–particle version of Proposition D.1 in the Appendix.

2.5. **The fate of zero-energy solutions for short range potentials.** Without a long–range repulsive tail of the potential one can still do a similar analysis as for long–range repulsive potentials, using now an additional boost coming from the kinetic energy. We say that a potential V is *short range* if

$$|V(x)| \lesssim \frac{1}{|x|^2 \ln^q(|x|)} \quad \text{for } |x| \gtrsim 1 \text{ and some } q > 2\,, \tag{2.39}$$

or if

$$|V(x)| \leq \frac{c}{|x|^2 \ln^2(|x|)} \quad \text{for } |x| \gtrsim 1 \text{ and some } c < \frac{1}{4} \tag{2.40}$$

Let $H = -\Delta + V$ be defined via quadratic forms. A function $\psi \in H^1_{\mathrm{loc}}(\mathbb{R}^d)$ is a (weak) zero energy solution if $\langle \varphi, H\psi\rangle = \langle \nabla\varphi, \nabla\psi\rangle + \langle \varphi, V\psi\rangle = 0$ for all $\varphi \in \mathcal{C}_0^\infty(\mathbb{R}^d)$. Clearly, this extends to all $\varphi \in H^1(\mathbb{R}^d)$ with compact support.

Theorem 2.8. *Assume that $\psi \in H^1_{loc}(\mathbb{R}^d)$ is a zero energy bound state of a one–particle Schrödinger operator $H = -\Delta + V$ with a short–range potential V in dimension $d \geq 3$ and*

$$\liminf_{L\to\infty} \frac{1}{L^2} \int_{L\leq |x| \leq \alpha L} |\psi(x)|^2\, dx = 0 \tag{2.41}$$

for some $\alpha > 1$. Then

$$x \mapsto \frac{(1+|x|)^{(d-4)/2}}{\ln(2+|x|)}\psi(x) \in L^2(\mathbb{R}^d) \tag{2.42}$$

Remark 2.9. The condition (2.41) poses a weak condition on the decay of ψ at infinity. In particular, ψ does not need to be in L^2. The bound (2.42) shows that if d ≥ 5, then $\psi \in L^2(\mathbb{R}^d)$, i.e., ψ is a zero energy eigenfunction of H. If $d = 4$, then $x \mapsto (\ln(2+|x|))^{-1}\psi(x) \in L^2(\mathbb{R}^4)$, i.e., ψ barely misses to be L^2 and in three dimensions one sees that $x \mapsto |x|^{-1/2}(\ln(2+|x|))^{-1}\psi(x) \in L^2(\mathbb{R}^3)$. This is consistent with the known behavior of zero-energy resonances of Schrödinger operators. A series of sharp criteria for the existence/absence of zero energy ground states for one–particle Schrödinger operators in any dimension can be found in [22].

Theorem 2.8 is an extension of results on L^2 bounds for zero energy eigenfunctions and resonances of one–particle Schrödinger operators in [7, Theorem 2.1]. As already shown in [7], the above bound has the following consequence: Assume that the potential V is infinitesimally form bounded with respect to $-\Delta$ and that the one–particle Schrödinger operators $H = -\Delta + V$, defined via quadratic forms, has a virtual level at zero, that is, $H \geq 0$ and, with $H_\delta = -(1-\delta) + V$,

$$\inf \sigma(H_\delta) < 0$$

for all $0 < \delta < 1$. Then in dimensions $d \geq 5$, zero is a simple eigenvalue of H. The proof uses Theorem 2.8, or better a slight extension of it to H_δ, and tightness and weak convergence arguments to show that the ground states of H_δ with $\delta = 1/(2n)$, $n \in \mathbb{N}$, yield a sequence which converges strongly to the ground of H. Similar arguments are given in Appendix C and D, for the existence of a ground state for helium–type atoms with a critical repulsion with finite or infinite nuclear mass.

Proof of Theorem 2.8. Let F be a function which is bounded and differentiable outside some compact set and whose gradient is bounded by $|\nabla F(x)| \lesssim |x|^{-1}$ for large $|x|$. Let $\widetilde{\chi} \in \mathcal{C}_0^\infty(\mathbb{R}^d)$ with $0 \leq \widetilde{\chi} \leq 1$, $\widetilde{\chi}(x) = 1$ if $|x| \leq 1$, and $\widetilde{\chi}(x) = 0$ if $|x| \geq 2$. We use the scaled version $\widetilde{\chi}_L(x) = \widetilde{\chi}(x/L)$, which is a smoothed out projection inside a centered ball of radius $\sim L$.

Use again $\xi = \chi_R e^F$ with χ_R from (2.8) and now also $\zeta_L = \widetilde{\chi}_L \xi$. Then $\zeta_L^2\psi$ is in H^1 and has compact support. The weak form of the eigenvalue equation and the IMS localization formula again show

$$0 = \langle \zeta_L^2\psi, H\psi\rangle = \langle \zeta_L\psi, H\zeta_L\psi\rangle - \langle \psi, |\nabla\zeta_L|^2\psi\rangle\,. \tag{2.43}$$

One calculates

$$\begin{aligned}
|\nabla\zeta_L|^2 &= |\nabla F|^2\widetilde{\chi}_L^2\chi_R^2e^{2F} + \widetilde{\chi}_L^2e^{2F}\left(|\nabla\chi_R|^2 + 2\chi_R\nabla\chi_R\nabla F\right) + \chi_R^2e^{2F}|\nabla\widetilde{\chi}_L|^2 \\
&\quad + 2\chi_R\widetilde{\chi}_L\nabla\widetilde{\chi}_L\left(\nabla\chi_R + \chi_R\nabla F\right)e^{2F} \\
&= |\nabla F|^2\zeta_L^2 + e^{2F}\left(|\nabla\chi_R|^2 + 2\chi_R\nabla\chi_R\nabla F\right) + \xi^2\left(|\nabla\widetilde{\chi}_L|^2 + 2\widetilde{\chi}_L\nabla\widetilde{\chi}_L\nabla F\right)
\end{aligned}$$

where the last equality holds for $L > R$, since then $\nabla\widetilde{\chi}_L$ and $\nabla\chi_R$ have disjoint supports and $\widetilde{\chi}_L = 1$ on the support of $\nabla\chi_R$. Reshuffling terms in (2.43) we get

$$\begin{aligned}
\langle \zeta_L\psi, \left(H - |\nabla F|^2\right)\zeta_L\psi\rangle &= \langle \psi, e^{2F}\left(|\nabla\chi_R|^2 + 2\chi_R\nabla\chi_R\nabla F\right)\psi\rangle \\
&\quad + \langle \psi, \xi^2\left(|\nabla\widetilde{\chi}_L|^2 + 2\widetilde{\chi}_L\nabla\widetilde{\chi}_L\nabla F\right)\psi\rangle\,.
\end{aligned} \tag{2.44}$$

An improvement of Hardy's inequality outside large balls given in [30] shows

$$\langle \nabla\varphi, \nabla\varphi\rangle \geq \langle \varphi, \Big(\big(\frac{d-2}{2}\big)^2 \frac{1}{|x|^2} + \frac{1}{4|x|^2 \ln^2(|x|)} \Big)\varphi\rangle \tag{2.45}$$

for any $\varphi \in H_0^1(B_t(0)^c)$ and t large enough. Thus

$$\langle \zeta_L\psi, \left(H - |\nabla F|^2\right) \zeta_L\psi\rangle \geq \langle \zeta_L\psi, \frac{c}{|x|^2\ln^2(|x|)}\zeta_L\psi\rangle \tag{2.46}$$

for some $c > 0$, if the potential V is short range and if

$$|\nabla F(x)| \leq \frac{d-2}{2|x|} \tag{2.47}$$

for all large $|x|$. Note that if F is bounded then $\xi = \chi_R e^F$ is bounded and if (2.47) holds then

$$|\langle \psi, \xi^2 \left(|\nabla\widetilde{\chi}_L|^2 + 2\widetilde{\chi}_L\nabla\widetilde{\chi}_L\nabla F\right)\psi\rangle| \lesssim \|\xi\|_\infty^2 \frac{1}{L^2}\int_{L\leq|x|\leq\alpha L} |\psi(x)|^2\, dx \tag{2.48}$$

since $|\nabla\widetilde{\chi}_L|^2$ and $|\nabla\widetilde{\chi}_L\nabla F| \lesssim L^{-2}\mathbf{1}_{\{L\leq|x|\leq\alpha L\}}$.

Using (2.46) and (2.48) together with Fatou's lemma in (2.44) one arrives at

$$\begin{aligned}
\langle \xi\psi, \frac{c}{|x|^2\ln^2(|x|)}\xi\psi\rangle &\leq \liminf_{L\to\infty}\langle \zeta_L\psi, \frac{c}{|x|^2\ln^2(|x|)}\zeta_L\psi\rangle \\
&\leq \langle \psi, e^{2F}\left(|\nabla\chi_R|^2 + 2\chi_R\nabla\chi_R\nabla F\right)\psi\rangle \\
&\leq C_{F,R}\int_{R/2\leq|x|\leq R} |\psi(x)|^2\, dx
\end{aligned} \tag{2.49}$$

with the same constant $C_{F,R}$ as in (2.5), since $|\nabla\chi_R| \leq \frac{4}{R}\mathbf{1}_{\{R/2\leq|x|\leq R\}}$.

Now let $F(x) = \frac{d-2}{2}\ln(|x|)$, so that (2.47) holds. In the definition of ξ, replace F by F_δ given in (2.11) for $\delta > 0$, i.e., use $\xi = \chi_R e^{F_\delta}$ in the above argument. Then, since $|\nabla F_\delta| \leq |\nabla F|$ we see that

$$\langle \chi_R e^{F_\delta}\psi, \frac{c}{|x|^2\ln^2(|x|)}\chi_R e^{F_\delta}\psi\rangle \leq C_{F,R}\int_{R/2\leq|x|\leq R} |\psi(x)|^2\, dx\,.$$

In addition, F_δ converges monotonically to F and $e^{F(x)} = |x|^{(d-2)/2}$, so monotone convergence gives

$$\begin{aligned}
c\int_{|x|\geq R}\frac{|x|^{d-4}}{\ln^2(|x|)}|\psi(x)|^2\, dx &= \lim_{\delta\to 0}\langle \chi_R e^{F_\delta}\psi, \frac{c}{|x|^2\ln^2(|x|)}\chi_R e^{F_\delta}\psi\rangle \\
&\leq C_R\int_{R/2\leq|x|\leq R} |\psi(x)|^2\, dx\,.
\end{aligned} \tag{2.50}$$

with constant C_R given by

$$C_R = 8\sup_{R/2\leq|x|\leq R} e^{2F(x)}\left(2R^{-2} + R^{-1}|\nabla F(x)|\right) \leq 8dR^{d-4}$$

Since ψ is locally L^2, this proves (2.42). ∎

Remark 2.10. In dimensions $2 \leq d \leq 4$ a repulsive tail of the potential V of the form

$$V(x) \geq \frac{\omega}{|x|^2} \quad \text{for } |x| \gg 1 \tag{2.51}$$

stabilizes zero energy bound states. In this case we can use (2.45) to see that

$$\langle \nabla\varphi, \nabla\varphi\rangle + \langle \varphi, V\varphi\rangle \geq \Big\langle \varphi, \Big(\Big(\Big(\frac{d-2}{2}\Big)^2 + \omega\Big) \frac{1}{|x|^2} + \frac{1}{4|x|^2 \ln^2(|x|)} \Big) \varphi \Big\rangle$$

for all $\varphi \in H^1$ with support outside a large enough centered ball in $\mathbb{R}^d$. Then the same analysis which yields (2.50), but now with the weight $F(x) = \big(((d-2)/2)^2 + \omega\big)^{1/2} \ln|x|$, leads to

$$c \int_{|x|\geq R} \frac{|x|^\sigma}{\ln^2(|x|)} |\psi(x)|^2 \, dx \leq C \int_{R/2 \leq |x| \leq R} |\psi(x)|^2 \, dx \tag{2.52}$$

with $\sigma = 2\big(((d-2)/2)^2 + \omega\big)^{1/2} - 2$ and some constant C depending on R and ω. Thus $\psi \in L^2(\mathbb{R}^d)$ as soon as $\sigma > 0$ and the last condition is equivalent to

$$\omega > \frac{d(4-d)}{4} \,. \tag{2.53}$$

Clearly $d(4-d)$ is positive if $d \leq 3$, zero if $d = 4$, and negative if $d \geq 5$. So a repulsive part stabilizes zero energy bound state in dimensions $d \leq 4$ and in dimensions $d \geq 5$ the potential V can be purely attractive and still have zero energy eigenstates. The results of [22] show that a repulsive part is needed in dimensions $d \leq 4$. Dimension $d = 4$ is critical in the sense that the repulsive part can be weaker in dimension four than for $d \leq 3$.

3. Local energy bound for Helium–type system in paraboloidal regions

In the following sections, we consider a helium–type atom consisting of an infinitely heavy nucleus at the origin and two indistinguishable electrons. In this section, we prove a local energy bound for these systems, which is the main tool for the proof of the sharp anisotropic upper bounds on the asymptotic behavior of the ground state in later sections. Our local energy bound for the helium–type operator H_U on $L^2(\mathbb{R}^6)$ are independent of the statistics of the particles and one can easily include the spin. The importance of such a local energy bound was already emphasized by Agmon in his work on non-isotropic upper bounds on the decay of eigenfunctions of multiparticle Schrödinger operators in [1].

We denote by x_j the position of the j^{th} particle, by P_j^2 its kinetic energy, where $P_j = -i\nabla_{x_j}$ is its momentum operator, and $j = 1, 2$. The Hamiltonian of this system is given by

$$H_U = P_1^2 + P_2^2 - \frac{1}{|x_1|} - \frac{1}{|x_2|} + \frac{U}{|x_1 - x_2|} \,. \tag{3.1}$$

It is well-defined and self-adjoint on the Sobolev space $\mathcal{D}(H_U) = H^2(\mathbb{R}^6) \subset L^2(\mathbb{R}^6)$. In the following, it will be very convenient to consider the quadratic form induced by H_U on the Sobolev space $H^1(\mathbb{R}^6)$. With a slight abuse of notation, we denote this quadratic form by

$$\langle \varphi, H_U \varphi\rangle \coloneqq \langle P_1\varphi, P_1\varphi\rangle + \langle P_2\varphi, P_2\varphi\rangle + \langle \varphi, V_U\varphi\rangle \tag{3.2}$$

where

$$V_U(x) = V_U(x_1, x_2) = -\frac{1}{|x_1|} - \frac{1}{|x_2|} + \frac{U}{|x_1 - x_2|} \,. \tag{3.3}$$

The proofs of our lower bounds in Sections 7 and 8 use the sesquilinear version of this quadratic form. Our local energy bound for Helium follows from a suitable localization in position space and the IMS localization formula. However, our localization is quite different from the usual approach in many-particle physics, where one localizes into conical regions, see for example [14]. For our derivation of the sharp upper and lower bounds, it turns out to be crucial to use paraboloidal regions.

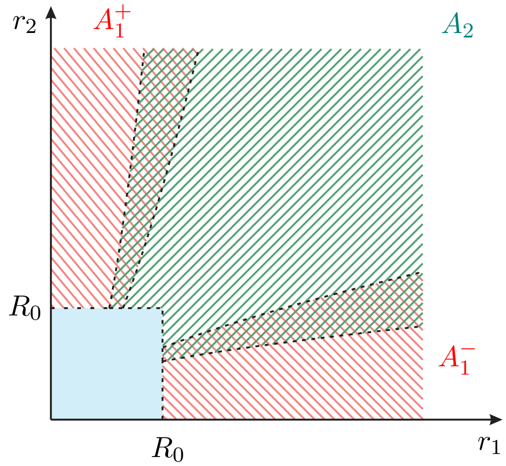

FIGURE 3.1. Sketch of the paraboloidal regions A_1, A_2.

Recall that for $x = (x_1, x_2) \in \mathbb{R}^3 \times \mathbb{R}^3$ we set $|x| = |(x_1, x_2)| = (|x_1|^2 + |x_2|^2)^{1/2}$, $|x|_0 = \min(|x_1|, |x_2|)$, and $|x|_\infty = \max(|x_1|, |x_2|)$. For $R_0 > 0$ and $0 < \gamma \le 1$ we define the following paraboloidal regions

Region 0: $A_0 := \{x \in \mathbb{R}^6 : |x| < 2R_0\}$.

Region 1: $A_1 := \{x \in \mathbb{R}^6 : |x| > R_0 \text{ and } |x|_0 < 2|x|_\infty^\gamma\}$.

Region 2: $A_2 := \{x \in \mathbb{R}^6 : |x| > R_0 \text{ and } |x|_0 > |x|_\infty^\gamma\}$.

We do not write explicitly the dependence of these regions on the parameters R_0 and γ. The inner region A_0 cuts out a ball centered around the nucleus. It is only necessary in order to have a bounded localization error in the IMS localization formula near the nucleus and will be irrelevant for our bounds on eigenstates. All regions above are invariant under permutation of the particles. In order to control the localization error, we will eventually choose the parameter $1/2 < \gamma < 1$.

In the region A_0 both particles are close to the nucleus and in A_2 both particles will be far from the nucleus. In these two cases, the local energy bound will be easy. The *tricky region* is A_1. At critical coupling U_c this region is critical in the sense that inside this region one particle stays much closer to the nucleus compared to the other particle, which can escape to infinity with no apparent energy cost, since the ionization energy is zero.

For large R_0 the tricky region A_1 is the union of two disjoint paraboloid regions

$$A_1^- = \{x \in \mathbb{R}^6 : |x| > R_0 \text{ and } |x_2| < 2|x_1|^\gamma\},$$
$$A_1^+ = \{x \in \mathbb{R}^6 : |x| > R_0 \text{ and } |x_1| < 2|x_2|^\gamma\}.$$

which are "above" and "below" the diagonal $|x_1| = |x_2|$, respectively.

To construct suitable cut–off functions which localize into the regions A_0, A_1, and A_2, take any two functions $0 \le \tilde{u}, \tilde{v} \in \mathcal{C}^\infty([0,\infty))$ with $\tilde{u} = 1$ and $\tilde{v} = 0$ on $[0,1]$, $\tilde{u} = 0$ and $\tilde{v} = 1$ on $[2,\infty)$, $\tilde{u} > 0$ on $[0, 7/4]$, and $\tilde{v} > 0$ on $[5/4, \infty)$ and put

$$u := \frac{\tilde{u}}{(\tilde{u}^2 + \tilde{v}^2)^{1/2}}, \quad v := \frac{\tilde{v}}{(\tilde{u}^2 + \tilde{v}^2)^{1/2}}. \tag{3.4}$$

Since $\tilde{u}^2 + \tilde{v}^2 \ge c$ for some constant $c > 0$, the functions u, v are infinitely differentiable. Moreover, by construction, $0 \le u, v \le 1$, $u = 1$ and $v = 0$ on $[0,1]$, $u = 0$ and $v = 1$ on $[2, \infty)$, and

$$u^2 + v^2 = 1 \tag{3.5}$$

Note that one can always find u, v with $\|u'\|_\infty \le 2$ and $\|v'\|_\infty \le 2$. Given u and v we set

$$\begin{aligned}\chi_0(x) &:= u\Big(|x|/R_0\Big)\,,\\ \chi_1(x) &:= v\Big(|x|/R_0\Big)u\Big(|x|_0/|x|_\infty^\gamma\Big)\,,\\ \chi_2(x) &:= v\Big(|x|/R_0\Big)v\Big(|x|_0/|x|_\infty^\gamma\Big)\,.\end{aligned} \tag{3.6}$$

By construction

$$\sum_{j=0}^{2}\chi_j^2 = 1. \tag{3.7}$$

In addition, we clearly have $\chi_0 \in \mathcal{C}_0^\infty(\mathbb{R}^6)$. This is less obvious for χ_1 and χ_2. For large enough R_0 the support of χ_1, which is contained in the tricky region, separates into two disjoint sets (contained in $A_1^\pm$) and on each of these sets χ_1 is infinitely differentiable. So we have $\chi_1 \in \mathcal{C}^\infty(\mathbb{R}^6)$ for large R_0 and a moment of reflection shows that also $\chi_2 \in \mathcal{C}^\infty(\mathbb{R}^6)$ for all large enough R_0. The gradients in $\mathbb{R}^6$ of χ_0 and χ_1 are given by

$$\nabla\chi_0(x) = R_0^{-1}u'\big(|x|/R_0\big)\frac{x}{|x|}\,, \tag{3.8}$$

$$\begin{aligned}\nabla\chi_1(x) &= R_0^{-1}v'\big(|x|/R_0\big)u\big(|x|_0/|x|_\infty^\gamma\big)\frac{x}{|x|}\\ &\quad + v\big(|x|/R_0\big)u'\big(|x|_0/|x|_\infty^\gamma\big)\begin{pmatrix}\big(\frac{1}{|x_2|^\gamma}\mathbf{1}_{\{|x_2|>|x_1|\}} - \gamma\frac{|x_2|}{|x_1|^{\gamma+1}}\mathbf{1}_{\{|x_2|<|x_1|\}}\big)\frac{x_1}{|x_1|}\\ \big(\frac{1}{|x_1|^\gamma}\mathbf{1}_{\{|x_1|>|x_2|\}} - \gamma\frac{|x_1|}{|x_2|^{\gamma+1}}\mathbf{1}_{\{|x_1|<|x_2|\}}\big)\frac{x_2}{|x_2|}\end{pmatrix}.\end{aligned} \tag{3.9}$$

Thus, abbreviating $s = |x|/R_0$ and $t = |x|_0/|x|_\infty^\gamma$,

$$|\nabla\chi_0(x)|^2 \le R_0^{-2}\big(u'(s)\big)^2 \le R_0^{-2}\|u'\|_\infty^2\mathbf{1}_{\{R_0\le|x|\le 2R_0\}} \tag{3.10}$$

and

$$\begin{aligned}|\nabla\chi_1(x)|^2 &= R_0^{-2}v'(s)^2u(t)^2 + 2R_0^{-1}v'(s)v(s)u'(t)u(t)|x|^{-1}(t-\gamma t)\\ &\quad + v(s)^2u'(t)^2|x|_\infty^{-2\gamma}\Big(1+\gamma^2t^2\Big)\,.\end{aligned} \tag{3.11}$$

For $\nabla\chi_2$ we note that a similar formula as for $\nabla\chi_1$ holds, just with u replaced by v. Collecting terms we get

$$\begin{aligned}&|\nabla\chi_1(x)|^2 + |\nabla\chi_2(x)|^2\\ &\quad = R_0^{-2}v'(s)^2\big(u(t)^2+v(t)^2\big) + 2R_0^{-1}v'(s)v(s)\big(u'(t)u(t)+v'(t)v(t)\big)|x|^{-1}(1-\gamma)t\\ &\qquad + v(s)^2\big(u'(t)^2+v'(t)^2\big)|x|_\infty^{-2\gamma}\Big(1+\gamma^2t^2\Big)\\ &\quad = R_0^{-2}v'(s)^2 + v(s)^2\Big(u'(t)^2+v'(t)^2\Big)|x|_\infty^{-2\gamma}\Big(1+\gamma^2t^2\Big)\end{aligned}$$

where we also used $u^2+v^2 = 1$ and $2(u'u+v'v) = (u^2+v^2)' = 0$. Hence

$$\begin{aligned}\sum_{j=0}^{2}|\nabla\chi_j(x)|^2 &= R_0^{-2}\big(v'(|x|/R_0)^2 + u'(|x|/R_0)^2\big)\\ &\quad + v(|x|/R_0)^2\big(u'\big(|x|_0/|x|_\infty^\gamma\big)^2 + v'\big(|x|_0/|x|_\infty^\gamma\big)^2\big)\Big(\frac{1}{|x|_\infty^{2\gamma}} + \frac{\gamma^2|x|_0^2}{|x|_\infty^{2\gamma+2}}\Big)\,.\end{aligned} \tag{3.12}$$

This yields the following bound on the localization error for localizing into paraboloidal regions.

Corollary 3.1. *The localization error* $\sum_{j=0}^{2}|\nabla\chi_j|^2$ *for the localizing functions* χ_j *constructed above, is bounded from above by*

$$\sum_{j=0}^{2}|\nabla\chi_j(x)|^2 \le \|(u')^2+(v')^2\|_\infty \left(R_0^{-2}\mathbf{1}_{\{R_0\le|x|\le 2R_0\}} + \frac{1+\gamma^2}{|x|_\infty^{2\gamma}}\mathbf{1}_{\{|x|\ge R_0\}}\right) \tag{3.13}$$

for $0<\gamma\le 1$ *and* $R_0>0$.

Proof. This follows immediately from (3.12) because $0\le u,v\le 1$, $R_0\le|x|\le 2R_0$ on the support of $v'(|x|/R_0)$, $|x|\ge R_0$ on the support of $v(|x|/R_0)$, and $|x|_0\le|x|_\infty$. ∎

Remark 3.2. In order to make $\|(u')^2+(v')^2\|_\infty$ small, a convenient choice is to pick

$$u(s)=\begin{cases} 1, & \text{for } 0\le s\le 1\\ \cos(\pi(s-1)/2), & \text{for } 1<s\le 2\\ 0, & \text{for } s>2\end{cases}$$

and $v=\sqrt{1-u^2}$, in which case $\|(u')^2+(v')^2\|_\infty=\pi^2/4$. Making this choice for u and v does not yield smooth cut-off function, however. Nevertheless, the set on which χ_j is not differentiable, is a Lebesgue measure zero Lipshitz hypersurface in $\mathbb{R}^6$, so Lemma A.1 shows that $\chi_j\in W^{1,\infty}(\mathbb{R}^6)$ and this is all one needs to use a suitable quadratic form version of the IMS localization formula, see the discussion in Appendix A.

Given a wave function φ in the quadratic form domain of H_U, which is the Sobolev space $H^1(\mathbb{R}^6)$, we can use (3.7) and the fact that $\langle\varphi,H_U\varphi\rangle$ is real together with the IMS localization formula (A.8) to get

$$\langle\varphi,H_U\varphi\rangle=\sum_{j=0}^{2}\mathrm{Re}\langle\chi_j^2\varphi,H_U\varphi\rangle=\sum_{j=0}^{2}\langle\chi_j\varphi,H_U\chi_j\varphi\rangle-\sum_{j=0}^{2}\langle\varphi,|\nabla\chi_j|^2\varphi\rangle\,. \tag{3.14}$$

Corollary 3.1 allows us to control the localization error. To bound the local energies $\langle\chi_j\varphi,H_U\chi_j\varphi\rangle$, where each $\chi_j\varphi$ is supported on A_j, the following bounds will be useful.

Lemma 3.3. *Let* V_U *be the Coulomb potential*

$$V_U(x)=-\frac{1}{|x_1|}-\frac{1}{|x_2|}+\frac{U}{|x_1-x_2|} \tag{3.15}$$

on $\mathbb{R}^6$. *Then for* $0<\gamma<1$ *we have*

$$V_U(x)\ge-\frac{1}{|x|_0}+\frac{U-1}{|x|_\infty}-\frac{2U}{|x|_\infty^{2-\gamma}}\quad \textit{for all } x\in A_1\,, \tag{3.16}$$

$$V_U(x)\ge-\frac{1}{|x|_0}-\frac{1}{|x|_\infty}\quad \textit{for all } x\in A_2\,. \tag{3.17}$$

Remark 3.4. Recall that $A_1=\{|x|\ge R_0 \text{ and } |x|_0\le 2|x|_\infty^\gamma\}$ is the *tricky region*, where one particle stays close to the nucleus, and the other one can escape. Due to (3.16) this will have a *local energy cost* of order $(U-1)/|x|_\infty$, which makes the classically forbidden region *stickier*. This is a key input for our a-priori bounds on the decay of ground states at critical coupling. A similar boost was already noted in [14, 19], however, due to the use of conical regions for the cutoff functions in [14], which is quite common in many–body quantum mechanics, their bound for the Coulomb interaction is worse than our bound in Lemma 3.3: It is *essential to use paraboloidal regions* in order to get the additional positive term $\frac{U-1}{|x|_\infty}$ with the *sharp constant* $U-1$ in the lower bound for two–particle Coulomb potential in the tricky region.

Proof. The bound on $A_2 = \{|x| > R_0, |x|_0 > |x|_\infty^\gamma\}$ follows by dropping the positive Coulomb repulsion. On A_1 we have $|x|_0 < 2|x|_\infty^\gamma$, thus

$$|x_1 - x_2| \le |x_1| + |x_2| \le |x|_\infty + 2|x|_\infty^\gamma$$

and

$$\frac{U}{|x_1 - x_2|} \ge \frac{U}{|x|_\infty + 2|x|_\infty^\gamma} = \frac{U}{|x|_\infty} - \frac{2U}{|x|_\infty^{2-\gamma}(1 + 2|x|_\infty^{\gamma-1})} .$$

This implies (3.16). ∎

In the following, we take any two functions u and v as above. Then Corollary 3.1 shows that there exists a constant $C_l = C_l(u, v) < \infty$ such that for any $0 < \gamma \le 1$ the localization error is bounded from above by

$$\sum_{j=0}^{2} |\nabla \chi_j(x)|^2 \le \frac{C_l}{\max(|x|_\infty^{2\gamma}, R_0^{2\gamma})} \text{ for all } x \in \mathbb{R}^6 . \tag{3.18}$$

For this constant C_l we set

$$W_0(x) := -\frac{1}{2} - \frac{C_l}{R_0^{2\gamma}} , \tag{3.19}$$

$$W_1(x) := -\frac{1}{4} + \frac{U-1}{|x|_\infty} - \frac{2U}{|x|_\infty^{2-\gamma}} - \frac{C_l}{|x|_\infty^{2\gamma}} , \tag{3.20}$$

and

$$W_2(x) := -\frac{1}{|x|_\infty} - \frac{1}{|x|_0} - \frac{C_l}{|x|_\infty^{2\gamma}} . \tag{3.21}$$

Lemma 3.3 and the IMS formula lead to

Proposition 3.5 (Local energy bound)**.** *For large enough R_0 and all φ in the quadratic form domain of H_U*

$$\langle \varphi, H_U \varphi \rangle \ge \sum_{j=0}^{2} \langle \chi_j \varphi, W_j \chi_j \varphi \rangle . \tag{3.22}$$

Remark 3.6. The localized functions $\chi_j\varphi$, $j = 0, 1, 2$, have the same permutation symmetry as φ, since the χ_j are symmetric under permurtation of the particles.

Proof. Set $L_{\mathrm{err}}(x) = \frac{C_l}{\max(|x|_\infty^{2\gamma}, R_0^{2\gamma})}$. From (3.14), Corollary 3.1, and (3.18) we get

$$\langle \varphi, H_U \varphi \rangle \ge \sum_{j=0}^{2} \langle \chi_j \varphi, H_U \chi_j \varphi \rangle - \langle \varphi, L_{\mathrm{err}} \varphi \rangle = \sum_{j=0}^{2} \langle \chi_j \varphi, H_U \chi_j \varphi \rangle - \sum_{j=0}^{2} \langle \chi_j \varphi, L_{\mathrm{err}} \chi_j \varphi \rangle$$

since L_{err} is multiplication by a function and $\sum_{j=0}^{2} \chi_j^2 = 1$. So it is enough to show

$$\langle \chi_j \varphi, H_U \chi_j \varphi \rangle \ge \langle \chi_j \varphi, \widetilde{W}_j \chi_j \varphi \rangle \tag{3.23}$$

for each $j = 0, 1, 2$, where $\widetilde{W}_j = W_j + L_{\mathrm{err}}$. Using that $\chi_2\varphi$ is supported in the region A_2, we can use Lemma 3.3 and immediately get (3.23) for $j = 2$ by dropping the kinetic energy term $P_1^2 + P_2^2$ in $\langle \chi_2 \varphi, H_U \chi_2 \varphi \rangle$.

For $j = 0$ we again drop the Coulomb repulsion term and use

$$H_U \ge P_1^2 - \frac{1}{|x_1|} + P_2^2 - \frac{1}{|x_2|} \ge -1/2$$

to get (3.23), since the ground state energy of hydrogen is $-1/4$ in the atomic units we use.

When $j = 1$, the particles are localized in the tricky region. For large enough R_0 the localization function χ_1 is a sum $\chi_1 = \chi_1^- + \chi_1^+$, where $\chi_1^\pm$ are smooth and have supports in $A_1^\pm$. In particular, their supports are disjoint for all large R_0. Using Lemma 3.3 and dropping P_1^2 we get

$$\begin{aligned}\langle \chi_1^-\varphi, H_U\chi_1^-\varphi\rangle &\geq \langle \chi_1^-\varphi, \left(P_2^2 - \frac{1}{|x_2|} + \frac{U-1}{|x_1|} - \frac{2U}{|x_1|^{2-\gamma}}\right)\chi_1^-\varphi\rangle \\ &\geq \langle \chi_1^-\varphi, \left(-\frac{1}{4} + \frac{U-1}{|x_1|} - \frac{2U}{|x_1|^{2-\gamma}}\right)\chi_1^-\varphi\rangle \\ &= \langle \chi_1^-\varphi, \widetilde{W}_1\chi_1^-\varphi\rangle\end{aligned}$$

since $P_2^2 - \frac{1}{|x_2|} \geq -1/4$. Similarly one sees

$$\langle \chi_1^+\varphi, H_U\chi_1^+\varphi\rangle \geq \langle \chi_1^+\varphi, \widetilde{W}_1\chi_1^+\varphi\rangle\,.$$

Since the supports of χ_1^- and χ_1^+ do not overlap when R_0 is large enough, we get

$$\begin{aligned}\langle \chi_1\varphi, H_U\chi_1\varphi\rangle &= \langle \chi_1^-\varphi, H_U\chi_1^-\varphi\rangle + \langle \chi_1^+\varphi, H_U\chi_1^+\varphi\rangle \\ &\geq \langle \chi_1^-\varphi, \widetilde{W}_1\chi_1^-\varphi\rangle + \langle \chi_1^+\varphi, \widetilde{W}_1\chi_1^+\varphi\rangle = \langle \chi_1\varphi, \widetilde{W}_1\chi_1\varphi\rangle\end{aligned}$$

which is (3.23) for $j = 1$. ∎

4. Isotropic upper bounds on the asymptotic decay of bound states

Before we start the proof of the sharp anisotropic upper bound in the next section, we give a proof of a simple isotropic bound. Such an upper bound is already quite useful, since it is *uniform* in the energy $E \leq -1/4$, i.e. up to the bottom of the essential spectrum. It allows for an easy proof of the *existence of a bound state* at critical coupling: The infimum of the spectrum of H_{U_c} is a simple eigenvalue, see Appendix D, even though it is embedded at the edge of the essential spectrum of H_{U_c}.

Our main tools are the local energy bounds from Section 3 and the quadratic form version of the IMS localization formula from Appendix A. For the simple isotropic upper bound on the asymptotic decay of eigenfunctions of H_U we use the weight function

$$F_1(r) = 2(U-1)^{1/2}r^{1/2} - Kr^\kappa \tag{4.1}$$

for $1 < U \leq U_c$, $K > 0$, and $1/6 < \kappa < 1/2$. The reason why we have to take $\kappa > 1/6$ in the isotropic upper bound will follow from the proof, in particular, (4.9). Note that the leading order term in F_1 is given by $2(U-1)^{1/2}r^{1/2}$, the other term is a *lower order correction* for any $K > 0$ and $1/6 < \kappa < 1/2$.

When $x = (x_1, x_2) \in \mathbb{R}^3 \times \mathbb{R}^3$, $|x|_\infty = \max(|x_1|, |x_2|)$, we will identify $F_1(x) = F_1(|x|_\infty)$, by a slight abuse of notation. For simplicity of notation, we do not explicitly write the dependence of F_1 on its parameters.

Recall that $\psi \in L^2(\mathbb{R}^6)$ is a bound state of H_U with energy E, if it is a weak solution of the eigenvalue equation $H_U\psi = E\psi$. That is, $\psi \in H^1(\mathbb{R}^6)$ and

$$\langle \varphi, H_U\psi\rangle = E\langle \varphi, \psi\rangle \tag{4.2}$$

as quadratic forms for all $\varphi \in H^1$.

Theorem 4.1 (Isotropic L^2 upper bound near critical coupling)**.** *If ψ_U is a bound state of H_U with energy $E_U \leq -\frac{1}{4}$ then for any $K > 0$ and $1/6 < \kappa < 1/2$*

$$e^{F_1}\psi_U \in L^2(\mathbb{R}^6) \tag{4.3}$$

Moreover, for normalized ψ_U, the function $e^{F_1}\psi_U$ is L^2 uniformly in the parameter range $1+\mu \le U \le U_c$ for any small fixed $0<\mu<U_c-1$.

Before we give the proof, we want to explain where the usual strategy fails. Let ψ be a bound state of a Schrödinger operator H_U with energy E. Take any bounded, real valued function $\xi \in H^1$. Since E is real we can use $\varphi = \xi^2\psi$ in (4.2) together with the IMS localization formula (A.7) and the local energy bound from Proposition 3.5 to see

$$\begin{aligned} E\|\xi\psi\|^2 &= \mathrm{Re}(E\langle \xi^2\psi,\psi\rangle) = \mathrm{Re}\langle \xi^2\psi, H_U\psi\rangle = \langle \xi\psi, H_U\xi\psi\rangle - \langle \psi, |\nabla\xi|^2\psi\rangle \\ &\ge \sum_{j=0}^{2}\langle \chi_j\xi\psi, W_j\chi_j\xi\psi\rangle - \langle \psi, |\nabla\xi|^2\psi\rangle\,, \end{aligned}$$

where χ_j, defined in (3.6), are the functions localizing in the regions A_j, $j=0,1,2$.

Now choose $\chi=\chi_R$ to be another smooth cutoff function outside of a centered ball of radius $R>2R_0$ and make the ansatz $\xi=\chi e^F$ for some bounded function $F\in H^1$. Then

$$|\nabla\xi|^2 = \xi^2|\nabla F|^2 + 2\chi e^{2F}\nabla\chi\cdot\nabla F + e^{2F}|\nabla\chi|^2\,,$$

hence

$$\sum_{j=1}^{2}\langle \chi_j\chi e^F\psi, (W_j - E - |\nabla F|^2)\chi_j\chi e^F\psi\rangle \le \langle \psi, e^{2F}(2\chi\nabla\chi\nabla F + |\nabla\chi|^2)\psi\rangle\,, \tag{4.4}$$

since χ_0 and χ have disjoint supports, the missing $l=0$ term in the sum on the left hand side above is zero.

The usual strategy for using (4.4) is to assume $W_j - E \ge c > 0$. That is, one needs a spectral gap for the operator $H_U - E$ *near infinity* (outside large enough balls), to have a safety distance to the essential spectrum. Under such an assumption, one gets from (4.4)

$$\delta c\|\chi e^F\psi\|^2 \le \langle \psi, e^{2F}(2\chi\nabla\chi\nabla F + |\nabla\chi|^2)\psi\rangle \le C_{F,\chi}\|\psi\|^2\,,$$

for the exponentially weighted bound state $e^F\psi$ on the support of χ, as long as $|\nabla F|^2 \le (1-\delta)c$ for some small $\delta>0$. This condition allows F to grow like $\sqrt{(1-\delta)c}|x|$. Of course, one has to remove the requirement that F is bounded. This is easy, since the constant $C_{F,\chi}$ depends on F and χ only on the support of $\nabla\chi$, which is compact. See the argument in the proof of Theorem 4.1 below, in particular (4.6).

However, the local energy bound $W_1 - E_{U_c} = W_1 + 1/4$ goes to zero at infinity in the *tricky region* A_1. Thus $c=0$, i.e., there is no safety distance to the essential spectrum anymore, when $E_U=-1/4$ or when E_U approaches $-1/4$ from below as $U \nearrow U_c$, and the above argument does not allow to control $e^F\psi$ anymore. So we have to be more careful.

Proof of Theorem 4.1. Let $a=(U-1)_+^{1/2}$, $1/6<\kappa<1/2$, $K>0$, and put

$$G(r) := 2ar^{1/2} - Kr^{\kappa}/2\,. \tag{4.5}$$

We use $K/2$ instead of K in the definition of G to have some wiggle room which allows us to absorb error terms later, see (4.12) and (4.13) below. Note that $G(r)$ is positive when r is large enough, so its regularized version

$$G_\delta(r) = \frac{G(r)}{1+\delta G(r)} \tag{4.6}$$

is well defined and bounded for all large enough r and all $\delta>0$. We also denote $G(x) = G(|x|_\infty)$ and the same for G_δ, with a slight abuse of notation. Note that G and G_δ are continuous on $\mathbb{R}^6$ and continuously differentiable on $\{|x_1|\ne|x_2|, |x|>R\}$ for large enough R.

Furthermore, let $0 \le \chi \le 1$ be a smooth function on $[0,\infty)$ with $\chi(r) = 0$ for $0 \le r \le 1$, $\chi(r) = 1$ for $r \ge 2$, $|\chi'| \le 2$, and put $\chi_R(x) = \chi(x/R)$. Lemma A.1 shows that $\xi = \chi_R e^{G_\delta}$ is in the Sobolev space $W^{1,\infty}(\mathbb{R}^6)$ and multiplication with ξ and ξ^2 leaves the quadratic form domain of H_U invariant. Setting $r = |x|_\infty$ one calculates

$$\nabla G(x) = (ar^{-1/2} - K\kappa r^{\kappa-1}/2)\begin{pmatrix} \frac{x_1}{|x_1|}\mathbf{1}_{\{|x_1|>|x_2|\}} \\ \frac{x_2}{|x_2|}\mathbf{1}_{\{|x_2|>|x_1|\}} \end{pmatrix}, \tag{4.7}$$

$$\nabla G_\delta = \frac{\nabla G}{(1+\delta G)^2}.$$

Thus

$$|\nabla G_\delta|^2 \le |\nabla G|^2 = \big(a|x|_\infty^{-1/2} - K\kappa |x|_\infty^{\kappa-1}/2\big)^2,$$

for large enough $|x|_\infty$. Using (4.4) with F replaced by G_δ and taking R such that $G(x) > 0$ for all x in the support of χ_R one gets

$$\begin{aligned}\sum_{j=1}^{2}&\langle \chi_j\chi_R e^{G_\delta}\psi, (W_j - E - |\nabla G|^2)\chi_j\chi_R e^{G_\delta}\psi\rangle \\ &\le \langle \psi, e^{2G}(2|\nabla\chi_R||\nabla G| + |\nabla \chi_R|^2)\psi\rangle \le C_R\|\psi\|^2\end{aligned} \tag{4.8}$$

where we also used that $G_\delta(x) \le G(x)$ and $|\nabla G_\delta(x)| \le |\nabla G(x)|$ once $G(x) > 0$. The constant C_R is given by

$$C_R = 4\sup_{R\le s\le 2R} e^{2G(s)}\big(|G'(s)|/R + 1/R^2\big) < \infty,$$

since $\nabla\chi_R$ is supported on the annulus $R \le |x| \le 2R$ and $|\nabla\chi_R| \le \|\chi'\|_\infty/R \le 2/R$.

In the following, we will use C for a generic constant, which may change from line to line. Recall that $0 \le \varepsilon_U = -1/4 - E_U$ is the ionization energy. On A_2 we have

$$W_2(x) - E_U - |\nabla G(x)|^2 \ge \frac14 + \varepsilon_U - \frac{1}{|x|_\infty} - \frac{1}{|x|_\infty^\gamma} - \frac{C}{|x|_\infty^{2\gamma}} - |\nabla G(x)|^2 \ge \frac18$$

for large enough $|x|_\infty$. On A_1 we get

$$\begin{aligned} W_1(x) - E_U - |\nabla G(x)|^2 &\ge \varepsilon_U + \frac{U-1}{|x|_\infty} - \frac{2U}{|x|_\infty^{2-\gamma}} - \frac{C}{|x|_\infty^{2\gamma}} - |\nabla G(x)|^2 \\ &\ge \varepsilon_U + aK\kappa|x|_\infty^{\kappa-3/2} - (K\kappa/2)^2|x|_\infty^{2(\kappa-1)} - 2U|x|_\infty^{\gamma-2} - C|x|_\infty^{-2\gamma} \\ &\ge \varepsilon_U + \frac34 aK\kappa|x|_\infty^{\kappa-3/2} - 2U|x|_\infty^{\gamma-2} - C|x|_\infty^{-2\gamma}\end{aligned} \tag{4.9}$$

for all large enough $|x|_\infty$, since $\kappa < 1/2$, which implies $\kappa - 3/2 > 2(\kappa-1)$. The minimum of $\max(\gamma-2, -2\gamma)$ is attained at $\gamma = 2/3$. The choice $\gamma = 2/3$ gives $\gamma - 2 = -2\gamma = -4/3$, which leads to the lower bound

$$W_1(x) - E_U - |\nabla G(x)|^2 \ge \varepsilon_U + \frac34 aK\kappa|x|_\infty^{\kappa-3/2} - (2U+C)|x|_\infty^{-4/3} \ge \varepsilon_U + \frac{aK\kappa}{2}|x|_\infty^{\kappa-3/2}$$

uniformly in $1+\mu \le U \le U_c \le 2$ for large enough $|x|_\infty$, since $\kappa > 1/6$. Putting everything together, we see that

$$\sum_{j=1}^{2}\chi_R\chi_j(W_j - E_U - |\nabla G|^2)\chi_j\chi_R \ge \big(\varepsilon_U + \frac{aK\kappa}{2}|x|_\infty^{\kappa-3/2}\big)\chi_R^2 \ge \frac{\varepsilon_U + aK}{12}|x|_\infty^{-4/3}\chi_R^2 \tag{4.10}$$

for large enough R and all bound state energies $E_U \le -1/4$, i.e., $\varepsilon_U \ge 0$. Using (4.10) in (4.8) we get

$$\langle \chi_R e^{G_\delta}\psi, |x|_\infty^{-4/3} \chi_R e^{G_\delta}\psi\rangle \le \frac{12C_R}{\varepsilon_U + (U-1)_+^{1/2}K}\|\psi\|^2 \tag{4.11}$$

for all $\delta > 0$. The right hand side of (4.11) is independent of $\delta > 0$, so

$$\langle \chi_R e^{G}\psi, |x|_\infty^{-4/3} \chi_R e^{G}\psi\rangle = \lim_{\varepsilon\to 0}\langle \chi_R e^{G_\delta}\psi, |x|_\infty^{-4/3} \chi_R e^{G_\delta}\psi\rangle \le \frac{12C_R}{\varepsilon_U + (U-1)_+^{1/2}K}\|\psi\|^2$$

by monotone convergence. Since arbitrary positive multiples of r^κ control any logarithmic term $\ln r$ for large r, we have

$$F_1(r) = 2ar^{1/2} - Kr^\kappa \le 2ar^{1/2} - Kr^\kappa/2 - \frac{2}{3}\ln r = G(r) - \frac{2}{3}\ln r \tag{4.12}$$

for r large. This shows

$$\|\chi_R e^{F_1}\psi\|^2 \le \langle \chi_R e^{G}\psi, |x|_\infty^{-4/3} \chi_R e^{G}\psi\rangle \le \frac{12C_R}{\varepsilon_U + (U-1)_+^{1/2}K}\|\psi\|^2 \tag{4.13}$$

for any $0 \le U \le U_c$. It is easy to see that $U \mapsto \varepsilon_U$ is decreasing and the discussion in the introduction shows that $\varepsilon_1 > 0$. So $\varepsilon_U + (U-1)_+^{1/2}K \gtrsim 1$ uniformly in $0 \le U \le U_c$, hence (4.13) proves the theorem. ∎

Our isotropic upper bound also allows for a simple proof for the existence of a ground state at critical coupling, see Propsotion D.1 in the appendix. In the infinite mass approximation, the existence of a bound state at critical coupling had been proven first in [19] with PDE methods and in [14] with variational methods.

Corollary 4.2. *At critical coupling the operator H_{U_c} has a simple eigenvalue at the edge of its essential spectrum. That is, there exists a bound state $\psi_c \in L^2(\mathbb{R}^6)$ with energy $-1/4$ of H_{U_c} which is unique up to a phase.*

5. First anisotropic upper bound

In this section we prove a preliminary version of the anisotropic upper bound from Theorem 1.1. This will be done in two steps: First we prove a L^2 version and convert this into a pointwise bound in a second step. Our first anisotropic upper bound given in Proposition 5.2 is *suboptimal in a transition region where* $|x_2| \sim |x_1|^\gamma$, for suitable $1/2 < \gamma < 1$. However, it has the *correct asymptotics* in the *tricky region* and in the region *near the diagonal*, i.e., where $|x_2| \sim |x_1|$ are large. This provides essential a-priori information for the proof of the sharp global anisotropic upper bound in the next section.

Recall that we set $a = a_U := (U-1)_+^{1/2}$ and $\varepsilon = \varepsilon_U := -\frac{1}{4} - E_U \ge 0$, where E_U is the ground state energy of H_U. Define

$$F_U(r) := \big(\varepsilon + \frac{a^2}{r}\big)^{1/2} r + \frac{a}{\varepsilon}\ln\left[\Big(1 + \frac{\varepsilon r}{a^2}\Big)^{1/2} + \frac{\sqrt{\varepsilon r}}{a}\right] \tag{5.1}$$

and

$$F_{2,U}(r_1, r_2) = F_U(r_1) - K_1 r_1^{\kappa_1} + \frac{1}{2}\big(r_2 - K_2 r_2^{\kappa_2} - 2r_1^\gamma\big)_+ . \tag{5.2}$$

With a slight abuse of notation, we also use $F_{2,U}(x) = F_{2,U}(|x|_\infty, |x|_0)$ for $(x_1, x_2) = x \in \mathbb{R}^6$.

Remark 5.1. The specific form of F_U is not important, the one thing which matters is that $F_U' = \big(\varepsilon + \frac{a^2}{r}\big)^{1/2}$. For $U = U_c$ we have

$$F_{2,U_c}(r_1, r_2) = 2(U_c - 1)^{1/2} r_1^{1/2} - K_1 r_1^{\kappa_1} + \frac{1}{2}\big(r_2 - K_2 r_2^{\kappa_2} - 2r_1^{\gamma}\big)_+ ,$$

see Remark 2.7.

Proposition 5.2 (First global anisotropic L^2 upper bound at critical coupling)**.** *Choose parameters $K_1, K_2 > 0$, $1/6 < \kappa_1 < 1/2$ and $1/2 - \kappa_1 < \kappa_2 < 1$, as well as $(3 - 2\kappa_1)/4 < \gamma < \min((\kappa_2 + 1)/2, \kappa_1 + 1/2)$. Then the ground state ψ_U of helium-type atoms at coupling U has the L^2 upper bound*

$$e^{F_{2,U}} \psi_U \in L^2(\mathbb{R}^6) \tag{5.3}$$

for all $0 \le U \le U_c$ and with $F_{2,U}$ defined in (5.2). Moreover, in the range $0 \le U \le U_c - \mu$ for some small $\mu > 0$, the bound (5.3) holds with any choice of parameters $0 < \kappa_1, \kappa_2 < 1$ and $1/2 < \gamma < (\kappa_2 + 1)/2$.

Remark 5.3. The most important part of Proposition 5.2 is of course the statement which holds uniformly in $0 \le U \le U_c$. By this we mean that for any choice of ground state ψ_U, which is normalized, i.e., $\|\psi_U\| = 1$, we have

$$\sup_{0 \le U \le U_c} \|e^{F_{2,U}} \psi_U\| < \infty .$$

A simple calculation shows that $(3 - 2\kappa_1)/4 < \min((\kappa_2 + 1)/2, \kappa_1 + 1/2)$ is equivalent to $\kappa_1 > 1/6$ and $\kappa_2 > 1/2 - \kappa_1$. So the range of allowed values for γ in Proposition 5.2 is not empty. Moreover, for any such choice we have $\gamma > (3 - 2\kappa_1)/4 > 1/2$, since $\kappa_1 < 1/2$. The bound is uniform in $0 \le U \le U_c$ and the implicit constant depends only on the parameters $K_1, K_2 > 0$, $1/6 < \kappa_1 < 1/2$ and $1/2 - \kappa_1 < \kappa_2 < 1$.

Proof. As in the proof of the isotropic bound, we use a modified version of $F_{2,U}$,

$$G_2(r_1, r_2) \coloneqq F_U(r_1) - K_1 r_1^{\kappa_1}/2 + \frac{1}{2}\big(r_2 - K_2 r_2^{\kappa_2} - 2r_1^{\gamma}\big)_+ \tag{5.4}$$

replacing K_1 by $K_1/2$. In the remainder, we will use $\partial_1 = \partial_{r_1}$, respectively, $\partial_2 = \partial_{r_2}$ and also freely abbreviate $a = a_U$.

We again use the smooth cut–off functions χ_R, which projects outside of large balls of radius R centered at zero and whose gradient $\nabla\chi_R$ is supported on the annulus $R \le |x| \le 2R$ and bounded by $|\nabla\chi_R| \lesssim R^{-1}$.

We also put $G_2(x) = G_2(|x|_\infty, |x|_0)$ as a function on $\mathbb{R}^6$, with a slight abuse of notation. Note that $G_2(x) \ge 0$ for all x in the support of χ_R as long as R is large enough, so we can regularize G_2 by using

$$G_{2,\delta} = \frac{G_2}{1 + \delta G_2} \tag{5.5}$$

which is then well defined on the support of χ_R and bounded for all $\varepsilon > 0$. Clearly $G_{2,\delta}$ is continuous on and differentiable on $\{|x|_0 - K_2|x|_0^{\kappa_2} - 2|x|_\infty^{\gamma} > 0\} \cap \{|x| > R_0\}$ and $\{|x|_0 - K_2|x|_0^{\kappa_2} - 2|x|_\infty^{\gamma} < 0\} \cap \{|x| > R_0\}$, for all large enough R_0. Up to the smooth zero Lebesgue measure surface $\{|x|_0 - K_2|x|_0^{\kappa_2} - 2|x|_\infty^{\gamma} = 0, |x| > R_0\}$ these two sets cover $\{|x| > R_0\}$. Hence Lemma A.1 shows that the exponential weight $\xi = \chi_R e^{G_{2,\delta}}$ has, for all large enough R, a bounded weak derivative on $\mathbb{R}^6$, which is almost everywhere given by its classical gradient and we can use ξ in the IMS localization formula.

As in the proof of the isotropic upper bound, see (4.4), one deduces from the IMS localization formula and the local energy bound from Proposition 3.5 that

$$\sum_{j=1}^{2}\langle\chi_j\chi_R e^{G_{2,\delta}}\psi,(W_j-E_U-|\nabla G_2|^2)\chi_j\chi_R e^{G_{2,\delta}}\psi\rangle\le\langle\psi,e^{2G_2}(2|\nabla\chi_R||\nabla G_2|+|\nabla\chi_R|^2)\psi\rangle\,,\tag{5.6}$$

by choosing $\varphi=(\chi_R e^{G_{2,\delta}})^2\psi$ as a test function in the quadratic form version of the eigenvalue equation. W_1 and W_2 are given in (3.20) and (3.21). Similar to the derivation of (4.8), we used $|\nabla G_{2,\delta}(x)|\le|\nabla G_2(x)|$ and $G_{2,\delta}(x)\le G_2(x)$ when $|x|_\infty$ is large and there is no $j=0$ term in (5.6) since $\chi_0\chi_R=0$ for all $R>2R_0$.

Recall that χ_1 localizes into the tricky region $A_1=\{|x|_0<2|x|_\infty^\gamma,|x|>R_0\}$. Clearly $G_2(x)=2a|x|_\infty^{1/2}-K_1|x|_\infty^{\kappa_1}/2$ for $x\in A_1$. Thus, setting $r_1=|x|_\infty$,

$$\nabla G_2(x)=\begin{pmatrix}\partial_1G_2\frac{x_1}{|x_1|}\mathbf{1}_{\{|x_1|>|x_2|\}}\\ \partial_1G_2\frac{x_2}{|x_2|}\mathbf{1}_{\{|x_2|>|x_1|\}}\end{pmatrix}=((\varepsilon+a^2/r_1)^{1/2}-K_1\kappa_1r_1^{\kappa_1-1}/2)\begin{pmatrix}\frac{x_1}{|x_1|}\mathbf{1}_{\{|x_1|>|x_2|\}}\\ \frac{x_2}{|x_2|}\mathbf{1}_{\{|x_2|>|x_1|\}}\end{pmatrix}\tag{5.7}$$

for all $x\in A_1$. Using $-E_U=\frac14+\varepsilon$ we have on the support of χ_1

$$\begin{aligned}W_1(x)-&E_U-|\nabla G_2|^2\\&\ge\varepsilon+a^2r_1^{-1}-2Ur_1^{\gamma-2}-((\varepsilon+a^2/r_1)^{1/2}-K_1\kappa_1r_1^{\kappa_1-1}/2)^2-Cr_1^{-2\gamma}\\&=K_1\kappa_1r_1^{\kappa_1-1}\big(2(\varepsilon+a^2/r_1)^{1/2}-K_1\kappa_1r_1^{\kappa_1-1}/2)\big)/2-2Ur_1^{\gamma-2}-Cr_1^{-2\gamma}\,.\end{aligned}$$

If $0\le U\le U_c-\mu$ then $\varepsilon=\varepsilon_U\ge c>0$ for some constant depending on $\mu>0$. In this case we get

$$\begin{aligned}W_1(x)-&E_U-|\nabla G_2|^2\\&\ge K_1\kappa_1r_1^{\kappa_1-1}\big(2c^{1/2}-K_1\kappa_1r_1^{\kappa_1-1}/2)\big)/2-2Ur_1^{\gamma-2}-Cr_1^{-2\gamma}\\&\gtrsim r_1^{\kappa_1-1}-r_1^{\gamma-2}-r_1^{-2\gamma}\gtrsim r_1^{\kappa_1-1}\ge r_1^{-1}\end{aligned}$$

for large enough r_1, i.e., large enough R_0, as long as $\kappa_1-1>\max(\gamma-2,-2\gamma)$, which is equivalent to $(1-\kappa_1)/2<\gamma<1+\kappa_1$.

In the range $0\le U\le U_c$, we note that when $r_1\ge1$ we have $\varepsilon+a^2/r_1=\varepsilon_U+a_U^2/r_1\ge(\varepsilon_U+(U-1)_+)/r_1\ge c/r_1$, with $c=\inf_{0\le U\le U_c}\big(\varepsilon_U+(U-1)_+\big)>0$. So uniformly in $0\le U\le U_c$ we have

$$\begin{aligned}W_1(x)-E_U-|\nabla G_2|^2&\ge K_1\kappa_1r_1^{\kappa_1-1}\big(2(c/r_1)^{1/2}-K_1\kappa_1r_1^{\kappa_1-1}/2)\big)/2-2Ur_1^{\gamma-2}-Cr_1^{-2\gamma}\\&\gtrsim r_1^{\kappa_1-3/2}-r_1^{\gamma-2}-r_1^{-2\gamma}\gtrsim r_1^{\kappa_1-3/2}\ge r_1^{-4/3}\end{aligned}$$

for large enough r_1, i.e., large enough R_0, as long as $\kappa_1-3/2>\max(\gamma-2,-2\gamma)$, which is equivalent to $(3-2\kappa_1)/4<\gamma<\kappa_1+1/2$. We also used that $\kappa_1>1/6$ in the last bound.

For the energy bound on the support of $\chi_2\subset A_2$, we split A_2 into the two regions $A_2^-=\{|x_1|^\gamma<|x_2|<|x_1|,|x_1|>R_0\}$ and $A_2^+=\{|x_2|^\gamma<|x_1|<|x_2|,|x_2|>R_0\}$ which cover A_2 up to a null set within the diagonal $\{|x_1|=|x_2|\}$. It is enough to provide a lower bound for $W_2-E_U-|\nabla G_2|^2$ on A_2^-, the same bound will then also hold on A_2^+, by symmetry, Since null sets are irrelevant such a bound will then hold on the support of χ_2.

For the same reason, we can also disregard the null set $\{|x_2|-K_2|x_2|^{\kappa_2}-2|x_1|^\gamma=0\}\cap A_2^-$, on which the classical gradient of G_2 does not exist.

On $\{|x_2|-K_2|x_2|^{\kappa_2}-2|x_1|^\gamma<0\}\cap A_2^-$ we again have $G_2(x)=2a|x_1|^{1/2}-K_1|x_1|^{\kappa_1}$. Thus

$$W_2(x)-E_U-|\nabla G_2(x)|^2$$

$$
\begin{aligned}
&\geq \frac{1}{4} + \varepsilon - r_1^{-1} - r_1^{-\gamma} - ((\varepsilon + a^2/r_1)^{1/2} - K_1\kappa_1 r_1^{\kappa_1-1}/2)^2 - Cr_1^{-2\gamma} \\
&\geq \frac{1}{4} - (1+a^2)r_1^{-1} - r_1^{-\gamma} - (K_1\kappa_1 r_1^{\kappa_1-1}/2)^2 \geq \frac{1}{8}
\end{aligned}
$$

on this set and all large enough $R > 0$.

For $x \in \{|x_2| - K_2|x_2|^{\kappa_2} - 2|x_1|^\gamma > 0\} \cap A_2^-$, we have

$$
G_2(x) = F_U(r_1) - K_1 r_1^{\kappa_1}/2 + \frac{1}{2}\big(r_2 - K_2 r_2^{\kappa_2} - 2r_1^\gamma\big) \tag{5.8}
$$

with $r_1 = |x_1|$ and $r_2 = |x_2|$. Hence

$$
\nabla G_2(x) = \begin{pmatrix} \partial_1 G_2 \frac{x_1}{|x_1|} \\ \partial_2 G_2 \frac{x_2}{|x_2|} \end{pmatrix} = \begin{pmatrix} \big((\varepsilon_U + a^2/r_1)^{1/2} - K_1\kappa_1 r_1^{\kappa_1-1}/2 - \gamma r_1^{\gamma-1}\big)\frac{x_1}{|x_1|} \\ \frac{1}{2}\big(1 - K_2\kappa_2 r_2^{\kappa_2-1}\big)\frac{x_2}{|x_2|} \end{pmatrix} \tag{5.9}
$$

which implies

$$
\begin{aligned}
&W_2(x) - E_U - |\nabla G_2(x)|^2 \geq W_2(x) + \frac{1}{4} + \varepsilon - |\nabla G_2(x)|^2 \\
&\quad = \frac{1}{4} - \frac{1}{4}\left(1 - K_2\kappa_2 r_2^{\kappa_2-1}\right)^2 - r_1^{-1} - r_2^{-1} \\
&\qquad + \varepsilon - \left((\varepsilon + a^2/r_1)^{1/2} - K_1\kappa_1 r_1^{\kappa_1-1}/2 - \gamma r_1^{\gamma-1}\right)^2 - Cr_1^{-2\gamma} \\
&\quad \geq \frac{1}{4}K_2\kappa_2 r_2^{\kappa_2-1}\left(2 - K_2\kappa_2 r_2^{\kappa_2-1}\right) - r_1^{-1} - r_2^{-1} - \frac{a^2}{r_1} \\
&\qquad + \left(\frac{\varepsilon + a^2}{r_1}\right)^{1/2}\left(K_1\kappa_1 r_1^{\kappa_1-1} + 2\gamma r_1^{\gamma-1}\right) - \left(K_1\kappa_1 r_1^{\kappa_1-1}/2 + \gamma r_1^{\gamma-1}\right)^2 - Cr_1^{-2\gamma}.
\end{aligned}
$$

Using again $\varepsilon + a^2 = \varepsilon_U + (U-1)_+ \gtrsim 1$ uniformly in $0 \leq U \leq U_c$ and also that $\gamma > 1/2 > \kappa_1$, so terms such as $r_1^{\gamma-1}$ control $r_1^{\kappa_1-1}$ for large r_1, we arrive at the lower bound

$$
\begin{aligned}
&W_2(x) - E_U - |\nabla G_2(x)|^2 \\
&\quad \geq \frac{1}{4}K_2\kappa_2 r_2^{\kappa_2-1}\left(2 - K_2\kappa_2 r_2^{\kappa_2-1}\right) - r_1^{-1} - r_2^{-1} - \frac{a^2}{r_1} \\
&\qquad + \left(\frac{\varepsilon + a^2}{r_1}\right)^{1/2}\left(K_1\kappa_1 r_1^{\kappa_1-1} + 2\gamma r_1^{\gamma-1}\right) - \left(K_1\kappa_1 r_1^{\kappa_1-1/2} + \gamma r_1^{\gamma-1}\right)^2 - Cr_1^{-2\gamma} \\
&\quad \gtrsim r_2^{\kappa_2-1} - r_2^{-1} + r_1^{\gamma-3/2} - r_1^{2(\gamma-1)} - r_1^{-2\gamma} \geq r_2^{\kappa_2-1} - r_2^{-1} + r_1^{\gamma-3/2} - r_2^{2(\gamma-1)} - r_1^{-2\gamma} \\
&\quad \geq r_2^{\kappa_2-1} \geq r_1^{\kappa_2-1} \geq r_1^{-1}
\end{aligned}
$$

for all $r_1^\gamma < r_2 \leq r_1$, and large enough r_1, as long as $0 < \kappa_2 < 1$, $\kappa_2 - 1 > 2(\gamma - 1)$, and $\gamma - 3/2 > -2\gamma$, which is equivalent to $1/2 < \gamma < (\kappa_2 + 1)/2$.

It is straightforward to check that $1/2 < \gamma < (\kappa_2+1)/2$ and $(3 - 2\kappa_1)/4 < \gamma < \kappa_1 + 1/2$ is equivalent to $(3 - 2\kappa_1)/4 < \gamma < \min((\kappa_2 + 1)/2, \kappa_1 + 1/2)$, since $(3 - 2\kappa_1)/4 > 1/2$ when $\kappa_1 < 1/2$. This is the condition on the parameter γ for the range $0 \leq U \leq U_c$.

One also easily checks that $(1-\kappa_1)/2 < \gamma < 1+\kappa_1$ and $1/2 < \gamma < (\kappa_2+1)/2$ is equivalent to $1/2 < \gamma < (\kappa_2 + 1)/2$ for $0 < \kappa_1, \kappa_2 < 1$. This is the condition on the parameter γ when U stays away from the critical coupling.

Collecting the lower bounds on $\frac{1}{4} + W_j - |\nabla G_2|^2$ on the supports of χ_1 and χ_2 and plugging this into (5.6), one arrives at

$$
\langle \chi_R e^{G_{2,\delta}}\psi, |x|_\infty^{-4/3}\chi_R e^{G_{2,\delta}}\psi\rangle \leq C\|\psi\|^2.
$$

The constant C is uniform in $\varepsilon > 0$, since G_2 is bounded on the support of $\nabla\chi_R$ for any fixed $R > 0$. Hence we can again use the monotone convergence theorem to conclude

$$\langle \chi_R e^{G_2}\psi, |x|_\infty^{-4/3}\chi_R e^{G_2}\psi\rangle = \lim_{\varepsilon\to 0}\langle \chi_R e^{G_{2,\delta}}\psi, |x|_\infty^{-4/3}\chi_R e^{G_{2,\delta}}\psi\rangle \le C\|\psi\|^2$$

which proves the theorem since $G_2(x) - \frac{2}{3}\ln|x|_\infty \ge F_2(x)$ for all large $|x|_\infty$. ∎

Corollary 5.4 (Pointwise version of Proposition 5.2)**.** *Given parameters $K_1, K_2 > 0$, $1/6 < \kappa_1 < 1/2$, and $1/2 - \kappa_1 < \kappa_2 < 1$, as well as $(3 - 2\kappa_1)/4 < \gamma < \min((\kappa_2 + 1)/2, \kappa_1 + 1/2)$, there exists a constant $C > 0$, depending only on the above parameters such that for any normalized ground state ψ_U of the helium–type system Hamiltonian H_U we have*

$$\psi_U(x) \le C\exp[-F_{2,U}(|x|_\infty, |x|_0)] \quad \text{for all } x \in \mathbb{R}^6\,, \tag{5.10}$$

uniformly in $0 \le U \le U_c$, with F_2 defined in (5.2).

Moreover, in the subcritical range $0 \le U \le U_c - \mu$ for some small $\mu > 0$, the bound (5.10) holds with any choice of parameters $0 < \kappa_1, \kappa_2 < 1$ and $1/2 < \gamma < (\kappa_2 + 1)/2$.

Proof. Proposition D.1 shows that H_U has a unique ground state ψ_U for any $0 \le U \le U_c$, which up to a phase can be chosen positive. The subsolution estimate of Trudinger [42] in the version of Aizenman and Simon [4], see also [36, Theorem C.1.3] shows that for any $r > 0$ and $x \in \mathbb{R}^6$

$$|\psi_U(x)| \le C_1 \int_{|x-y|\le r} |\psi_U(y)|\, dy \tag{5.11}$$

since the Coulomb potential is in the Kato class. The constant C_1 depends only on r and the Kato norm of the potential, see, e.g., [36, Section C.1]. Thus, with $|B_1^d|$ the volume of the unit ball in $\mathbb{R}^d$,

$$\begin{aligned} e^{F_{2,U}(x)}|\psi_U(x)| &\le C_1|B_1^d|^{1/2}\left(\int_{|x-y|\le 1} e^{2F_{2,U}(x)}|\psi_U(y)|^2\, dy\right)^{1/2} \\ &\le C_1|B_1^d|^{1/2}\sup_{|x-y|\le 1} e^{F_{2,U}(x)-F_{2,U}(y)}\|e^{F_{2,U}}\psi_U\| \end{aligned} \tag{5.12}$$

for all $x \in \mathbb{R}^6$. One easily checks that for all $|r_1 - s_1|, |r_2 - s_2| \le 1$

$$\begin{aligned} &F_{2,U}(r_1, r_2) - F_{2,U}(s_1, s_2) \\ &\lesssim |r_1^{1/2} - s_1^{1/2}| + |r_1^{\kappa_1} - s_1^{\kappa_1}| + |r_1 - s_1| + |r_2^{\kappa_2} - s_2^{\kappa_2}| + |r_1^{\gamma} - s_1^{\gamma}| \\ &\lesssim t^{-1/2} + t^{\kappa_1 - 1} + 1 + u^{\kappa_2 - 1} + t^{\gamma - 1} \end{aligned}$$

with $t = \max(r_1, s_1)$, $u = \max(r_2, s_2)$. Hence

$$C_2 \coloneqq \sup_{x\in\mathbb{R}^6}\sup_{|x-y|\le 1} |F_{2,U}(x) - F_{2,U}(y)| < \infty\,. \tag{5.13}$$

So (5.12) gives the pointwise exponential upper bound

$$|\psi_U(x)| \le CC_1C_2|B_1^d|^{1/2}e^{-F_{2,U}(x)} \quad \text{for all } x \in \mathbb{R}^6 \tag{5.14}$$

for the ground state ψ_U, where C is the constant from the L^2 upper bound of Proposition 5.2. This proves Corollary 5.4. ∎

6. Global anisotropic upper bound

In this section we give the proof of Theorem 1.1 and the proof of the upper bound from Theorem 1.6. Recall that the function F_+ is given by

$$F_+(r_1, r_2) = 2(U_c - 1)^{1/2} r_1^{1/2} - K_1 r_1^{\kappa_1} + \frac{1}{2} r_2 - K_2 r_2^{\kappa_2} \tag{6.1}$$

and the function F_+^U is given by

$$F_+^U(r_1, r_2) = F_U(r_1) - K_1 r_1^{\kappa_1} + \frac{1}{2} r_2 - K_2 r_2^{\kappa_2} \tag{6.2}$$

for $r_1, r_2 \geq 0$ with F_U defined in (1.8). We also set $F_+(x) = F_+(|x|_\infty, |x|_0)$ and the same for F_+^U. We choose ψ_U to be the unique positive ground state of H_U. We want to use the comparison principle from Theorem B.3 to show that there exist a constant $0 < C < \infty$, depending only on the parameters $\kappa_1, \kappa_2, K_1, K_2$ in the definition of F_+^U such that

$$\psi_U(x) \leq C \exp(-F_+^U(|x|_\infty, |x|_0)) \tag{6.3}$$

for all $x \in \mathbb{R}^6$ and all $0 \leq U \leq U_c$. Since ψ_U is bounded by Proposition D.1 and $\exp(-F_+^U)$ is bounded away from zero on compact sets uniformly in U, it is enough to assume that $|x|_\infty > R$ for some large $R > 0$. In this section, we abbreviate

$$f_U \coloneqq \exp(-F_+^U) \tag{6.4}$$

and note that, similarly as for F_+^U, we will not explicitly write the dependence of f_U on the other parameters except U, for simplicity of notation.

Remark 6.1. Note that F_+^U, hence also f, is twice continuously differentiable for all $0 < |x|_0 < |x|_\infty$. However, it is not twice differentiable on any neighborhood of the diagonal $|x_2| = |x_1|$, since the gradient of F_+^U has a jump discontinuity across the diagonal. Nevertheless, we could use Agmon's quadratic form version of the comparison principle, see Theorem B.3, as long as one could control certain boundary terms on the diagonal $|x_1| = |x_2|$, which appear from integration by parts. However, as the proof of the *global lower bound* in Section 8, in particular, the proof of Lemma 8.6, will show, the boundary terms have the *wrong sign and cannot be discarded.* This is why we cannot apply the comparison theorem directly. Instead, one has to apply the comparison theorem separately on $\{R^\alpha < |x_2| < |x_1|\}$ and $\{R^\alpha < |x_1| < |x_2|\}$, for large enough R. This forces us to have *very precise a-priori information* about the asymptotic behavior of ψ_U at infinity near the diagonal $|x|_0 = |x|_\infty$, since we need the a–priori information that $\psi_U(x) \lesssim f_U(x)$ near the diagonal $|x_1| = |x_2|$. Fortunately this is exactly what Corollary 5.4 provides. We summarize the necessary a-priori information about the asymptotic decay of ψ_c near the diagonal and within the tricky region in the following

Lemma 6.2. *Given any $K_1, K_2 > 0$, $1/6 < \kappa_1 < 1/2$, $0 < \alpha < \kappa_1$, and $3/4 - \kappa_1/2 < \kappa_2 < 1$, there exist a constant $0 < C < \infty$ such that*

$$\psi_U(x) \leq C f_U(x) \tag{6.5}$$

on the sets $\{|x|_0 \leq |x|_\infty^\alpha, |x|_\infty \geq R\}$ and $\{|x|_\infty - 1 \leq |x|_0 \leq |x|_\infty, |x|_\infty \geq R\}$ for all large enough $R > 0$ and all $0 \leq U \leq U_c$.

Moreover, in the subcritical range $0 \leq U \leq U_c - \mu$ for some small $\mu > 0$, for any choice of parameters $0 < \kappa_1, \kappa_2 < 1$, $\max(\kappa_1, \kappa_2) > 1/2$, $0 < \alpha < \min(\kappa_1, 1/2)$, and $K_1, K_2 > 0$, there exist $R > 0$ such that the bound (6.5) holds on the above sets and the constant C is again independent of $0 \leq U \leq U_c - \mu$.

Remark 6.3. Note that Lemma 6.2 provides the sharp upper bound on the asymptotic behavior of the ground state ψ_U, in particular in the critical case when $U = U_c$ in the regions $\{|x|_0 \leq |x|_\infty^\alpha, |x|_\infty \geq R\}$, which is within the tricky region, where one particle tries to escape and the other one stays close to the nucleus, and $\{|x|_\infty - 1 \leq |x|_0 \leq |x|_\infty, |x|_\infty \geq R\}$, which is a neighborhood of the diagonal, when both particles try to escape to infinity.

Proof. The conditions $1/6 < \kappa_1$ and $3/4 - \kappa_1/2 < \kappa_2$ are equivalent to

$$(3 - 2\kappa_1)/4 < \min(\kappa_2, \kappa_1 + 1/2)\,.$$

Since $\kappa_2 < 1$, we also have $\kappa_2 < (\kappa_2+1)/2$, so any γ with $(3-2\kappa_1)/4 < \gamma < \min(\kappa_2, \kappa_1+1/2)$ fulfills the condition of Corollary 5.4 in the whole range $0 \leq U \leq U_c$.

In the subcritical range where U stays away from U_c, we choose $1/2 < \gamma < \max(\kappa_1, \kappa_2)$. Note that for this choice the conditions of Corollary 5.4 for the subcritical case are also satisfied since $\kappa_2 < (\kappa_2 + 1)/2$.

Given the parameters $\kappa_1, \kappa_2, \gamma$ and $K_1, K_2 > 0$ we use the exponential weight $F_{2,U}$ from Corollary 5.4, but with K_1 replaced by $K_1/2$, that is, with a slight abuse of notation, we use

$$F_{2,U}(r_1, r_2) = F_U(r_1) - K_1 r_1^{\kappa_1}/2 + \frac{1}{2}\left(r_2 - K_2 r_2^{\kappa_2} - 2r_1^\gamma\right)_+\,.$$

Due to $\alpha < 1/2 < \gamma$, we have $F_{2,U}(r_1, r_2) = F_U(r_1) - \frac{K_1}{2} r_1^{\kappa_1}$ when $r_2 \leq r_1^\alpha$ and r_1 is large. In particular,

$$\begin{aligned} F_{2,U}(r_1, r_2) = F_U(r_1) - \frac{K_1}{2} r_1^{\kappa_1} &\geq F_U(r_1) - K_1 r_1^{\kappa_1} + \frac{1}{2} r_2 - K_2 r_2^{\kappa_2} + \frac{K_1}{2} r_1^{\kappa_1} - \frac{1}{2} r_2 \\ &\geq F_+^U(r_1, r_2) + \frac{K_1}{2} r_1^{\kappa_1} - \frac{1}{2} r_1^\alpha > F_+^U(r_1, r_2) \end{aligned}$$

if $r_2 \leq r_1^\alpha$ and r_1 is large enough since $\alpha < \kappa_1$. Similarly,

$$\begin{aligned} F_{2,U}(r_1, r_2) &= F_U(r_1) - \frac{K_1}{2} r_1^{\kappa_1} + \frac{1}{2} r_2 - \frac{K_2}{2} r_2^{\kappa_2} - r_1^\gamma \\ &\geq F_+^U(r_1, r_2) + \frac{K_1}{2} r_1^{\kappa_1} + \frac{K_2}{2}(r_1 - 1)^{\kappa_2} - r_1^\gamma > F_+^U(r_1, r_2) \end{aligned}$$

when $r_1 - 1 < r_2 \leq r_1$ and r_1 is large, since $\gamma < \kappa_2$ in the critical case and $\gamma < \max(\kappa_1, \kappa_2)$ in the subcritical case. From Corollary 5.4 we get, the pointwise upper bound

$$\psi_U(x) \leq C \exp[-F_{2,U}(x)] \leq C \exp[-F_+^U(x)] = C f_U(x) \tag{6.6}$$

in the regions $|x|_0 \leq |x|_\infty^\alpha$, respectively, $|x|_\infty - 1 < |x|_0 \leq |x|_\infty$, when $|x|_\infty$ is large enough. ∎

The next Lemma shows that f_U is a supersolution on a set "sandwiched between" the sets $\{|x|_0 \leq |x|_\infty^\alpha, |x|_\infty \geq R\}$ and $\{|x|_\infty - 1 \leq |x|_0 \leq |x|_\infty, |x|_\infty \geq R\}$.

Lemma 6.4. *Let $0 < \kappa_1 < 1/2 < \kappa_2 < 1$, $K_1, K_2 > 0$, and $0 < \alpha < 1$. Then the function $f_U = \exp(-F_+^U)$, with F_+^U given in (6.1), is a classical supersolution of H_U at energy E_U on the set*

$$B_R = \{|x|_\infty^\alpha - 1 < |x|_0 < |x|_\infty, |x|_\infty > R\} \tag{6.7}$$

for all large enough $R > 0$. That is,

$$(H_U - E_U) f_U \geq 0 \text{ pointwise in } B_R\,. \tag{6.8}$$

In particular, f_U is a supersolution in the quadratic form sense a la Agmon: for large enough R and all $0 \le \varphi \in \mathcal{C}_0^\infty(B_R)$ we have the quadratic form inequality

$$\langle \varphi, (H_U - E_U) f_U \rangle \ge 0 \,. \tag{6.9}$$

Moreover, in the subcritical range, where $0 \le U \le U_c - \mu$ for some small $\mu > 0$, for any choice of parameters $0 < \kappa_1, \kappa_2 < 1$, and $0 < \alpha < 1$, there exists $R > 0$ such that the function f_U is a classical supersolution in the set B_R.

Proof. In order to be able to control the errors, it will be important that both particles are far from the nucleus in B_R. For large enough $R > 0$, the set B_R is the disjoint union of $B_R^- := \{|x_1|^\alpha - 1 < |x_2| < |x_1|, |x_1| > R\}$, the part of B_R "below the diagonal" $|x_2| = |x_1|$, and the part B_R^+ above the diagonal, defined similarly as B_R^- but with x_1 and x_2 interchanged. By symmetry of f_U, which is clear from the symmetry of F_+^U, it is enough to show that f_U is a classical supersolution of H_U at energy E_U on B_R^-.

Let ∇ be the gradient and Δ the Laplacian on $\mathbb{R}^6$. We abbreviate $F = F_+^U$ and $f = f_U$. Since they are twice differentiable on B_R^- we clearly have

$$-\Delta f = f\big[- |\nabla F|^2 + \Delta F \big]$$

on B_R^-. Also recall that $\varepsilon = -\frac{1}{4} - E_U \ge 0$ is the ionization energy (which is zero when $U = U_c$) and we also abbreviate $a = (U-1)_+^{1/2}$, so $F_U'(r_1) = (\varepsilon + a^2/r_1)^{1/2}$. Moreover, we have $f(x) = \exp(-F(r_1, r_2))$ with $r_1 = |x_1|$ and $r_2 = |x_2|$ on B_R^-, so one easily calculates

$$\nabla F(x) = \begin{pmatrix} \partial_1 F \frac{x_1}{|x_1|} \\ \partial_2 F \frac{x_2}{|x_2|} \end{pmatrix} = \begin{pmatrix} \big(F_U'(r_1) - K_1 \kappa_1 r_1^{\kappa_1 - 1}\big) \frac{x_1}{|x_1|} \\ \big(\frac{1}{2} - K_2 \kappa_2 r_2^{\kappa_2 - 1}\big) \frac{x_2}{|x_2|} \end{pmatrix} \quad \text{on } B_R^- \tag{6.10}$$

and

$$\Delta F(x) = \partial_1^2 F + \partial_1 F \frac{2}{|x_1|} + \partial_2^2 F + \partial_2 F \frac{2}{|x_2|} \quad \text{on } B_R^- \,. \tag{6.11}$$

Thus

$$-\Delta f = f \left[-|\partial_1 F|^2 - |\partial_2 F|^2 + \partial_1^2 F + \partial_1 F \frac{2}{|x_1|} + \partial_2^2 F + \partial_2 F \frac{2}{|x_2|} \right],$$

on B_R^-, hence also

$$\begin{aligned} (H_U - E_U) f &= f \Big[\varepsilon - |\partial_1 F|^2 + \frac{1}{4} - |\partial_2 F|^2 + \partial_1^2 F + \partial_1 F \frac{2}{|x_1|} + \partial_2^2 F + \partial_2 F \frac{2}{|x_2|} \\ &\qquad - \frac{1}{|x_1|} - \frac{1}{|x_2|} + \frac{U}{|x_1 - x_2|} \Big] \\ &\ge f \Big[\varepsilon - |\partial_1 F|^2 + \frac{1}{4} - |\partial_2 F|^2 + \partial_1^2 F + \partial_2 F \frac{2}{r_2} - \frac{1}{r_1} - \frac{1}{r_2} \Big], \end{aligned}$$

where we dropped the positive terms $\partial_2^2 F$, $U/|x_1 - x_2|$, and also $\partial_1 F \frac{2}{r_1}$, which is positive for large enough r_1. Furthermore, using $F_U'(r_1) = (\varepsilon + a^2/r_1)^{1/2} \ge (\varepsilon + a^2)^{1/2} r_1^{-1/2} \ge c r_1^{-1/2}$ with the constant $c^2 = \inf_{0 \le U \le U_c} (\varepsilon_U + a_U^2) > 0$ we have

$$\begin{aligned} \varepsilon - |\partial_1 F|^2 &= \varepsilon - \Big(F_U'(r_1) - K_1 \kappa_1 r_1^{\kappa_1 - 1} \Big)^2 \\ &= -a^2 r_1^{-1} + 2 K_1 \kappa_1 F_U'(r_1) r_1^{\kappa_1 - 1} - (K_1 \kappa_1 r_1^{\kappa_1 - 1})^2 \\ &\gtrsim -r_1^{-1} + r_1^{\kappa_1 - 3/2} - r_1^{2(\kappa_1 - 1)} \gtrsim -r_1^{-1} + r_1^{\kappa_1 - 3/2}, \end{aligned}$$

since $\kappa_1 - 3/2 > 2(\kappa_1 - 1)$. Moreover,

$$\frac{1}{4} - |\partial_2 F|^2 = K_2\kappa_2 r_2^{\kappa_2-1}(1 - K_2\kappa_2 r_2^{\kappa_2-1}) \sim r_2^{\kappa_2-1}\,,$$

$$\begin{aligned}\partial_1^2 F &= F_U''(r_1) + K_1\kappa_1(1-\kappa_1)r_1^{\kappa_1-2} = -\frac{a^2}{r_1^2}\left(\varepsilon + a^2/r_1\right)^{-1/2} + K_1\kappa_1(1-\kappa_1)r_1^{\kappa_1-2}\\ &\geq -\frac{a^2}{r_1^2}\frac{r_1^{1/2}}{c} + K_1\kappa_1(1-\kappa_1)r_1^{\kappa_1-2} \gtrsim -r_1^{-3/2}\,,\end{aligned}$$

$$\partial_2 F\frac{2}{r_2} - r_2^{-1} = (\frac{1}{2} - K_2\kappa_2 r_2^{\kappa_2-1})\frac{2}{r_2} - r_2^{-1} \sim -r_2^{\kappa_2-2}$$

for all large enough r_1, r_2. So we get

$$\begin{aligned}(H_U - E_U)f &\gtrsim f\Big[-r_1^{-1} + r_1^{\kappa_1-3/2} + r_2^{\kappa_2-1} - r_1^{-3/2} - r_2^{\kappa_2-2}\Big] \gtrsim f\Big[-r_1^{-1} + r_2^{\kappa_2-1}\Big]\\ &\geq f\Big[-r_1^{-1} + r_1^{\kappa_2-1}\Big] \gtrsim f\, r_1^{\kappa_2-1} > 0\,,\end{aligned}$$

for all $x \in B_R^-$ and large enough R. The second inequality holds since $r_1^{\kappa_1-3/2} > r_1^{-3/2}$ for large r_1, the third because $r_2^{\kappa_2-1} \geq r_1^{\kappa_2-1}$ and the fourth, because $r_1^{\kappa_2-1} - r_1^{-1} = r_1^{\kappa_2-1}(1 - r_1^{-\kappa_2}) \gtrsim r_1^{\kappa_2-1}$. This proves Lemma 6.4 uniformly in $0 \leq U \leq U_c$.

In the subcritical case, when $0 \leq U \leq U_c - \mu$ for some fixed small $\mu > 0$, we have the bound

$$\varepsilon - |\partial_1 F|^2 \gtrsim -r_1^{-1} + r_1^{\kappa_1-1} - r_1^{2(\kappa_1-1)} \gtrsim r_1^{\kappa_1-1}\,,$$

uniformly in $0 \leq U \leq U_c - \mu$ and therefore

$$(H_U - E_U)f \gtrsim f\Big[r_1^{\kappa_1-1} + r_2^{\kappa_2-1} - r_1^{-3/2} - r_2^{\kappa_2-2}\Big] > 0\,,$$

since $0 < \kappa_1, \kappa_2 < 1$, $r_1 \geq R$, $r_2 \geq R^\alpha - 1$ and R is large enough, which proves the second claim. ∎

Now we come to the proof of the global upper bound.

Theorem 6.5 (Sharp upper bound, arbitrary coupling)**.** *For any choice of parameters $K_1, K_2 > 0$, $1/6 < \kappa_1 < 1/2$, and $(3 - 2\kappa_1)/4 < \kappa_2 < 1$ there exist constants C_+ depending only on κ_1, κ_2, K_1, and K_2, such that for the unique positive choice of the ground state of the helium-type operator H_U the pointwise bound*

$$\psi_U(x) \leq C_+ \exp\left(-F_+^U(|x|_\infty, |x|_0)\right) \tag{6.12}$$

holds uniformly in $0 \leq U \leq U_c$.

For the subcritical case, where for fixed small $\mu > 0$ the repulsion parameter U is allowed to vary uniformly in $0 \leq U \leq U_c - \mu$ assume that $0 < \kappa_1, \kappa_2 < 1$, $\max(\kappa_1, \kappa_2) > 1/2$, and $K_1, K_2 > 0$. Then there exist a constant $\widetilde{C}_+$, depending only on $\kappa_1, \kappa_2, K_1, K_2$, and also μ, such that the upper bound

$$\psi_U(x) \leq \widetilde{C}_+ \exp\left(-F_+^U(|x|_\infty, |x|_0)\right) \tag{6.13}$$

holds for all $0 \leq U \leq U_c - \mu$.

Remark 6.6. Note that Theorem 1.1 is a special case of Theorem 6.5 for $U = U_c$.

Proof of Theorem 6.5: Since ψ_U is bounded uniformly in $0 \leq U \leq U_c$, see Proposition D.1, and $f_U = \exp(-F_+^U)$ is bounded away from zero on compact sets uniformly in $0 \leq U \leq U_c$, we clearly have $\psi_U(x) \leq C f_U(x) = C\exp(-F_+^U(x))$ for all $|x|_\infty \leq R$ for some constant C, which might depend on R and the parameters but not on U.

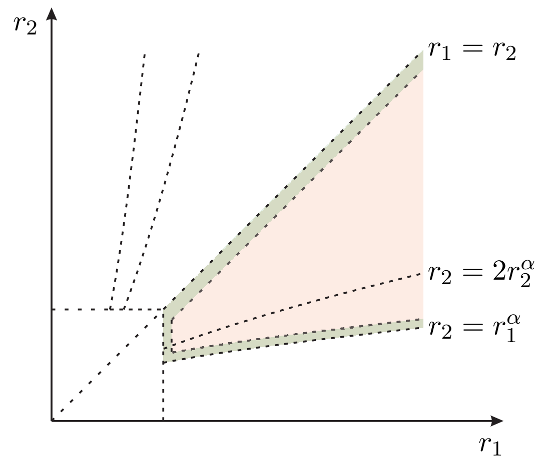

FIGURE 6.1. The intermediate region B_R^- and its boundary layer

So it is enough to show there exists some constant C such that $\psi_U(x) \le Cf_U(x)$ on $\{|x|_\infty > R\}$ for some $R > 0$. By symmetry, it is enough to prove that there exists a constant C such that

$$\psi_U(x) \le Cf_U(x) = C\exp(-F_+^U(x)) \tag{6.14}$$

for all $\{|x_2| \le |x_1|, |x_1| > R\}$ and large enough $R > 0$.

Fix any $0 < \alpha < \min(\kappa_1, 1/2)$. Due to the assumptions on the parameters $\kappa_1, \kappa_2, K_1, K_2$ in Theorem 1.6 the assumptions of Lemma 6.2 are satisfied with this choice of α. Hence the bound (6.14) holds for some constant C on the sets $B_{1,R} := \{|x_2| \le |x_1|^\alpha, |x_1| > R\}$ and $B_{2,R} := \{|x_1| - 1 \le |x_2| \le |x_1|, |x_1| > R\}$, both in the critical and subcritical case.

So we only have to prove the same bound on the intermediate region $B_R^- = \{|x_1|^\alpha - 1 < |x_2| < |x_1|, |x_1| > R\}$. Consider

$$\widetilde{\partial} B_R^1 := \{|x_1| - 1 \le |x_2| < |x_1|, |x_1| > R + 1\}$$
$$\widetilde{\partial} B_R^2 := \{|x_1|^\alpha - 1 < |x_2| \le |x_1|^\alpha, |x_1| > R + 1\}$$

and

$$\widetilde{\partial} B_R^0 := \{|x_1|^\alpha - 1 < |x_2| < |x_1|, R < |x_1| \le R + 1\}.$$

Then $\widetilde{\partial} B_R = \cup_{j=0}^2 \widetilde{\partial} B_R^j$ is a boundary layer of B_R^- in the sense of Definition B.2. Moreover, as already mentioned above, we know from Lemma 6.2 that (6.14) holds on the parts $\widetilde{\partial} B_R^1$ and $\widetilde{\partial} B_R^2$ when R is large enough. Since $f_U = \exp(-F_+^U)$ is bounded away from zero on any compact set and the closure of $\widetilde{\partial} B_R^0$ is bounded, we see that f_U is bounded away from zero on $\widetilde{\partial} B_R^0$. Using that ψ_U is bounded, shows that the bound (6.14) also holds on $\widetilde{\partial} B_R^0$ for some constant C. Thus, enlarging the constant if necessary, we see that the upper bound (6.14) holds on the boundary layer $\widetilde{\partial} B_R$ for some constant C. This constant only depends on the constant from Lemma 6.2, on uniform bounds on ψ_U from Proposition D.1, and lower bounds on f_U on compact sets, which are independent of U.

To finish the argument, we note that f_U is a classical supersolution, hence also in the quadratic form sense, of H_U at energy E_U on B_R^- by Lemma 6.4 (for the precise notion see the discussion in Appendix B). Moreover, $\psi_U \in H^1(\mathbb{R}^6)$ is a solution, hence also a subsolution, in the quadratic form sense a la Agmon on B_R^-. The subharmonic comparison principle given in Theorem B.3 then yields the upper bound (6.14) on all of B_R^-. This proves the upper bound from Theorem 1.6 in the critical and subcritical case. ∎

Remark 6.7. It is very convenient to have a quadratic form version of the subharmonic comparison principle, since it allows us to directly work with weak eigenfunctions, which are only in $H^1(\mathbb{R}^6)$ and not in $H^2(\mathbb{R}^6)$. To the best of our knowledge, the quadratic form version of the subharmonic comparison principle goes back to a beautiful paper by Agmon [2]. Theorem B.3 in the appendix is a slight extension of Agmon's original result. Agmon works on open sets which are neighborhoods of infinity, i.e., complements of compacts sets, while we have to work on unbounded sets, which are not necessarily neighborhoods of infinity.

7. Lower bound in the tricky region

Theorem 7.1 (Lower pointwise bound in the tricky region)**.** *Let H_U be the helium–type Schrödinger operator given in (1.1) and let $\psi_U \in L^2(\mathbb{R}^6)$ be the positive ground state of H_U for $0 \le U \le U_c$. Then for any $1/6 < \kappa < 1/2$ and any $0 < \gamma < \kappa + 1/2$ and any $K > 0$*

$$\psi_U(x) \gtrsim \exp\Big(- F_U(|x|_\infty) - K|x|_\infty^\kappa - \frac{1}{2}|x|_0\Big) \quad \text{for all } |x|_0 \le |x|_\infty^\gamma \tag{7.1}$$

with F_U defined in (1.8). Again we use $|x|_0 = \min\{|x_1|, |x_2|\}$, $|x|_\infty = \max\{|x_1|, |x_2|\}$. The implicit constant in the above bound depends on the parameters κ, γ, and K, but not on U in the range $0 \le U \le U_c$.

Moreover, in the subcritical case, i.e., when U stays away from U_c, the lower bound (7.1) holds for any fixed small μ uniformly in $0 \le U \le U_c - \mu$ and any $0 < \kappa < 1$ and $0 < \gamma < 1$.

Remark 7.2. Theorem 7.1 provides a lower bound for the ground state when one particle escapes while the other stays close to the nucleus. This is an important a-priori bound for our proof of the global lower bound.

Since the leading order behavior of $F_U(r)$ switches from linear to $r^{1/2}$ at $U = U_c$, we need the restriction $\kappa < 1/2$ in the first case, so that r^κ is a lower order correction compared to the leading order term $F_U(r)$, uniformly in $0 \le U \le U_c$.

When U stays away from U_c, the leading order term $F_U(r)$ is always linear in r, which allows for a larger range for κ and γ.

Proof. For $0 < \gamma < 1$ define $\widetilde{A} = \{|x|_0 \le |x|_\infty^\gamma\}$. For large enough R, the regions $\widetilde{A}_R^- = \{|x_2| \le |x_1|^\gamma, |x_1| > R\}$ and $\widetilde{A}_R^+ = \{|x_1| \le |x_2|^\gamma, |x_2| > R\}$ are disjoint. By symmetry, a lower bound of the form (7.1) on the set $\widetilde{A}_R^-$, for some $R > 0$ implies the same bound on $\widetilde{A}_R^+$. The set $\widetilde{A} \setminus (\widetilde{A}_R^- \cup \widetilde{A}_R^+) = \{|x|_0 \le |x|_\infty^\gamma \le R^\gamma\}$ is a compact subset of $\mathbb{R}^6$. Clearly the right hand side of (7.1) bounded above on compact sets and, because of Proposition D.1, ψ_U is bounded away from zero on compact sets. Hence there is some constant $C > 0$ with

$$\psi_U(x) \ge C \exp\Big(- F_U(|x|_\infty) - K|x|_\infty^\kappa - \frac{1}{2}|x|_0\Big) \quad \text{for all } x \in \widetilde{A} \setminus (\widetilde{A}_R^- \cup \widetilde{A}_R^+)\,.$$

Thus, shrinking the involved constant, if necessary, one sees that the lower bound (7.1) holds on $\widetilde{A}$ iff it holds on $\widetilde{A}_R^-$ for some $R > 0$.

For technical reasons, we need to work on the slightly larger set

$$A_R^- := \{|x_2| < 2|x_1|^\gamma, |x_1| \ge R\}.$$

which is just the (lower) tricky region from Section 3. Recall that $a = (U-1)_+^{1/2}$ and $\varepsilon = -\frac{1}{4} - E_U$ is the ionization energy. F_U, defined in (1.8), depends on these two parameters.

Finally we define

$$
\begin{aligned}
F_{3,U}(r_1,r_2) &= F_U(r_1) + K r_1^\kappa - \tfrac{1}{2} r_2 \quad \text{for } r_1, r_2 \geq 0\,, \\
\Phi(s) &:= \begin{cases} 1\,, & 0 \leq s \leq 1 \\ \cos\left(\frac{\pi}{2}(s-1)\right)\,, & 1 < s < 2 \\ 0\,, & 2 \leq s \end{cases} \\
\chi(x) &:= \Phi\Big(\frac{|x_2|}{|x_1|^\gamma}\Big) \quad \text{for } x = (x_1,x_2) \in A_R^-
\end{aligned}
\tag{7.2}
$$

and

$$
g_U(x) := \chi(x) \exp(-F_{3,U}(|x_1|,|x_2|)) \quad \text{for } x = (x_1,x_2) \in A_R^-\,. \tag{7.3}
$$

We will suppress the dependence of $F_{3,U}$ and g_U on the other parameters, except on U, for simplicity of notation. Note that $\chi(x) = 1$ on $\widetilde{A}_R^-$, so the bound (7.1) will hold on $\widetilde{A}_R^-$, hence also on $\widetilde{A}$, once we show that $\psi_U \geq C g_U$ on A_R^- for some $R > 0$ and some constant $C > 0$, which can depend on all the parameters, but not on U.

The boundary ∂A_R^- is the union of the unbounded part $\partial A_{R,1}^- = \{|x_2| = 2|x_1|^\gamma, |x_1| \geq R\}$ and the compact set $\partial A_{R,2}^- = \{|x_1| = R, |x_2| \leq 2R^\gamma\}$. We clearly have $\psi_U(x) > 0 = g_U(x)$ for all $x \in \partial A_{R,1}^-$. By continuity of ψ_U and g_U, there exists an open neighborhood O_1 of $\partial A_{R,1}^-$ such that $\psi_U(x) > g_U(x)$ for all $x \in O_1$. Hence $\psi_U \geq g_U$ on $O_1 \cap A_R^-$.

Moreover, $\psi_U > 0$ is bounded from below by a positive constant on compact subsets of $\mathbb{R}^6$, uniformly in $0 \leq U \leq U_c$, see Proposition D.1 and $g_U \geq 0$ is continuous and depends continuously on the parameters. Thus, since $\partial A_{R,2}^-$ is compact, there exists a constant $C > 0$ such that $\psi_U \geq 2C g_U > C g_U$ on $\partial A_{R,2}^-$ for all $0 \leq U \leq U_c$. By continuity, there exist an open neighborhood O_2 of $\partial A_{R,2}^-$ such that $\psi_U > C g_U$ on O_2, hence $\psi_U > C g_U$ on $O_2 \cap A_R^-$. Thus

$$
\psi_U \geq \min(C,1) g_U \text{ on the boundary layer } (O_1 \cup O_2) \cap A_R^-\,.
$$

Now assume that $1/6 < \kappa < 1/2$ and $(3-2\kappa)/4 < \gamma < \kappa + 1/2$. In Lemma 7.3 we show that under these conditions there exists $R > 0$ such that g_U is a subsolution of H_U at energy E_U in A_R^-, for all $0 \leq U \leq U_c$, in the quadratic form sense a la Agmon. Moreover, it is easy to see that $g_U \in L^2(\mathbb{R}^6)$. Hence we can apply Theorem B.3 to conclude that $\psi_U \geq C g_U$ on all of A_R^-, hence on all of $\{|x|_0 \leq |x|_\infty^\gamma\}$.

It remains to get rid of the lower bound on γ. Note that the sets $\{|x|_0 \leq |x|_\infty^\gamma\}$ are increasing in $0 < \gamma < 1$, i.e., once the bound (7.1) holds for some $(3-2\kappa)/4 < \gamma < \kappa + 1/2$ it holds for all $0 < \gamma \leq \kappa + 1/2$. This finishes the proof of Theorem 7.1. ∎

It remains to prove that for suitable choices of the parameters, the function g_U defined in (7.3) is a classical subsolution in the tricky region.

Lemma 7.3. *Let $\kappa > 1/6$ and $(3-2\kappa)/4 < \gamma < \min(\kappa + 1/2, 1)$. Then there exists $R > 0$ such that the function g_U defined in (7.3) is a classical subsolution of H_U at energy $E_U = -1/4 - \varepsilon_U \leq -1/4$ on the set $A_R = \{|x|_0 < 2|x|_\infty^\gamma, |x|_\infty > R\}$, that is,*

$$
(H_U - E_U) g_U \leq 0 \quad \textit{pointwise in } A_R \tag{7.4}
$$

for any $0 \leq U \leq U_c$. In particular, it is a subsolution in the quadratic form sense a la Agmon: for large enough R and all $0 \leq \varphi \in \mathcal{C}_0^\infty(A_R)$ we have the quadratic form inequality

$$
\langle \varphi, (H_U - E_U) g_U \rangle \leq 0\,. \tag{7.5}
$$

Moreover, in the subcritical case, i.e., when U stays away from U_c, the same holds for any fixed small μ uniformly in $0 \le U \le U_c - \mu$ and any $\kappa > 0$ and $\max((1-\kappa)/2, 0) < \gamma < 1$.

Remark 7.4. It is easy to see that $(3-2\kappa)/4 < \kappa + 1/2$ is equivalent to $\kappa > 1/6$. So the set of allowed values for γ is not empty iff $\kappa > 1/6$.

Proof. The bound (7.5) immediately follows from (7.4) by integration by parts, since φ has compact support inside A_R and is non–negative on A_R. Moreover, since A_R splits into the regions $A_R^- = \{|x_2| < 2|x_1|^\gamma, |x_1| > R\}$ and $A_R^+ = \{|x_1| < 2|x_2|^\gamma, |x_2| > R\}$, which are disjoint for large enough R. So it is enough to prove (7.4) on A_R^-, by symmetry.

In the remainder of the proof, we will work only on A_R^-, abbreviate $F = F_{3,U}$ and $g = g_U$, and also identify the function F with $F(|x_1|, |x_2|)$, for simplicity of notation.

Clearly, F is twice continuously differentiable on A_R^-. Moreover, Φ is twice differentiable on $[0, 2)$ and one easily checks that $g \in H_0^1(A_R^-) \cap H^2(A_R^-)$. Since $\nabla g = \nabla\chi e^{-F} - \chi\nabla F e^{-F}$, we have

$$-\Delta g = e^{-F}\left[\chi\Delta F - \chi|\nabla F|^2 - \Delta\chi + 2\nabla\chi\nabla F\right].$$

From the definition of F and χ, setting $r_1 = |x_1|$, $r_2 = |x_2|$, and recalling $\partial_1 = \partial_{r_1}$, $\partial_2 = \partial_{r_2}$, one calculates

$$\nabla F(x) = \begin{pmatrix} \partial_1 F \frac{x_1}{|x_1|} \\ \partial_2 F \frac{x_2}{|x_2|} \end{pmatrix} = \begin{pmatrix} \left(F_U'(r_1) + K\kappa r_1^{\kappa-1}\right)\frac{x_1}{|x_1|} \\ \frac{1}{2}\frac{x_2}{|x_2|} \end{pmatrix}$$

with $F_U'(r_1) = (\varepsilon + a^2/r_1)^{1/2}$ and $\varepsilon = 1/4 - E_U \ge 0$ and $a = (U-1)_+^{1/2}$. Moreover,

$$\nabla\chi(x) = \Phi'\Big(\frac{r_2}{r_1^\gamma}\Big)\begin{pmatrix} -\gamma\frac{r_2}{r_1^{\gamma+1}}\frac{x_1}{|x_1|} \\ \frac{1}{r_1^\gamma}\frac{x_2}{|x_2|} \end{pmatrix}.$$

Thus

$$\nabla\chi(x)\nabla F(x) = \Phi'\Big(\frac{r_2}{r_1^\gamma}\Big)\left[\partial_2 F r_1^{-\gamma} - \gamma\partial_1 F\, r_2 r_1^{-\gamma-1}\right]$$

and

$$\Delta\chi(x) = \Phi''\Big(\frac{r_2}{r_1^\gamma}\Big)\left(\gamma^2 r_2^2 r_1^{-2\gamma-2} + r_1^{-2\gamma}\right) + \Phi'\Big(\frac{r_2}{r_1^\gamma}\Big)\left(2r_1^{-\gamma}r_2^{-1} - \gamma(1-\gamma)r_2 r_1^{-\gamma-2}\right),$$

so

$$\begin{aligned} 2\nabla\chi(x)&\nabla F(x) - \Delta\chi(x) \\ &= -\Phi''\Big(\frac{r_2}{r_1^\gamma}\Big)\left(\gamma^2 r_2^2 r_1^{-2\gamma-2} + r_1^{-2\gamma}\right) \\ &\quad + \Phi'\Big(\frac{r_2}{r_1^\gamma}\Big) r_1^{-\gamma}\left[2\partial_2 F - 2\gamma\partial_1 F\, r_2 r_1^{-1} + \gamma(1-\gamma)r_2 r_1^{-2} - 2r_2^{-1}\right]. \end{aligned} \tag{7.6}$$

Note that $\Phi' \le 0$ and since the support of Φ' is contained in the interval $[1, 2]$, we have $r_1^\gamma \le r_2 \le 2r_1^\gamma$ for the second term on the right hand side above. Thus we get the lower bound

$$2\partial_2 F - 2\gamma\partial_1 F\, r_2 r_1^{-1} + \gamma(1-\gamma)r_2 r_1^{-2} - 2r_2^{-1} \ge 2\partial_2 F - 4\gamma\partial_1 F\, r_1^{\gamma-1} - 2r_2^{-\gamma} \gtrsim 1$$

since $2\partial_2 F = 1$ and $\partial_1 F$ is bounded at infinity uniformly in $0 \le U \le U_c$.

So we can again use $\Phi' \le 0$ to drop the second term on the right hand side of (7.6) to arrive at

$$2\nabla\chi(x)\nabla F(x) - \Delta\chi(x) \le -\Phi''\Big(\frac{r_2}{r_1^\gamma}\Big)\left(\gamma^2 r_2^2 r_1^{-2\gamma-2} + r_1^{-2\gamma}\right) \le \frac{\pi^2}{4}\chi(x)\left(4\gamma^2 r_1^{-2} + r_1^{-2\gamma}\right)$$

for all large enough r_1, where we also used that $-\Phi'' \leq \frac{\pi^2}{4}\Phi$ on $[0,2)$ by definition of Φ. Hence

$$-\Delta g \leq g\big[\Delta F - |\nabla F|^2 + \frac{\pi^2}{4}(4\gamma^2 r_1^{-2} + r_1^{-2\gamma})\big] \quad \text{on } A_R^- . \tag{7.7}$$

for large enough R.

Now the rest of the argument is easy: One checks

$$\Delta F = \partial_1^2 F + \partial_1 F \frac{2}{r_1} + \partial_2^2 F + \partial_2 F \frac{2}{r_2} = \partial_1^2 F + \partial_1 F \frac{2}{r_1} + \frac{1}{r_2}$$

since $\partial_2 F = 1/2$. Using this, $1/4 - (\partial_2 F)^2 = 0$, and (7.7), we get

$$(H_U - E_U)g \leq g\left[\varepsilon - (\partial_1 F)^2 + \frac{U}{|x_1 - x_2|} - \frac{1}{r_1} + \partial_1^2 F + \partial_1 F \frac{2}{r_1} + \frac{\pi^2}{4}(4\gamma^2 r_1^{-2} + r_1^{-2\gamma})\right] \tag{7.8}$$

On A_R^- we have $|x_2| \leq 2|x_1|^\gamma$, so $|x_1 - x_2| \geq |x_1| - |x_2| \geq r_1 - 2r_1^\gamma$. Thus

$$\frac{U}{|x_1 - x_2|} - \frac{1}{r_1} \leq \frac{U}{r_1 - 2r_1^\gamma} - \frac{1}{r_1} = \frac{U-1}{r_1} + \frac{2Ur_1^{\gamma-2}}{1 - 2r_1^{\gamma-1}} \quad \text{on } A_R^-$$

for large enough R. Since $\partial_1 F = F_U'(r_1) + K\kappa r_1^{\kappa-1}$ and $\gamma < 1$, we have

$$\varepsilon - (\partial_1 F)^2 + \frac{U}{|x_1 - x_2|} - \frac{1}{r_1} \leq -2K\kappa_1 F_U'(r_1) r_1^{\kappa-1} + 4Ur_1^{\gamma-2}$$

for all $r_1 > 0$ such that $1 - 2r_1^{\gamma-1} \geq 1/2$. The bound $F_U'' \leq 0$ implies

$$\begin{aligned}\partial_1^2 F + \partial_1 F \frac{2}{r_1} &= F_U''(r_1) + K\kappa(\kappa+1) r_1^{\kappa-2} + 2F_U'(r_1) r_1^{-1} \\ &\leq 2F_U'(r_1) r_1^{-1} + K\kappa(\kappa+1) r_1^{\kappa-2}\end{aligned}$$

which leads to

$$\begin{aligned}\varepsilon - (\partial_1 F)^2 + \frac{U}{|x_1 - x_2|} - \frac{1}{r_1} + \partial_1^2 F + \partial_1 F \frac{2}{r_1} \\ \lesssim -F_U'(r_1) r_1^{\kappa-1} + r_1^{\gamma-2} + r_1^{\kappa-2} \lesssim -r_1^{\kappa-3/2} + r_1^{\gamma-2}\end{aligned}$$

for large r_1, using again the bound $F_U'(r_1) \geq cr_1^{-1/2}$ with some constant $c > 0$, uniformly in $0 \leq U \leq U_c$. Thus from (7.8) we get

$$(H_U - E_U)g \lesssim g\left[-r_1^{\kappa-3/2} + r_1^{\gamma-2} + r_1^{-2} + r_1^{-2\gamma}\right] \leq 0 \quad \text{in } A_R^-$$

for all large enough R, under the condition that $\kappa - 3/2 > \max(\gamma - 2, -2\gamma)$, which is equivalent to $(3 - 2\kappa)/4 < \gamma < \kappa + 1/2$. Since we have the constraint $\gamma < 1$, this is equivalent to the condition on the parameters in the range $0 \leq U \leq U_c$.

In the subcritical case we use that $F_U'(r_1) \gtrsim c_\mu > 0$, for any $0 \leq U \leq U_c - \mu$ so $F_U'(r_1) r_1^{\kappa-1} \gtrsim r_1^{\kappa-1}$ uniformly in $0 \leq U \leq U_c - \mu$. Using this as before, we see that $(H_U - E_U)g \leq 0$ on A_R^- for all large enough R, under the condition that $\kappa - 1 > \max(\gamma - 2, -2\gamma)$. This is equivalent to $(1-\kappa)/2 < \gamma < \kappa + 1$. Since we have the constraint $0 < \gamma < 1$, this is equivalent to the condition on the parameters in the subcritical case. ∎

8. Global lower bound

In this section we prove the global pointwise lower bound for the ground state of helium type atoms, including the critical coupling. The Coulomb repulsion of the particles, which can become *arbitrary large* when the particles are close to each other, requires a considerably more complicated ansatz for the subsolution compared to the proof of the lower bound in the *tricky region* in Section 7. On the other hand, since we already proved a lower bound in Theorem 7.1 in the tricky region, we can now assume that both $|x|_0$ and $|x|_\infty$ are large, which helps to control the errors.

Recall that for non-negative constants $\kappa_1, \kappa_2, K_1, K_2$, and $s, r_1, r_2 \geq 0$ the weight function F_-^U is given by

$$F_-^U(r_1, r_2) := F_U(r_1) + \frac{1}{2} r_2 + K_1 r_1^{\kappa_1} + K_2 r_2^{\kappa_2} \tag{8.1}$$

with F_U defined in (1.8) and we consider the couplings in the range $\mu \leq U \leq U_c$ for some positive μ. Moreover, we will use

$$\theta(s) := \frac{1}{1+s} \tag{8.2}$$

$$h(s, r_2) := s\,\theta(r_2^{-\nu} s) \tag{8.3}$$

for some $0 < \nu < 1$. Recall also $1 < U_c \leq 2$. Furthermore, we will use

$$L_U(x) = L_U(x_1, x_2) := F_-^U(|x|_\infty, |x|_0) - h(|x_1 - x_2|, |x|_0) \tag{8.4}$$

and abbreviate $g_U = \exp(-L_U)$ in the remainder of this section. Again, for simplicity of notation, we do not indicate the dependence of L_U and g_U on the other parameters except for U, in our notation. Note that $g_U \in H^1(\mathbb{R}^6)$, but its gradient has a jump discontinuity along the diagonal $|x_1| = |x_2|$, so it is not even locally in $H^2(U)$ for any open set $U \cap \{|x_1| = |x_2|\} \neq \emptyset$. Fortunately, the subharmonic comparison principle which we will use does not require local H^2 regularity.

Proposition 8.1. *For all $0 < \beta, \nu < 1$, $0 < \kappa_1 < \kappa_2 < 1$, $\max(\nu, 1-\nu) < \kappa_2$, and $K_1, K_2 > 0$, the function $g_U = \exp(-L_U)$ is a subsolution of H_U at energy E_U in the sense of Agmon in the region*

$$C_{R,\beta} := \left\{ |x|_0 > |x|_\infty^\beta, |x|_\infty > R \right\} \tag{8.5}$$

for all large enough R uniformly in $0 \leq U \leq U_c$. That is, for all $0 \leq \varphi \in H^1(C_{R,\beta})$ one has, as quadratic forms,

$$\langle \varphi, (H_U - E_U) g_U \rangle \leq 0 \tag{8.6}$$

and R depends on the parameters κ_1, κ_2, and ν, but not on U in the range $0 \leq U \leq U_c$.

Moreover, if $0 < \beta, \nu, \kappa_1, \kappa_2 < 1$, $\max(\nu, 1-\nu) < \kappa_2$, and $0 < \mu < U_c$ then there exists $R > 0$ independent of U in the range $\mu \leq U \leq U_c$ such that (8.6) again holds.

Proof. The proof of Proposition 8.1 follows directly from Lemma 8.6 and 8.8 at the end of this section. ∎

Remark 8.2. The additional term h is needed to control the Coulomb repulsion between the particles. We believe that our choice is not only considerably simpler than the one used by Thomas Hoffmann–Ostenhof in [20] in his derivation of exponential lower bounds for the ground state of subcritical helium but it also allows us to get the *sharp coefficients* of the leading order terms in the lower bound!

Moreover, the proof shows that one has considerable flexibility in the choice of θ. The only properties of θ which we need are: $\theta \geq 0$ is continuous on $[0, \infty)$ and twice differentiable on

$(0,\infty)$, $\theta(0) > 1/2$, $s \mapsto s\theta(s)$ is increasing and bounded on $[0,\infty)$, and $s \mapsto (1+s+s^2)\theta'(s)$, $s \mapsto (s+s^2+s^3)\theta''(s)$ are bounded on $(0,\infty)$.

Assuming Proposition 8.1 and given the quadratic form version of the sub-harmonic comparison principle, the proof of the following lower bound is relatively straightforward.

Theorem 8.3. *Let ψ_U be the positive ground state of helium–type operator H_U, i.e, $H_U\psi_U = E_U\psi_U$, in the quadratic form sense. Then for $1/6 < \kappa_1 < \frac{1}{2}$, $0 < \nu < 1$, $\max(\nu, 1-\nu) < \kappa_2 < 1$, and $K_1, K_2 > 0$, we have the lower bound*

$$\psi_U(x) \geq C \exp\big(-L_U(x)\big) \tag{8.7}$$

for all $x \in \mathbb{R}^6$ where L_U is defined in (8.4), the constant C depends on the parameters κ_1, κ_2, ν, and K_1, K_2 but not on U in the range $0 \leq U \leq U_c$.

Moreover, if $0 < \nu, \kappa_1 < 1$, $\max(\nu, 1-\nu) < \kappa_2 < 1$, $K_1, K_2 > 0$, and $\mu > 0$ is small enough, then we again have the bound (8.7) for some constant C, depending on the parameters κ_1, κ_2, ν, K_1, K_2, and μ but not on U in the range $\mu \leq U \leq U_c - \mu$.

Proof. The lower bound given in Theorem 7.1 shows that uniformly in $0 \leq U \leq U_c$ and for all fixed $1/6 < \kappa_1 < 1/2$, $0 < \gamma < \kappa_1 + 1/2$, and $K_1 > 0$

$$\psi_U(x) \gtrsim \exp\Big(-F_U(|x|_\infty) - \frac{K_1}{2}|x|_\infty^{\kappa_1} - \frac{1}{2}|x|_0\Big). \tag{8.8}$$

for all $|x|_0 \leq |x|_\infty^\gamma$. Since $s\theta(s) \leq 1$, one sees $0 < h(s, r_2) = s\theta(r_2^{-\nu}s) \leq r_2^\nu$ uniformly in $s \geq 0$. Thus, since $0 < \nu < \kappa_2$,

$$F_U(r_1) + K_1 r_1^{\kappa_1} + \frac{1}{2}r_2 \leq F_-^U(r_1, r_2) - h(s, r_2) + r_2^\nu - K_2 r_2^{\kappa_2} \leq F_-^U(r_1, r_2) - h(s, r_2) + C$$

for all $s, r_1, r_2 \geq 0$ and some constant $0 \leq C < \infty$. This proves the lower bound (8.7) in the tricky region $\widetilde{A} = \{|x|_0 \leq |x|_\infty^\gamma\}$ for any $0 < \gamma < \kappa_1 + 1/2$.

The same argument applies, for subcritical U uniformly in the range $0 \leq U \leq U_c - \mu$, for small fixed $\mu > 0$, for all fixed $0 < \gamma, \kappa_1 < 1$ and $0 < \nu < \kappa_2$.

Let $0 < \beta < \gamma$ and abbreviate $C_R = C_{R,\beta} = \{|x|_0 > |x|_\infty^\beta, |x|_\infty > R\}$ for the remainder of this proof. Its boundary is given by $\partial C_R = \partial C_R^1 \cup \partial C_R^2$ with $\partial C_R^1 = \{R^\beta \leq |x|_0 \leq R, |x|_\infty = R\}$, which is compact, and $\partial C_R^2 = \{|x|_0 = |x|_\infty^\beta, |x|_\infty > R\}$, which is *unbounded*. Since the bound (8.7) holds on the tricky region $\widetilde{A}$ it clearly holds on ∂C_R^2, that is, there exist a constant $C_1 > 0$ such that

$$\psi_U(x) \geq C_1 g_U(x) \quad \text{for all } x \in \partial C_R^2$$

where the constant C_1 does not depend on U. Moreover, since ψ_U is bounded away from zero uniformly in $0 \leq U \leq U_c$ on compact sets, see Proposition D.1, and g_U is continuous and ∂C_R^1 is compact, there exist a constant $C_2 > 0$ such that

$$\psi_U(x) \geq C_2 g_U(x) \quad \text{for all } x \in \partial C_R^1,$$

with C_2 independent of U. Hence, for some constant $C > 0$ we have $\psi_U(x) \geq 2C g_U(x)$ for all $x \in \partial C_R$. By continuity of ψ_U and g_U, there exists a boundary layer $\widetilde{\partial C}_R$ such that

$$\psi_U(x) \geq C g_U(x) \quad \text{for all } x \in \widetilde{\partial C}_R. \tag{8.9}$$

Such a boundary layer is an open subset of C_R near the boundary ∂C_R with $\operatorname{dist}(x, \partial C_R) > 0$ for all $x \in C_R \setminus \widetilde{\partial C}_R$, see Appendix B.

Due to Proposition 8.1 we can use Theorem B.3, to extend the bound (8.9) to almost all $x \in C_R$. Since ψ_U and $g_U = \exp(-L_U)$ are continuous, this lower bound clearly holds for all $x \in C_R$ and since we already showed that the same type of lower bound holds in the region $\widetilde{A} = \{|x|_0 \le |x|_\infty^\gamma\}$, it holds on $C_R \cup \widetilde{A}$.

The complement of $C_R \cup \widetilde{A}$ in $\mathbb{R}^6$ is bounded, hence its closure is compact. Using Proposition D.1 one sees that ψ_U is bounded away from zero on compact sets and since g_U is bounded uniformly in $0 \le U \le U_c$, a bound of the form $\psi_U \ge C g_U$ also holds on $\mathbb{R}^6 \setminus (C_R \cup \widetilde{A})$. Thus, at the expense of decreasing the constant $C > 0$, if necessary, the lower bound (8.7) holds globally uniformly in in the critical range $0 \le U \le U_c$.

In the subcritical case, the same arguments apply, but now we have to restrict the range of allowed parameters U to $\mu \le U \le U_c - \mu$ for arbitrary but fixed small μ, due to the additional lower bound on U in Proposition 8.1. ∎

Now we come to the proof of the global lower bound.

Theorem 8.4 (Sharp lower bound, arbitrary coupling)**.** *For any choice of parameters $K_1, K_2 > 0$, $1/6 < \kappa_1 < 1/2$, and $1/2 < \kappa_2 < 1$ there exist a constant C_- depending only on κ_1, κ_2, K_1, and K_2, such that for the unique positive choice of the ground state of the helium-type operator H_U the pointwise bound*

$$\psi_U(x) \ge C_- \exp\left(-F_-^U(|x|_\infty, |x|_0)\right) \tag{8.10}$$

holds uniformly in $\mu \le U \le U_c$.

For the subcritical case let $0 < \kappa_1 < 1$, $1/2 < \kappa_2 < 1$, $K_1, K_2 > 0$, and $0 < \mu < U_c/2$ be arbitrary. Then there exist a constant $\widetilde{C}_-$, depending only on $\kappa_1, \kappa_2, K_1, K_2$, and also on μ, such that the lower bound

$$\psi_U(x) \ge \widetilde{C}_- \exp\left(-F_-^U(|x|_\infty, |x|_0)\right) \tag{8.11}$$

holds for all $\mu \le U \le U_c - \mu$.

Remark 8.5. Note that Theorem 1.3 is a special case of Theorem 8.4 for $U = U_c$.

Proof of Theorem 8.4: Theorem 8.3 gives the global lower bound $\psi_U \ge C\exp(-L_U) = C\exp(-F_-^U + h) \ge C\exp(-F_-^U)$, since $h \ge 0$ with the constant C from Theorem 8.3 which does not depend on U in the range $0 \le U \le U_c$. The same argument applies for the subcritical range $\mu \le U \le U_c - \mu$. ∎

We still have to give the proof of Proposition 8.1. This will be done in two steps. We split the region $C_{R,\beta}$ in two subregions

$$C_{R,\beta}^- := \left\{|x_1|^\beta < |x_2| < |x_1|,\, |x_1| > R\right\}, \tag{8.12}$$

$$C_{R,\beta}^+ := \left\{|x_2|^\beta < |x_1| < |x_2|,\, |x_2| > R\right\}, \tag{8.13}$$

and the diagonal

$$D_R := \left\{|x_1| = |x_2| > R\right\}. \tag{8.14}$$

While e^{-L_U} with L_U defined in (8.4) is not $H^2(C_{R,\beta})$, due to the jump of the gradient of L_U along the diagonal D_R, it is twice differentiable in $C_{R,\beta}^\pm$. The next lemma shows that e^{-L_U} is a subsolution on $C_{R,\beta}$ in the quadratic form sense a la Agmon , see [2] and Appendix B, as soon as it is a classical subsolution locally on $C_{R,\beta}^\pm$, that is, $(H_U - E_U)e^{-L_U} \le 0$ on $C_{R,\beta}^+$ and on $C_{R,\beta}^-$ separately.

Lemma 8.6. *Let $0 < \beta < 1$ and assume that $g_U := e^{-L_U}$ is a classical subsolution of H_U at energy E_U, i.e., $(H_U - E_U)g_U \le 0$ pointwise, both in $C_{R,\beta}^+$ and $C_{R,\beta}^-$.*

If $0<\nu,\kappa_1<\kappa_2<1$, then g_U is a subsolution in the quadratic form sense a la Agmon on $C_{R,\beta}$ for any large enough $R>0$ independent of $0\le U\le U_c$. That is

$$\langle \varphi, (H_U - E_U) g_U\rangle \le 0 \tag{8.15}$$

for all $0\le\varphi\in\mathcal{C}_0^\infty(C_{R,\beta})$.

Moreover, if $0<\nu,\kappa_1,\kappa_2<1$ and $0<\mu<U_c$ then there exists $R>0$ independent of U in the range $\mu\le U\le U_c$ such that (8.15) again holds.

Proof. We will write g, L, and F for g_U, L_U, respectively, F_-^U in the remainder of this proof, for simplicity of notation. The contribution of the Coulomb potential is local. So we only have to show that for R large enough,

$$\langle\nabla\varphi,\nabla g\rangle_{L^2(C_{R,\beta})} \le \langle\varphi,-\Delta g\rangle_{L^2(C^+_{R,\beta})} + \langle\varphi,-\Delta g\rangle_{L^2(C^-_{R,\beta})} \tag{8.16}$$

for all $\varphi\in\mathcal{C}_0^\infty(C_{R,\beta})$, since then for all $\varphi\ge 0$ the pointwise bounds $(H_U-E_U)g\le 0$ in $C^\pm_{R,\beta}$ together with (8.16) will imply (8.15). The bound (8.16) follows from splitting the domain $C_{R,\beta}$ into two pieces along the diagonal $D_R=\{|x_2|=|x_1|>R\}$ and integration by parts, since the boundary term on D_R has the right sign when R is large enough, as we will show in a moment. Thus we can drop the boundary term to get (8.16).

Given $x=(x_1,x_2)\in D_R$, the vectors

$$n_-(x) := \frac{1}{\sqrt{2}}\begin{pmatrix}\frac{-x_1}{|x_1|}\\ \frac{x_2}{|x_2|}\end{pmatrix} \quad\text{and } n_+(x) := \frac{1}{\sqrt{2}}\begin{pmatrix}\frac{x_1}{|x_1|}\\ \frac{-x_2}{|x_2|}\end{pmatrix} \tag{8.17}$$

are the outer normals of $C^-_{R,\beta}$, respectively $C^+_{R,\beta}$, on the diagonal D_R. To see this simply note that level sets $\{N(x)=\lambda\}\cap C^-_{R,\beta}$ with $\lambda<1$ of the function $N(x)=|x_2|/|x_1|$ converge to the diagonal D_R from within $C^-_{R,\beta}$ as $\lambda\nearrow 1$. The gradient of N points into the direction of the largest increase, hence the vector $n_-(x)$ is a positive, and $n_+(x)$ a negative, multiple of $\nabla N(x)$ when $x=(x_1,x_2)\in D_R$. This proves (8.17), because

$$\nabla N(x) = \begin{pmatrix}\frac{-|x_2|}{|x_1|^2}\frac{x_1}{|x_1|}\\ \frac{1}{|x_1|}\frac{x_2}{|x_2|}\end{pmatrix} = \frac{1}{|x_1|}\begin{pmatrix}\frac{-x_1}{|x_1|}\\ \frac{x_2}{|x_2|}\end{pmatrix}$$

when $|x_1|=|x_2|$. Since

$$\langle\nabla\varphi,\nabla g\rangle_{L^2(C_{R,\beta})} = \langle\nabla\varphi,\nabla g\rangle_{L^2(C^-_{R,\beta})} + \langle\nabla\varphi,\nabla g\rangle_{L^2(C^+_{R,\beta})}, \tag{8.18}$$

Gauß' formula, i.e., integration by parts, gives

$$\langle\nabla\varphi,\nabla g\rangle_{L^2(C^-_{R,\beta})} = \langle\varphi,-\Delta g\rangle_{L^2(C^-_{R,\beta})} + \int_{D_R}\varphi\nabla g\cdot n_-\,dS \tag{8.19}$$

where S is 5-dimensional Hausdorff (surface) measure on D_R. There are no contributions from the other parts of the boundary of $C_{R,\beta}$, since φ vanishes there. Similarly,

$$\langle\nabla\varphi,\nabla g\rangle_{L^2(C^+_{R,\beta})} = \langle\varphi,-\Delta g\rangle_{L^2(C^+_{R,\beta})} + \int_{D_R}\varphi\nabla g\cdot n_+\,dS\,. \tag{8.20}$$

Thus (8.16) will follow once the boundary integrals in (8.19) and (8.20) are non-positive for all $\varphi\ge 0$ and large enough R. By symmetry, it is enough to show this for the boundary integral in (8.19).

Clearly $\nabla g = -e^{-L}\nabla L$. Using $\varphi\ge 0$ and $e^{-L}\ge 0$, one sees that the second term in (8.19) is non-positive as soon as

$$\nabla L\cdot n_- \ge 0 \quad \text{on } D_R\,. \tag{8.21}$$

On $C^-_{R,\beta}$ the function L is given by

$$L(x) = F(|x_1|, |x_2|) - h(|x_1 - x_2|, |x_2|) \tag{8.22}$$

with $h(s, r_2) = s\theta(s^{-\nu}s)$. So

$$\nabla L = \begin{pmatrix} \nabla_{x_1}(F-h) \\ \nabla_{x_2}(F-h) \end{pmatrix} = \begin{pmatrix} \partial_1 F \frac{x_1}{|x_1|} - \partial_s h \frac{x_1 - x_2}{|x_1 - x_2|} \\ \partial_2 F \frac{x_2}{|x_2|} - \partial_2 h \frac{x_2}{|x_2|} - \partial_s h \frac{x_2 - x_1}{|x_1 - x_2|} \end{pmatrix}, \tag{8.23}$$

hence on D_R we have

$$\begin{aligned} \sqrt{2}\nabla L \cdot n_- &= -\partial_1 F + \partial_s h \frac{x_1(x_1 - x_2)}{|x_1||x_1 - x_2|} + \partial_2 F - \partial_2 h - \partial_s h \frac{x_2(x_2 - x_1)}{|x_2||x_1 - x_2|} \\ &= -\partial_1 F + \partial_2 F - \partial_2 h + \partial_s h \frac{x_1(x_1 - x_2) - x_2(x_2 - x_1)}{|x_1||x_1 - x_2|} \end{aligned} \tag{8.24}$$

using also $|x_1| = |x_2|$ on D_R. Since $x_1(x_1 - x_2) - x_2(x_2 - x_1) = x_1^2 - x_2^2 = 0$ on D_R this simplifies to

$$\sqrt{2}\nabla L \cdot n_- = -\partial_1 F + \partial_2 F - \partial_2 h\,. \tag{8.25}$$

Also

$$0 \le \partial_2 h = \partial_2(s\theta(r_2^{-\nu}s)) = -\nu r_2^{\nu-1}(r_2^{-\nu}s)^2\theta'(r_2^{-\nu}s) \lesssim r_2^{\nu-1} \tag{8.26}$$

by our choice of θ. Thus, with $r_1 = |x_1| = |x_2| = r_2$, we get for all large enough r_1

$$\begin{aligned} \sqrt{2}\nabla L \cdot n_- &\ge -\partial_1 F + \partial_2 F - \partial_2 h \ge -F_U'(r_1) - K_1\kappa_1 r_1^{\kappa_1 - 1} + \frac{1}{2} + K_2\kappa_2 r_2^{\kappa_2 - 1} - Cr_1^{\nu-1} \\ &= -\left(\varepsilon + \frac{a^2}{r_1}\right)^{1/2} + \frac{1}{2} - K_1\kappa_1 r_1^{\kappa_1 - 1} + K_2\kappa_2 r_1^{\kappa_2 - 1} - Cr_1^{\nu-1} > 0 \end{aligned}$$

where we used the bound (8.27) below, $r_2 = r_1$ is large, and $0 < \nu, \kappa_1 < \kappa_2 < 1$ uniformly in $0 \le U \le U_c$. If U stays away from zero, we also get $\sqrt{2}\nabla L \cdot n_- \ge 0$ uniformly in U in the range $\mu \le U \le U_c$ for large r_1, any small $\mu > 0$, and $0 < \nu, \kappa_1, \kappa_2 < 1$, using (8.28).

Thus the second term in (8.19), hence by symmetry also the second term in (8.20), is non-positive when R is large enough. ■

Remark 8.7. In the proof above, and also in the proof of Lemma 8.8 below the inequality

$$\sup_{0 \le U \le U_c} \left(\varepsilon_U + \frac{a_U^2}{r_1}\right) \le \frac{1}{4} \tag{8.27}$$

for all large enough r_1 plays an important role. Moreover, we have

$$\limsup_{r_1 \to \infty} \sup_{\mu \le U \le U_c} \left(\varepsilon_U + \frac{a_U^2}{r_1}\right) < \frac{1}{4} \tag{8.28}$$

for any small $\mu > 0$. This can be seen as follows: Since the Coulomb repulsion is positive and the ground state energy of H_0 is $-1/2$ (twice the energy of hydrogen), we clearly have $E_U \ge E_0 = -1/2$, so $\varepsilon_U = -1/4 - E_U \le 1/4$, always. Since E_U is strictly increasing in $0 \le U \le U_c$, by the Hellman-Feynman formula, we also have $\varepsilon_U = -1/4 - E_U < -1/4 - E_{U'} = \varepsilon U' < 1/4$ for any $U > U' > 0$. Since $a_U = (U-1)_+^{1/2}$, this immediately implies (8.28). Moreover, we have

$$\varepsilon_U + \frac{a_U^2}{r_1} = \varepsilon_U \le \frac{1}{4}$$

if $0 \le U \le 1$ and all $r_1 > 0$. Moreover, we know that $U_c \le 2$, so if $1 \le U \le U_c$, we have

$$\varepsilon_U + \frac{a_U^2}{r_1} \le \varepsilon_1 + \frac{1}{r_1} \le \frac{1}{4}$$

for all large enough r_1, independently of $1 \le U \le U_c$, since $\varepsilon_U \le \varepsilon_1 < 1/4$ for $U \ge 1$. This proves (8.27).

Lemma 8.8. *Assume $0 < \beta, \nu < 1$, $0 < \kappa_1 < \kappa_2 < 1$ and $\max(\nu, 1-\nu) < \kappa_2$ and L_U given by (8.4). Then $g_U = e^{-L_U}$ is a classical subsolution of H_U at energy E_U on $C^{\pm}_{R,\beta}$ for all large R independently of $0 \le U \le U_c$.*

Moreover, if $0 < \beta, \nu, \kappa_1, \kappa_2 < 1$, $\max(\nu, 1-\nu) < \kappa_2$, and $0 < \mu < U_c$ then there exists $R > 0$ independent of U in the range $\mu \le U \le U_c$ such that g_U is again a classical subsolution of H_U at energy E_U on $C^{\pm}_{R,\beta}$.

Proof. Again, we abbreviate $g = g_U$, $L = L_U$, and $F = F^U_-$. Clearly, L and hence $g = e^{-L}$ is $\mathcal{C}^2$ on $C^{\pm}_{R,\beta}$ and the derivatives of g up to order two are in $L^2(C^{\pm}_{R,\beta})$ for large enough R. Moreover, we only have to show the pointwise bound $(H_U - E_U)g \le 0$ in $C^-_{R,\beta}$, since by symmetry the same bound then also holds on $C^+_{R,\beta}$.

From $\nabla g = -e^{-L}\nabla L$, one gets

$$-\Delta g = g\left[-|\nabla L|^2 + \Delta L\right] . \tag{8.29}$$

On $C^-_{R,\beta}$ we have $L(x) = F(|x_1|, |x_2|) - h(|x_1 - x_2|, |x_2|)$. Using formula (8.23) for ∇L we have

$$\begin{aligned}
\Delta L &= \nabla_{x_1}\left(\partial_1 F \frac{x_1}{|x_1|} - \partial_s h \frac{x_1 - x_2}{|x_1 - x_2|}\right) \\
&\quad + \nabla_{x_2}\left(\partial_2 F \frac{x_2}{|x_2|} - \partial_2 h \frac{x_2}{|x_2|} - \partial_s h \frac{x_2 - x_1}{|x_1 - x_2|}\right) \\
&= \partial_1^2 F + \partial_1 F \frac{2}{|x_1|} + \partial_2^2 F + \partial_2 F \frac{2}{|x_2|} - \partial_2^2 h - \partial_2 h \frac{2}{|x_2|} - 2\partial_s^2 h \\
&\quad - 2\partial_2\partial_s h \frac{x_2(x_2 - x_1)}{|x_2||x_1 - x_2|} - \partial_s h \frac{4}{|x_1 - x_2|} .
\end{aligned} \tag{8.30}$$

The term $\partial_s h \frac{4}{|x_1 - x_2|}$ will allow us to control the Coulomb repulsion between the electrons. Dropping the positive term $(\partial_s h)^2$ we also get from (8.23)

$$\begin{aligned}
|\nabla L|^2 &= |\nabla_{x_1} L|^2 + |\nabla_{x_2} L|^2 \\
&\ge (\partial_1 F)^2 - 2\partial_s h \partial_1 F \frac{x_1(x_1 - x_2)}{|x_1||x_1 - x_2|} + (\partial_2 F - \partial_2 h)^2 - 2(\partial_2 F - \partial_2 h)\partial_s h \frac{x_2(x_2 - x_1)}{|x_2||x_1 - x_2|}
\end{aligned}$$

hence

$$
\begin{aligned}
\big(H_U - E_U\big)g &= \big(-\Delta - \frac{1}{|x_1|} - \frac{1}{|x_2|} + \frac{U}{|x_1 - x_2|} + \frac{1}{4} + \varepsilon\big)g \\
&\le g\Big[\underbrace{\varepsilon - (\partial_1 F)^2}_{\mathrm{I}} + \underbrace{\frac{1}{4} - (\partial_2 F - \partial_2 h)^2}_{\mathrm{II}} \\
&\qquad + \underbrace{2\partial_s h(\partial_1 F \frac{x_1(x_1 - x_2)}{|x_1||x_1 - x_2|} + (\partial_2 F - \partial_2 h)\frac{x_2(x_2 - x_1)}{|x_2||x_1 - x_2|}}_{\mathrm{III}} \\
&\qquad + \underbrace{\partial_1^2 F + \partial_1 F \frac{2}{|x_1|} - \frac{1}{|x_1|}}_{\mathrm{IV}} + \underbrace{\partial_2^2 F + \partial_2 F \frac{2}{|x_2|} - \frac{1}{|x_2|}}_{\mathrm{V}} \qquad (8.31) \\
&\qquad \underbrace{- \partial_2^2 h - \partial_2 h \frac{2}{|x_2|} - 2\partial_s^2 h}_{\mathrm{VI}} \underbrace{- 2\partial_2 \partial_s h \frac{x_2(x_2 - x_1)}{|x_2||x_1 - x_2|}}_{\mathrm{VII}} \\
&\qquad + \underbrace{\frac{U}{|x_1 - x_2|} - \partial_s h \frac{4}{|x_1 - x_2|}}_{\mathrm{VIII}}\Big].
\end{aligned}
$$

Abbreviating $r_1 = |x_1|, r_2 = |x_2|, s = |x_1 - x_2|$, we have

$$\partial_1 F = F_U'(r_1) + K_1 \kappa_1 r_1^{\kappa_1 - 1},$$

and since $F_U'(r_1) = \big(\varepsilon + a^2/r_1\big)^{1/2} \ge 0$ we have $\varepsilon - (F_U'(r_1))^2 \le 0$. Hence

$$\mathrm{I} \le 0\,.$$

Moreover,

$$
\begin{aligned}
\partial_2 F &= \frac{1}{2} + K_2 \kappa_1 r_2^{\kappa_2 - 1}\,, \\
\partial_2 h &= -\nu r_2^{\nu - 1}(r_2^{-\nu} s)^2 \theta'(r_2^{-\nu} s) \le \nu r_2^{\nu - 1}\,,
\end{aligned}
$$

where the last bound holds since $0 \le t \mapsto t^2|\theta'(t)| \le 1$. Since $\nu < \kappa_2 < 1$, we get

$$
\begin{aligned}
\mathrm{II} &= \big(\frac{1}{2} - \partial_2 F + \partial_2 h\big)\big(\frac{1}{2} + \partial_2 F - \partial_2 h\big) \\
&\le -\big(K_2 \kappa_2 r_2^{\kappa_2 - 1} - \nu r_2^{\nu - 1}\big)\big(1 + K_2 \kappa_2 r_2^{\kappa_2 - 1} - \nu r_2^{\nu - 1}\big) \lesssim -r_2^{\kappa_2 - 1}
\end{aligned}
$$

for $r_2 \gg 1$.

The bound for the third term III is tricky, since neither $\partial_1 F$, $\partial_2 F$ nor $\partial_s h$ go to zero as $r_1, r_2 \to \infty$. We will do this one last and bound the other terms first. Since $\partial_1 F = F_U'(r_1) + K_1 \kappa_1 r_1^{\kappa_1 - 1}$ we get

$$\partial_1^2 F = F_U''(r_1) - K_1 \kappa_1 (1 - \kappa_1) r_1^{\kappa_1 - 2} \le 0\,,$$

since $\kappa_1 < 1$ and $F_U'' \le 0$. Thus

$$\mathrm{IV} \le (2F_U'(r_1) - 1)r_1^{-1} = \left(2\big(\varepsilon + \frac{a^2}{r_1}\big)^{1/2} - 1\right) r_1^{-1} \le 0$$

for $r_1 \gg 1$ because of (8.27). Similarly,

$$\mathrm{V} = K_2 \kappa_2 (\kappa_2 - 1) r_2^{\kappa_2 - 2} + \big(\frac{1}{2} + K_2 \kappa_2 r_2^{\kappa_2 - 1}\big)\frac{2}{r_2} - r_2^{-1} = K_2 \kappa_2 (\kappa_2 + 1) r_2^{\kappa_2 - 2}\,.$$

Moreover, with $t = r_2^{-\nu}s$, we have

$$|\partial_2^2 h| \lesssim r_2^{\nu-2}\big(|t^2|\theta'(t)| + t^3|\theta''(t)|\big) \lesssim r_2^{\nu-2}\,,$$
$$|\partial_s^2 h| = r_2^{-\nu}\big|2\theta'(t) + t\theta''(t)\big| \lesssim r_2^{-\nu}$$

since $\theta'(t)$ and $t\theta''(t)$ are bounded for $t \geq 0$. Thus we get

$$\mathrm{VI} \lesssim r_2^{\nu-2} + r_2^{-\nu}$$

for all $r_2 \gg 1$ and since

$$|\partial_2\partial_s h| = \nu r_2^{-1}\big|2t\theta'(t) + t^2\theta''(t)\big| \lesssim r_2^{-1}$$

we have

$$\mathrm{VII} \lesssim r_2^{-1}\,.$$

For the term VIII which contains the Coulomb repulsion, we have

$$\mathrm{VIII} = \frac{1}{s}\big(U - 4\theta(r_2^{-\nu}s)\big) - 4r_2^{-\nu}\theta'(r_2^{-\nu}s) \leq \frac{1}{s}\big(2 - 4\theta(r_2^{-\nu}s)\big) + 4r_2^{-\nu}\,.$$

Recall that $U \leq U_c \leq 2$. If $r_2^{-\nu}s \leq 1$, we have $\theta(r_2^{-\nu}s) \geq 1/2$, hence also $2 - 4\theta((r_2^{-\nu}s)) \leq 0$. If $r_2^{-\nu}s \geq 1$ we have $s^{-1}(2 - 4\theta(r_2^{-\nu}s)) \leq 2r_2^{-\nu}$. Altogether,

$$\mathrm{VIII} \leq 2r_2^{-\nu} + 4r_2^{-\nu} = 6r_2^{-\nu}$$

for all $r_2 > 0$.

Now we come to the term III, which is the hardest term to bound. Recall that $|\partial_2 h| \lesssim r_2^{\nu-1}$. Moreover, $\partial_s h = \theta(r_2^{\nu}s) + r_2^{-\nu}s\theta'(r_2^{-\nu}s) \geq 0$, so $|\partial_s h| \lesssim 1$. Thus

$$\begin{aligned}\mathrm{III} &= 2\partial_s h\left(\partial_1 F\frac{x_1(x_1-x_2)}{|x_1||x_1-x_2|} + \partial_2 F\frac{x_2(x_2-x_1)}{|x_2||x_1-x_2|}\right) - \partial_s h\partial_2 h\frac{x_2(x_2-x_1)}{|x_2||x_1-x_2|}\\ &\leq 2\partial_s h\left(\partial_1 F\frac{x_1(x_1-x_2)}{|x_1||x_1-x_2|} + \partial_2 F\frac{x_2(x_2-x_1)}{|x_2||x_1-x_2|}\right) + Cr_2^{\nu-1}\,.\end{aligned}$$

Note also

$$x_1(x_1-x_2) = \frac{1}{2}\left(x_1^2 - x_2^2 + |x_1-x_2|^2\right)$$

and

$$x_2(x_2-x_1) = \frac{1}{2}\left(x_2^2 - x_1^2 + |x_1-x_2|^2\right)\,,$$

so with $r_1^2 = x_1^2 \geq r_2^2 = x_2^2$ we have

$$\partial_1 F\frac{x_1(x_1-x_2)}{|x_1||x_1-x_2|} + \partial_2 F\frac{x_2(x_2-x_1)}{|x_2||x_1-x_2|} = \left(\frac{\partial_1 F}{2r_1} - \frac{\partial_2 F}{2r_2}\right)\frac{r_1^2 - r_2^2}{|x_1-x_2|} + \left(\frac{\partial_1 F}{2r_1} + \frac{\partial_2 F}{2r_2}\right)|x_1-x_2|\,.$$

Due to $r_2 \leq r_1$, we have

$$\begin{aligned}\frac{\partial_1 F}{r_1} - \frac{\partial_2 F}{r_2} &= \frac{(\varepsilon + \frac{a^2}{r_1})^{1/2}}{r_1} + K_1\kappa_1 r_1^{\kappa_1-2} - \frac{1}{2r_2} - K_2\kappa_2 r_2^{\kappa_2-2}\\ &\leq r_1^{-1}\left[\left(\varepsilon + \frac{a^2}{r_1}\right)^{1/2} - \frac{1}{2} + K_1\kappa_1 r_1^{\kappa_1-1} - K_2\kappa_2 r_1^{\kappa_2-1}\right] \leq 0\end{aligned}$$

for all large r_1, since $0 < \kappa_1 < \kappa_2 < 1$ and using (8.27), uniformly in $0 \leq U \leq U_c$. If U stays away from zero, we again get $\frac{\partial_1 F}{r_1} - \frac{\partial_2 F}{r_2} \leq 0$ uniformly in U in the range $\mu \leq U \leq U_c$ for large r_1, any small $\mu > 0$ and $0 < \kappa_1, \kappa_2 < 1$, using now (8.28).

Thus with $s = |x_1 - x_2|$ we see that

$$\mathrm{III} \le s\partial_s h \left(\frac{\partial_1 F}{r_1} + \frac{\partial_2 F}{r_2} \right) + C r_2^{\nu-1}$$

for large r_1. Since $\partial_s h = \theta(r_2^{-\nu}s) + r_2^{-\nu}s\theta'(r_2^{-\nu}s) \ge 0$ we have

$$s\partial_s h = r^{\nu}\left((r_2^{-\nu}s)\theta(r_2^{-\nu}s) + (r_2^{-\nu}s)^2\theta'(r_2^{-\nu}s)\right) \lesssim r_2^{\nu}$$

uniformly in $s \ge 0$. Moreover, $\partial_1 F r_1^{-1} \lesssim r_1^{-1} + r_1^{\kappa_1-2}$ and $\partial_2 F r_1^{-1} \lesssim r_2^{-1} + r_2^{\kappa_2-2}$, so we arrive at

$$\mathrm{III} \lesssim r_2^{\nu}\left[r_1^{-1} + r_1^{\kappa_1-2} + r_2^{-1} + r_2^{\kappa_2-2}\right] \lesssim r_2^{\nu-1} + r_2^{\nu+\kappa_1-2} + r_2^{\nu+\kappa_2-2}$$

since $\kappa_1, \kappa_2 < 1$ and $r_2 \le r_1$.

Collecting the above bounds in (8.31) we finally arrive at

$$\begin{aligned}(H_U + E_U)g &\lesssim g\left[-r_2^{\kappa_2-1} + r_2^{\nu-1} + r_2^{\nu+\kappa_1-2} + r_2^{\nu+\kappa_2-2} + r_2^{\kappa_2-2} + r_2^{\nu-2} + r_2^{-\nu} + r_2^{-1}\right] \\ &\le g r_2^{\kappa_2-1}\left[-1 + r_2^{\nu-\kappa_2} + r_2^{\nu+\kappa_1-\kappa_2-1} + r_2^{\nu-1} + r_2^{-1} + r_2^{\nu-1-\kappa_2} + r_2^{1-\nu-\kappa_2} + r_2^{-\kappa_2}\right] \\ &< 0\end{aligned}$$

for all large enough r_2, since $0 < \nu, \kappa_1, \kappa_2 < 1$ and $\max(\nu, 1-\nu) < \kappa_2 < 1$. This proves the lemma. ∎

9. Finite nuclear mass

We can also treat the case of a finite nuclear mass, i.e., avoid the Born-Oppenheimer approximation. The three particle system is described by

$$H_U = \frac{p_1^2}{m} + \frac{p_2^2}{m} + \frac{p_N^2}{M} - \frac{1}{|x_1 - x_N|} - \frac{1}{|x_2 - x_N|} + \frac{U}{|x_1 - x_2|} \tag{9.1}$$

where $p_N = -i\partial_N$ is the momentum of the nucleus, M is its mass and x_N is its position. The other two particles have mass m and their position are given by x_1 respectively x_2 The domain of the operator (9.1) is $\mathcal{D}(H_U) = H^2(\mathbb{R}^6) \otimes H^2(\mathbb{R}^3)$.

Remark 9.1. We do not require the nucleus to be heavy and the other two particles to be light. We only need that the "nucleus" attracts the other two, which repel each other. For example two protons orbiting an electron.

In order to discuss bound states, we need to work in the center–of–mass frame. One way is to choose so-called atomic coordinates. However such a choice of coordinates creates the so–called *Hughes-Eckart terms* [33, Chapter XI.5]. We will therefore use Jacobi-Coordinates instead.

9.1. Jacobi-Coordinates.

We define two sets of coordinates (ξ_i, R_i) with $i \in \{1, 2\}$. The first set is given by

$$\xi_1 := x_1 - x_N\,, \qquad R_1 := \frac{1}{M+m}(Mx_N + mx_1)\,,$$

where R_1 is the center of mass of the electron-nucleus two-particle system. The second set of coordinates is

$$\xi_2 := x_2 - R_1\,, \qquad R_2 := \frac{1}{M+2m}((M+m)R_1 + mx_2)\,.$$

Note that R_2 describes the center of mass of the whole three-particle system. Hence the first set of coordinates describes a system of a nucleus with one electrons. The second

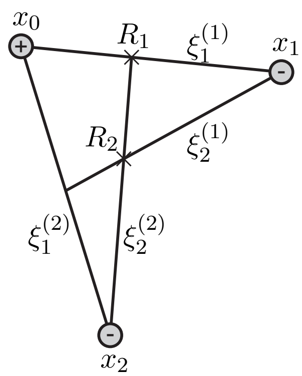

FIGURE 9.1. Jacobi Coordinates for three particle system, where the particles are positioned at x_N, x_1 and x_2. The vectors R_1 and R_2 indicate the center of mass of the two body system $\{x_N, x_1\}$ and the center of mass of the three body system $\{x_N, x_1, x_2\}$, respectively.

pair of coordinates describes a system consisting of a second electron and the compound nucleus-electron system from the first set of coordinates, see Figure 9.1.

In order to obtain the new representation of H_U in the new coordinates we first write the position operators in the new coordinates.

$$x_1 = R_1 + \frac{M}{M+m}\xi_1\,, \quad x_N = R_1 - \frac{m}{M+m}\xi_1\,, \quad x_2 = R_2 + \frac{M+m}{M+2m}\xi_2\,.$$

In these coordinates distances between the particles and the nucleus is given by

$$x_2 - x_1 = \xi_2 - \frac{M}{M+m}\xi_1\,, \qquad x_2 - x_N = \xi_2 + \frac{m}{M+m}\xi_1\,.$$

To write the Hamiltonian H_U in the center-of-mass coordinates, we decompose $L^2(\mathbb{R}^9) = L^2(\mathbb{R}^3) \otimes L^2(\mathbb{R}^6)$ and define a corresponding tensor decomposition

$$\tilde{H} = h_{\mathrm{CM}} \otimes \mathbf{1} + \mathbf{1} \otimes H_{\mathrm{CM}}$$

where the kinetic energy of the center of mass is

$$h_{\mathrm{CM}} = -\left(\frac{2}{m} + \frac{1}{M}\right)^{-1} \Delta_{R_2}\,.$$

The three particle system with the center-of-mass motion removed is given by

$$\tilde{H}_{\mathrm{CM}} = -\frac{1}{\nu_1}\Delta_{\xi_1} - \frac{1}{\nu_2}\Delta_{\xi_2} - \frac{1}{|\xi_1|} - \frac{1}{|\xi_2 + \frac{m}{M+m}\xi_1|} + \frac{U}{|\xi_2 - \frac{M}{M+m}\xi_1|}$$

where $\nu_1 := \left(\frac{1}{m} + \frac{1}{M}\right)^{-1}$ and $\nu_2 := \left(\frac{1}{M+m} + \frac{1}{m}\right)^{-1}$ are the so–called effective masses, see, e.g., [33, Chapter XI.5].

9.2. **Local energy bound.** By fixing the total center of mass $R_2 = a \in \mathbb{R}^3$ the three-body system is completely described by internal degrees of freedom $(\xi_1, \xi_2) \in \mathbb{R}^6$. For simplicity, we can use translation invariance to choose $R_2 = 0$ for the rest of this section.

We want to get similar local energy bounds as in Section 3 in order to get similar isotropic upper bounds as in Section 4. So we need to split $\mathbb{R}^6$, i.e., the internal degrees of freedom, into similar regions. For this note that

$$|x_N - R_2|^2 + |x_1 - R_2|^2 + |x_2 - R_2|^2 \leq 2\left(|\xi_1|^2 + |\xi_2|^2\right)\,.$$

Hence if $|\xi_1|$ and $|\xi_2|$ are small all particles need to be close to the total center of mass.

Next we use the same cut–off functions u and v as in Section 3 so that u, v are infinitely often differentiable, $0 \leq u, v, \leq 1$, $u = 1$ and $v = 0$ on $[0, 1]$, $u = 0$ and $v = 1$ on $[2, \infty)$ and $u^2 + v^2 = 1$. We also define, for large $R_0 > 0$, and $x = (\xi_1, \xi_2)$, the localization functions

$$\chi_a(x) = u\left(|x|/R_0\right), \qquad \text{and} \qquad \overline{\chi}_a(x) = v\left(|x|/R_0\right),$$

so that $\chi_a^2 + \overline{\chi}_a^2 = 1$ and χ_a, $\overline{\chi}_a \in C^\infty(\mathbb{R}^6)$. As before their gradients in $\mathbb{R}^6$ are given by

$$\nabla\chi_a(x) = R_0^{-1} u'(|x|/R_0)\frac{x}{|x|}, \qquad \nabla\overline{\chi}_a(x) = R_0^{-1} v'(|x|/R_0)\frac{x}{|x|}.$$

Therefore

$$\begin{aligned}
|\nabla\chi_a(x)|^2 &\leq R_0^{-2}\|u'\|_\infty^2 \mathbf{1}_{\{R_0 \leq |x| \leq 2R_0\}}, \\
|\nabla\overline{\chi}_a(x)|^2 &\leq R_0^{-2}\|v'\|_\infty^2 \mathbf{1}_{\{R_0 \leq |x| \leq 2R_0\}}.
\end{aligned}$$

Hence we can bound the localization error Loc_1 for this first localization into regions where either both electrons and the nucleus are near to center–of–mass or the complement of this region by

$$\mathrm{Loc}_1(x) \leq C\mathbf{1}_{\{R_0 \leq |x| \leq 2R_0\}} \tag{9.2}$$

where the constant depends on the effective masses ν_1, ν_2. Next we further split the "outside region" corresponding to the support of $\overline{\chi}_a$. Recall, that this is the region where at least one of the particles is far away from the center–of–mass. Obviously one way how this happens is if the electron at x_2 is much further away from the two–particle cluster of a particle at x_1 and the nucleus at x_N with respect to the inter–cluster distance, see Figure 9.1. In the Jacobi–Coordinates above we can easily represent this region. Let $0 < \gamma \leq 1$

$$\chi_b = u\left(|\xi_1|/|\xi_2|^\gamma\right) \qquad \text{and} \qquad \overline{\chi}_b = v\left(|\xi_1|/|\xi_2|^\gamma\right).$$

By our choice of u and v, we have $\chi_b^2 + \overline{\chi}_b^2 = 1$. We again calculate the corresponding localization errors. We start with

$$\begin{aligned}
\nabla_{\xi_1}\chi_b &= u'(|\xi_1|/|\xi_2|^\gamma)\frac{1}{|\xi_2|^\gamma}\frac{\xi_1}{|\xi_1|}, \\
\nabla_{\xi_2}\chi_b &= -\gamma u'(|\xi_1|/|\xi_2|^\gamma)\frac{1}{|\xi_2|^\gamma}\frac{\xi_2}{|\xi_2|},
\end{aligned}$$

and obtain

$$\begin{aligned}
|\nabla_{\xi_1}\chi_b|^2 &\leq \|u'\|_\infty^2 \frac{1}{|\xi_2|^{2\gamma}}\mathbf{1}_{\{|\xi_1| < |\xi_2|^\gamma\}}(x), \\
|\nabla_{\xi_2}\chi_b|^2 &\leq \|u'\|_\infty^2 \frac{1}{|\xi_2|^{2\gamma}}\mathbf{1}_{\{|\xi_1| < |\xi_2|^\gamma\}}(x),
\end{aligned}$$

where the last inequality follows since $0 < \gamma \leq 1$. Similarly we calculate the corresponding gradients for $\overline{\chi}_b$ and arrive at

$$\begin{aligned}
\mathrm{Loc}_2(x) &= C\left(|\nabla_{\xi_1}\chi_b(x)|^2 + |\nabla_{\xi_2}\chi_b(x)|^2 + |\nabla_{\xi_1}\overline{\chi}_b(x)|^2 + |\nabla_{\xi_2}\overline{\chi}_b(x)|^2\right) \\
&\leq C\left(\|u'\|_\infty^2 + \|v'\|_\infty^2\right)\frac{1}{|\xi_2|^{2\gamma}}\mathbf{1}_{\{|\xi_1| < |\xi_2|^\gamma\}}(x)
\end{aligned}$$

where the constant C might change from line to line and depends on the effective masses ν_1, ν_2. Note that on the support of Loc_2 we have $|\xi_1| \leq |\xi_2|^\gamma \ll |\xi_2|$.

Using the IMS localization formula twice, we see that

$$\langle\psi, H_{CM}\psi\rangle = \langle\left(\chi_a^2 + \overline{\chi}_a^2\right)\psi, H_{CM}\psi\rangle = \langle\chi_a\psi, H_{CM}\chi_a\psi\rangle + \langle\overline{\chi}_a\psi, H_{CM}\overline{\chi}_a\psi\rangle - \langle\psi, \mathrm{Loc}_1(x)\psi\rangle$$

$$= \langle \chi_a\psi, (H_{CM} - \mathrm{Loc}_1(x))\, \chi_a\psi\rangle + \langle \chi_b\overline{\chi}_a\psi, (H_{CM} - \mathrm{Loc}_1(x) - \mathrm{Loc}_2(x))\, \chi_b\overline{\chi}_a\psi\rangle$$
$$+ \langle \overline{\chi}_b\overline{\chi}_a\psi, (H_{CM} - \mathrm{Loc}_1(x) - \mathrm{Loc}_2(x))\, \overline{\chi}_b\overline{\chi}_a\psi\rangle \tag{9.3}$$

Summarising, in the spirit of Section 3, we have so far split $\mathbb{R}^6$ into regions where either

1) all particles are close to the center–of–mass,
2) the region where the particle at x_2 is far away from the nucleus with respect to the second particle. This is one part of the *tricky region*,
3) and the rest of the configuration space given by the support of $\overline{\chi}_b\overline{\chi}_a$.

Next we have to identify the remaining part of the full *tricky region* in the support of $\overline{\chi}_b\overline{\chi}_a$. For this we introduce a new set of Jacobi coordinates, which is adapted to the situation where the nucleus and the particle at x_2 stay close to each other and the particle at x_1 might try to escape.

$$\xi_1^{(2)} := x_2 - x_N\,, \quad R_1^{(2)} := \frac{1}{m+M}\,(Mx_N - mx_2)$$

and

$$\xi_2^{(2)} := x_1 - R_1^{(2)}\,, \quad R_2^{(2)} := R_2\,.$$

The center–of–mass does not change since we only rename the two particles with this coordinate transformation. However in the new coordinate system we can now identify the 'tricky region' in the support of $\overline{\chi}_b\overline{\chi}_a$ in the same way as we did in the previous step. We define

$$\chi_c = u\left(|\xi_1^{(2)}|/|\xi_2^{(2)}|^\gamma\right) \quad \text{and} \quad \overline{\chi}_c = v\left(|\xi_1^{(2)}|/|\xi_2^{(2)}|^\gamma\right)\,.$$

Exactly as before we calculate the corresponding localization error to see that

$$\mathrm{Loc}_3(x) \le C\left(\|u'\|_\infty^2 + \|v'\|_\infty^2\right) \frac{1}{|\xi_2^{(2)}|^{2\gamma}}\mathbf{1}_{\{|\xi_1^{(2)}|<|\xi_2^{(2)}|^\gamma\}}(x)$$

where the constant depends on the effective masses ν_1, ν_2. Now note that if R_0 is large enough, the supports of χ_b and χ_c do not overlap, i.e. $\chi_c\overline{\chi}_b = \chi_c$ and $\langle \chi_c\overline{\chi}_a\psi, \chi_b\overline{\chi}_a\psi\rangle = 0$. In particular $\chi_1 := (\chi_b + \chi_c)\,\overline{\chi}_a$ corresponds to the *tricky region* where either the electron at x_1 or the electron at x_2 are far away and the respective other electron is "next" to the nucleus at x_N. We also define $\chi_0 := \chi_a$ and $\chi_2 := \overline{\chi}_c\overline{\chi}_b\overline{\chi}_a$.

Note that the localization functions χ_j for $j = 0, 1, 2$ are invariant under permutation of the particles at x_1 and x_2, so the energy bounds below hold for any choice of statistics of the two particles of mass m. Applying the IMS localization formula once more for the last term in the right hand side of (9.3) one sees

$$\begin{aligned}\langle \psi, H_{CM}\psi\rangle \ge{}& \langle \chi_0\psi, (H_{CM} - \mathrm{Loc}_1(x))\, \chi_0\psi\rangle \\ &+ \langle \chi_1\psi, (H_{CM} - \mathrm{Loc}_1(x) - \mathrm{Loc}_2(x) - \mathrm{Loc}_3(x))\, \chi_1\psi\rangle \\ &+ \langle \chi_2\psi, (H_{CM} - \mathrm{Loc}_1(x) - \mathrm{Loc}_2(x) - \mathrm{Loc}_3(x))\, \chi_2\psi\rangle \\ \ge{}& \sum_{j=0}^{2} \langle \chi_i\psi\, (H_{CM} - \mathrm{Loc}_1(x) - \mathrm{Loc}_2(x) - \mathrm{Loc}_3(x))\, \chi_i\psi\rangle\,.\end{aligned}$$

To find suitable energy bounds in the regions χ_1 and χ_2, we proceed as in Section 3. We start with the support of χ_2, i.e., outside of the *tricky region*. Dropping the kinetic terms as well as the positive Coulomb repulsion between the two electrons and using that

$$\frac{-1}{|x_N - x_1|} = \frac{-1}{|\xi_1|} > \frac{-1}{|\xi|_\infty^\gamma}\,, \qquad \frac{-1}{|x_N - x_2|} = \frac{-1}{|\xi_1^{(2)}|} > \frac{-1}{|\xi|_\infty^\gamma}$$

with

$$|\xi|_\infty^\gamma := \max\left(|\xi_2|^\gamma, |\xi_2^{(2)}|^\gamma\right),$$

we obtain

$$\langle \chi_2\psi, H_{CM}\chi_2\psi\rangle \geq -\langle \chi_2\psi, \frac{2}{|\xi|_\infty^\gamma}\chi_2\psi\rangle\,.$$

Now let $E_{\mathrm{H}}^{\mathrm{CM}}$ denote the re-scaled energy of a hydrogen atom with effective mass $\nu_1 = \frac{Mm}{M+m}$. Then on the support of $\chi_1 := (\chi_b + \chi_c)\,\overline{\chi}_a$ we have for big enough R_0

$$\langle \chi_b\overline{\chi}_a\psi, \left(\frac{1}{\nu_1}\Delta_{\xi_1} - \frac{1}{|\xi_1|}\right)\chi_b\overline{\chi}_a\psi\rangle \geq \langle \chi_b\overline{\chi}_a\psi, E_{\mathrm{H}}^{\mathrm{CM}}\chi_b\overline{\chi}_a\psi\rangle$$

respectively

$$\langle \chi_c\overline{\chi}_a\psi, \left(\frac{1}{\nu_1}\Delta_{\xi_1^{(2)}} - \frac{1}{|\xi_1^{(2)}|}\right)\chi_c\overline{\chi}_a\psi\rangle \geq \langle \chi_c\overline{\chi}_a\psi, E_{\mathrm{H}}^{\mathrm{CM}}\chi_c\overline{\chi}_a\psi\rangle\,.$$

By a calculation similar as the one done in Section 3 to bound the Coulomb potential in the tricky region,

$$-\frac{1}{|\xi_2|} - \frac{1}{|\xi_2 + \frac{m}{M+m}\xi_1|} + \frac{U}{|\xi_2 - \frac{M}{M+m}\xi_1|} \geq \frac{U-1}{|\xi_2|} - \frac{C}{|\xi_2|^{2-\gamma}}$$

for $|\xi_1| \leq 2|\xi_2|^\gamma$ and $|\xi_2| \geq R_0$, the part of the tricky region where the nucleus and the particle at x_1 form a cluster and the particle at x_2 is trying to escape. The constant is given by $C = 4\frac{UM+m}{M+m}$, the precise form is not important, but one should note that it depends on the masses and is bounded for bounded U.

By symmetry, the same bound holds for the system, where the second particle stays close to the nucleus and the first one wants to escape.

Since the supports of χ_b and χ_c are disjoint we obtain

$$\langle \chi_1\psi, H_{CM}\chi_1\psi\rangle \geq \langle \chi_1\psi, \big(E_{\mathrm{H}}^{\mathrm{CM}} + \frac{U-1}{|\xi|_\infty} - \frac{C}{|\xi|_\infty^{2-\gamma}}\big)\chi_1\psi\rangle$$

with $|\xi|_\infty = \max(|\xi_2|, |\xi_2^{(2)}|)$. These estimates are of the same form as the corresponding estimates for the regions A_1 and A_2 in the proof of Theorem 4.1. Hence using now a multiplier of the form $\chi_R e^F$, with suitable F and χ_R smoothly cutting off outside a large ball centered at the total center–of–mass we can again easily derive isotropic subexponential upper bounds for the decay of any eigenfunction of H_{CM} without Born-Oppenheimer approximation *uniformly in the energy* E below, or at the ionization threshold E_H^{CM}.

Theorem 9.2. *If ψ is a bound state for H_{CM} with energy $E \leq E_H^{CM}$ then for any $K > 0$ and $1/6 < \kappa < 1/2$*

$$e^{F_{\mathrm{CM}}}\psi_{\mathrm{CM}} \in L^2(\mathbb{R}^6)$$

where $F_{\mathrm{CM}}(|\xi|_\infty) := 2\sqrt{\frac{(M+m)m}{M+2m}(U-1)_+}\,|\xi|_\infty^{1/2} - K|\xi|_\infty^\kappa$.

Corollary 9.3. *For finite nuclear mass and $U_c > 1$, the Helium–type operator 9.1 has a ground state for critical coupling. The energy of this state is embedded at the edge of the essential spectrum. It is unique, up to a global phase, and can be chosen to be positive.*

Remark 9.4. As for the infinite nuclear mass case, the coupling parameter U is bounded from above when ground states exist. Moreover, a result of Hill [18] shows that (9.1) has a ground state in the center–of–mass frame for some $U > 1$, when the mass ration

$m/M \leq 0.2101$. So $1 < U_c < \infty$ in this case. Furthermore numerical calculations in [26] indicate that even for ratio $m/M = 1$ the critical coupling is still above 1.0848, which covers the case of $e^-e^-e^+$ systems.

Proof of Corollary 9.3. The existence follows from the same argument as in the infinite nuclear mass approximation, by choosing a sequence of couplings $U_n \nearrow U_c$ and using weakly convergent subsequences and a tightness argument, now based on Theorem 9.2. Uniqueness and the other properties of such a ground state follows from the results in [32, Chapter XIII.12]. ∎

Remark 9.5.

- A corresponding anisotropic upper bound as in Section 6 is also possible to prove. The rate function at critical coupling should have the same form
$$F = 2\sqrt{\nu_2(U_c-1)_+}|\xi|_\infty^{1/2} - K_1|\xi|_\infty^{\kappa_1} + \sqrt{E_{\mathrm{H}}^{\mathrm{CM}}\nu_1}|\xi|_0 - K_2|\xi|_0^{\kappa_2}$$
with $|\xi|_\infty = \max(|\xi_2|, |\xi_2^{(2)}|)$ and $|\xi|_0 = \min(|\xi_1|, |\xi_1^{(2)}|)$ and where $K_1, K_2, \kappa_1, \kappa_2$ are choose similarly to Theorem 1.1.
Here $\nu_1 = \frac{Mm}{M+m}$ is the effective mass of the two–particle subsystem and $\nu_2 = \frac{(M+m)m}{M+2m}$ the effective mass of the full three–particle system. Note that $\nu_2|\xi|_\infty/m$ is precisely the distance of the farthest of the two particles with mass m from the total center–of–mass of the three–particle system.
- Finding corresponding lower bounds is a much harder task. The main ideas for lower bounds from Sections and 7 and 8 should still work.

Appendix A. A quadratic form version of the IMS localization formula

In this section we derive the well-known IMS localization formula under rather weak assumptions on the localization functions. Our derivation is motivated by [16] who used quadratic form methods to derive an IMS localization formula for pseudo–relativistic Schrödinger operators under weak assumptions on the localization functions. While we believe that the result for non-relativistic Schrödinger operators is known, at least to the experts, we could not find any reference in the literature for the version we need.

In the following, we consider the momentum operator $P = -i\nabla$ on $\mathbb{R}^d$ and acting in $L^2(\mathbb{R}^d)$ for general $d \in \mathbb{N}$. The domain of P is the Sobolev space $\mathcal{D}(P) = H^1(\mathbb{R}^d) = H^1$. The kinetic energy is given by the the quadratic form $\langle P\varphi, P\varphi\rangle$, which is a closed quadratic form on $\mathcal{D}(P)$. In order to be able to even formulate the IMS localization formula, on needs to have weight functions $\xi : \mathbb{R}^d \to \mathbb{R}$ such that $\xi^2\varphi, \xi\varphi \in \mathcal{D}(P)$ for any $\varphi \in \mathcal{D}(P)$.

Lemma A.1. *Assume that $\xi : \mathbb{R}^d \to \mathbb{R}$ is bounded and continuous and there exist $k \in \mathbb{N}$ and pairwise disjoint open sets U_j, $j = 1, \dots, k$ with Lipshitz boundary, such that $\mathbb{R}^d = \cup_j \overline{U_j}$ and*
$$\xi\big|_{U_j} \in W^{1,\infty}(U_j) \quad \text{for all } j = 1, \dots, k \tag{A.1}$$
that is, the weak derivative $\nabla\xi$ is bounded on each U_j, $j = 1, \dots, k$. Then for all $\varphi \in \mathcal{D}(P)$ we have $\xi^2\varphi, \xi\varphi \in \mathcal{D}(P)$, that is, as multiplication operators ξ^2 and ξ map $\mathcal{D}(P)$ into itself.

Proof. First, we show that the weak derivative of ξ exists and is given by the function $\widetilde{\nabla\xi}$ defined by $\widetilde{\nabla\xi} := \nabla\xi$ on U_j and $\widetilde{\nabla\xi}(x) := 0$ if $x \notin \cup_j U_j$. Of course, we can set $\widetilde{\nabla\xi}(x)$ equal to an arbitrary fixed vector in $\mathbb{R}^d$ for $x \notin \cup_j U_j$.

Since the boundary ∂U_j is Lipshitz regular it has zero d-dimensional Lebesgue measure. By definition of the distributional derivative, we get

$$\langle \nabla \xi, \varphi\rangle = -\langle \xi, \nabla\varphi\rangle = -\sum_{j=1}^k \int_{U_j} \overline{\xi}\nabla\varphi \,\mathrm{d}x = \sum_{j=1}^k \left(\int_{U_j} \overline{\nabla\xi}\varphi\, dx - \int_{\partial U_j} \overline{\xi}\varphi\nu_j \mathrm{d}H^{d-1}\right) \tag{A.2}$$

for any test function $\varphi \in \mathcal{C}_0^\infty(\mathbb{R}^d)$, where the last equality follows from the weak form of Gauß's theorem, see [5, Theorem A6.8] or [13, Theorem 1 in Chapter 5.8], H^{d-1} is $d-1$ dimensional Hausdorff measure, and ν_j is the outer normal, which is well defined H^{d-1} almost everywhere on ∂U_j, see [5, Section 6.5] or [13, Section 5.1].

Since in the sum over j each part of the boundaries ∂U_j comes in pairs with *opposite* direction of their corresponding normals and the integrand $\overline{\xi}\varphi$ is the same on each of these pairs, we have

$$\sum_{j=1}^k \int_{\partial U_j} \overline{\xi}\varphi\nu_j \mathrm{d}H^{d-1} = 0\,. \tag{A.3}$$

Thus

$$-\langle \xi, \nabla\varphi\rangle = \sum_{j=1}^k \int_{U_j} \overline{\nabla\xi}\varphi\, dx = \langle \widetilde{\nabla\xi}, \varphi\rangle \tag{A.4}$$

for any test function $\varphi \in \mathcal{C}_0^\infty(\mathbb{R}^d)$, so $\xi \in W^{1,\infty}(\mathbb{R}^d)$.

Now we check that $\xi : \mathcal{D}(P) \to \mathcal{D}(P)$: Clearly, since ξ is bounded, $\|\xi\varphi\| \le \|\xi\|_\infty \|\varphi\|$. Since ξ has weak derivative in $W^{1,\infty}$ we have

$$\nabla(\xi\varphi) = (\nabla\xi)\varphi + \xi\nabla\varphi \tag{A.5}$$

for all $\varphi \in \mathcal{D}(P)$. Thus

$$\begin{aligned}\|P(\xi\varphi)\| &\le \|(\nabla\xi)\varphi\| + \|\xi P\varphi\| \le \|\nabla\xi\|_\infty\|\varphi\| + \|\xi\|_\infty\|P\varphi\| \\ &\le (\|\nabla\xi\|_\infty + \|\xi\|_\infty)\|\varphi\|_{H^1}\end{aligned}$$

which shows that the multiplication operator $\xi : \mathcal{D}(P) \to \mathcal{D}(P)$ is bounded.

This argument shows also that $\xi^2 : \mathcal{D}(P) \to \mathcal{D}(P)$ is bounded, since replacing ξ by ξ^2 in the argument leading to (A.4) shows $\xi^2 \in W^{1,\infty}(\mathbb{R}^d)$ as soon as ξ is bounded and continuous, with bounded weak derivatives on U_j, since on each component U_j we clearly have $\nabla(\xi^2) = 2\xi\nabla\xi \in W^{1,\infty}(U_j)$. Thus, by what we already proved, $\xi^2 \in W^{1,\infty}(\mathbb{R}^d)$ and $\xi^2 : \mathcal{D}(P) \to \mathcal{D}(P)$ is bounded. ∎

Remark A.2. As the proof shows, the continuity assumption on ξ can be weakened to ξ is continuous in a neighborhood of the boundary set $\cup_j \partial U_j$ and this can also be further weakened using the appropriate notion of traces, see, e.g., [5, Section A.6]. Furthermore, the natural regularity assumption on the boundary of U_j is that U_j has locally finite perimeter, see [13, Chapter 5], so that a suitable integration–by–parts formula holds.

Our version of the famous IMS localization formula is

Lemma A.3 (IMS localization formula, quadratic form version)**.** *Let $\xi : \mathbb{R}^d \to \mathbb{R}$ be bounded and continuous and assume that there exist $k \in \mathbb{N}$ and pairwise disjoint open sets U_j, $j = 1, \ldots, k$ with a Lipshitz boundary, such that $\mathbb{R}^d = \cup_j \overline{U_j}$ and*

$$\xi\big|_{U_j} \in W^{1,\infty}(U_j) \quad \textit{for all } j = 1, \ldots, k\,. \tag{A.6}$$

Then for all $\varphi \in \mathcal{D}(P) = H^1(\mathbb{R}^d)$ *we have*

$$\mathrm{Re}\langle \nabla(\xi^2\varphi), \nabla\varphi\rangle = \langle \nabla(\xi\varphi), \nabla(\xi\varphi)\rangle - \langle \varphi, |\nabla\xi|^2\varphi\rangle\,. \tag{A.7}$$

In particular, for a Schrödinger operator $H = P^2 + V$*, defined in the sense of quadratic forms with a local potential* V*, we have*

$$\mathrm{Re}\langle \xi^2\varphi, H\varphi\rangle = \langle \xi\varphi, H\xi\varphi\rangle - \langle \varphi, |\nabla\xi|^2\varphi\rangle\,. \tag{A.8}$$

Remark A.4. A natural choice for ξ is $\xi^2 = 1 = \sum_j \chi_j^2$ for suitable "partition of unity" given by cut–off functions χ_j. A second choice, which is useful to derive weighted L^2 bounds, is given by an exponentially weighted function $\xi = \chi e^F$ for some (bounded) function F. Our version of the IMS localization formula allows us to have rather minimal, weak regularity properties on the involved functions χ_j, χ, and F, which is very convenient for the proof of our upper bounds.

Proof. Lemma A.1 shows that $\xi^2\varphi$ and $\xi\varphi$ are in $H^1(\mathbb{R}^d)$ as soon as φ is. So both sides of (A.7) are well defined. Given $\varphi \in H^1$ and using that ξ is real-valued, a short calculation reveals

$$\begin{aligned}
\mathrm{Re}\langle \nabla(\xi^2\varphi), \nabla\varphi\rangle &= \mathrm{Re}\langle \xi\nabla(\xi\varphi) + (\nabla\xi)\xi\varphi, \nabla\varphi\rangle = \mathrm{Re}\langle \nabla(\xi\varphi), \xi\nabla\varphi\rangle + \mathrm{Re}\langle (\nabla\xi)\varphi, \xi\nabla\varphi\rangle \\
&= \mathrm{Re}\langle \nabla(\xi\varphi), \nabla(\xi\varphi) - (\nabla\xi)\varphi\rangle + \mathrm{Re}\langle (\nabla\xi)\varphi, \xi\nabla\varphi\rangle \\
&= \langle \nabla(\xi\varphi), \nabla(\xi\varphi)\rangle - \mathrm{Re}\langle (\nabla\xi)\varphi + \xi\nabla\varphi, (\nabla\xi)\varphi\rangle + \mathrm{Re}\langle (\nabla\xi)\varphi, \xi\nabla\varphi\rangle \\
&= \langle \nabla(\xi\varphi), \nabla(\xi\varphi)\rangle - \langle (\nabla\xi)\varphi, (\nabla\xi)\varphi\rangle
\end{aligned}$$

since also $\mathrm{Re}\langle (\nabla\xi)\varphi, \xi\nabla\varphi\rangle = \mathrm{Re}\langle \xi\nabla\varphi, (\nabla\xi)\varphi\rangle$. Thus (A.7) holds.

The formula (A.8) follows immediately from (A.7) since the potential V is a local multiplication operator, hence we have $\langle \xi^2\varphi, V\varphi\rangle = \langle \xi\varphi, V\xi\varphi\rangle$ for the quadratic form. ∎

Appendix B. Sub– and supersolution bounds a la Agmon

Let $H = -\Delta + V$ be a Schrödinger operator defined by the quadratic form

$$\langle \varphi, H\psi\rangle := \langle \nabla\varphi, \nabla\psi\rangle + \langle \varphi, V\psi\rangle \tag{B.1}$$

for $\varphi, \psi \in H^1(\mathbb{R}^d)$ and an infinitesimally form small perturbation by a real-valued function V. Here we define $\langle \varphi, V\psi\rangle = \langle \mathrm{sgn}(V)|V|^{1/2}\varphi, |V|^{1/2}\psi\rangle$ where $\mathrm{sgn}(t) = t/|t|$ when $t \neq 0$ and $\mathrm{sgn}(0) := 0$.

Definition B.1 (Sub– and supersolutions in the quadratic form sense a la Agmon)**.** Let Ω be an open subset of $\mathbb{R}^d$. Then a real-valued function $\psi \in H^1_{\mathrm{loc}}(\Omega)$ is a *supersolution* of H at energy $E \in \mathbb{R}$ in Ω if

$$\langle \varphi, (H - E)\psi\rangle \geq 0 \tag{B.2}$$

and ψ is a *subsolution* if

$$\langle \varphi, (H - E)\psi\rangle \leq 0 \tag{B.3}$$

for all non-negative $\varphi \in \mathcal{C}_0^\infty(\Omega)$.

For our slight extension of a beautiful result of Agmon [2] we need one more notation.

Definition B.2. Let $\Omega \subset \mathbb{R}^d$ be an open set with boundary $\partial\Omega$. We call a closed set $\widetilde{\partial\Omega}$ an (inner) boundary layer of Ω if it is a subset of the closure of Ω which contains the boundary $\partial\Omega$ of Ω in such a way that $\Omega \setminus \widetilde{\partial\Omega}$ has locally positive distance from the boundary $\partial\Omega$. More precisely, for any compact set $K \subset \mathbb{R}^d$ we have

$$\mathrm{dist}(\partial\Omega, (K \cap \Omega) \setminus \widetilde{\partial\Omega}) > 0\,. \tag{B.4}$$

In other words, a boundary layer $\widetilde{\partial\Omega}$ provides locally a safety distance to the boundary: For any $R > 0$ there exist $\delta > 0$ such that

$$\operatorname{dist}(x, \partial\Omega) \geq \delta$$

uniformly in $x \in \Omega \setminus \widetilde{\partial\Omega}$ with $|x| \leq R$.

Theorem B.3. *Let Ω be an open subset of $\mathbb{R}^d$, f a positive supersolution and g a subsolution of H at energy E in Ω. Assume that for some $\lambda > 1$*

$$\liminf_{L\to\infty} L^{-2} \int_{\Omega\cap\{L\leq|x|\leq\lambda L\}} g_+^2 \, dx = 0 \tag{B.5}$$

where $g_+ = \sup(g, 0)$ is the positive part of g, and

$$f \geq g \quad \text{for (almost) all } x \in \widetilde{\partial\Omega} \tag{B.6}$$

where $\widetilde{\partial\Omega}$ is an (inner) boundary layer of Ω. Then $f \geq g$ almost everywhere in Ω.

Remark B.4. We would like to stress that this is basically Theorem 2.7 in [2]. It is a slight extension of Agmon's result, since he considers neighborhoods of infinity, i.e., complements of compact subsets of $\mathbb{R}^d$. We need to work with more general unbounded domains which contain infinity but are not necessarily neighborhoods of infinity.

Proof. We give a sketch of the proof, for the convenience of the reader. Since f is a positive supersolution and g is a subsolution in Ω, the function

$$u \coloneqq (g - f)_+ \tag{B.7}$$

is a subsolution of H at energy E in Ω, see [2, 2.9 Lemma] whose proof also shows that one only needs $V \in L^1_{\mathrm{loc}}(\mathbb{R}^d)$ for this. So for any real-valued $\xi \in \mathcal{C}_0^\infty(\Omega)$ we can choose $\varphi = \xi^2 u$ as a testfunction in the IMS localization formula (A.7) to get

$$\langle \xi u, (H - E)\xi u\rangle - \langle u, |\nabla\xi|^2 u\rangle = \operatorname{Re}\langle \xi^2 u, (H - E)u\rangle = \langle \xi^2 u, (H - E)u\rangle \leq 0\,.$$

That is, we have

$$\langle \xi u, (H - E)\xi u\rangle \leq \langle u, |\nabla\xi|^2 u\rangle \quad \text{for all } \xi \in \mathcal{C}_0^\infty(\Omega)\,. \tag{B.8}$$

Extend u by zero to Ω^c, by a slight abuse of notation, we continue to use u for this extension. Since u vanishes on the boundary layer $\widetilde{\partial\Omega}$, i.e, within a safety–distance to the boundary $\partial\Omega$, this extension of u is in the Sobolev space $H^1(\mathbb{R}^d)$. Moreover, thanks to u being zero on the boundary layer $\widetilde{\partial\Omega}$, it is easy to see that (B.8) continues to hold for all real-valued $\xi \in \mathcal{C}_0^\infty(\mathbb{R}^d)$, since the both sides of the inequality (B.8) depend only on the values of ξ on the support of u. So

$$\langle \xi u, (H - E)\xi u\rangle \leq \langle u, |\nabla\xi|^2 u\rangle \quad \text{for all } \xi \in \mathcal{C}^\infty(\mathbb{R}^d)\,. \tag{B.9}$$

By assumption, $f > 0$ is a supersolution of H at energy E in Ω. Thus for any real-valued $\xi \in \mathcal{C}_0^\infty(\mathbb{R}^d)$ we can choose $\varphi = \rho^2 f$, with $\rho = \xi u/f$, as a positive test function with support in Ω to get, from the definition of a supersolution,

$$0 \leq \langle \varphi, (H - E)f\rangle = \langle \rho^2 f, (H - E)f\rangle = \langle \xi u, (H - E)\xi u\rangle - \langle f, \big|\nabla\big(\frac{\xi u}{f}\big)\big|^2 f\rangle \tag{B.10}$$

where we again used the IMS localization formula. Together with (B.9) this yields

$$\langle f, \Big|\nabla\Big(\frac{\xi u}{f}\Big)\Big|^2 f\rangle \leq \langle u, |\nabla\xi|^2 u\rangle \quad \text{for all } \xi \in \mathcal{C}^\infty(\mathbb{R}^d)\,. \tag{B.11}$$

Now pick $\chi \in \mathcal{C}_0^\infty(\mathbb{R}^d)$ with $0 \le \chi \le 1$, $\chi(x) = 1$ for $|x| \le 1$, $\chi(x) = 0$ for $|x| \ge 2$, and use the scaled version $\xi(x) = \xi_L(x) = \chi(x/L)$ in (B.11). Since $\xi_L \to 1$ pointwise as $L \to \infty$, Fatou's lemma and (B.11) imply

$$\begin{aligned}\langle f, \left|\nabla\Big(\frac{u}{f}\Big)\right|^2 f\rangle &\le \liminf_{L\to\infty} \langle f, \left|\nabla\big(\frac{\xi_L u}{f}\big)\right|^2 f\rangle \le \liminf_{L\to\infty} \langle u, |\nabla \xi_L|^2 u\rangle \\ &\le \liminf_{L\to\infty} \int_\Omega |\nabla \xi_L|^2 g_+^2 \, dx = 0\end{aligned} \tag{B.12}$$

where in the second inequality we used $u = (g-f)_+ \le g_+$, which follows from $f > 0$ in Ω. The last equality in (B.12) is due to the bound $\nabla \xi_L \le \|\nabla \chi\|_\infty^2 L^{-2} \mathbf{1}_{\{L \le |x| \le \lambda L\}}$ and assumption (B.5).

Clearly, (B.12) implies that $u = cf$ in Ω for some constant c. Since $f > 0$ in Ω and $u = 0$ on the boundary layer $\widetilde{\partial\Omega}$, we must have $c = 0$. Thus $u = (g-f)_+ = 0$ almost everywhere in Ω, which proves the lemma. ∎

Appendix C. A tightness argument

In this section we show how one can prove a simple tightness argument for weakly convergent sequences in $L^2(\mathbb{R}^d)$ from [23]. Of course, such results are well-known using, for example, the locally compact embedding of the Sobolev space H^1 into suitable L^p spaces. Our point is that one can work with a pure L^2–space version. The tightness argument we use is based on the following equivalence.

Theorem C.1. ([23]) *Let $(\psi_n)_{n\in\mathbb{N}}$ be a sequence in $L^2(\mathbb{R}^d)$ and $(\widehat{\psi}_n)_{n\in\mathbb{N}}$ the sequence of Fourier transforms. Then the following are equivalent.*

1) *The sequence $(\psi_n)_{n\in\mathbb{N}}$ is converging strongly,*
2) *The sequence $(\psi_n)_{n\in\mathbb{N}}$ is converging weakly and satisfies*

$$\lim_{R\to\infty} \limsup_{n\to\infty} \int_{|x|>R} |\psi_n(x)|^2 \, dx = 0\,, \tag{C.1}$$

$$\lim_{L\to\infty} \limsup_{n\to\infty} \int_{|k|>L} |\hat{\psi}_n(k)|^2 \, dk = 0\,, \tag{C.2}$$

3) *The sequence $(\psi_n)_{n\in\mathbb{N}}$ is converging weakly and there exist functions $H, F \ge 0$ with $\lim_{|x|\to\infty} H(x) = \infty = \lim_{|k|\to\infty} F(k)$ such that*

$$\limsup_{n\to\infty} \int_{\mathbb{R}^d} H(x) |\psi_n(x)|^2 \, dx < \infty\,, \tag{C.3}$$

$$\limsup_{n\to\infty} \int_{\mathbb{R}^d} F(k) |\hat{\psi}_n(k)|^2 \, dk < \infty\,. \tag{C.4}$$

Remark C.2. It is straightforward to see that conditions (C.1) and (C.3), respectively, conditions (C.2) and (C.4), are equivalent.

Proof. For the convenience of the reader, we give a sketch of the proof. The equivalence of part 1 and 2 of Theorem C.1 was already shown in [23]. The easy argument is as follows: It is clear that part 1 implies part 2. For the converse assume that ψ_n converges weakly to zero in L^2, without loss of generality. Let $P_L = \mathbf{1}_{\{|P|\le L\}}$ be a Fourier cutoff onto momenta $|\eta| \le L$ in Fourier space and $Q_R = \mathbf{1}_{\{|x|\le R\}}$ be a cutoff in x-space. Then it is easy to see that $P_L Q_R$ has a square integrable kernel, i.e., it is a Hilbert–Schmidt operator on L^2, hence compact, [37]. Since

$$\psi_n = P_L\psi_n + (1-P_L)\psi_n = P_L Q_R \psi_n + P_L(1-Q_R)\psi_n + (1-P_L)\psi_n$$

and P_L is an orthogonal projection we get

$$\limsup_{n\to\infty} \|\psi_n\| \le \limsup_{n\to\infty} \|(1-Q_R)\psi_n\| + \limsup_{n\to\infty} \|(1-P_L)\psi_n\| \tag{C.5}$$

using that $\lim_{n\to\infty} \|P_L Q_R \psi_n\| = 0$, by compactness of $P_L Q_R$ for all fixed L, R. Now simply note that the two terms on the right hand side of (C.5) go to zero as $R, L \to \infty$ due to (C.1), respectively (C.2).

Clearly part 3 implies part 2 using the Chebycheff–Markov inequality. For the converse assume that (C.3) holds and take an increasing sequence of radii $R_k \to \infty$ with

$$\limsup_{n\to\infty} \int_{|x|>R_k} |\psi_n(x)|^2 \mathrm{d}x \le 2^{-2k} \tag{C.6}$$

for all $k \in \mathbb{N}$. Setting

$$H(x) = \sum_{k:R_k<|x|}^{\infty} 2^k \tag{C.7}$$

we get

$$\limsup_{n\to\infty} \int H(x)|\psi_n(x)|^2\, dx \le \sum_{k=0}^{\infty} 2^k \limsup_{n\to\infty} \int_{|x|>R_k} |\psi_n(x)|^2\, dx \le \sum_{k=0}^{\infty} 2^{-k} = 1.$$

i.e., (C.3) holds. Similarly one shows that (C.2) implies (C.4). ■

Appendix D. Basic properties of the ground state

In this appendix we gather some basic properties of the ground state and the ground state energy. We call $E_U = \inf \sigma(H_U)$ the ground state energy, although, technically, it is only the ground state energy when a ground state exists.

A result of Lieb [29], based on a clever idea of Benguria, but now applied for the case that the electron–electron repulsion term contains a coupling constant U, shows that a single atom with nuclear charge Z can only bind

$$N < \frac{2Z}{U} + 1 \tag{D.1}$$

particles, independent of the statistics of the particles. That is, if the ground state energy is strictly below the essential spectrum, then (D.1) holds. For $N = 2$ and $Z = 1$ this shows that $E_U < -1/4 = \sigma_{\mathrm{ess}}(H_U)$ implies $U < 2$. Thus, for the operator given by (1.1), the critical coupling U_c is bounded by

$$1 < U_c \le 2\,. \tag{D.2}$$

These simple rigorous bounds give are rough, but not bad, estimate for the critical coupling U_c. As discussed in the introduction, calculations by quantum chemists predict $U_c \sim 1.09766$. Moreover, Hill showed that even for finite nuclear mass M the Hamiltonian (9.1) has a ground state in the center–of–mass frame for some $U > 1$ as long as the mass ration $m/M \le 0.2101$. Also Lieb's argument, with some less explicit constants carries over to the case of an atom with finite nuclear mass. So $1 < U_c < \infty$ also in this case.

To not be puzzled by the numbers in the proposition below, we want to emphazise that for infinite nuclear mass, we scaled the mass m of the light particles out, putting them to $m = 1/2$, see the easy scaling argument in the beginning of the introduction. Without the Born-Oppenheimer we do not scale out the mass m of the two particles and denote the mass of the nucleus by M.

Proposition D.1. *Given a helium-type operator H_U, with infinite nuclear mass, or with finite nuclear mass in the center of mass frame, let $E_U = \inf\sigma(H_U)$ be its ground state energy. Then*

1) *$U \mapsto E_U$ is concave and continuous. It is strictly increasing on $[0, U_c]$, constant on $[U_c, \infty)$, and*

$$E_U < -\frac{1}{4} \quad \text{for } 0 \le U < U_c, \quad E_{U_c} = -\frac{1}{4} \quad (\textit{infinite nuclear mass}), \tag{D.3}$$

$$E_U < -\frac{Mm}{2(M+m)} \text{ for } 0 \le U < U_c,\ E_{U_c} = -\frac{Mm}{2(M+m)} \ (\textit{finite nuclear mass}). \tag{D.4}$$

Moreover, E_U is differentiable in $U < U_c$ with a positive derivative. At U_c its left derivative exists and is positive.

2) *At critical coupling the energy $E_{U_c} = -1/4$ (infinite nuclear mass), respectively, $E_{U_c} = -\frac{Mm}{2(M+m)}$ (finite nuclear mass) is a simple eigenvalue at the edge of the essential spectrum. The corresponding ground state $\psi_c = \psi_{U_c} \in L^2$ is unique and positive up to a global phase factor.*

3) *Choosing all ground states ψ_U for $0 \le U \le U_c$ normalized, there exist constant $C < \infty$ such that for any $2 \le p \le \infty$ we have*

$$\sup_{0 \le U \le U_c} \|\psi_U\|_p \le C\,. \tag{D.5}$$

Moreover, the map $[0, U_c] \ni U \mapsto \psi_U$ is continuous in L^p for all $2 \le p \le \infty$.

4) *For any compact set $K \subset \mathbb{R}^6$ (or the center of mass frame) there exists a constant $C_K > 0$ such that*

$$\inf_{0 \le U \le U_c} \inf_{x \in K} \psi_U(x) \ge C_K\,. \tag{D.6}$$

Proof. Let H_0 be the operator H_U with $U = 0$. Since $H_U = H_0 + \frac{U}{|x_1 - x_2|}$ is linear in the perturbation, one sees that $E_U = \inf_{\|\psi\|=1}\langle\psi, H_U\psi\rangle$ is an infimum of linear functions, hence concave. Since $-\infty < E_U < \infty$ for all $U \in \mathbb{R}$, it is continuous.

At critical coupling and above, the energy E_U is equal to the infimum of the essential spectrum, which by the HVZ theorem is given by the ground state energy of hydrogen. This gives the values for E_U for finite nuclear mass and in the infinite nuclear mass limit when $U \ge U_c$.

When $U < U_c$, perturbation theory [32] applies. First order perturbation theory, the so-called Feynman–Hellmann formula, shows

$$\partial_U E_U = \langle\psi_U, \frac{dH_U}{dU}\psi_U\rangle = \langle\psi_U, \frac{1}{|x_1 - x_2|}\psi_U\rangle > 0 \tag{D.7}$$

for all $U < U_c$. Moreover, this formula also holds, as soon as a normalizable ground ψ_U state exists, for critical coupling $U = U_c$, when one replaces the derivative $\partial_U E_U$ with the left derivative $\partial_U^- E_U = \lim_{U \nearrow U_c} \frac{E_U - E_{U_c}}{U - U_c}$, see [35]. This prove claim 1.

The Coulomb potential V_U is in the so–called Kato–class, for a definition see [4, 10, 36], for any coupling $U \in \mathbb{R}$. Moreover, $V_U \ge V_0$ for all $U \ge 0$, so [36, Theorem B.1.1] and monotonicity of the Schrödinger semigroup in the potential gives

$$\|\psi_U\|_p = \|\mathrm{e}^{tE_U} e^{-tH_U}\psi_U\|_p \le e^{tE_U}\|e^{-tH_U}\|_{2\to p}\|\psi_U\| \le e^{tE_U}\|e^{-tH_0}\|_{2\to p}\|\psi_U\|\,.$$

So for fixed $t > 0$ and with $C_p = e^{tE_U}\|e^{-tH_0}\|_{2\to p}$ we have $\|\psi_U\|_p \le C_p\|\psi_U\|$ for all $2 \le p \le \infty$. The Riesz–Thorin interpolation theorem also shows $C_p \le C_2^{\Theta} C_\infty^{1-\Theta}$ for any

$1/p = \Theta/2 + (1-\Theta)/\infty = \Theta/2$ and $0 \le \Theta \le 1$. Hence $C_p \le \max(C_2, C_\infty) =: C$ and we arrive at

$$\sup_{0\le U<U_c} \|\psi_U\|_p \le C \tag{D.8}$$

when $\|\psi_U\| = 1$ for $0 \le U < U_c$.

Take a sequence $1 < U_n < U_c$ which converges monotonically to U_c and consider the corresponding sequence of normalized bound states ψ_n of $H_n = H_{U_n}$ with energies $E_n < -1/4$. The Coulomb potential V_U is relatively form bounded with respect to the Laplacian $-\Delta$ in $\mathbb{R}^6$ with relative form bound zero, thus

$$|\langle\psi, V_U\psi\rangle| \le a\|\nabla\psi\|^2 + b\|\psi\|^2$$

for some constants $0 < a < 1$ and $b > 0$ uniformly in $0 \le U \le U_c$ for all $\psi \in H^1(\mathbb{R}^6)$. So for ψ_n we get

$$E_n = \langle\psi_n, H_n\psi_n\rangle = \langle\nabla\psi_n, \nabla\psi_n\rangle + \langle\psi_n, V_U\psi_n\rangle \ge (1-a)\|\nabla\psi_n\|^2 - b\|\psi_n\|^2$$

which implies

$$\|\nabla\psi_n\|^2 \le \frac{b}{1-a}\|\psi_n\|^2$$

since the energy E_n of the minimizing sequence is bounded. So

$$\|\psi_n\|^2_{H^1(\mathbb{R}^6)} = \|(1-\Delta)^{1/2}\psi_n\|^2 \le \frac{b}{1-a}\|\psi_n\|^2 + \|\psi_n\|^2 \le \frac{b+1}{1-a} < \infty$$

uniformly in $n \in \mathbb{N}$, since ψ_n is normalized. Thus the sequence ψ_n is bounded in H^1, hence there exists a subsequence, which we also denote by ψ_n, which converges weakly to some $\psi_c \in H^1(\mathbb{R}^6)$. We claim that ψ_c is a normalized ground state of H_{U_c}, i.e., $\|\psi_c\| = 1$, $\psi_c \in H^1(\mathbb{R}^6)$, and $\langle\varphi, H_{U_c}\psi_c\rangle = -1/4\langle\varphi, \psi_c\rangle$ for all $\varphi \in H^1(\mathbb{R}^6)$.

Since ψ_n is a bounded sequence in $H^1(\mathbb{R}^6)$ it is tight in momentum space,

$$\lim_{L\to\infty} \sup_{n\in\mathbb{N}} \int_{|\eta|\ge L} |\widehat{\psi_n}|^2 \mathrm{d}\eta = 0\,. \tag{D.9}$$

Moreover, the upper bound from Theorem 4.1, which only needs the bound (D.8) for $\psi_n = \psi_{U_n}$ with subcritical $U_n < U_c$, easily implies also tightness of the sequence ψ_n in position space,

$$\lim_{R\to\infty} \sup_{n\in\mathbb{N}} \int_{|\eta|\ge L} |\psi_n|^2 \mathrm{d}\eta = 0 \tag{D.10}$$

and standard compactness results, for example Theorem C.1, show that ψ_n converges to ψ_c strongly in $L^2(\mathbb{R}^6)$, so $\|\psi_c\| = \lim_{n\to\infty} \|\psi_n\| = 1$.

Weak lower semicontinuity of the H^1-norm implies $\|\psi_c\|_{H^1} \le \liminf_{n\to\infty} \|\psi_n\|_{H^1}$. Hence the strong L^2 convergence of ψ_n implies lower semicontinuity of the kinetic energy,

$$\langle\nabla\psi_c, \nabla\psi_c\rangle \le \liminf_{n\to\infty} \langle\nabla\psi_n, \nabla\psi_n\rangle \tag{D.11}$$

where ∇ is the gradient in $\mathbb{R}^6$.

One easily checks that strong convergence in L^2 and boundedness in H^1 of ψ_n imply $\langle\psi_c, V_{U_c}\psi_c\rangle = \lim_{n\to\infty}\langle\psi_n V_{U_n}\psi_n\rangle$ which together with (D.11) shows

$$-\frac{1}{4} \le \langle\psi_c, H_{U_c}\psi_c\rangle \le \liminf_{n\to\infty} \langle\psi_n, H_{U_n}\psi_n\rangle = -\frac{1}{4}\,. \tag{D.12}$$

where we also used that ψ_c is normalized and $H_{U_c} \ge -\frac{1}{4}$, as quadratic forms. By the variational principle, ψ_c is a weak eigenfunction of H_{U_c}: $\langle\varphi, H_{U_c}\psi_c\rangle = -\frac{1}{4}\langle\varphi, \psi_c\rangle$ for all

$\varphi \in H^1(\mathbb{R}^6)$. The uniqueness, up to a global phase, follows from the usual arguments, [32, Theorem XII44] since the semigroup e^{-tH_U} is positivity improving, i,e. $e^{-tH_U}f > 0$ if $f \geq 0$ and $f \neq 0$. This proves claim 2.

Having the existence of ψ_U at $U = U_c$, the same argument which proved (D.8) can be used to prove (D.5). Continuity of ψ_U in $U < U_c$ with respect to the L^2 norm follow from perturbation theory. Take any sequence U_n converging to U_c from below. Let n_j be an arbitrary subsequence and $U_j^1 = U_{n_j}$. Then the above argument shows that there exists a further subsequence $U_k^2 = U_{j_k}^1$ such that with $\psi_{U_k^2}$ converges in L^2 to ψ_c, which is the unique ground state of H_{U_c}. Thus any subsequence of ψ_{U_n} has a further subsequence which converges to the same limit, i.e., ψ_{U_n} converges in L^2 to ψ_{U_c} for any sequence $U_n \nearrow U_c$. Hence $[0, U_c] \ni U \mapsto \psi_U$ is continuous in L^2.

The Coulomb potential V_U is in the Kato–class and it is continuous in U in the Kato–norm (for definitions, see [36, Section A.2]). Thus [36, Theorem B.10.1] shows that

$$\|e^{-tH_U} - e^{-tH_{U_0}}\|_{2\to p} \to 0$$

as $U \to U_0$ for any fixed $t > 0$ and $2 \leq p \leq \infty$. Define $\widetilde{H}_U = H_U - E_U$. Then continuity of E_U in U shows that also $\|e^{-t\widetilde{H}_{U'}} - e^{-t\widetilde{H}_U}\|_{2\to p} \to 0$ as $U' \to U$ for any fixed $t > 0$ and $2 \leq p \leq \infty$. Using $\widetilde{H}_U\psi_U = 0$, we have $\psi_U = e^{-t\widetilde{H}_U}\psi_U$ for all $U \leq U_c$. Hence

$$\psi_{U'} - \psi_U = e^{-t\widetilde{H}_{U'}}\psi_{U'} - e^{-t\widetilde{H}_U}\psi_U = \left(e^{-t\widetilde{H}_{U'}} - e^{-t\widetilde{H}_U}\right)\psi_{U'} + e^{-t\widetilde{H}_U}\left(\psi_{U'} - \psi_U\right)$$

and with the L^2 normalization $\|\psi_U\| = 1$ and the L^2 continuity of ψ_U in $U \in [0, U_c]$ we have

$$\|\psi_{U'} - \psi_U\|_p \leq \|e^{-t\widetilde{H}_{U'}} - e^{-t\widetilde{H}_U}\|_{2\to p} + \|e^{-t\widetilde{H}_U}\|_{2\to p}\|\psi_{U'} - \psi_U\| \to 0$$

as $U' \to U$ for any fixed $t > 0$ and $2 \leq p \leq \infty$. This finishes the proof of claim 3.

Let ψ_U be the strictly positive ground state, which exists for any $U \leq U_c$ (both in the infinite and finite nuclear mass cases). Since V_U is in the Kato–class, any eigenfunction of H_U is continuous [36, Theorem B.3.1]. So for any compact set $K \subset \mathbb{R}^6$ (respectively the center–of–mass frame)

$$c(K, U) \coloneqq \inf_{x\in K} \psi_U(x) > 0\,. \tag{D.13}$$

By continuity, there exists open sets $O_U \subset \mathbb{R}$ such that

$$\|\psi_{U'} - \psi_U\|_\infty < \frac{1}{2}c(K, U) \quad \text{for all } U' \in [0, U_c] \cap O_U\,. \tag{D.14}$$

Clearly

$$\inf_{x\in K} \psi_{U'}(x) \geq \inf_{x\in K} \psi_U(x) - \|\psi_{U'} - \psi_U\|_\infty \geq \frac{1}{2}c(K, U)$$

for all $U' \in [0, U_c] \cap O_U$. Clearly, $[0, U_c] \subset \cup_{U\in[0,U_c]} O_U$. Since $[0, U_c]$ is compact, there exist finitely many $O_j = O_{U_j}$, $j = 1, \dots, N$ such that $[0, U_c] \subset \cup_{j=1}^N O_j$. So with $c_j(K) = c(K, U_j)$, we get

$$\inf_{0\leq U\leq U_c} \inf_{x\in K} \psi_U(x) \geq \frac{1}{2} \min_{j=1,\dots,N} c_j(K) =: C_K > 0\,,$$

which proves the last claim.

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