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Two-particle bound states at interfaces and corners

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A R T I C L E   I N F O

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A B S T R A C T

We study two interacting quantum particles forming a bound state in d-dimensional free space, and constrain the particles in k directions to $(0,\infty)^k \times \mathbb{R}^{d-k}$, with Neumann boundary conditions. First, we prove that the ground state energy strictly decreases upon going from k to $k+1$. This shows that the particles stick to the corner where all boundary planes intersect. Second, we show that for all k the resulting Hamiltonian, after removing the free part of the kinetic energy, has only finitely many eigenvalues below the essential spectrum. This paper generalizes the work of Egger, Kerner and Pankrashkin (2020) [6] to dimensions $d > 1$.

1. Introduction and main results

We consider two interacting quantum particles in d-dimensional space that form a bound state in free space. We constrain the particles in k directions to $(0,\infty)^k \times \mathbb{R}^{d-k}$ for some $k \in \{1,\ldots,d\}$ and impose Neumann boundary conditions. The goal of this paper is to show that at low energy the particles will stick to the boundary of the domain. In fact, the particles want to be close to as many boundary planes as possible.

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In particular, they stick to the corner where all boundary planes intersect. Neumann boundary conditions can be interpreted as representing perfect mirrors. It is remarkable that while such boundary conditions are not sufficiently attractive to capture single particles, mutually bound pairs are always attracted to the boundary.

In order to justify the picture of particles sticking to the boundary, we show that introducing a boundary plane lowers the ground state energy. Then it is energetically favorable for the particles to localize at a finite distance to the new boundary plane. Moving the particles away from that boundary plane would reduce the boundary effects and raise the energy to reach the previous ground state energy, which is strictly higher. Since moving just one of the particles to infinity would increase the potential energy between them, both particles stick to the boundary.

This problem was already studied (for particles with equal masses) in the case $d = k = 1$. Kerner and Mühlenbruch [9] considered a hard-wall interaction between the particles. (For a higher-dimensional version of this problem, which is different from the one we consider here, however, see [3].) More general interactions were studied by Egger, Kerner and Pankrashkin in [6]. Additionally, they showed that the Hamiltonian has only finitely many eigenvalues below the essential spectrum. We show here that this also holds true for particles with different masses and all dimensions d and numbers of boundary planes k. The finiteness of the number of bound states is a consequence of the fact that the effective attractive interaction with the boundary decays exponentially with distance, a decay that is inherited from the corresponding one of the ground state wave function in free space.

Let x^a and x^b be the coordinates of the particles. The Hamiltonian of the system is

$$H = -\frac{1}{2m_a}\Delta_{x^a} - \frac{1}{2m_b}\Delta_{x^b} + V(x^a - x^b) \tag{1.1}$$

acting in $L^2\left((0,\infty)^k \times \mathbb{R}^{d-k}\right) \otimes L^2\left((0,\infty)^k \times \mathbb{R}^{d-k}\right)$, where $V : \mathbb{R}^d \to \mathbb{R}$ is the interaction potential. We change to relative and center-of-mass coordinates $y = x^a - x^b$ and $z = \frac{m_a x^a + m_b x^b}{M}$, where $M = m_a + m_b$ is the total mass. The conditions $x^a_j > 0$ and $x^b_j > 0$ for $1 \leq j \leq k$ result in the coordinates $(z_1, ..., z_k, y_1, ..., y_k)$ lying in the domain

$$Q_k = \left\{ (z_1, ..., z_k, y_1, ..., y_k) \in \mathbb{R}^{2k} \mid \forall j \in \{1, ..., k\} : z_j > 0 \text{ and } -\frac{M}{m_b} z_j < y_j < \frac{M}{m_a} z_j \right\}, \tag{1.2}$$

while $(z_{k+1}, ..., z_d)$ and $(y_{k+1}, ..., y_d)$ lie in $\mathbb{R}^{d-k}$. In these coordinates, the Hamiltonian becomes $H = -\frac{1}{2\mu}\Delta_y - \frac{1}{2M}\Delta_z + V(y)$, where $\mu = \frac{m_a m_b}{M}$ is the reduced mass. Separating the variables $(z_{k+1}, ..., z_d)$ from the rest, we write the Hamiltonian as $H = H_k \otimes \mathbb{I} + \mathbb{I} \otimes q$, where $q = -\frac{1}{2M}\Delta$ on $H^2(\mathbb{R}^{d-k})$ and

$$H_k = -\frac{1}{2\mu}\Delta_y - \frac{1}{2M}\sum_{j=1}^{k} \frac{\partial^2}{\partial z_j^2} + V(y) \tag{1.3}$$

acting in $L^2(Q_k \times \mathbb{R}^{d-k})$. To be precise, we define the Hamiltonian H_k via the quadratic form

$$h_k[\psi] = \int\limits_{Q_k \times \mathbb{R}^{d-k}} \left(\frac{1}{2\mu}|\nabla_y \psi|^2 + \frac{1}{2M} \sum_{j=1}^{k} \left| \frac{\partial \psi}{\partial z_j} \right|^2 + V(y)|\psi|^2 \right) \mathrm{d}z_1 ... \mathrm{d}z_k \mathrm{d}y_1 ... \mathrm{d}y_d \quad (1.4)$$

with domain $D[h_k] = H^1(Q_k \times \mathbb{R}^{d-k})$. Due to the free part of the kinetic energy q, the Hamiltonian H has no discrete spectrum if $k < d$. We remove this free part and work with H_k instead of H.

We impose the following conditions on the interaction potential V.

Assumption 1.1. We assume that

(i) $V = v + w$ for some $v \in L^r(\mathbb{R}^d)$ and $w \in L^\infty(\mathbb{R}^d)$, where

$$r = 1 \quad \text{if } d = 1, \quad (1.5)$$

$$r > 1 \quad \text{if } d = 2, \quad (1.6)$$

$$r \geq \frac{d}{2} \quad \text{if } d \geq 3, \quad (1.7)$$

(ii) the operator $H_0 = -\frac{1}{2\mu}\Delta_y + V(y)$ in $L^2(\mathbb{R}^d)$ has a ground state ψ_0 with energy $E^0 < 0$,

(iii) $\liminf_{|y|\to\infty} V(y) \geq 0$,

(iv) V is invariant under permutation of the d coordinates $(y_1, ..., y_d) \in \mathbb{R}^d$.

Remark 1.2. Condition (i) implies that in the quadratic form h_k the interaction term is infinitesimally form bounded with respect to the kinetic energy, see Proposition A.3 in the Appendix. The KLMN theorem (see e.g. Theorem 6.24 in [13]) then guarantees that there is a unique self-adjoint operator H_k corresponding to h_k, which is bounded from below. Assumption (ii) means that the particles form a bound state in free space. Condition (iii) is a rather strong form of decay of the negative part at infinity. Presumably some weaker assumptions would be sufficient, but in our proofs this version is convenient. Also the assumptions on the positive part of V can probably be relaxed. Assumption (iv) is imposed for convenience as it implies that it is irrelevant which coordinates are restricted, and without loss of generality we pick the first k. However, our methods easily extend to the general case.

Our first result is that the ground state energy strictly decreases upon adding a Neumann boundary that cuts space in half, i.e. when going from $k \to k+1$. Moreover, the essential spectrum after dividing space starts at the previous ground state energy.

Theorem 1.3. *Let V satisfy Assumptions 1.1. Then for every $k \in \{1, ..., d\}$, the bottom of the spectrum of the operator H_k is an isolated eigenvalue $E^k = \inf \sigma(H_k)$. Moreover, the essential spectrum of H_k is $\sigma_{\text{ess}}(H_k) = [E^{k-1}, \infty)$. In particular, the ground state energies form a decreasing sequence $E^d < E^{d-1} < ... < E^0 < 0$.*

Our second result is that the operators H_k have only finitely many bound states.

Theorem 1.4. *Let $1 \le k \le d$. Then H_k has a finite number of eigenvalues below the essential spectrum.*

In the one-dimensional case $d = k = 1$ with equal masses $m_a = m_b$, Theorems 1.3 and 1.4 were proved in [6]. While we follow their main ideas, several new ingredients are needed to extend the results to general d and k. In particular, the localization procedure in the proofs is more complicated and requires several additional steps.

Remark 1.5. At various places it will be convenient to switch back to the particle coordinates in the first k components, while keeping the relative coordinate in the last $d-k$ components. We shall from now on use the notation $x^a = (x_1^a, ..., x_k^a)$, $x^b = (x_1^b, ..., x_k^b)$ for the first k components of the particle coordinates and $\tilde{y} = (y_{k+1}, ..., y_d)$ for the remaining components of the relative coordinate. In this notation, $y = (x^a - x^b, \tilde{y})$ and

$$h_k[\psi] = \int\limits_{[0,\infty)^{2k}\times\mathbb{R}^{d-k}} \Big(\frac{1}{2m_a}|\nabla_{x^a}\psi|^2 + \frac{1}{2m_b}|\nabla_{x^b}\psi|^2 + \frac{1}{2\mu}|\nabla_{\tilde{y}}\psi|^2 + V(x^a - x^b, \tilde{y})|\psi|^2 \Big) \mathrm{d}x^a \mathrm{d}x^b \mathrm{d}\tilde{y} \quad (1.8)$$

with domain $D[h_k] = H^1((0,\infty)^{2k} \times \mathbb{R}^{d-k})$.

Remark 1.6. By Corollary 5.1 in [7], if H_k has a ground state, it is non-degenerate and we can choose the corresponding wave function to be positive almost everywhere.

The remainder of this paper is structured as follows. Section 2 contains the proof of Theorem 1.3. In Section 3, we prove Theorem 1.4. The Appendix contains an explicit example for $d = 1$ in A.1, the proof of Lemma 2.3 in A.2, as well as technical details of the proofs in A.3. The exponential decay of Schrödinger eigenfunctions needed in the proof is discussed in Appendix B by Rupert L. Frank.

2. Proof of Theorem 1.3

We shall prove the following two statements.

Proposition 2.1. *Let $k \in \{1, ..., d\}$. If H_{k-1} has a ground state with energy $E^{k-1} \le ... \le E^0$ the essential spectrum of H_k is $[E^{k-1}, \infty)$.*

Proposition 2.2. *Let $k \in \{1, ..., d\}$. If H_{k-1} has a ground state ψ_{k-1} with energy E^{k-1} the spectrum of H_k satisfies*

$$E^k = \inf \sigma(H_k) \leq E^{k-1} - \frac{J^2 M}{8\mu^2} \left(1 + 2\max\left\{\frac{m_a}{m_b}, \frac{m_b}{m_a}\right\}\right)^{-1} < E^{k-1}, \tag{2.1}$$

where $J = \int_{Q_{k-1}\times\mathbb{R}^{d-k+1}} \delta(y_k)|\psi_{k-1}|^2 \mathrm{d}z\mathrm{d}y > 0$ with δ the Dirac delta-function.

The assumption $E^{k-1} \leq ... \leq E^0$ in the first Proposition holds as a consequence of the second Proposition. These two propositions combined yield Theorem 1.3.

Proof of Theorem 1.3. We proceed by induction. The claim is that H_k has a ground state, and that the ground state energies form a strictly decreasing sequence $E^d < ... < E^0$. For $k = 0$ the former is true by Assumption 1.1(ii). For the induction step we apply Propositions 2.1 and 2.2. Assuming that the claim is true for $k - 1$, Proposition 2.2 implies that H_k has spectrum below E^{k-1}. By Proposition 2.1 this part of the spectrum must consist of eigenvalues. Since H_k is bounded from below by Proposition A.3, it must have a ground state. The ground state energy E^k is strictly smaller than E^{k-1} by Proposition 2.2. □

2.1. Proof of Proposition 2.1

In order to compute the essential spectrum of H_k, we follow the proof of Proposition 2.1 in [6]. For the inclusion $[E^{k-1}, \infty) \subset \sigma_{\mathrm{ess}}(H_k)$ we use Weyl's criterion (see Section 6.4 in [13]). For the opposite inclusion, we bound the essential spectrum of H_k from below by introducing additional Neumann boundaries. They split the particle domain into several regions. One of them is bounded, so it does not contribute to the essential spectrum. In another, the interaction potential is larger than E^{k-1}, and hence there is no essential spectrum below E^{k-1}. In the remaining regions, the Hamiltonian can be bounded from below by approximately $H_{k-1} \otimes \mathbb{I}$. For this operator the essential spectrum starts at E^{k-1}.

Proof of Proposition 2.1. For the inclusion $[E^{k-1}, \infty) \subset \sigma_{\mathrm{ess}}(H_k)$ we construct a Weyl sequence. Remark 1.6 allows us to choose the ground state wave function ψ_{k-1} of H_{k-1} to be normalized and positive almost everywhere. Let $l \in [0, \infty)$ and let $\tau : \mathbb{R} \to \mathbb{R}$ be a smooth function satisfying $0 \leq \tau \leq 1$ with $\tau(x) = 0$ for $x \leq 1$ and $\tau(x) = 1$ for $x \geq 2$. Let us write $\delta = M/\max\{m_a, m_b\}$. For integers $n \geq 5$, choose $\varphi_n(z_1, ..., z_k, y_1, ..., y_d) = f_n(z_1, ..., z_{k-1}, y_1, ..., y_d)g_n(z_k)$ for $(z, y) \in Q_k \times \mathbb{R}^{d-k}$ with

$$f_n(z_1, ..., z_{k-1}, y_1, ..., y_d) = \psi_{k-1}(z_1, ..., z_{k-1}, y_1, ..., y_d)\tau(n - |y_k|/\delta) \tag{2.2}$$

and

$$g_n(z_k) = \cos(lz_k)\tau(z_k - n)\tau(2n - z_k). \tag{2.3}$$

Using the properties of τ, we observe that $g_n(z_k) = \cos(lz_k)$ for $z_k \in [n+2, 2n-2]$. Moreover, for $|y_k| < \delta(n-2)$ we have $f_n = \psi_{k-1}$. Note that for $(z, y) \in Q_k \times \mathbb{R}^{d-k}$ with $z_k \geq n+2$, the variable y_k can take all values satisfying $|y_k| \leq \delta(n+2)$. Therefore,

$$\|\varphi_n\|^2_{L^2(Q_k \times \mathbb{R}^{d-k})} \geq \left(\int\limits_{Q_{k-1}\times[\delta(-n+2),\delta(n-2)]\times\mathbb{R}^{d-k}} \psi_{k-1}^2 \right) \left(\int\limits_{n+2}^{2n-2} \cos^2(lz_k)\mathrm{d}z_k \right). \tag{2.4}$$

Since ψ_{k-1} is normalized, the first integral converges to 1 as $n \to \infty$. The second integral is greater than some constant times n. Thus, $\|\varphi_n\|^2_{L^2(Q_k\times\mathbb{R}^{d-k})} \geq C_1 n$ for some constant $C_1 > 0$.

Using the eigenvalue equation for ψ_{k-1}, we have

$$\left(H_k - E^{k-1} - \frac{l^2}{2M} \right) \varphi_n = f_n \Psi_n + \Phi_n g_n \tag{2.5}$$

with

$$\Psi_n(z_k) = \frac{1}{M} l \sin(lz_k) \left[\tau'(z_k - n)\tau(2n - z_k) - \tau(z_k - n)\tau'(2n - z_k)\right]$$
$$-\frac{1}{2M}\cos(lz_k)\left[\tau''(z_k - n)\tau(2n - z_k) - 2\tau'(z_k - n)\tau'(2n - z_k) + \tau(z_k - n)\tau''(2n - z_k)\right] \tag{2.6}$$

and

$$\Phi_n(z_1, ..., z_{k-1}, y_1, ..., y_d) = \frac{1}{\delta\mu}\partial_{y_k}\psi_{k-1}\mathrm{sgn}(y_k)\tau'(n - |y_k|/\delta) - \frac{1}{2\delta^2\mu}\psi_{k-1}\tau''(n - |y_k|/\delta). \tag{2.7}$$

By choice of the function τ, we have $\operatorname{supp}\Psi_n \subset [n+1, n+2] \cup [2n-2, 2n-1]$ and $\operatorname{supp}\Phi_n \subset Q_{k-1} \times [\delta(-n+1), \delta(-n+2)] \cup [\delta(n-2), \delta(n-1)] \times \mathbb{R}^{d-k}$. Since both τ' and τ'' are bounded, there is a constant $C_2 > 0$ independent of n such that $|\Phi_n| \leq C_2 \left(|\partial_{y_k}\psi_{k-1}| + |\psi_{k-1}|\right)$ and $\|\Psi_n\|_\infty \leq C_2$. With the aid of the Schwarz inequality, we therefore have

$$\left\| \left(H_k - E^{k-1} - \frac{l^2}{2M} \right) \varphi_n \right\|^2_{L^2(Q_k\times\mathbb{R}^{d-k})}$$
$$\leq 2 \int\limits_{Q_{k-1}\times\mathbb{R}^{d-k+1}} f_n^2 \int\limits_{[n+1,n+2]\cup[2n-2,2n-1]} \Psi_n^2 + 2 \int\limits_{Q_{k-1}\times\mathbb{R}^{d-k+1}} \Phi_n^2 \int\limits_{n+1}^{2n-1} g_n^2$$

$$\leq 4C_2^2 \left(1 + (n-2) \int\limits_{Q_{k-1}\times[\delta(-n+1),\delta(-n+2)]\cup[\delta(n-2),\delta(n-1)]\times\mathbb{R}^{d-k}} \left((\partial_{y_k}\psi_{k-1})^2 + \psi_{k-1}^2\right)\right) \tag{2.8}$$

where we used $\|\psi_{k-1}\|_{L^2} = 1$ in the last step. Since $\psi_{k-1} \in H^1(Q_{k-1} \times \mathbb{R}^{d-k+1})$, we obtain

$$\begin{aligned} &\lim_{n\to\infty} \frac{\|(H_k - E^{k-1} - \frac{l^2}{2M})\varphi_n\|^2_{L^2(Q_k\times\mathbb{R}^{d-k})}}{\|\varphi_n\|^2_{L^2(Q_k\times\mathbb{R}^{d-k})}} \\ &\quad\leq \frac{4C_2^2}{C_1} \lim_{n\to\infty} \int\limits_{Q_{k-1}\times[\delta(-n+1),\delta(-n+2)]\cup[\delta(n-2),\delta(n-1)]\times\mathbb{R}^{d-k}} \left((\partial_{y_k}\psi_{k-1})^2 + \psi_{k-1}^2\right) = 0. \end{aligned} \tag{2.9}$$

By Weyl's criterion, we obtain $E^{k-1} + \frac{l^2}{2M} \in \sigma(H_k)$ for all $l \geq 0$. Since the interval $[E^{k-1}, \infty)$ has no isolated points, it belongs to the essential spectrum of H_k.

For the opposite inclusion $\sigma_{\text{ess}}(H_k) \subset [E^{k-1}, \infty)$, we partition the domain $Q_k \times \mathbb{R}^{d-k}$ into $k+2$ subsets. By Assumption 1.1(iii) there is a number L_0 such that for all $y \in \mathbb{R}^d$ with $|y| > L_0$ the potential satisfies $V(y) > E^0$. For $L > L_0$ and $1 \leq l \leq k$ let

$$\Omega_l := \left\{(z,y) \in Q_k \times \mathbb{R}^{d-k} \;\middle|\; z_l > \frac{L}{\delta}, |y_l| < L, \forall 1 \leq j < l : z_j < \frac{L}{\delta}\right\}, \tag{2.10}$$

$$\Omega_{k+1} := \left\{(z,y) \in Q_k \times \mathbb{R}^{d-k} \;\middle|\; \forall 1 \leq j \leq k : z_j < \frac{L}{\delta}, \forall j > k : |y_j| < L\right\}, \tag{2.11}$$

$$\Omega_{k+2} := \Omega_0 \setminus \bigcup_{l=1}^{k+1} \overline{\Omega_l}. \tag{2.12}$$

These sets are sketched in Fig. 1. The set Ω_{k+1} is bounded. For $(z,y) \in \Omega_{k+2}$, we always have $|y| > L$. Moreover, in Ω_l the range of y_l is independent of z_l.

For $1 \leq l \leq k+2$, we define the quadratic forms $a_l : H^1(\Omega_l) \to \mathbb{R}$ as

$$a_l[\psi] := \int\limits_{\Omega_l} \left(\frac{1}{2M}|\nabla_z\psi|^2 + \frac{1}{2\mu}|\nabla_y\psi|^2 + V(y)|\psi|^2\right) \mathrm{d}z\mathrm{d}y. \tag{2.13}$$

For $1 \leq l \leq k+1$, the potential term in a_l is infinitesimally bounded with respect to the kinetic energy term, as will be shown in Lemma A.4. For a_{k+2} the potential is bounded from below. Thus, by the KLMN theorem there is a corresponding self-adjoint operator A_l for all $1 \leq l \leq k+2$. Let $A = \bigoplus_{l=1}^{k+2} A_l$. There is an isometry $\iota : H^1(\Omega_0) \to \bigoplus_l H^1(\Omega_l)$, $\varphi \mapsto \{\varphi|_{\Omega_l}\}$. Let $\{\varphi_n\}$ be a normalized Weyl sequence such

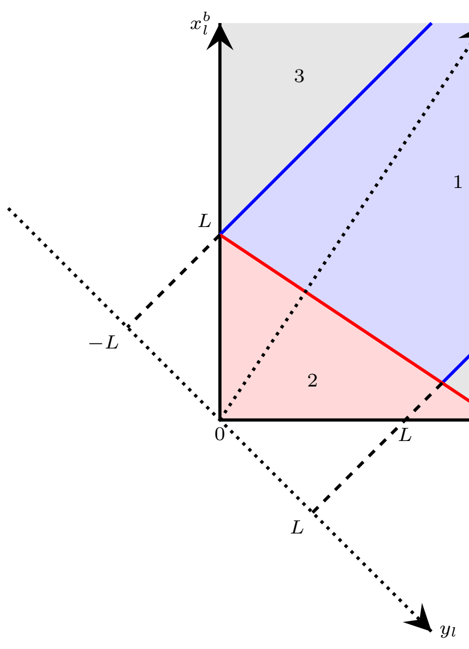

Fig. 1. In the case $d = k = 1$, the areas labeled 1, 2, and 3 are precisely $\Omega_1, \Omega_2, \Omega_3$, respectively. In higher dimensions, region 1 (blue) is the domain of the lth component of z and y for $(z, y) \in \Omega_l$, $l \leq k$. In particular, the domain of y_l is independent of z_l. The (red) triangular area 2 corresponds to the domain of z_j and y_j for $(z, y) \in \Omega_l$ and $j < l \leq k + 1$. (For interpretation of the colors in the figure(s), the reader is referred to the web version of this article.)

that $\lim_{n\to\infty} \|(H_k - \inf \sigma_{\text{ess}}(H_k))\varphi_n\| = 0$. Then $\{\iota(\varphi_n)\}$ is an orthonormal sequence with $\lim_{n\to\infty} \langle \iota(\varphi_n)|A\iota(\varphi_n)\rangle = \inf \sigma_{\text{ess}}(H_k)$. By the min-max principle,

$$\inf \sigma_{\text{ess}}(H_k) \geq \inf \sigma_{\text{ess}}(A) = \min_l \inf \sigma_{\text{ess}}(A_l). \tag{2.14}$$

We shall now analyze $\inf \sigma_{\text{ess}}(A_l)$ for all $1 \leq l \leq k+2$. Since Ω_{k+1} is a bounded Lipschitz domain, $H^1(\Omega_{k+1})$ is compactly embedded in $L^2(\Omega_{k+1})$ by the Rellich–Kondrachov theorem [1]. Therefore, A_{k+1} has compact resolvent and the spectrum of A_{k+1} is discrete. In Ω_{k+2}, always at least one of the y_j is larger than L. Therefore, $\inf \sigma(A_{k+2}) \geq \inf_{|y|>L} V(y) \geq E^0$.

Consider now A_l with $l \leq k$. In order to separate the variable z_l from the rest, let q be the quadratic form $q[\varphi] = \frac{1}{2M}\int_{L/\delta}^{\infty} |\varphi'(z_l)|^2 \, \mathrm{d}z_l$ with domain $H^1((L/\delta, \infty))$. The remaining variables lie in

$$\Omega_{k-1}^{L,l} := \Big\{ (z_1, ..., \widehat{z_l}, ..., z_k, y_1, ..., y_d) \in \mathbb{R}^{d+k-1} \;\Big|\; \forall 1 \leq j < l : 0 < z_j < \frac{L}{\delta}, \forall j > l : z_j > 0,$$
$$\forall 1 \leq j \neq l \leq k : -\frac{M}{m_b} z_j < y_j < \frac{M}{m_a} z_j, |y_l| < L \Big\} \tag{2.15}$$

where the hat means that the z_l variable is omitted. Note that for $L \to \infty$ the set $\Omega_{k-1}^{L,l}$ becomes $Q_{k-1} \times \mathbb{R}^{d-k+1}$ with l and k components swapped. Define the quadratic form

$$h_{k-1}^{L,l}[\psi] = \int\limits_{\Omega_{k-1}^{L,l}} \left(\frac{1}{2M} \sum_{\substack{j=1 \\ j \neq l}}^{k} \left| \frac{\partial \psi}{\partial z_j} \right|^2 + \frac{1}{2\mu} |\nabla_y \psi|^2 + V(y)|\psi|^2 \right) \mathrm{d}z_1 ... \widehat{\mathrm{d}z_l} ... \mathrm{d}z_k \mathrm{d}y \tag{2.16}$$

with domain $D[h_{k-1}^{L,l}] = H^1(\Omega_{k-1}^{L,l})$. In Lemma A.4, we show that there is a self-adjoint operator $H_{k-1}^{L,l}$ corresponding to the quadratic form $h_{k-1}^{L,l}$. By Assumption 1.1(iv), the quadratic form $h_{k-1}^{L,l}$ resembles h_{k-1} with l and k components swapped, up to the constraints imposed by the finite number L.

We can decompose

$$a_l = h_{k-1}^{L,l} \otimes \mathbb{I} + \mathbb{I} \otimes q. \tag{2.17}$$

It is well-known that the self-adjoint operator corresponding to q has purely essential spectrum $[0, \infty)$. Therefore, we obtain $\inf \sigma_{\mathrm{ess}}(A_l) = \inf \sigma(H_{k-1}^{L,l})$. Using localization arguments, one can easily prove the following.

Lemma 2.3. *Let $1 \leq l \leq k \leq d$ and assume that $E^{k-1} \leq ... \leq E^0$. The self-adjoint operator $H_{k-1}^{L,l}$ defined through the quadratic form (2.16) satisfies $\liminf_{L\to\infty} \inf \sigma(H_{k-1}^{L,l}) \geq E^{k-1}$.*

The proof of Lemma 2.3 is rather straightforward and follows similar arguments as in the one-dimensional case in Proposition A.5 in [6]. For completeness, we carry it out in Appendix A.2.

Collecting all estimates and applying (2.14), we see that

$$\inf \sigma_{\mathrm{ess}}(H_k) \geq \min\{E^0, \inf \sigma(H_{k-1}^{L,l})\} \tag{2.18}$$

for all $L > L_0$. With Lemma 2.3 and since $E^0 \geq E^{k-1}$, it follows that $\sigma_{\mathrm{ess}}(H_k) \subset [E^{k-1}, \infty)$. □

2.2. Proof of Proposition 2.2

The goal is to find a trial function ψ such that $(\psi, H_k \psi) < E^{k-1} \|\psi\|_2^2$. Then $\inf \sigma(H_k) < E^{k-1}$ by the min-max principle.

We denote the ground state of H_{k-1} by ψ_{k-1} and choose it normalized and positive a.e. (see Remark 1.6). Since we expect the ground state of H_k to stick to the boundary, we pick the trial function

$$\psi(z_1, ..., z_k, y_1, ..., y_d) = \psi_{k-1}(z_1, ..., z_{k-1}, y_1, ..., y_d) e^{-\gamma z_k} \tag{2.19}$$

for $\gamma > 0$. We start with a preliminary computation.

Lemma 2.4. *Let* $f(y_k) = \chi_{(-\infty,0)}(y_k)e^{-2\gamma m_b|y_k|/M} + \chi_{(0,\infty)}(y_k)e^{-2\gamma m_a|y_k|/M}$*, where* χ *denotes the characteristic function. We have*

$$A := \frac{1}{2}(f\psi_{k-1}, \psi_{k-1}) = \gamma\|\psi\|_2^2. \tag{2.20}$$

Proof. Carrying out the integration over z_k, we have

$$\begin{aligned} &\|\psi\|_2^2 \\ &= \int_{Q_{k-1}\times\mathbb{R}^{d-k+1}} \mathrm{d}z_1 ... \mathrm{d}z_{k-1}\mathrm{d}y \int_0^\infty \mathrm{d}z_k\ \chi_{\{-\frac{M}{m_b}z_k<y_k<\frac{M}{m_a}z_k\}}\psi_{k-1}^2(z_1,...,z_{k-1},y_1,...,y_d)e^{-2\gamma z_k} \\ &= \frac{1}{2\gamma}\int_{Q_{k-1}\times\mathbb{R}^{d-k+1}} \mathrm{d}z_1 ... \mathrm{d}z_{k-1}\mathrm{d}y\ \psi_{k-1}^2(z_1,...,z_{k-1},y_1,...,y_d)f(y_k) \\ &= \frac{1}{2\gamma}(f\psi_{k-1},\psi_{k-1}) = \frac{1}{\gamma}A. \quad \square \end{aligned} \tag{2.21}$$

Proof of Proposition 2.2. We have

$$\begin{aligned} h_k[\psi] = \int_{Q_k\times\mathbb{R}^{d-k}} \mathrm{d}z_1 ... \mathrm{d}z_k\mathrm{d}y_1 ... \mathrm{d}y_d \Bigg(\frac{1}{2M}|\nabla_z\psi_{k-1}|^2 + \frac{1}{2\mu}|\nabla_y\psi_{k-1}|^2 \\ + \frac{\gamma^2}{2M}\psi_{k-1}^2 + V(y)\psi_{k-1}^2\Bigg)e^{-2\gamma z_k}. \end{aligned} \tag{2.22}$$

We rewrite this as

$$\begin{aligned} h_k[\psi] &= \frac{\gamma^2\|\psi\|_2^2}{2M} + \int_{Q_{k-1}\times\mathbb{R}^{d-k+1}} \mathrm{d}z_1 ... \mathrm{d}z_{k-1}\mathrm{d}y_1 ... \mathrm{d}y_d \\ &\times \int_0^\infty \mathrm{d}z_k \chi_{\{-\frac{M}{m_b}z_k<y_k<\frac{M}{m_a}z_k\}}\left(\frac{1}{2M}|\nabla_z\psi_{k-1}|^2 + \frac{1}{2\mu}|\nabla_y\psi_{k-1}|^2 + V(y)\psi_{k-1}^2\right)e^{-2\gamma z_k}. \end{aligned} \tag{2.23}$$

Integrating over z_k as in the proof of Lemma 2.4, we obtain

$$h_k[\psi] = \frac{\gamma^2\|\psi\|_2^2}{2M} + \frac{1}{2\gamma}\int_{Q_{k-1}\times\mathbb{R}^{d-k+1}} \mathrm{d}z_1 ... \mathrm{d}z_{k-1}\mathrm{d}y_1 ... \mathrm{d}y_d \left(\frac{1}{2M}|\nabla_z\psi_{k-1}|^2\right.$$

$$+\frac{1}{2\mu}|\nabla_y\psi_{k-1}|^2+V(y)\psi_{k-1}^2\Big)f(y_k). \quad (2.24)$$

We pull the function f into the gradients and write

$$h_k[\psi]=\frac{\gamma^2\|\psi\|_2^2}{2M}+\frac{1}{2\gamma}\int\limits_{Q_{k-1}\times\mathbb{R}^{d-k+1}}\Bigg(\frac{1}{2M}\nabla_z(f\psi_{k-1})\nabla_z\psi_{k-1}+\frac{1}{2\mu}\nabla_y(f\psi_{k-1})\nabla_y\psi_{k-1}$$
$$+\frac{\gamma}{\mu M}\left(-m_b\chi_{(-\infty,0)}e^{-2\gamma\frac{m_b}{M}|y_k|}+m_a\chi_{(0,\infty)}e^{-2\gamma\frac{m_a}{M}|y_k|}\right)\psi_{k-1}\partial_{y_k}\psi_{k-1}+V(y)f\psi_{k-1}^2\Bigg). \quad (2.25)$$

Let us write $h_k[\cdot,\cdot]$ for the sesquilinear form associated to the quadratic form h_k. The previous equation reads

$$h_k[\psi]=\frac{\gamma^2\|\psi\|_2^2}{2M}+\frac{1}{2\gamma}h_{k-1}[f\psi_{k-1},\psi_{k-1}]+B, \quad (2.26)$$

where

$$B=\frac{1}{2\mu M}\int\limits_{Q_{k-1}\times\mathbb{R}^{d-k+1}}\left(-m_b\chi_{(-\infty,0)}e^{-2\gamma\frac{m_b}{M}|y_k|}+m_a\chi_{(0,\infty)}e^{-2\gamma\frac{m_a}{M}|y_k|}\right)\psi_{k-1}\partial_{y_k}\psi_{k-1}. \quad (2.27)$$

Since ψ_{k-1} is the minimizer of the functional $\frac{h_{k-1}[\phi]}{\|\phi\|_2^2}$, for all functions $g\in H^1(Q_{k-1}\times\mathbb{R}^{d-k+1})$ it holds that $h_{k-1}[g,\psi_{k-1}]=E^{k-1}(g,\psi_{k-1})$. With $g=f\psi_{k-1}$ and Lemma 2.4, we obtain

$$h_k[\psi]=\left(\frac{\gamma^2}{2M}+E^{k-1}\right)\|\psi\|_2^2+B. \quad (2.28)$$

We now simplify the integral in B. By the Sobolev embedding theorem (Theorem 4.12 in [1]), the restriction of an H^1-function to a hyperplane is an L^2-function. Therefore, one can restrict the function ψ_{k-1} to $y_k=0$ and obtain a finite number $J:=\int_{Q_{k-1}\times\mathbb{R}^{d-k}}\left(\psi_{k-1}|_{y_k=0}\right)^2$. Integration by parts with respect to y_k gives

$$\begin{aligned}2\mu MB=&-m_b\int\limits_{Q_{k-1}\times(-\infty,0)\times\mathbb{R}^{d-k}}e^{-2\gamma\frac{m_b}{M}|y_k|}\psi_{k-1}\partial_{y_k}\psi_{k-1}\\&+m_a\int\limits_{Q_{k-1}\times(0,\infty)\times\mathbb{R}^{d-k}}e^{-2\gamma\frac{m_a}{M}|y_k|}\psi_{k-1}\partial_{y_k}\psi_{k-1}\\=&-\frac{m_b}{2}\int\limits_{Q_{k-1}\times\mathbb{R}^{d-k}}\left(\psi_{k-1}|_{y_k=0}\right)^2+\gamma\frac{m_b^2}{M}\int\limits_{Q_{k-1}\times(-\infty,0)\times\mathbb{R}^{d-k}}e^{-2\gamma\frac{m_b}{M}|y_k|}\psi_{k-1}^2\end{aligned}$$

$$
\begin{aligned}
&- \frac{m_a}{2} \int\limits_{Q_{k-1}\times\mathbb{R}^{d-k}} \left(\psi_{k-1}|_{y_k=0}\right)^2 + \gamma \frac{m_a^2}{M} \int\limits_{Q_{k-1}\times(0,\infty)\times\mathbb{R}^{d-k}} e^{-2\gamma\frac{m_a}{M}|y_k|}\psi_{k-1}^2 \\
=& - \frac{M}{2} J \\
&+ \frac{\gamma}{M} \int\limits_{Q_{k-1}\times\mathbb{R}^{d-k+1}} \left(m_b^2 \chi_{(-\infty,0)}(y_k) e^{-2\gamma\frac{m_b}{M}|y_k|} + m_a^2 \chi_{(0,\infty)}(y_k) e^{-2\gamma\frac{m_a}{M}|y_k|}\right)\psi_{k-1}^2.
\end{aligned} \tag{2.29}
$$

The last integral is bounded from above by $2\max\{m_a^2, m_b^2\}A$. With (2.28), Lemma 2.4 and the min-max principle we obtain

$$
\inf \sigma(H_k) \leq \frac{h_k[\psi]}{\|\psi\|_2^2} \leq E^{k-1} + \frac{\gamma}{A}\left(\left(\frac{1}{2} + \max\left\{\frac{m_a}{m_b}, \frac{m_b}{m_a}\right\}\right)\frac{\gamma A}{M} - \frac{J}{4\mu}\right). \tag{2.30}
$$

This holds for all $\gamma > 0$. Minimizing with respect to γ yields

$$
\inf \sigma(H_k) \leq E^{k-1} - \frac{J^2 M}{32\mu^2 A^2}\left(1 + 2\max\left\{\frac{m_a}{m_b}, \frac{m_b}{m_a}\right\}\right)^{-1}. \tag{2.31}
$$

Moreover, since ψ_{k-1} is normalized we have

$$
A = \frac{1}{2} \int\limits_{Q_{k-1}\times\mathbb{R}^{d-k+1}} f\psi_{k-1}^2 \leq \frac{1}{2} \int\limits_{Q_{k-1}\times\mathbb{R}^{d-k+1}} \psi_{k-1}^2 = \frac{1}{2}. \tag{2.32}
$$

This yields (2.1).

We are left with showing that $J > 0$. Suppose that $J = 0$. Define a new function $\widetilde{\psi}_{k-1} = \psi_{k-1}\left(\chi_{y_k<0} - \chi_{y_k>0}\right)$. Since $J = 0$, the function $\widetilde{\psi}_{k-1} \in H^1(Q_{k-1} \times \mathbb{R}^{d-k+1})$. Moreover, $\widetilde{\psi}_{k-1}$ is a ground state of H_{k-1} because $\frac{h_{k-1}[\widetilde{\psi}_{k-1}]}{\|\widetilde{\psi}_{k-1}\|_2^2} = \frac{h_{k-1}[\psi_{k-1}]}{\|\psi_{k-1}\|_2^2}$. Since ψ_{k-1} and $\widetilde{\psi}_{k-1}$ are linearly independent, this contradicts the uniqueness of the ground state (Remark 1.6). Hence, $J > 0$ and $\inf \sigma(H_k) < E^{k-1}$. □

3. Finiteness of the discrete spectrum

In this section we shall give the proof of Theorem 1.4. An important ingredient will be the exponential decay of the ground state wave function ψ_k of H_k. In fact, the Agmon estimate (Corollary 4.2. in [2]) implies that for any $a < \sqrt{\inf \sigma_{\mathrm{ess}}(H_k) - E^k}$ we have

$$
\int\limits_{Q_k\times\mathbb{R}^{d-k}} |\psi_k|^2 e^{2a\sqrt{2M|z|^2+2\mu|y|^2}} \mathrm{d}z\mathrm{d}y < \infty. \tag{3.1}
$$

Strictly speaking, the assumptions on the interaction potential stated in [2] are slightly stronger than ours. However, the Agmon estimate only requires V to be form-bounded with respect to the kinetic energy with form bound less than 1, as shown in Theorem B.1 in Appendix B by Rupert Frank. As we argue in Proposition A.3, this is the case given Assumptions 1.1.

In order to derive (3.1) from Theorem B.1, we remove the boundaries in the particle domain via mirroring and consider the operator $\widetilde{H}_k$ acting on $H^1(\mathbb{R}^{d+k})$ (see Proposition A.1). It suffices to prove the exponential decay for the ground state $\widetilde{\psi}_k$ of $\widetilde{H}_k$. We rescale the variables to remove the masses in front of the Laplacians using the unitary transform $U\varphi(z,y) = \sqrt{2M}^k \sqrt{2\mu}^d \varphi(\sqrt{2M}z, \sqrt{2\mu}y)$ on $H^1(\mathbb{R}^{d+k})$. Switching to relative and center of mass coordinates and writing $\widetilde{V}(z,y) = V((|x_j^a| - |x_j^b|)_{j=1}^k, \tilde{y})$ and $\widetilde{V}_U(z,y) = \widetilde{V}(z/\sqrt{2M}, y/\sqrt{2\mu})$ we have

$$\widetilde{H}_k = -\frac{1}{2M}\Delta_z - \frac{1}{2\mu}\Delta_y + \widetilde{V} = U\left(-\Delta_z - \Delta_y + \widetilde{V}_U\right)U^\dagger. \tag{3.2}$$

The ground state φ_k of $-\Delta_z - \Delta_y + \widetilde{V}_U$ satisfies $\widetilde{\psi}_k = U\varphi_k$. For any $a < \sqrt{\inf \sigma_{\mathrm{ess}}(H_k) - E^k} = \sqrt{\inf \sigma_{\mathrm{ess}}(\widetilde{H}_k) - E^k}$, we thus have

$$\int_{\mathbb{R}^{d+k}} |\widetilde{\psi}_k|^2 e^{2a\sqrt{2M|z|^2+2\mu|y|^2}} \mathrm{d}z\mathrm{d}y = \int_{\mathbb{R}^{d+k}} |\varphi_k|^2 e^{2a\sqrt{|z|^2+|y|^2}} \mathrm{d}z\mathrm{d}y < \infty \tag{3.3}$$

by Theorem B.1. Hence (3.1) holds.

Definition 3.1. Let $n \in \mathbb{Z}^{\geq 0}$ and A be a self-adjoint operator with corresponding quadratic form a. We define

$$E_n(A) := \inf_{\substack{V\subset D[a]\\ \dim V = n+1}} \sup_{\substack{\varphi\in V\\ \varphi\neq 0}} \frac{a[\varphi]}{\|\varphi\|^2}. \tag{3.4}$$

By the min-max principle, if n is larger than the number of eigenvalues below the essential spectrum, we have $E_n(A) = \inf \sigma_{\mathrm{ess}}(A)$. Otherwise, E_{n-1} is the n-th eigenvalue of A below the essential spectrum counted with multiplicities.

Definition 3.2. For a self-adjoint operator A and a number $\lambda \in \mathbb{R}$, let $N(A,\lambda)$ denote the number of eigenvalues in $(-\infty, \lambda)$ if $\sigma_{\mathrm{ess}}(A) \cap (-\infty, \lambda) = \emptyset$. Otherwise, set $N(A,\lambda) = \infty$. When $N(A,\lambda) \neq 0$, one can write

$$N(A,\lambda) = \sup\left\{n \in \mathbb{Z}^{\geq 1} | E_{n-1}(A) < \lambda\right\}. \tag{3.5}$$

In the case $k = d = 1$, Theorem 1.4 was already shown in [6]. We generalize the proof using similar ideas. The overall strategy is to construct localized operators A and bound $N(H_k, E^{k-1})$ using $N(A, E^{k-1})$. The localized operators fall into three categories. First, they can have compact resolvent or second, the corresponding potential is larger than

E^{k-1}. In these cases, the number of eigenvalues below E^{k-1} is certainly finite (or even zero). In the third category, the operator is of the form $\mathbb{I}\otimes H_{k-1} - \frac{1}{2M}\Delta_{z_j}\otimes\mathbb{I} - K$, where K is a well behaved error term. One estimates this operator by projecting onto $L^2(\mathbb{R})\otimes\psi_{k-1}$ and its orthogonal complement. This reduces the problem to a one-dimensional operator. Then, (3.1) and the Bargmann estimate [4] imply that the number of eigenvalues is finite.

Proof of Theorem 1.4. Let $\chi_1, \chi_2 : \mathbb{R} \to [0,1]$ and $\chi_3 : \mathbb{R}^2 \to [0,1]$ be continuously differentiable functions satisfying $\chi_1(t) = 0$ for $t \geq 2$, $\chi_1(t) = 1$ for $t \leq 1$, $\chi_1(t)^2 + \chi_2(t)^2 = 1$ for all t and $\chi_3(s,t)^2 + \chi_2(s)^2\chi_2(t)^2 = 1$ for all t and s. Note that for $j = 1,2,3$ we have $\|(\nabla\chi_j)^2\|_\infty < \infty$.

Let $\Omega_0 = (0,\infty)^{2k} \times \mathbb{R}^{d-k}$. The boundary of the particle domain consists of k orthogonal $d-1$-dimensional hyperplanes. We start by localizing into two separate regions, distinguishing whether there is a particle close to all the hyperplanes, or whether both particles are far from some hyperplane. For $R > 0$, let

$$\begin{aligned}\Omega_1 &= \left\{(x^a, x^b, \tilde{y}) \in \Omega_0 | x^a \in (0,2R)^k \text{ or } x^b \in (0,2R)^k\right\} \\ &= \left\{(x^a, x^b, \tilde{y}) \in \Omega_0 | \max\{x_1^a, ..., x_k^a\} < 2R \text{ or } \max\{x_1^b, ..., x_k^b\} < 2R\right\}, \quad (3.6)\\ \Omega_2 &= \left\{(x^a, x^b, \tilde{y}) \in \Omega_0 | x^a \notin [0,R]^k \text{ and } x^b \notin [0,R]^k\right\} \\ &= \left\{(x^a, x^b, \tilde{y}) \in \Omega_0 | \max\{x_1^a, ..., x_k^a\} > R \text{ and } \max\{x_1^b, ..., x_k^b\} > R\right\}. \quad (3.7)\end{aligned}$$

We define the functions

$$f_1^R(x^a, x^b) = \chi_3\left(\frac{\max\{x_1^a, ..., x_k^a\}}{R}, \frac{\max\{x_1^b, ..., x_k^b\}}{R}\right), \quad (3.8)$$

$$f_2^R(x^a, x^b) = \chi_2\left(\frac{\max\{x_1^a, ..., x_k^a\}}{R}\right)\chi_2\left(\frac{\max\{x_1^b, ..., x_k^b\}}{R}\right). \quad (3.9)$$

Note that for all functions $\varphi \in L^2(\Omega_0)$ we have support $\operatorname{supp} f_j^R\varphi \subset \Omega_j$. By the IMS localization formula we have for all $\varphi \in H^1(\Omega_0)$ that

$$h_k[f_1^R\varphi] + h_k[f_2^R\varphi] = h_k[\varphi] + \int\limits_{(0,\infty)^{2k}\times\mathbb{R}^{d-k}} W_R|\varphi|^2 \, \mathrm{d}x^a \mathrm{d}x^b \mathrm{d}\tilde{y}, \quad (3.10)$$

where

$$\begin{aligned}W_R(x^a, x^b, \tilde{y}) = \frac{1}{R^2}\Bigg[&\frac{1}{2m_a}(\nabla_{x^a}\chi_3)\left(\frac{\max\{x_1^a, ..., x_k^a\}}{R}, \frac{\max\{x_1^b, ..., x_k^b\}}{R}\right)^2 \\ &+ \frac{1}{2m_b}(\nabla_{x^b}\chi_3)\left(\frac{\max\{x_1^a, ..., x_k^a\}}{R}, \frac{\max\{x_1^b, ..., x_k^b\}}{R}\right)^2 \\ &+ \frac{1}{2m_a}\chi_2'\left(\frac{\max\{x_1^a, ..., x_k^a\}}{R}\right)^2\chi_2\left(\frac{\max\{x_1^b, ..., x_k^b\}}{R}\right)^2\end{aligned}$$

$$+ \frac{1}{2m_b}\chi_2\left(\frac{\max\{x_1^a,...,x_k^a\}}{R}\right)^2 \chi_2'\left(\frac{\max\{x_1^b,...,x_k^b\}}{R}\right)^2\Bigg]. \tag{3.11}$$

Note that there is a constant $c_1 > 0$ such that $\|W_R\|_\infty \leq \frac{c_1}{R^2}$. For $j = 1, 2$, define the quadratic forms

$$a_j[\varphi] = \int_{\Omega_j}\Bigg(\frac{1}{2m_a}|\nabla_{x^a}\varphi|^2 + \frac{1}{2m_b}|\nabla_{x^b}\varphi|^2 + \frac{1}{2\mu}|\nabla_{\tilde{y}}\varphi|^2 + \left(V(x^a - x^b, \tilde{y}) - W_R(x^a, x^b, \tilde{y})\right)|\varphi|^2\Bigg)\mathrm{d}x^a\mathrm{d}x^b\mathrm{d}\tilde{y} \tag{3.12}$$

with domains

$$D[a_1] = \left\{\varphi \in H^1(\Omega_0) | \varphi(x^a, x^b, \tilde{y}) = 0 \text{ if } \max\{x_1^a,...,x_k^a\} \geq 2R \text{ and } \max\{x_1^b,...,x_k^b\} \geq 2R\right\}, \tag{3.13}$$

$$D[a_2] = \left\{\varphi \in H^1(\Omega_0) | \varphi(x^a, x^b, \tilde{y}) = 0 \text{ if } \max\{x_1^a,...,x_k^a\} \leq R \text{ or } \max\{x_1^b,...,x_k^b\} \leq R\right\}. \tag{3.14}$$

For all quadratic forms a_j in this proof, let A_j denote the corresponding self-adjoint operator. In Lemma A.5, we verify that these operators exist. For $\varphi \in D[h_k]$, the restriction of the function $f_j^R\varphi$ to Ω_j belongs to $D[a_j]$. With $(f_1^R)^2 + (f_2^R)^2 = 1$, it follows that $h_k[\varphi] = a_1[f_1^R\varphi] + a_2[f_2^R\varphi]$. Let $\hat{A}$ denote the operator $\hat{A} = A_1 \oplus A_2$. The map $J : H^1(\Omega_0) \to H^1(\Omega_0) \oplus H^1(\Omega_0), \varphi \mapsto (f_1^R\varphi, f_2^R\varphi)$ is an L^2-isometry and thus injective. By the min-max principle, we have

$$E_n(H_k) = \inf_{\substack{V \subset D[h_k] \\ \dim V = n+1}} \sup_{\substack{\varphi \in V \\ \varphi \neq 0}} \frac{h_k[\varphi]}{\|\varphi\|^2_{L^2(\Omega_0)}} = \inf_{\substack{V \subset D[h_k] \\ \dim V = n+1}} \sup_{\substack{\varphi \in V \\ \varphi \neq 0}} \frac{\hat{a}[J\varphi]}{\|J\varphi\|^2_{L^2(\Omega_0)\oplus L^2(\Omega_0)}}$$
$$= \inf_{\substack{V \subset JD[h_k] \\ \dim V = n+1}} \sup_{\substack{\varphi \in V \\ \varphi \neq 0}} \frac{\hat{a}[\varphi]}{\|\varphi\|^2_{L^2(\Omega_0)\oplus L^2(\Omega_0)}} \geq \inf_{\substack{V \subset D[\hat{a}] \\ \dim V = n+1}} \sup_{\substack{\varphi \in V \\ \varphi \neq 0}} \frac{\hat{a}[\varphi]}{\|\varphi\|^2_{L^2(\Omega_0)\oplus L^2(\Omega_0)}} = E_n(\hat{A}) \tag{3.15}$$

for all $n \in \mathbb{Z}^{\geq 0}$. Thus, $N(H_k, E^{k-1}) \leq N(\hat{A}, E^{k-1}) = N(A_1, E^{k-1}) + N(A_2, E^{k-1})$.

Let

$$\tilde{\Omega}_{1,\mathrm{int}} = \left\{(x^a, x^b, \tilde{y}) \in \Omega_0 | (x^a - x^b, \tilde{y}) \in (-R, R)^d\right\} \quad \text{and} \tag{3.16}$$

$$\tilde{\Omega}_{1,\mathrm{ext}} = \left\{(x^a, x^b, \tilde{y}) \in \Omega_0 | (x^a - x^b, \tilde{y}) \notin [-R, R]^d\right\}. \tag{3.17}$$

Moreover, let $\Omega_{1,\bullet} = \tilde{\Omega}_{1,\bullet} \cap \Omega_1$ for $\bullet \in \{\mathrm{int}, \mathrm{ext}\}$. Define quadratic forms $a_{1,\mathrm{int}}, a_{1,\mathrm{ext}}$ through expression (3.12) with domain

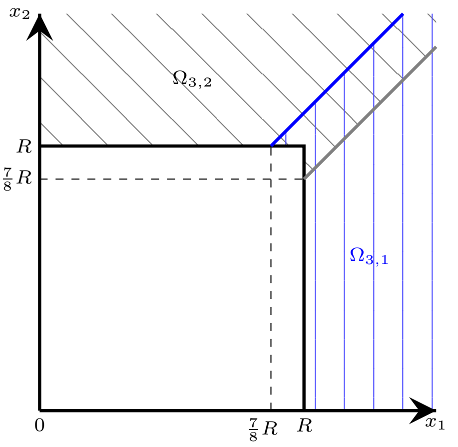

Fig. 2. Let $k = 2$. In Ω_2 both x^a and x^b lie outside the square $(0, R)^2$. If x^a lies below the upper diagonal, the configuration belongs to $\Omega_{3,1}$. If x^a lies above the lower diagonal, the configuration belongs to $\Omega_{3,2}$.

$$D[a_{1,\bullet}] = \left\{\varphi \in H^1(\tilde{\Omega}_{1,\bullet}) | \varphi(x^a, x^b, \tilde{y}) = 0 \text{ if } \max\{x_1^a, ..., x_k^a\} \geq 2R \text{ and } \max\{x_1^b, ..., x_k^b\} \geq 2R\right\}, \tag{3.18}$$

for $\bullet \in \{\text{int}, \text{ext}\}$. Again, there is an isometry

$$D[a_1] \to D[a_{1,\text{int}}] \oplus D[a_{1,\text{ext}}], \varphi \mapsto (\varphi|_{\tilde{\Omega}_{1,\text{int}}}, \varphi|_{\tilde{\Omega}_{1,\text{ext}}}), \tag{3.19}$$

and therefore, $N(A_1, E^{k-1}) \leq N(A_{1,\text{int}}, E^{k-1}) + N(A_{1,\text{ext}}, E^{k-1})$. Since the negative part of V vanishes at infinity by Assumption 1.1(iii) and since $\|W_R\|_\infty \leq \frac{c_1}{R^2}$, there is a $R_0 > 0$ such that for $R \geq R_0$ and $|(x^a - x^b, \tilde{y})| \geq R_0$ we have $V(x^a - x^b, \tilde{y}) - W_R(x^a, x^b, \tilde{y}) > E^{k-1}$. Choosing $R \geq R_0$, we have $N(A_{1,\text{ext}}, E^{k-1}) = 0$. Since $\Omega_{1,\text{int}}$ is a bounded Lipschitz domain, $A_{1,\text{int}}$ has purely discrete spectrum. As $A_{1,\text{int}}$ is bounded from below, we have $N(A_{1,\text{int}}, E^{k-1}) < \infty$.

We are left with showing that $N(A_2, E^{k-1}) < \infty$. For $k = 1$, wave functions in the support of A_2 are localized away from the boundary. Effectively, the boundary has thus disappeared and one can directly make a comparison with $H_{k-1} = H_0$. For $k > 1$, the domain Ω_2 is more complicated and we need to continue localizing in order to effectively eliminate one of the boundary planes. For now, assume $k > 1$ and let $r = R/8$. We localize x^a in the k sectors

$$\Omega_{3,j} = \{(x^a, x^b, \tilde{y}) \in \Omega_2 | x_j^a > \max\{x_1^a, ..., x_k^a\} - r\} \quad \text{for } 1 \leq j \leq k. \tag{3.20}$$

In the sector $\Omega_{3,j}$, the largest component of x^a is x_j^a up to the constant r. The domains are sketched in Fig. 2 for the case $k = 2$. For the localization, we need functions $f_{3,j}^r$ on Ω_2 which are supported in $\Omega_{3,j}$, satisfy $\sum_{j=1}^k (f_{3,j}^r)^2 = 1$, and their derivatives scale as $1/r$. We construct auxiliary functions $f_{3,j}$ corresponding to the case $r = 1$ and set

$$f^r_{3,j}(x^a, x^b, \tilde{y}) = f_{3,j}(x^a/r). \tag{3.21}$$

The idea behind the construction of the auxiliary functions is as follows. We want that $f_{3,1}$ equals 1 on $\Omega_{3,1}$ apart from the boundary region which overlaps with other $\Omega_{3,j}$. The expression $\max\{x^a_2, ..., x^a_k\} - x^a_1$ measures the distance to the boundary of $\Omega_{3,1}$ and is large outside $\Omega_{3,1}$. Hence, to define $f_{3,1}$, we apply χ_1 to this expression (up to some constants). For the sum condition to hold, the remaining $f_{3,j}$ will contain the corresponding factor χ_2. This χ_2 factor takes care of the behavior at the boundary towards large x^a_1. For the next function $f_{3,2}$, we proceed analogously to before, but ignoring the x^a_1 direction. Inductively, for $x^a \in (0, \infty)^k$ and $1 \le j \le k-1$ we define

$$\begin{aligned} f_{3,j}(x^a) &= \chi_1\left(\frac{k}{2}\left(\max\{x^a_{j+1}, ..., x^a_k\} - x^a_j\right) + \frac{3}{2}\right) \\ &\quad \times \prod_{l=1}^{j-1} \chi_2\left(\frac{k}{2}\left(\max\{x^a_{l+1}, ..., x^a_k\} - x^a_l\right) + \frac{3}{2}\right), \\ f_{3,k}(x^a) &= \prod_{l=1}^{k-1} \chi_2\left(\frac{k}{2}\left(\max\{x^a_{l+1}, ..., x^a_k\} - x^a_l\right) + \frac{3}{2}\right), \end{aligned} \tag{3.22}$$

where the product in the first line has to be understood as 1 for $j = 1$. Note that for all $1 \le j \le k$ the derivatives are bounded, i.e. $\|(\nabla f_{3,j})^2\|_\infty < \infty$. By construction, we have $\sum_{j=1}^k (f_{3,j})^2 = 1$. That the functions $f^r_{3,j}$ indeed have the correct support is the content of the following Lemma, which is proved at the end of this section.

Lemma 3.3. *For $1 \le j \le k$, the functions $f^r_{3,j}$ defined through (3.21) and (3.22) satisfy*

$$\operatorname{supp} f^r_{3,j} \cap \Omega_2 \subset \overline{\Omega_{3,j}}. \tag{3.23}$$

Moreover,

$$\begin{aligned} &\operatorname{supp} \nabla f^r_{3,j} \cap \Omega_2 \subset \\ &\{(x^a, x^b, \tilde{y}) \in \Omega_2 |\max\{x^a_1, ..., \widehat{x^a_j}, ..., x^a_k\} - r \le x^a_j \le \max\{x^a_1, ..., \widehat{x^a_j}, ..., x^a_k\} + r\}, \end{aligned} \tag{3.24}$$

where $\widehat{x^a_j}$ means that this variable is omitted.

By the IMS formula, we have for all $\varphi \in D[a_2]$

$$\sum_{j=1}^k a_2[f^r_{3,j}\varphi] = a_2[\varphi] + \int_{\Omega_2} F_r(x^a, x^b, \tilde{y})|\varphi|^2 \mathrm{d}x^a \mathrm{d}x^b \mathrm{d}\tilde{y}, \tag{3.25}$$

where

$$F_r(x^a, x^b, \tilde{y}) = \frac{1}{r^2} \sum_{j=1}^{k} \frac{1}{2m_a} (\nabla f_{3,j})^2 (x^a/r) \,. \tag{3.26}$$

For $1 \leq j \leq k$, define the quadratic forms

$$a_{3,j}[\varphi] = \int\limits_{\Omega_{3,j}} \Bigg(\frac{1}{2m_a} |\nabla_{x^a} \varphi|^2 + \frac{1}{2m_b} |\nabla_{x^b} \varphi|^2 + \frac{1}{2\mu} |\nabla_{\tilde{y}} \varphi|^2 + \left(V(x^a - x^b, \tilde{y}) - W_R(x^a, x^b, \tilde{y}) - F_r(x^a, x^b, \tilde{y}) \right) |\varphi|^2 \Bigg) \mathrm{d}x^a \mathrm{d}x^b \mathrm{d}\tilde{y} \tag{3.27}$$

with domains

$$D[a_{3,j}] = \Big\{ \varphi \in H^1(\Omega_0) | \varphi(x^a, x^b, \tilde{y}) = 0 \quad \text{if} \quad \max\{x_1^a, ..., x_k^a\} \leq R \text{ or } \max\{x_1^b, ..., x_k^b\} \leq R \text{ or } x_j^a \leq \max\{x_1^a, ..., x_k^a\} - r \Big\}. \tag{3.28}$$

Again we have $N(A_2, E^{k-1}) \leq \sum_{j=1}^{k} N(A_{3,j}, E^{k-1})$. We will show that $N(A_{3,k}, E^{k-1}) < \infty$. For $1 \leq j < k$, by Assumption 1.1(iv) the same argument with vector components $k \leftrightarrow j$ swapped gives $N(A_{3,j}, E^{k-1}) < \infty$.

We localize x^b close and far from the domain of x^a. Define the sets

$$\Omega_4 = \left\{ (x^a, x^b, \tilde{y}) \in \Omega_{3,k} | x_k^b > \max\{x_1^b, ..., x_{k-1}^b\} - 4r \right\} \quad \text{and} \tag{3.29}$$

$$\Omega_5 = \left\{ (x^a, x^b, \tilde{y}) \in \Omega_{3,k} | x_k^b < \max\{x_1^b, ..., x_{k-1}^b\} - 2r \right\}. \tag{3.30}$$

For $k = 2$, they are sketched in Fig. 3. Let $f_4^r(x^b) = \chi_1 \left(\frac{\max\{x_1^b, ..., x_{k-1}^b\} - x_k^b}{2r} \right)$ and $f_5^r(x^b) = \chi_2 \left(\frac{\max\{x_1^b, ..., x_{k-1}^b\} - x_k^b}{2r} \right)$. By the IMS formula, we have for all $\varphi \in D[a_{3,k}]$

$$a_{3,k}[f_4^r \varphi] + a_{3,k}[f_5^r \varphi] = a_{3,k}[\varphi] + \int\limits_{\Omega_{3,k}} G_r(x^a, x^b, \tilde{y}) |\varphi|^2 \mathrm{d}x^a \mathrm{d}x^b \mathrm{d}\tilde{y}, \tag{3.31}$$

where

$$G_r(x^a, x^b, \tilde{y}) = \frac{1}{4r^2 m_b} \left[\chi_1' \left(\frac{\max\{x_1^b, ..., x_{k-1}^b\} - x_k^b}{2r} \right)^2 + \chi_2' \left(\frac{\max\{x_1^b, ..., x_{k-1}^b\} - x_k^b}{2r} \right)^2 \right]. \tag{3.32}$$

For $j = 4, 5$, define the quadratic forms

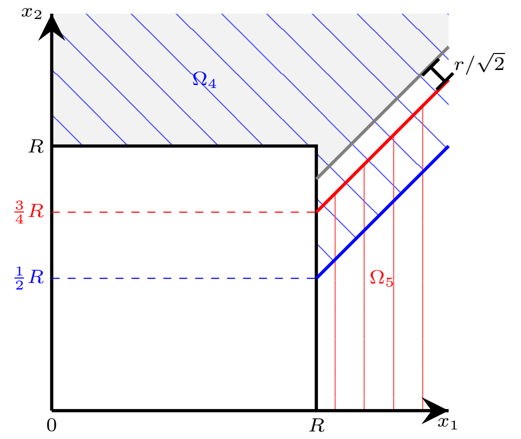

Fig. 3. In $\Omega_{3,2}$, the first particle's coordinate x^a lies in the shaded area, while the second particle at x^b lies outside the square $(0, R)^2$. If x^b lies above the lowest diagonal (blue), the configuration belongs to Ω_4. If x^b lies below the middle diagonal (red), the configuration belongs to Ω_5. Note that for any configuration in Ω_5, the particles are separated by at least distance $r/\sqrt{2}$.

$$a_j[\varphi] = \int_{\Omega_j} \left(\frac{1}{2m_a} |\nabla_{x^a}\varphi|^2 + \frac{1}{2m_b} |\nabla_{x^b}\varphi|^2 + \frac{1}{2\mu} |\nabla_{\tilde{y}}\varphi|^2 + \left(V(x^a - x^b, \tilde{y}) - W_R(x^a, x^b, \tilde{y}) - F_r(x^a, x^b, \tilde{y}) - G_r(x^a, x^b, \tilde{y}) \right) |\varphi|^2 \right) \mathrm{d}x^a \mathrm{d}x^b \mathrm{d}\tilde{y} \tag{3.33}$$

with domains

$$D[a_4] = \{\varphi \in H^1(\Omega_0) | \varphi(x^a, x^b, \tilde{y}) = 0 \quad \text{if} \quad \max\{x_1^a, ..., x_k^a\} \leq R \text{ or } \max\{x_1^b, ..., x_k^b\} \leq R \text{ or } x_k^a \leq \max\{x_1^a, ..., x_{k-1}^a\} - r \text{ or } x_k^b \leq \max\{x_1^b, ..., x_{k-1}^b\} - 4r\}, \tag{3.34}$$

$$D[a_5] = \{\varphi \in H^1(\Omega_0) | \varphi(x^a, x^b, \tilde{y}) = 0 \quad \text{if} \quad \max\{x_1^a, ..., x_k^a\} \leq R \text{ or } \max\{x_1^b, ..., x_k^b\} \leq R \text{ or } x_k^a \leq \max\{x_1^a, ..., x_{k-1}^a\} - r \text{ or } x_k^b \geq \max\{x_1^b, ..., x_{k-1}^b\} - 2r\}. \tag{3.35}$$

Again, we have $N(A_{3,k}, E^{k-1}) \leq N(A_4, E^{k-1}) + N(A_5, E^{k-1})$.

For $(x^a, x^b, \tilde{y}) \in \Omega_5$, we claim that

$$|(x^a - x^b, \tilde{y})| \geq r/\sqrt{2} = R/(8\sqrt{2}). \tag{3.36}$$

Let l be the index such that $x_l^b = \max\{x_1^b, ..., x_{k-1}^b\}$. We estimate

$$|(x^a - x^b, \tilde{y})|^2 \geq (x_l^a - x_l^b)^2 + (x_k^a - x_k^b)^2 \geq \frac{1}{2} \left(x_l^a - x_k^a - x_l^b + x_k^b \right)^2. \tag{3.37}$$

Since $\max\{x_1^a, ..., x_{k-1}^a\} \geq x_l^a$ we have in the set Ω_5 (see (3.30) and (3.20))

$$x_k^a > x_l^a - r \quad \text{and} \quad x_k^b < x_l^b - 2r \qquad \Leftrightarrow \qquad x_l^a - x_k^a < r \quad \text{and} \quad x_l^b - x_k^b > 2r. \quad (3.38)$$

Combining this with (3.37) yields (3.36). Moreover, we have $\|W_R\|_\infty + \|F_r\|_\infty + \|G_r\|_\infty \le \frac{c_2}{R^2}$. By Assumption 1.1(iii), there is $R_1 > 0$ such that for $R > R_1$ we have $a_5 > E^{k-1}$. Choosing R large enough, we thus have $N(A_5, E^{k-1}) = 0$.

For $k = 1$, we set $F_r = G_r = 0$ and $a_4 = a_2$. For any choice of $k \ge 1$, we now just need to show $N(A_4, E^{k-1}) < \infty$. At the boundaries which constrain the kth component of x^a and x^b, the operator A_4 has Dirichlet boundary conditions. The idea is to extend the domain of x_k^a and x_k^b to $\mathbb{R}$, which leads to the new operator $\hat{A}_4$ defined below. In $\hat{A}_4$, the boundary hyperplane in the kth direction has disappeared. This makes it possible to compare the operator $\hat{A}_4$ to the Hamiltonian H_{k-1} of the problem with $k-1$ boundary hyperplanes. Let us write $K_R = (W_R + F_r + G_r)\chi_{(0,\infty)^{2k} \times \mathbb{R}^{d-k}}$. Let $\hat{\Omega}_4 = \left((0,\infty)^{k-1} \times \mathbb{R}\right)^2 \times \mathbb{R}^{d-k}$ and define the quadratic form

$$\hat{a}_4[\varphi] = \int_{\hat{\Omega}_4} \Bigg(\frac{1}{2m_a} |\nabla_{x^a}\varphi|^2 + \frac{1}{2m_b}|\nabla_{x^b}\varphi|^2 + \frac{1}{2\mu}|\nabla_{\tilde{y}}\varphi|^2 + \left(V(x^a - x^b, \tilde{y}) - K_R(x^a, x^b, \tilde{y})\right)|\varphi|^2 \Bigg) \mathrm{d}x^a \mathrm{d}x^b \mathrm{d}\tilde{y} \quad (3.39)$$

with domain $D[\hat{a}_4] = H^1(\hat{\Omega}_4)$. We have $N(A_4, E^{k-1}) \le N(\hat{A}_4, E^{k-1})$.

Let us change to relative and center-of-mass coordinates $y = (x^a - x^b, \tilde{y})$ and $z = \frac{m_a x^a + m_b x^b}{M}$. Then

$$\hat{a}_4[\varphi] = \int_{\mathbb{R}} \mathrm{d}z_k \int_{Q_{k-1}\times\mathbb{R}^{d-k+1}} \mathrm{d}z_1..\mathrm{d}z_{k-1}\mathrm{d}y \Bigg(\frac{1}{2\mu}|\nabla_y \varphi|^2 + \frac{1}{2M}|\nabla_z\varphi|^2 + \left[V(y) - K_R\left(z + \frac{m_b}{M}(y_1,...,y_k), z - \frac{m_a}{M}(y_1,...,y_k), \tilde{y}\right)\right]|\varphi|^2 \Bigg) \quad (3.40)$$

with $D[\hat{a}_4] = H^1(\mathbb{R} \times Q_{k-1} \times \mathbb{R}^{d-k+1})$. Note that we can separate z_k from the other variables and write the corresponding operator as $\hat{A}_4 = \mathbb{I} \otimes H_{k-1} - \frac{1}{2M}\Delta_{z_k} \otimes \mathbb{I} - K_R$. Recall that H_{k-1} has the ground state ψ_{k-1} with energy E^{k-1}. Let Π denote the orthogonal projection onto $L^2(\mathbb{R}) \otimes \psi_{k-1}$ in $L^2(\mathbb{R} \times Q_{k-1} \times \mathbb{R}^{d-k+1})$, and $\Pi^\perp := \mathbb{I} - \Pi$. For $\varphi \in H^1(\mathbb{R} \times Q_{k-1} \times \mathbb{R}^{d-k+1})$ both $\Pi\varphi$ and $\Pi^\perp\varphi$ belong to $H^1(\mathbb{R} \times Q_{k-1} \times \mathbb{R}^{d-k+1})$. We have

$$\hat{a}_4[\varphi] = \hat{a}_4[\Pi\varphi] + \hat{a}_4[\Pi^\perp\varphi] - 2K_R[\Pi^\perp\varphi, \Pi\varphi], \quad (3.41)$$

where

$$K_R[\varphi,\psi] = \int\limits_{\mathbb{R}\times Q_{k-1}\times\mathbb{R}^{d-k+1}} \overline{\varphi(z,y)} K_R\left(z+\frac{m_b}{M}(y_1,...,y_k), z-\frac{m_a}{M}(y_1,...,y_k), \tilde{y}\right)\psi(z,y)$$

$$\mathrm{d}z_k\mathrm{d}z_1...\mathrm{d}z_{k-1}\mathrm{d}y. \quad (3.42)$$

Using the Schwarz inequality, we estimate

$$|2K_R[\Pi^\perp\varphi,\Pi\varphi]| \leq R\|K_R\Pi\varphi\|^2_{L^2(\mathbb{R}\times Q_{k-1}\times\mathbb{R}^{d-k+1})} + \frac{1}{R}\|\Pi^\perp\varphi\|^2_{L^2(\mathbb{R}\times Q_{k-1}\times\mathbb{R}^{d-k+1})}. \quad (3.43)$$

Since E^{k-1} is a discrete and non-degenerate eigenvalue of H_{k-1}, we have $E_1^{k-1} = \inf(\sigma(H_{k-1})\setminus\{E^{k-1}\}) > E^{k-1}$, and $(\mathbb{I}\otimes h_{k-1})[\Pi^\perp\varphi] \geq E_1^{k-1}\|\Pi^\perp\varphi\|^2_{L^2(\mathbb{R}\times Q_{k-1}\times\mathbb{R}^{d-k+1})}$. Together with the positivity of $-\Delta_{z_k}\otimes\mathbb{I}$ and $\|K_R\|_\infty \leq \frac{c_2}{R^2}$ it follows that

$$\hat{a}_4[\Pi^\perp\varphi] \geq \left(E_1^{k-1} - \frac{c_2}{R^2}\right)\|\Pi^\perp\varphi\|^2_{L^2(\mathbb{R}\times Q_{k-1}\times\mathbb{R}^{d-k+1})}. \quad (3.44)$$

In total, we have

$$\hat{a}_4[\varphi] \geq \hat{a}_4[\Pi\varphi] - R\|K_R\Pi\varphi\|^2_{L^2(\mathbb{R}\times Q_{k-1}\times\mathbb{R}^{d-k+1})} + \left(E_1^{k-1} - \frac{1}{R} - \frac{c_2}{R^2}\right)\|\Pi^\perp\varphi\|^2_{L^2(\mathbb{R}\times Q_{k-1}\times\mathbb{R}^{d-k+1})}. \quad (3.45)$$

We choose R large enough such that $E_1^{k-1} - E^{k-1} > \frac{1}{R} + \frac{c_2}{R^2}$. Let B_1 be the self-adjoint operator corresponding to

$$b_1[\varphi] = \hat{a}_4[\varphi] - R\|K_R\varphi\|^2_{L^2(\mathbb{R}\times Q_{k-1}\times\mathbb{R}^{d-k+1})} \quad (3.46)$$

in ran Π. Then $N(\hat{A}_4, E^{k-1}) \leq N(B_1, E^{k-1})$ by the min-max principle.

We can write any function $\varphi \in$ ran Π as $\varphi(z,y) = f(z_k)\psi_{k-1}(z_1,...,z_{k-1},y)$ for some $f \in H^1(\mathbb{R})$. Integrating over $z_1,...,z_{k-1},y$, we have

$$\hat{a}_4[f\otimes\psi_{k-1}] = \int\limits_{\mathbb{R}}\left(\frac{1}{2M}|f'(z_k)|^2 + (E^{k-1} - U_R(z_k))f(z_k)^2\right)\mathrm{d}z_k, \quad (3.47)$$

where

$$U_R(z_k) = \int\limits_{Q_{k-1}\times\mathbb{R}^{d-k+1}} K_R\left(z+\frac{m_b}{M}(y_1,...,y_k), z-\frac{m_a}{M}(y_1,...,y_k), \tilde{y}\right)\psi_{k-1}(z_1,...z_{k-1},y)^2$$

$$\mathrm{d}z_1...\mathrm{d}z_{k-1}\mathrm{d}y. \quad (3.48)$$

Moreover,

$$\|K_R(f \otimes \psi_{k-1})\|^2_{L^2(\mathbb{R}\times Q_{k-1}\times\mathbb{R}^{d-k+1})} = \int_{\mathbb{R}} V_R(z_k) f(z_k)^2 \mathrm{d}z_k \tag{3.49}$$

with

$$V_R(z_k) = \int_{Q_{k-1}\times\mathbb{R}^{d-k+1}} K_R\left(z + \frac{m_b}{M}(y_1, ..., y_k), z - \frac{m_a}{M}(y_1, ..., y_k), \tilde{y}\right)^2 \psi_{k-1}(z_1, ..., z_{k-1}, y)^2 \mathrm{d}z_1...\mathrm{d}z_{k-1}\mathrm{d}y. \tag{3.50}$$

Let $Z_R = U_R + RV_R$. With

$$b_2[f] = \int_{\mathbb{R}} \left(\frac{1}{2M}|f'(z)|^2 - Z_R(z)f(z)^2\right) \mathrm{d}z, \tag{3.51}$$

we can write $b_1[f \otimes \psi_{k-1}] = E^{k-1}\|f\|^2_{L^2(\mathbb{R})} + b_2[f]$. Therefore, $N(B_1, E^{k-1}) = N(B_2, 0)$.

In the following, we bound the function Z_R from above by an exponentially decaying function. With this bound it is easy to see that $N(B_2, 0) < \infty$ using e.g. the Bargmann estimate (see Chapter 2, Theorem 5.3 in [4]). This concludes the proof of $N(H_k, E^{k-1}) < \infty$.

To bound Z_R, first use that K_R is bounded to obtain

$$Z_R(z_k) \leq \left(\|K\|_\infty + R\|K\|^2_\infty\right) I(z_k), \tag{3.52}$$

where

$$I(z_k) = \int_{Q_{k-1}\times\mathbb{R}^{d-k+1}} \chi_{\operatorname{supp} K_R}(z, y)\psi^2_{k-1}\mathrm{d}z_1...\mathrm{d}z_{k-1}\mathrm{d}y. \tag{3.53}$$

By construction, $I(z_k) = 0$ for $z_k < 0$. We shall show that $I(z_k)$ decays exponentially for $z_k \geq 0$. In fact, if z_k is large and $K_R(z, y) \neq 0$, then necessarily one of the remaining coordinates $z_1, ..., z_{k-1}, y_1, ..., y_d$ has to be large as well. This is essentially the content of the following Lemma.

Lemma 3.4. *Let $a > 0$. For $z_k \geq 2R$ the function*

$$\alpha(z, y) = e^{a\sqrt{2M|z_1|^2+...+2M|z_{k-1}|^2+2\mu|y|^2}}\chi_{\operatorname{supp} K_R}(z, y) \tag{3.54}$$

satisfies $\alpha(z, y) \geq e^{ac(z_k-2R)}\chi_{\operatorname{supp} K_R}(z, y)$ with $c = \sqrt{2M}(1 + 2\max\{\frac{m_a}{m_b}, \frac{m_b}{m_a}\})^{-1/2}$.

The Agmon estimate (3.1) tells us that there is a constant $a > 0$ such that

$$c_3 := \int\limits_{Q_{k-1}\times\mathbb{R}^{d-k+1}} \psi_{k-1}^2 e^{a\sqrt{2M|z_1|^2+...+2M|z_{k-1}|^2+2\mu|y|^2}} \mathrm{d}z_1...\mathrm{d}z_{k-1}\mathrm{d}y < \infty. \tag{3.55}$$

We apply Lemma 3.4 with this constant a and conclude that

$$\chi_{\operatorname{supp} K_R}(z,y) \le e^{-c_4(z_k-2R)}\alpha(z,y) \tag{3.56}$$

for $z_k \ge 2R$ and suitable constant $c_4 > 0$. In particular,

$$\begin{aligned} I(z_k) &\le e^{-c_4(z_k-2R)} \int\limits_{Q_{k-1}\times\mathbb{R}^{d-k+1}} \alpha(z,y)\psi_{k-1}(z_1,...,z_{k-1},y)^2 \mathrm{d}z_1...\mathrm{d}z_{k-1}\mathrm{d}y \\ &\le c_3 e^{-c_4(z_k-2R)} \end{aligned} \tag{3.57}$$

for $z_k \ge 2R$. Recall that Z_R vanishes on $(-\infty, 0)$ and $\|Z_R\|_\infty < \infty$. With (3.52) we thus conclude the desired exponentially decaying bound. □

It remains to give the proof of Lemmas 3.3 and 3.4.

Proof of Lemma 3.4. Recall the definitions of W_R, F_r and G_r in (3.11), (3.26) and (3.32), respectively. Since $\operatorname{supp} K_R \subset \operatorname{supp} W_R \cup \operatorname{supp} F_r \cup \operatorname{supp} G_r$, we estimate α on each of these three sets. In $\operatorname{supp} W_R$, at least one particle is close to the corner, i.e. in the hypercube $(0, 2R)^k$. If z_k is large, this means that the two particles are far apart and y_k is large. To be precise, using $x_j^a = z_j + \frac{m_b}{M} y_j$ and $x_j^b = z_j - \frac{m_a}{M} y_j$ we have

$$\begin{aligned} \operatorname{supp} W_R &\subset \left\{ (z,y) \in Q_k \times \mathbb{R}^{d-k} | 0 \le \frac{z_k + \frac{m_b}{M} y_k}{R} \le 2 \text{ or } 0 \le \frac{z_k - \frac{m_a}{M} y_k}{R} \le 2 \right\} \\ &\subset \left\{ (z,y) \in Q_k \times \mathbb{R}^{d-k} | z_k - 2R \le \frac{\max\{m_a, m_b\}}{M} |y_k| \right\}. \end{aligned} \tag{3.58}$$

For $(z, y) \in \operatorname{supp} W_R$ with $z_k \ge 2R$, we therefore have

$$M \sum_{j=1}^{k-1} |z_j|^2 + \mu \sum_{j=1}^{k} |y_k|^2 \ge \frac{\mu M^2 (z_k - 2R)^2}{\max\{m_a^2, m_b^2\}} = \frac{M(z_k - 2R)^2}{\max\{\frac{m_a}{m_b}, \frac{m_b}{m_a}\}}, \tag{3.59}$$

which implies the desired bound on α.

For $k = 1$, both F_r and G_r are identically zero, hence to estimate α on their support we can restrict our attention to the case $k > 1$. Observe that in $\operatorname{supp} F_r$ every coordinate x_j^a for $1 \le j \le k$ is smaller than or similar in magnitude to the largest of the other coordinates x_i^a, $i \ne j$; in particular, this applies to $j = k$. Intuitively, for large z_k either

x_k^a or $|y_k|$ needs to be large. If x_k^a is large, also some other x_j^a with $j < k$ has to be large. Phrased precisely, by Lemma 3.3 we have

$$\begin{aligned}
&\operatorname{supp} F_r \subset \\
&\bigcup_{j=1}^{k} \left\{ (z,y) \in Q_k \times \mathbb{R}^{d-k} | \max_{\substack{1\le l\le k,\\ l\neq j}} \{z_l + \frac{m_b}{M} y_l\} - r \le z_j + \frac{m_b}{M} y_j \le \max_{\substack{1\le l\le k,\\ l\neq j}} \{z_l + \frac{m_b}{M} y_l\} + r \right\} \\
&\qquad \subset \left\{ (z,y) \in Q_k \times \mathbb{R}^{d-k} | z_k - r \le -\frac{m_b}{M} y_k + \max_{1\le j\le k-1} \{ \frac{m_b}{M} y_j + z_j \} \right\} =: S_F. \quad (3.60)
\end{aligned}$$

The constraint in S_F can be written as $z_k - r \le (\sqrt{M} z, \sqrt{\mu} y) \cdot e$ for a vector $e \in \mathbb{R}^{k+d}$. A simple Schwarz inequality therefore shows that on the set S_F we have

$$M \sum_{j=1}^{k-1} |z_j|^2 + \mu \sum_{j=1}^{k} |y_k|^2 \ge \frac{(z_k - r)^2}{\|e\|^2} = \frac{M(z_k - r)^2}{1 + 2\frac{m_b}{m_a}} \quad (3.61)$$

as long as $z_k \ge r$, which yields the desired bound on α.

Similarly to the previous case, in $\operatorname{supp} G_r$ the coordinate x_k^b is of similar magnitude as the largest of the other coordinates x_j^b. We have

$$\begin{aligned}
\operatorname{supp} G_r &\subset \left\{ (z,y) \in Q_k \times \mathbb{R}^{d-k} | 2r \le \max_{1\le j\le k-1} \{ z_j - \frac{m_a}{M} y_j \} + \frac{m_a}{M} y_k - z_k \le 4r \right\} \\
&\subset \left\{ (z,y) \in Q_k \times \mathbb{R}^{d-k} | z_k + 2r \le \max_{1\le j\le k-1} \{ z_j - \frac{m_a}{M} y_j \} + \frac{m_a}{M} y_k \right\} =: S_G.
\end{aligned} \quad (3.62)$$

Analogously to before, on the set S_G we have

$$M \sum_{j=1}^{k-1} |z_j|^2 + \mu \sum_{j=1}^{k} |y_k|^2 \ge \frac{M(z_k + 2r)^2}{1 + 2\frac{m_a}{m_b}}. \quad (3.63)$$

This concludes the proof. □

Proof of Lemma 3.3. Suppose $(x^a, x^b, \tilde{y}) \in \operatorname{supp} f_{3,j}^r$. If $j < k$, we need

$$k \frac{\max\{x_{j+1}^a, ..., x_k^a\} - x_j^a}{2r} + \frac{3}{2} \le 2 \quad (3.64)$$

for the factor χ_1 to be non-zero. This is equivalent to $\max\{x_{j+1}^a, ..., x_k^a\} \le x_j^a + \frac{r}{k}$. Thus, for any $1 \le j \le k$ we have $\max\{x_j^a, ..., x_k^a\} \le x_j^a + \frac{r}{k}$ on the support of $f_{3,j}^r$. Let us argue inductively why $\max\{x_1^a, ..., x_k^a\} \le x_j^a + r$. Suppose we know for some $1 < l \le j$ that $\max\{x_l^a, ..., x_k^a\} \le x_j^a + (j + 1 - l)\frac{r}{k}$. If $x_{l-1}^a \le \max\{x_l^a, ..., x_k^a\}$, we trivially have

$\max\{x_{l-1}^a, ..., x_k^a\} \leq x_j^a + (j+1-(l-1))\frac{r}{k}$. If $x_{l-1}^a > \max\{x_l^a, ..., x_k^a\}$, for the factor $\chi_2\left(k\frac{\max\{x_l^a,...,x_k^a\}-x_{l-1}^a}{2r} + \frac{3}{2}\right)$ not to vanish we have $\max\{x_l^a, ..., x_k^a\} + \frac{r}{k} \geq x_{l-1}^a$. Thus,

$$\max\{x_{l-1}^a, ..., x_k^a\} = x_{l-1}^a \leq \max\{x_l^a, ..., x_k^a\} + \frac{r}{k} \leq x_j^a + (j+1-(l-1))\frac{r}{k}. \tag{3.65}$$

Inductively, we see that for every j we have $\max\{x_1^a, ..., x_k^a\} \leq x_j^a + j\frac{r}{k} \leq x_j^a + r$. Thus, $\operatorname{supp} f_{3,j} \cap \Omega_2 \subset \Omega_{3,j}$.

For the support of $\nabla f_{3,j}$, we have

$$\begin{aligned} &\operatorname{supp} \nabla f_{3,j}^r \cap \Omega_2 \subset \operatorname{supp} f_{3,j}^r \cap \Omega_2 \subset \Omega_{3,j} \\ &= \{(x^a, x^b, \tilde{y}) \in \Omega_2 | x_j^a \geq \max\{x_1^a, ..., \widehat{x_j^a}, ..., x_k^a\} - r\}. \end{aligned} \tag{3.66}$$

Now, suppose $x_j^a > \max\{x_1^a, ..., \widehat{x_j^a}, ..., x_k^a\} + r$. It is sufficient to show that $f_{3,j}^r \equiv 1$ in this region. For $j < k$, we have

$$k\frac{\max\{x_{j+1}^a, ..., x_k^a\} - x_j^a}{2r} + \frac{3}{2} \leq k\frac{\max\{x_1^a, ..., \widehat{x_j^a}, ..., x_k^a\} - x_j^a}{2r} + \frac{3}{2} < -\frac{k}{2} + \frac{3}{2} \leq 1. \tag{3.67}$$

Thus, $\chi_1\left(k\frac{\max\{x_{j+1}^a,...,x_k^a\}-x_j^a}{2r} + \frac{3}{2}\right) = 1$. For $l < j \leq k$, we have

$$\begin{aligned} &k\frac{\max\{x_{l+1}^a, ..., x_k^a\} - x_l^a}{2r} + \frac{3}{2} \\ &= k\frac{x_j^a - x_l^a}{2r} + \frac{3}{2} \geq k\frac{x_j^a - \max\{x_1^a, ..., \widehat{x_j^a}, ..., x_k^a\}}{2r} + \frac{3}{2} > \frac{k}{2} + \frac{3}{2} \geq 2. \end{aligned} \tag{3.68}$$

Thus, $\chi_2\left(k\frac{\max\{x_{l+1}^a,...,x_k^a\}-x_l^a}{2r} + \frac{3}{2}\right) = 1$. In total, $f_{3,j} \equiv 1$ for $x_j^a > \max\{x_1^a, ..., \widehat{x_j^a}, ..., x_k^a\} + r$. □

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Appendix A

A.1. Explicit example in one dimension

To illustrate the effect of a boundary on two-particle bound states, we present an explicit example in one dimension. We consider particles with equal masses $m_a = m_b = \frac{1}{2}$ and with delta-interaction $V(y) = -\alpha\delta(y)$ for $\alpha > 0$. The full Hamiltonian is

$$H = -\left(\frac{\partial}{\partial x^a}\right)^2 - \left(\frac{\partial}{\partial x^b}\right)^2 - \alpha\delta(x^a - x^b), \tag{A.1}$$

either on $L^2(\mathbb{R}^2)$ or on $L^2((0,\infty)^2)$ with Neumann boundary conditions. In the first case, corresponding to $k = 0$, we look at the operator $H_0 = -2\frac{\partial^2}{\partial y^2} - \alpha\delta(y)$ on $L^2(\mathbb{R})$. It has the ground state $\psi_0(y) = e^{-\frac{\alpha}{4}|y|}$ with corresponding energy $E^0 = -\frac{\alpha^2}{8}$.

The second case corresponds to $k = 1$. To compute the ground state of $H = H_1$ on $L^2((0,\infty)^2)$, we mirror the problem along the $x^a = 0$ and $x^b = 0$ boundaries, and look for the ground state of the modified Hamiltonian

$$\widetilde{H}_1 = -\left(\frac{\partial}{\partial x^a}\right)^2 - \left(\frac{\partial}{\partial x^b}\right)^2 - \alpha\delta(x^a - x^b) - \alpha\delta(x^a + x^b) \tag{A.2}$$

on $L^2(\mathbb{R}^2)$. This is exactly the operator considered in Proposition A.1. Switching to relative and center of mass coordinates $y = x^a - x^b$ and $z = \frac{x^a + x^b}{2}$, we obtain

$$\widetilde{H}_1 = \left(-2\frac{\partial^2}{\partial y^2} - \alpha\delta(y)\right) + \frac{1}{2}\left(-\frac{\partial^2}{\partial z^2} - \alpha\delta(z)\right). \tag{A.3}$$

The ground state of $\tilde{H}_1$ is $\widetilde{\psi}_1(y,z) = \psi_0(y)e^{-\frac{\alpha}{2}|z|}$, which decays exponentially away from the Neumann boundary. The ground state energy $E^1 = -\frac{\alpha^2}{4}$ is strictly lower than E^0.

A.2. Proof of Lemma 2.3

Let $1 \le k \le d$. First, we shall prove that the claim is true for $l = 1$, i.e.

$$\lim_{L\to\infty} \inf \sigma(H^{L,1}_{k-1}) \ge E^{k-1}. \tag{A.4}$$

In $\Omega^{L,1}_{k-1}$, the first component of y is constrained to $|y_1| < L$. Apart from that, $\Omega^{L,1}_{k-1}$ is the same as $Q_{k-1}\times\mathbb{R}^{d-k+1}$ with components 1 and k swapped. We localize in the y_1 direction, analogously to the one-dimensional case in Proposition A.5 in [6]. For this, let $\chi_1, \chi_2 : \mathbb{R} \to [0,1]$ be continuously differentiable functions satisfying $\chi_1(t) = 0$ for $t \ge 1$, $\chi_1(t) = 1$ for $t \le \frac{1}{2}$, and $\chi_1(t)^2 + \chi_2(t)^2 = 1$ for all t. Note that $c := \max\{\|(\chi_1')^2\|_\infty, \|(\chi_2')^2\|_\infty\} < \infty$. We choose the localizing functions f_j on $\Omega^{L,1}_{k-1}$ as $f_j(z_2,\dots z_k, y) = \chi_j(|y_1|/L)$. By the IMS localization formula, we have for all $\psi \in H^1(\Omega^{L,1}_{k-1})$

$$h^{L,1}_{k-1}[\psi] = h^{L,1}_{k-1}[f_1\psi] + h^{L,1}_{k-1}[f_2\psi] - \frac{1}{2\mu}\int_{\Omega^{L,1}_{k-1}} \left((\nabla f_1)^2 + (\nabla f_2)^2\right)|\psi|^2. \tag{A.5}$$

Note that $(\nabla f_j)^2 = \frac{1}{L^2}(\chi_j'(|y_1|/L))^2 \le \frac{c}{L^2}$. Since $f_2\psi$ is nonzero only for $|y_1| > L/2$, for large enough L, we have $h^{L,1}_{k-1}[f_2\psi] \ge E^{k-1}\|f_2\psi\|_2^2$ by Assumption 1.1(iii). Furthermore, since $f_1\psi$ satisfies Dirichlet boundary conditions at $|y_1| = L$, we can extend the function by zero to $y_1 \in \mathbb{R}$. Additionally, let us swap the first and the kth components and call the function obtained this way $\iota(f_1\psi)$. Note that $\iota(f_1\psi) \in H^1(Q_{k-1} \times \mathbb{R}^{d-k+1})$ and $\|\iota(f_1\psi)\|_2^2 = \|f_1\psi\|_2^2$. Therefore,

$$\frac{h_{k-1}^{L,1}[f_1\psi]}{\|f_1\psi\|_2^2} = \frac{h_{k-1}[\iota(f_1\psi)]}{\|\iota(f_1\psi)\|_2^2} \geq E^{k-1}. \tag{A.6}$$

Combining the estimates, we obtain for large L that

$$\frac{h_{k-1}^{L,1}[\psi]}{\|\psi\|^2} \geq E^{k-1}\frac{\|f_1\psi\|^2 + \|f_2\psi\|^2}{\|\psi\|_2^2} - \frac{c}{\mu L^2} = E^{k-1} - \frac{c}{\mu L^2}. \tag{A.7}$$

Hence, $\inf \sigma(H_{k-1}^{L,1}) \geq E^{k-1} - \frac{c}{\mu L^2}$ and the claim follows.

Note that for $k = 1$, $l = 1$ was the only possible case. Consider $k \geq 2$. We proceed by induction. For $l \geq 2$, assume the claim holds for $l - 1$. The strategy is to bound $h_{k-1}^{L,l}$ using $h_{k-1}^{L,l-1}$ and $h_{k-2}^{L,l-1}$. In $\Omega_{k-1}^{L,l}$, each of the first $l-1$ components are restricted to the (red) triangular domain 2 in Fig. 1. Furthermore, $y_l \in (-L, L)$ while in the z-coordinate the lth component is omitted. In the components $l+1$ to k we have the full quadrant. Recall that $\delta = M/\max\{m_a, m_b\}$. In the $(l-1)$th component, we localize such that one function has Dirichlet boundary conditions along the (red) line $z_{l-1} = L/\delta$ in Fig. 1 and the other is localized at $L/2\delta < z_{l-1} < L/\delta$, with a Dirichlet boundary at $z_{l-1} = L/2\delta$. For this, we use the functions $f_j(z_1, \ldots, \hat{z}_l, \ldots, z_k, y) = \chi_j(\delta z_{l-1}/L)$. By the IMS localization formula, we have for all $\psi \in H^1(\Omega_{k-1}^{L,l})$

$$h_{k-1}^{L,l}[\psi] = h_{k-1}^{L,l}[f_1\psi] + h_{k-1}^{L,l}[f_2\psi] - \frac{1}{2M}\int\limits_{\Omega_{k-1}^{L,l}} \left((\nabla f_1)^2 + (\nabla f_2)^2\right)|\psi|^2. \tag{A.8}$$

Note that $(\nabla f_j)^2 = \frac{\delta^2}{L^2}(\chi_j'(\delta z_{l-1}/L))^2 \leq \frac{\delta^2 c}{L^2}$. Since $f_1\psi$ satisfies Dirichlet boundary conditions along $z_{l-1} = L/\delta$, one can extend the function by zero to the quadrant Q_1 in the $(l-1)$th component. Additionally swap y_{l-1} and y_l to define $\iota_1(f_1\psi) \in H^1(\Omega_{k-1}^{L,l-1})$. Then $\|\iota_1(f_1\psi)\|_2^2 = \|f_1\psi\|_2^2$ and hence

$$\frac{h_{k-1}^{L,l}[f_1\psi]}{\|f_1\psi\|_2^2} = \frac{h_{k-1}^{L,l-1}[\iota_1(f_1\psi)]}{\|\iota_1(f_1\psi)\|_2^2} \geq \inf \sigma(H_{k-1}^{L,l-1}). \tag{A.9}$$

To estimate $h_{k-1}^{L,l}[f_2\psi]$, we localize in the y_{l-1}-direction, such that the first function satisfies Dirichlet boundary conditions at $y_{l-1} = L/2$ and the second function is nonzero only for $y_{l-1} > L/4$. For this, we use the functions $g_j(z_1, \ldots, \hat{z}_l, \ldots, z_k, y) = \chi_j(2y_{l-1}/L)$. The IMS localization formula gives

$$h_{k-1}^{L,l}[f_2\psi] = h_{k-1}^{L,l}[g_1 f_2\psi] + h_{k-1}^{L,l}[g_2 f_2\psi] - \frac{1}{2\mu}\int\limits_{\Omega_{k-1}^{L,l}} \left((\nabla g_1)^2 + (\nabla g_2)^2\right)|f_1\psi|^2, \tag{A.10}$$

where $(\nabla g_j)^2 = \frac{4}{L^2}(\chi_j'(2|y_{l-1}|/L))^2 \leq \frac{4c}{L^2}$. For L large enough, by Assumption 1.1(iii), we have $h_{k-1}^{L,l}[g_2 f_2 \psi] \geq E^{k-1}\|g_2 f_2 \psi\|_2^2$. In the $(l-1)$th component, the function $g_1 f_2 \psi$ is supported in the parallelogram $(z_{l-1}, y_{l-1}) \in (L/2\delta, L/\delta) \times (-L/2, L/2)$ and satisfies Dirichlet boundary conditions at $|y_{l-1}| = L/2$ and $z_{l-1} = L/2\delta$. We extend the function $g_1 f_2 \psi$ by zero to $y_{l-1} \in \mathbb{R}$. Then we define $\iota_2(g_1 f_2 \psi)$ on $\Omega_{k-2}^{L,l-1} \times (L/2\delta, L/\delta)$ as

$$\begin{aligned} &\iota_2(g_1 f_2 \psi)(z_1 \ldots, \hat{z}_{l-1}, \ldots z_{k-1}, y, x) \\ &\quad = g_1 f_2 \psi(z_1, \ldots, z_{l-2}, x, z_l, \ldots, z_{k-1}, y_1, \ldots, y_{l-2}, y_k, y_{l-1}, \ldots, y_{k-1}, y_{k+1}, \ldots y_d). \end{aligned} \tag{A.11}$$

Observe that $h_{k-1}^{L,l}$ now can effectively be decomposed into $h_{k-2}^{L,l-1}$ plus a Laplacian in the x-direction

$$\frac{h_{k-1}^{L,l}[g_1 f_2 \psi]}{\|g_1 f_2 \psi\|_2^2} = \frac{(h_{k-2}^{L,l-1} \otimes \mathbb{I} + \mathbb{I} \otimes q)[\iota_2(g_1 f_2 \psi)]}{\|\iota_2(g_1 f_2 \psi)\|_2^2}, \tag{A.12}$$

where q is defined on $H^1((L/2\delta, L/\delta))$ through

$$q[\varphi] = \int_{L/2\delta}^{L/\delta} \frac{1}{2M}|\varphi'(x)|^2 \mathrm{d}x. \tag{A.13}$$

Since $\inf \sigma(H_{k-2}^{L,l-1} \otimes \mathbb{I} - \frac{1}{2M}\mathbb{I} \otimes \Delta_x) \geq \inf \sigma(H_{k-2}^{L,l-1})$, we obtain

$$\frac{h_{k-1}^{L,l}[g_1 f_2 \psi]}{\|g_1 f_2 \psi\|_2^2} \geq \inf \sigma(H_{k-2}^{L,l-1}). \tag{A.14}$$

Combining all the estimates, we obtain that for large L and all $\psi \in H^1(\Omega_{k-1}^{L,l})$

$$\frac{h_{k-1}^{L,l}[\psi]}{\|\psi\|^2} \geq \min\{\inf \sigma(H_{k-1}^{L,l-1}), \inf \sigma(H_{k-2}^{L,l-1}), E^{k-1}\} - \frac{\delta^2 c}{ML^2} - \frac{4c}{\mu L^2}. \tag{A.15}$$

Taking $L \to \infty$ the claim now follows from the induction hypothesis.

A.3. Technical details

By mirroring along the $x_j^a = 0$ and $x_j^b = 0$ hyperplanes, we can relate H_k to an operator $\widetilde{H}_k$ defined in $L^2(\mathbb{R}^{d+k})$.

Proposition A.1. *Let $\widetilde{H}_k$ be the operator defined by the quadratic form*

$$\widetilde{h}_k[\psi] = \int\limits_{\mathbb{R}^{d+k}} \left(\frac{1}{2m_a} |\nabla_{x^a}\psi|^2 + \frac{1}{2m_b}|\nabla_{x^b}\psi|^2 + \frac{1}{2\mu}|\nabla_{\tilde{y}}\psi|^2 + V((|x_j^a| - |x_j^b|)_{j=1}^k, \tilde{y})|\psi|^2 \right) \mathrm{d}x^a \mathrm{d}x^b \mathrm{d}\tilde{y} \quad \text{(A.16)}$$

with domain $D[\widetilde{h}_k] = H^1(\mathbb{R}^{d+k})$. *Then* $\inf \sigma(H_k) = \inf \sigma(\widetilde{H}_k)$ *and* $\inf \sigma_{ess}(H_k) = \inf \sigma_{ess}(\widetilde{H}_k)$. *Moreover, the function* ψ_k *is a ground state of* H_k *if and only if the function*

$$\widetilde{\psi}_k(x^a, x^b, \tilde{y}) = \psi_k((|x_j^a|)_{j=1}^k, (|x_j^b|)_{j=1}^k, \tilde{y}) \quad \text{(A.17)}$$

is a ground state of $\widetilde{H}_k$.

Proof. The operator $\widetilde{H}_k$ commutes with all reflections along the $x_j^a = 0$ or $x_j^b = 0$ hyperplanes. Reflections along different hyperplanes commute as well. Therefore, the Hilbert space $\mathbb{H} = L^2(\mathbb{R}^{d+k})$ splits into subspaces $\mathbb{H} = \bigoplus_r \mathbb{H}_r$ characterized by the eigenvalues ± 1 of these reflections. We can write $\widetilde{H}_k = \bigoplus_r \widetilde{H}_k^r$, where $\widetilde{H}_k^r$ is the restriction of $\widetilde{H}_k$ to $\mathbb{H}_r$. For the spectrum, we obtain $\inf \sigma(\widetilde{H}_k) = \min_r \inf \sigma(\widetilde{H}_k^r)$ and $\inf \sigma_{\text{ess}}(\widetilde{H}_k) = \min_r \inf \sigma_{\text{ess}}(\widetilde{H}_k^r)$.

The subspace that is symmetric under all reflections corresponds to Neumann boundary conditions on $[0, \infty)^{2k} \times \mathbb{R}^{d-k}$. The other subspaces $\mathbb{H}_r$ are antisymmetric under at least one reflection, so they have Dirichlet boundary conditions along the corresponding hyperplane. Thus, the domains of the quadratic forms for $\widetilde{H}_k^r$ satisfy $D[h_k^r] \subset D[h_k^{\text{sym}}]$. By the min-max principle, $E_n(\widetilde{H}_k^r) \geq E_n(\widetilde{H}_k^{\text{sym}})$. Therefore, both $\inf \sigma(\widetilde{H}_k) = \inf \sigma(\widetilde{H}_k^{\text{sym}})$ and $\inf \sigma_{\text{ess}}(\widetilde{H}_k) = \inf \sigma_{\text{ess}}(H_k^{\text{sym}})$.

Note that the map $U : L^2([0, \infty)^{2k} \times \mathbb{R}^{d-k}) \to L^2_{\text{sym}}(\mathbb{R}^{d+k})$ that maps ψ to $\widetilde{\psi}(x^a, x^b, \tilde{y}) = \frac{1}{2^k}\psi((|x_j^a|)_j, (|x_j^b|)_j, \tilde{y})$ is unitary. Since $\widetilde{H}_k^{\text{sym}} = UH_kU^{-1}$, the operators are unitarily equivalent and $\sigma(\widetilde{H}_k^{\text{sym}}) = \sigma(H_k)$. □

The next lemma follows from the Sobolev inequality, see e.g. Sections 8.8 and 11.3 in [10].

Lemma A.2. *Let* $\Omega \subset \mathbb{R}^d$ *be a domain satisfying the cone property (as defined in [10]) with radius* R *and opening angle* θ. *Let* V *satisfy Assumption 1.1(i). Then, for any* $0 < a < 1$ *there is a constant* $b \in \mathbb{R}$ *(depending only on* d, R, θ, V *and* a*) such that*

$$\int\limits_{\Omega} |V||f|^2 \leq a\|\nabla f\|^2_{L^2(\Omega)} + b\|f\|^2_{L^2(\Omega)}, \quad \text{(A.18)}$$

for all $f \in H^1(\Omega)$.

Proposition A.3. *Let* $0 \leq k \leq d$. *Assumption 1.1(i) implies that in the quadratic form* h_k *in* (1.4) *the interaction term is infinitesimally form bounded with respect to the kinetic* *energy. By the KLMN theorem, there is a unique self-adjoint operator H_k corresponding to h_k, and both h_k and H_k are bounded from below.*

Proof. The quadratic form $q_k : H^1([0,\infty)^{2k} \times \mathbb{R}^{d-k}) \to \mathbb{R}$ given by

$$q_k[\psi] = \int\limits_{[0,\infty)^{2k}\times\mathbb{R}^{d-k}} \left(\frac{1}{2m_a} |\nabla_{x^a}\psi|^2 + \frac{1}{2m_b} |\nabla_{x^b}\psi|^2 + \frac{1}{2\mu} |\nabla_y \psi|^2 \right) \mathrm{d}x^a \mathrm{d}x^b \mathrm{d}\tilde{y} \tag{A.19}$$

is closed and bounded from below. In order to apply the KLMN theorem, we need to show that there are constants $a < 1, b \in \mathbb{R}$ such that for all $\psi \in H^1([0,\infty)^{2k} \times \mathbb{R}^{d-k})$

$$K[\psi] := \left| \int\limits_{[0,\infty)^{2k}\times\mathbb{R}^{d-k}} V(x^a - x^b, \tilde{y}) |\psi|^2 \mathrm{d}x^a \mathrm{d}x^b \mathrm{d}\tilde{y} \right| \leq a q_k[\psi] + b\|\psi\|_2^2. \tag{A.20}$$

Let $\psi \in H^1([0,\infty)^{2k} \times \mathbb{R}^{d-k})$ and define $\widetilde{\psi}(x^a, x^b, \tilde{y}) = \frac{1}{2^k}\psi((|x^a_j|)_j, (|x^b_j|)_j, \tilde{y})$ for $(x^a, x^b, \tilde{y}) \in \mathbb{R}^k \times \mathbb{R}^k \times \mathbb{R}^{d-k}$. We have $\|\widetilde{\psi}\|_2^2 = \|\psi\|_2^2$ and $\|\nabla\widetilde{\psi}\|_2^2 = \|\nabla\psi\|_2^2$. Moreover, ψ and $2^k\widetilde{\psi}$ agree on $[0,\infty)^{2k} \times \mathbb{R}^{d-k}$. Hence,

$$K[\psi] \leq 4^k \int\limits_{[0,\infty)^{2k}\times\mathbb{R}^{d-k}} |V(x^a - x^b, \tilde{y})||\widetilde{\psi}(x^a, x^b, \tilde{y})|^2 \mathrm{d}x^a \mathrm{d}x^b \mathrm{d}\tilde{y}. \tag{A.21}$$

Since the integrand is nonnegative, extending the domain of integration from $[0,\infty)^{2k} \times \mathbb{R}^{d-k}$ to $\mathbb{R}^{2k} \times \mathbb{R}^{d-k}$ gives the upper bound

$$\begin{aligned} K[\psi] \leq 4^k &\int\limits_{\mathbb{R}^{2k}\times\mathbb{R}^{d-k}} |V(x^a - x^b, \tilde{y})||\widetilde{\psi}(x^a, x^b, \tilde{y})|^2 \mathrm{d}x^a \mathrm{d}x^b \mathrm{d}\tilde{y} \\ &= 4^k \int\limits_{\mathbb{R}^k\times\mathbb{R}^d} |V(y)||\widetilde{\psi}(w + (y_1, ..., y_k)/2, w - (y_1, ..., y_k)/2, \tilde{y})|^2 \mathrm{d}w\mathrm{d}y, \end{aligned} \tag{A.22}$$

where we changed to coordinates $w = \frac{x^a + x^b}{2}$ and y. For almost every $w \in \mathbb{R}^k$, the function $f(y) = \widetilde{\psi}(w + (y_1, ..., y_k)/2, w - (y_1, ..., y_k)/2, \tilde{y})$ lies in $H^1(\mathbb{R}^d)$ by Fubini's theorem. By Lemma A.2, for any $0 < \tilde{a}$ there is a constant b independent of f such that $\int_{\mathbb{R}^d} |V||f|^2 \leq \tilde{a}\|\nabla f\|_2^2 + b\|f\|_2^2$. Integrating over w then gives

$$K[\psi] \leq 4^k \left(\tilde{a} \int\limits_{\mathbb{R}^k\times\mathbb{R}^d} \left| \nabla_y \widetilde{\psi}(w + (y_1, ..., y_k)/2, w - (y_1, ..., y_k)/2, \tilde{y}) \right|^2 \mathrm{d}w\mathrm{d}y + b\|\widetilde{\psi}\|_2^2 \right). \tag{A.23}$$

For $1 \leq j \leq k$,

$$\left|\partial_{y_j}\widetilde{\psi}(w+(y_1,...,y_k)/2,w-(y_1,...,y_k)/2,\tilde{y})\right|^2$$
$$=\frac{1}{4}\left|\partial_{x_j^a}\widetilde{\psi}-\partial_{x_j^b}\widetilde{\psi}\right|^2\le\frac{1}{2}\left(\left|\partial_{x_j^a}\widetilde{\psi}\right|^2+\left|\partial_{x_j^b}\widetilde{\psi}\right|^2\right). \tag{A.24}$$

Therefore,

$$K[\psi]\le 4^k\left(\tilde{a}\|\nabla\widetilde{\psi}\|_2^2+b\|\widetilde{\psi}\|_2^2\right)=4^k\tilde{a}\|\nabla\psi\|_2^2+4^kb\|\psi\|_2^2. \tag{A.25}$$

For any $0<a<1$, pick $\tilde{a}=2^{-2k-1}\min(m_a^{-1},m_b^{-1})a$ to obtain $K[\psi]\le aq_k[\psi]+4^kb\|\psi\|_2^2$. □

Lemma A.4. *The quadratic forms defined in the proof of Proposition 2.1 in Eqs. (2.13) and (2.16) correspond to unique self-adjoint operators.*

Proof. In all cases we prove that the potential term in the quadratic form is infinitesimally bounded with respect to the kinetic energy term. The claim then follows from the KLMN theorem.

Let us begin with the quadratic form $h_{k-1}^{l,L}$ in (2.16). The idea is to use the same mirroring argument as in Proposition A.3 for the coordinate components from $l+1$ to k. In the first $l-1$ components, we extend the triangular domain in Fig. 1 via a suitable mirroring, in order to be able to apply Lemma A.2. To be precise, we define the map ϕ taking $(0,L/\delta)\times\left(-\frac{ML}{m_b\delta},\frac{ML}{m_a\delta}\right)$ to the triangular domain $\{(z,y)\in(0,L/\delta)\times\mathbb{R}|-\frac{M}{m_b}z<y<\frac{M}{m_a}z\}$ as

$$\phi(z,y)=(z,y)\qquad \text{if } x^a=z+\frac{m_b}{M}y\ge 0 \text{ and } x^b=z-\frac{m_a}{M}y\ge 0, \tag{A.26}$$

$$\phi(z,y)=\left(\frac{m_a}{M}y,\frac{M}{m_a}z\right)\qquad \text{if } x^b\le 0, \tag{A.27}$$

$$\phi(z,y)=\left(\frac{m_b}{M}y,\frac{M}{m_b}z\right)\qquad \text{if } x^a\le 0. \tag{A.28}$$

Let us use the notation $\phi=(\phi_1,\phi_2)$. Note that for a function f defined on the triangular domain, we have

$$\|f\circ\phi\|_2^2=2\|f\|_2^2, \tag{A.29}$$

where one contribution of $\|f\|_2^2$ comes from the triangular domain, and the second $\|f\|_2^2$ is the sum of the contributions with $x^b<0$ and $x^a<0$. In the region with $x^b<0$ we have

$$\int_0^{\frac{ML}{m_a\delta}} \mathrm{d}y \int_0^{\frac{m_a y}{M}} \mathrm{d}z |f(\phi(z,y))|^2 = \int_0^{\frac{ML}{m_a\delta}} \mathrm{d}y \int_0^{\frac{m_a y}{M}} \mathrm{d}z |f(m_a y/M, Mz/m_a)|^2$$
$$= \int_0^{L/\delta} \mathrm{d}\tilde{z} \int_0^{\frac{M\tilde{z}}{m_a}} \mathrm{d}\tilde{y} |f(\tilde{z},\tilde{y})|^2, \quad \text{(A.30)}$$

where we substituted $\tilde{z} = m_a y/M$ and $\tilde{y} = Mz/m_a$. Similarly, for $x^a < 0$

$$\int_{-\frac{ML}{m_b\delta}}^{0} \mathrm{d}y \int_0^{\frac{m_b y}{M}} \mathrm{d}z |f(\phi(z,y))|^2 = \int_0^{L/\delta} \mathrm{d}\tilde{z} \int_{-\frac{M\tilde{z}}{m_b}}^{0} \mathrm{d}\tilde{y} |f(\tilde{z},\tilde{y})|^2. \quad \text{(A.31)}$$

Moreover, if $f \in H^1$, then $f \circ \phi \in H^1$ by the Lipschitz continuity of ϕ.

Let us work in center of mass and relative coordinates in the first l components, and with the x^a and x^b coordinates in components $l+1$ to k. The kinetic part of $h_{k-1}^{l,L}$ is then

$$q_{k-1}^{l,L}[\psi] := \int_{\Omega_{k-1}^{l,L}} \left[\sum_{j=1}^{l-1} \left(\frac{1}{2M} |\nabla_{z_j}\psi|^2 + \frac{1}{2\mu} |\nabla_{y_j}\psi|^2 \right) + \frac{1}{2\mu} |\nabla_{y_l}\psi|^2 + \sum_{j=l+1}^{k} \left(\frac{1}{2m_a} |\nabla_{x_j^a}\psi|^2 \right.\right.$$
$$\left.\left. + \frac{1}{2m_b} |\nabla_{x_j^b}\psi|^2 \right) + \frac{1}{2\mu} |\nabla_{\tilde{y}}\psi|^2 \right] \mathrm{d}z_1 \ldots \mathrm{d}z_{l-1} \mathrm{d}x_{l+1}^a \ldots \mathrm{d}x_k^a \mathrm{d}y_1 \ldots \mathrm{d}y_l \mathrm{d}x_{l+1}^b \ldots \mathrm{d}x_k^b \mathrm{d}\tilde{y}. \quad \text{(A.32)}$$

For $\psi \in H^1(\Omega_{k-1}^{l,L})$ define $\widetilde{\psi}$ on

$$\widetilde{\Omega}_{k-1}^{l,L} := \left\{ (z_1, \ldots z_{l-1}, x_{l+1}^a, \ldots x_k^a, y_1, \ldots, y_l, x_{l+1}^b, \ldots x_k^b, \tilde{y}) | \forall j < l : z_j \in (0, L/\delta), \right.$$
$$\left. y_j \in \left(-\frac{ML}{m_b\delta}, \frac{ML}{m_a\delta} \right), y_l \in (-L,L), \forall l < j \leq k : x_j^a \in \mathbb{R}, x_j^b \in \mathbb{R}, \tilde{y} \in \mathbb{R}^{d-k} \right\} \quad \text{(A.33)}$$

as

$$\widetilde{\psi}(z,y) = \frac{1}{2^{(l-1)/2}} \frac{1}{2^{k-l}} \psi \left((\phi_1(z_j,y_j))_{j=1}^{l-1}, (|x_j^a|)_{j=l+1}^k, (\phi_2(z_j,y_j))_{j=1}^{l-1}, y_l, (|x_j^b|)_{j=l+1}^k, \tilde{y} \right). \quad \text{(A.34)}$$

By (A.29) we have $\|\widetilde{\psi}\|_2^2 = \|\psi\|_2^2$. Furthermore, $\|\nabla\widetilde{\psi}\|_2^2 \leq \left(\frac{M^2}{\min\{m_a,m_b\}^2} + 1 \right)^{l-1} \|\nabla\psi\|_2^2$.

Analogously to (A.21)-(A.22) we obtain

$$K[\psi] := \left| \int_{\Omega_{k-1}^{l,L}} V(y_1, \dots y_l, x_{l+1}^a - x_{l+1}^b, \dots x_k^a - x_k^b, \tilde{y}) |\psi|^2 \times \mathrm{d}z_1 \dots \mathrm{d}z_{l-1} \mathrm{d}x_{l+1}^a \dots \mathrm{d}x_k^a \mathrm{d}y_1 \dots \mathrm{d}y_l \mathrm{d}x_{l+1}^b \dots \mathrm{d}x_k^b \mathrm{d}\tilde{y} \right|$$

$$\leq 2^{l-1} 4^{k-l} \int_{\tilde{\Omega}_{k-1}^{l,L}} |V(y)| |\widetilde{\psi}(z_1, \dots z_{l-1}, (w_j + \frac{y_j}{2})_{j=l+1}^k, y_1, \dots, y_l, (w_j - \frac{y_j}{2})_{j=l+1}^k, \tilde{y})|^2 \times \mathrm{d}z_1 \dots \mathrm{d}z_{l-1} \mathrm{d}w_{l+1} \dots \mathrm{d}w_k \mathrm{d}y, \tag{A.35}$$

where we changed the coordinates x_j^a, x_j^b to $w_j = \frac{x^a + x^b}{2}$ and y_j. Let $D_y = \left(-\frac{ML}{m_b \delta}, \frac{ML}{m_a \delta}\right)^{l-1} \times (-L, L) \times \mathbb{R}^{d-k}$. For almost every $(z_1, \dots z_{l-1}, w_{l+1}, \dots w_k) \in (0, L/\delta)^{l-1} \times \mathbb{R}^{k-l}$, the function $f(y) = \widetilde{\psi}(z_1, \dots z_{l-1}, (w_j + \frac{y_j}{2})_{j=l+1}^k, y_1, \dots, y_l, (w_j - \frac{y_j}{2})_{j=l+1}^k, \tilde{y})$ lies in $H^1(D_y)$ by Fubini's theorem. Applying Lemma A.2 with $\Omega = D_y$ and integrating over z and w one obtains

$$K[\psi] \leq 2^{l-1} 4^{k-l} a \int_{\tilde{\Omega}_{k-1}^{l,L}} \left| \nabla_y \widetilde{\psi}(z_1, \dots z_{l-1}, (w_j + \frac{y_j}{2})_{j=l+1}^k, y_1, \dots, y_l, (w_j - \frac{y_j}{2})_{j=l+1}^k, \tilde{y}) \right|^2 \times \mathrm{d}z_1 \dots \mathrm{d}z_{l-1} \mathrm{d}w_{l+1} \dots \mathrm{d}w_k \mathrm{d}y + 2^{l-1} 4^{k-l} b \|\widetilde{\psi}\|_2^2 \tag{A.36}$$

for any $a > 0$ and a suitable constant b. As in (A.24) we have

$$K[\psi] \leq 2^{l-1} 4^{k-l} \left(a \|\nabla \widetilde{\psi}\|_2^2 + b \|\widetilde{\psi}\|_2^2 \right) \leq 2^{l-1} 4^{k-l} \left(\frac{M^2}{\min\{m_a, m_b\}^2} + 1 \right)^{l-1} a \|\nabla \psi\|_2^2 + 2^{l-1} 4^{k-l} b \|\psi\|_2^2. \tag{A.37}$$

Since a can be arbitrarily small, the interaction term is infinitesimally bounded w.r.t. $q_{k-1}^{l,L}$.

Let us now consider the quadratic form a_l in (2.13). For $l = k+2$, the potential term is bounded from below since $|y| > L$, and is hence infinitesimally bounded w.r.t. the kinetic energy.

The kinetic part of a_l is

$$q_l[\psi] := \int_{\Omega_l} \left[\sum_{j=1}^{l} \left(\frac{1}{2M} |\nabla_{z_j} \psi|^2 + \frac{1}{2\mu} |\nabla_{y_j} \psi|^2 \right) + \sum_{j=l+1}^{k} \left(\frac{1}{2m_a} |\nabla_{x_j^a} \psi|^2 + \frac{1}{2m_b} |\nabla_{x_j^b} \psi|^2 \right) \right.$$

$$+ \frac{1}{2\mu}|\nabla_{\tilde{y}}\psi|^2 \Bigg] \mathrm{d}z_1 \dots \mathrm{d}z_l \mathrm{d}x^a_{l+1} \dots \mathrm{d}x^a_k \mathrm{d}y_1 \dots \mathrm{d}y_l \mathrm{d}x^b_{l+1} \dots \mathrm{d}x^b_k \mathrm{d}\tilde{y}. \quad \text{(A.38)}$$

First, we consider $1 \leq l \leq k$. Then, a_l is closely related to $h^{l,L}_{k-1}$ through (2.17). Let $\psi \in H^1(\Omega_l)$. For every $z_l \in (L/\delta, \infty)$, the function $\psi(\cdot, \dots, z_l, \dots, \cdot)$ belongs to $H^1(\Omega^{l,L}_{k-1})$. In (A.35)-(A.37), we saw that for any $a > 0$ there is a constant b such that

$$\int_{\Omega^{l,L}_{k-1}} |V(y)|\,|\psi(z,y)|^2 \mathrm{d}y \mathrm{d}z_1 \dots \widehat{\mathrm{d}z_l} \dots \mathrm{d}z_k$$

$$\leq a q^{l,L}_{k-1}[\psi(\cdot, z_l, \cdot)] + b \int |\psi(z,y)|^2 \mathrm{d}y \mathrm{d}z_1 \dots \widehat{\mathrm{d}z_l} \dots \mathrm{d}z_k. \quad \text{(A.39)}$$

Integrating the inequality over z_l, we obtain

$$\int_{\Omega_l} |V(y)||\psi(z,y)|^2 \mathrm{d}y \mathrm{d}z \leq a \int_{L/\delta}^{\infty} q^{l,L}_{k-1}[\psi(\cdot, z_l, \cdot)] \mathrm{d}z_l + b\|\psi\|_2^2 \leq a q_l[\psi] + b\|\psi\|_2^2. \quad \text{(A.40)}$$

Hence, the potential term is infinitesimally bounded w.r.t. q_l.

For $l = k+1$, we use the map ϕ in the first k components. For $\psi \in H^1(\Omega_{k+1})$ define $\widetilde{\psi}$ on

$$\widetilde{\Omega}_{k+1} := (0, L/\delta)^k \times \left(-\frac{ML}{m_b\delta}, \frac{ML}{m_a\delta}\right)^k \times (-L, L)^{d-k} \quad \text{(A.41)}$$

as

$$\widetilde{\psi}(z,y) = \frac{1}{2^{k/2}} \psi\left((\phi_1(z_j, y_j))_{j=1}^k, (\phi_2(z_j, y_j))_{j=1}^k, \tilde{y}\right). \quad \text{(A.42)}$$

By (A.29) we have $\|\widetilde{\psi}\|_2^2 = \|\psi\|_2^2$. Furthermore, $\|\nabla\widetilde{\psi}\|_2^2 \leq \left(\frac{M^2}{\min\{m_a, m_b\}^2} + 1\right)^k \|\nabla\psi\|_2^2$. Analogously to (A.21)-(A.22) we obtain

$$K[\psi] := \left| \int_{\Omega_{k+1}} V(y)|\psi(z,y)|^2 \mathrm{d}z \mathrm{d}y \right| \leq 2^k \int_{\widetilde{\Omega}_{k+1}} |V(y)||\widetilde{\psi}(z,y)|^2 \mathrm{d}z \mathrm{d}y. \quad \text{(A.43)}$$

Let $D_y = \left(-\frac{ML}{m_b\delta}, \frac{ML}{m_a\delta}\right)^k \times (-L, L)^{d-k}$. For almost every $z \in (0, L/\delta)^k$, the function $f(y) = \widetilde{\psi}(z,y)$ lies in $H^1(D_y)$ by Fubini's theorem. Applying Lemma A.2 with $\Omega = D_y$ and integrating over z gives

$$K[\psi] \le 2^k a \int\limits_{\tilde{\Omega}_{k+1}} \left|\nabla_y \widetilde{\psi}(z,y)\right|^2 \mathrm{d}z\mathrm{d}y + 2^k b\|\widetilde{\psi}\|_2^2 \le 2^k a\|\nabla\widetilde{\psi}\|_2^2 + 2^k b\|\widetilde{\psi}\|_2^2 \tag{A.44}$$

for any $a > 0$ and a suitable constant b. Hence,

$$K[\psi] \le 2^k \left(\frac{M^2}{\min\{m_a, m_b\}^2} + 1\right)^k a\|\nabla\psi\|_2^2 + 2^k b\|\psi\|_2^2. \tag{A.45}$$

Since a can be arbitrarily close to zero, the interaction term is infinitesimally bounded w.r.t. q_{k+1}. □

Lemma A.5. *The quadratic forms defined in the proof of Theorem 1.4 in Eqs. (3.12), (3.18), (3.27), (3.33), (3.39), (3.46) and (3.51) correspond to unique self-adjoint operators.*

Proof. The quadratic forms a_j with $j \in \{1, 2, 4, 5\}$ in Eqs. (3.12) and (3.33) and the forms $a_{3,j}$ for $1 \le j \le k$ in (3.27) have the form

$$a_j[\varphi] = \int\limits_{\Omega_j} \Bigg(\frac{1}{2m_a}|\nabla_{x^a}\varphi|^2 + \frac{1}{2m_b}|\nabla_{x^b}\varphi|^2 + \frac{1}{2\mu}|\nabla_{\tilde{y}}\varphi|^2 + \left(V(x^a - x^b, \tilde{y}) + V_\infty(x^a, x^b, \tilde{y})\right)|\varphi|^2\Bigg)\mathrm{d}x^a\mathrm{d}x^b\mathrm{d}\tilde{y} \tag{A.46}$$

for some bounded potential V_∞. The quadratic form $q_j : H^1(\Omega_j) \to \mathbb{R}$ given by

$$q_j[\varphi] = \int\limits_{\Omega_j} \left(\frac{1}{2m_a}|\nabla_{x^a}\varphi|^2 + \frac{1}{2m_b}|\nabla_{x^b}\varphi|^2 + \frac{1}{2\mu}|\nabla_{\tilde{y}}\varphi|^2\right)\mathrm{d}x^a\mathrm{d}x^b\mathrm{d}\tilde{y} \tag{A.47}$$

is closed and bounded from below. Using that $\varphi \in D[a_j]$ vanishes outside $\overline{\Omega_j}$ and applying Proposition A.3, we obtain

$$\left|\int\limits_{\Omega_j} V(x^a - x^b, \tilde{y}) + V_\infty(x^a, x^b, \tilde{y})|\varphi|^2\right| \le \left|\int\limits_{Q_k\times\mathbb{R}^{d-k}} V(y)|\varphi|^2\right| + \|V_\infty\|_\infty\|\varphi\|_2^2 \le a q_j[\varphi] + (b + \|V_\infty\|_\infty)\|\varphi\|_2^2 \tag{A.48}$$

for some $a < 1$ and $b \in \mathbb{R}$. By the KLMN theorem, there is a unique self-adjoint operator A_j corresponding to a_j.

For $\hat{a}_4$ in (3.39), note that K_R is bounded. Adapting the argument in Proposition A.3, we show that the interaction term is infinitesimally bounded with respect to the kinetic part $\hat{q} : H^1(((0,\infty)^{k-1} \times \mathbb{R})^2 \times \mathbb{R}^{d-k}) \to \mathbb{R}$ given by

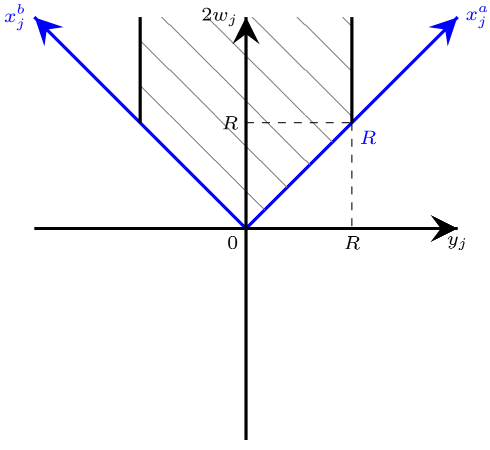

Fig. A.4. In the domain of ψ for $1 \le j \le k$, the coordinates (x^a_j, x^b_j) lie in the hatched set. We have $y_j = x^a_j - x^b_j$ and $w_j = \frac{x^a_j + x^b_j}{2}$.

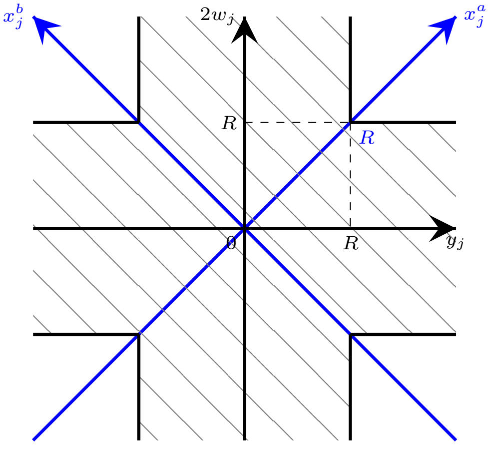

Fig. A.5. Mirroring ψ along $x^a_j = 0$ and $x^b_j = 0$ defines $\tilde{\psi}$. For $1 \le j \le k$, the coordinates (x^a_j, x^b_j) or equivalently (w_j, y_j) lie in the hatched set.

$$\hat{q}[\varphi] = \int_{\hat{\Omega}_4} \left(\frac{1}{2m_a} |\nabla_{x^a} \varphi|^2 + \frac{1}{2m_b} |\nabla_{x^b} \varphi|^2 + \frac{1}{2\mu} |\nabla_{\tilde{y}} \varphi|^2 \right) \mathrm{d}x^a \mathrm{d}x^b \mathrm{d}\tilde{y}. \tag{A.49}$$

For $\psi \in H^1(\hat{\Omega}_4)$, define $\widetilde{\psi}(x^a, x^b, \tilde{y}) = \frac{1}{2^{k-1}} \psi((|x^a_j|)_{j=1}^{k-1}, x^a_k, (|x^b_j|)_{j=1}^{k-1}, x^b_k, \tilde{y})$ for $(x^a, x^b, \tilde{y}) \in \mathbb{R}^k \times \mathbb{R}^k \times \mathbb{R}^{d-k}$. We have $\|\widetilde{\psi}\|_2^2 = \|\psi\|_2^2$ and $\|\nabla \widetilde{\psi}\|_2^2 = \|\nabla \psi\|_2^2$. Following the same steps as in Proposition A.3 from (A.21)-(A.25) with this adapted choice of $\tilde{\psi}$, we obtain that for any $0 < a$ there is a b such that

$$K[\psi] := \left| \int_{\hat{\Omega}_4} V(x^a - x^b, \tilde{y}) |\psi|^2 \mathrm{d}x^a \mathrm{d}x^b \mathrm{d}\tilde{y} \right| \le 4^{k-1} \left(a \|\nabla \widetilde{\psi}\|_2^2 + b \|\widetilde{\psi}\|_2^2 \right)$$
$$= 4^{k-1} a \|\nabla \psi\|_2^2 + 4^k b \|\psi\|_2^2. \tag{A.50}$$

By the KLMN theorem, $\hat{a}_4$ corresponds to a self-adjoint operator. Since b_1 in (3.46) differs from $\hat{a}_4$ by a bounded term, it also corresponds to a self-adjoint operator. For b_2 in (3.51) and $a_{1,\text{ext}}$ in (3.18), the potential is bounded. Thus, these forms also correspond to self-adjoint operators.

For $a_{1,\text{int}}$ in (3.18), we proceed similarly to Proposition A.3. Let $\psi \in D[a_{1,\text{int}}]$. The domain of ψ is sketched in Fig. A.4. Mirroring the domain along the $x^a_j = 0$ and $x^b_j = 0$ hyperplanes, we obtain the set $\tilde{\Omega}$ sketched in Fig. A.5. For $(x^a, x^b, \tilde{y}) \in \tilde{\Omega}$ define $\tilde{\psi}(x^a, x^b, \tilde{y}) = \frac{1}{2^k} \psi((|x^a_j|)_j, (|x^b_j|)_j, \tilde{y})$. We have $\|\tilde{\psi}\|_2^2 = \|\psi\|_2^2$ and $\|\nabla \tilde{\psi}\|_2^2 = \|\nabla \psi\|_2^2$. Using the triangle inequality and enlarging the domain of integration to $\tilde{\Omega}$, we have

$$K[\psi] := \left| \int_{\Omega_{1,\mathrm{int}}} V(x^a - x^b, \tilde{y}) |\psi(x^a, x^b, \tilde{y})|^2 \mathrm{d}x^a \mathrm{d}x^b \mathrm{d}\tilde{y} \right|$$
$$\leq 4^k \int_{\tilde{\Omega}} |V(x^a - x^b, \tilde{y})| |\tilde{\psi}(x^a, x^b, \tilde{y})|^2 \mathrm{d}x^a \mathrm{d}x^b \mathrm{d}\tilde{y}. \quad \text{(A.51)}$$

We change to coordinates $w = \frac{x^a + x^b}{2}$ and y. For every $w \in \mathbb{R}^k$, the set

$$\Omega_w = \{ \, y \in \mathbb{R}^d | (w + (y_1, ..., y_k)/2, w - (y_1, ..., y_k)/2, \tilde{y}) \in \tilde{\Omega} \} \quad \text{(A.52)}$$

is equal to $I_1 \times ... \times I_k \times \mathbb{R}^{d-k}$, where each $I_j \in \{\mathbb{R}, (-R, R)\}$ (Fig. A.5). Thus, there is an angle θ and radius r such that all the sets Ω_w satisfy the cone property with parameters θ, r. For almost every $w \in \mathbb{R}^k$, the function $f(y) = \widetilde{\psi}(w + (y_1, ..., y_k)/2, w - (y_1, ..., y_k)/2, \tilde{y})$ lies in $H^1(\Omega_w)$. By Lemma A.2, for any $0 < \tilde{a}$ there is a constant b independent of f_w and w such that

$$\int_{\Omega_w} |V(y)| |f(y)|^2 \mathrm{d}y \leq \tilde{a} \|\nabla f\|_2^2 + b \|f\|_2^2. \quad \text{(A.53)}$$

Integrating inequality (A.53) over w and using (A.24) gives

$$\int_{\tilde{\Omega}} |V(x^a - x^b, \tilde{y})| |\widetilde{\psi}(x^a, x^b, \tilde{y})|^2 \mathrm{d}x^a \mathrm{d}x^b \mathrm{d}\tilde{y} \leq \tilde{a} \|\nabla_y \widetilde{\psi}\|^2 + b \|\widetilde{\psi}\|_2^2 \leq \tilde{a} \|\nabla \widetilde{\psi}\|^2 + b \|\widetilde{\psi}\|_2^2. \quad \text{(A.54)}$$

In total, we thus have

$$K[\psi] \leq 4^k \tilde{a} \|\nabla \psi\|_2^2 + 4^k b \|\psi\|_2^2. \quad \text{(A.55)}$$

For any $0 < a < 1$, pick $\tilde{a} = 2^{-2k-1} \min(m_a^{-1}, m_b^{-1}) a$ to obtain $K[\psi] \leq a q_{1,\mathrm{int}}[\psi] + 4^k b \|\psi\|_2^2$. The KLMN theorem thus implies that there is a self-adjoint $A_{1,\mathrm{int}}$, which is bounded from below. □

Appendix B. Exponential decay of Schrödinger eigenfunctions (by Rupert L. Frank[1])

It is a folklore theorem that eigenfunctions of Schrödinger operators corresponding to eigenvalues below the bottom of their essential spectrum decay exponentially. This was

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raised to high art by Agmon [2] and others; see, for instance, the review [12]. It may be of interest to note that the most basic one of these bounds holds under rather minimal assumptions of the potential. This is what we record here.

Let $V \in L^1_{\mathrm{loc}}(\mathbb{R}^d)$ be real and set $V_\pm := \max\{\pm V, 0\}$. Given $\alpha \in [0,1]$, we say that V_- is $-\Delta$-form bounded with form bound α if there is a $C_\alpha < \infty$ such that

$$\int_{\mathbb{R}^d} V_-|\psi|^2\, dx \le \alpha \int_{\mathbb{R}^d} |\nabla\psi|^2\, dx + C_\alpha \int_{\mathbb{R}^d} |\psi|^2\, dx \qquad \text{for all } \psi \in H^1(\mathbb{R}^d)\,.$$

In this case, we define a quadratic form h by

$$D[h] := \left\{ \psi \in H^1(\mathbb{R}^d) : \int_{\mathbb{R}^d} V_+|\psi|^2\, dx < \infty \right\},$$

$$h[\psi] := \int_{\mathbb{R}^d} \left(|\nabla\psi|^2 + V|\psi|^2 \right) dx \qquad \text{for } \psi \in D[h]\,.$$

This quadratic form is lower semibounded in $L^2(\mathbb{R}^d)$ and, if $\alpha < 1$, closed. Thus, it corresponds to a selfadjoint, lower semibounded operator, which we denote by $-\Delta + V$. We abbreviate

$$E_\infty := \inf \sigma_{\mathrm{ess}}(-\Delta + V) \in \mathbb{R} \cup \{+\infty\}.$$

Theorem B.1. *Assume that $V_+ \in L^1_{\mathrm{loc}}(\mathbb{R}^d)$ and that V_- is $-\Delta$-form bounded with bound < 1. For every $E' < E_\infty$ there is a constant $C_{E'} < \infty$ such that if $E \le E'$ and if $\psi \in D(-\Delta + V)$ satisfies $(-\Delta + V)\psi = E\psi$, then*

$$\int_{\mathbb{R}^d} e^{2\sqrt{E'-E}\,|x|} \left(|\nabla\psi|^2 + V_+|\psi|^2 + (E'-E)|\psi|^2 \right) dx \le C_{E'}\, \|\psi\|^2\,. \tag{B.1}$$

We emphasize that E_∞ may be equal to $+\infty$, in which case E' may be taken arbitrarily large. If $E_\infty < \infty$, the decay exponent $\sqrt{E'-E}$ can be any number $< \sqrt{E_\infty - E}$.

Note that under the assumptions of the theorem, ψ is not necessarily bounded, so one cannot expect pointwise exponential decay bounds. The bounds in the theorem control the quantities that are natural from the definition of the operator in the form sense.

In order to prove Theorem B.1, we use a geometric characterization of the bottom of the essential spectrum due to Persson [11]. Let $K \subset \mathbb{R}^d$ be a compact set and define

$$E_1(-\Delta + V|_{\mathbb{R}^d\setminus K}) = \inf \left\{ \frac{h[\psi]}{\|\psi\|^2} :\ \psi \in D[h],\, \psi \equiv 0 \text{ on } K \right\}.$$

Clearly, $E_1(-\Delta + V|_{\mathbb{R}^d\setminus K})$ is nondecreasing in K and therefore its supremum over all compact $K \subset \mathbb{R}^d$ exists in $\mathbb{R} \cup \{+\infty\}$.

Theorem B.2. *Assume that $V_+ \in L^1_{\mathrm{loc}}(\mathbb{R}^d)$ and that V_- is $-\Delta$-form bounded with bound < 1. Then*

$$E_\infty = \sup_{K \subset \mathbb{R}^d \text{ compact}} E_1(-\Delta + V|_{\mathbb{R}^d \setminus K}) .$$

We first assume Theorem B.2 and show how it implies Theorem B.1. Then we will provide a proof of Theorem B.2 under our assumptions on V.

Proof of Theorem B.1. Fix $E_\infty > E'' > E'$. By Theorem B.2, there is an $R' > 0$ such that

$$h[u] \geq E'' \|u\|^2$$

for all $u \in D[h]$ with $u \equiv 0$ in $\overline{B_{R'/2}}$. Next, for an $R > 0$ to be specified, we choose two smooth, real-valued functions $\chi_<$ and $\chi_>$ on $\mathbb{R}^d$ such that

$$\operatorname{supp} \chi_< \subset \overline{B_{2R}} \quad \text{and} \quad \operatorname{supp} \chi_> \subset \mathbb{R}^d \setminus B_R \tag{B.2}$$

and such that $\chi_<^2 + \chi_>^2 \equiv 1$ on $\mathbb{R}^d$. By scaling an R-independent quadratic partition of unity, we may assume that

$$|\nabla \chi_<|^2 + |\nabla \chi_>|^2 \leq C R^{-2} \tag{B.3}$$

with a constant C independent of R. By increasing R' if necessary, we can make sure that $C(R')^{-2} \leq (E'' - E')/2 =: \epsilon$ with C from (B.3). Let $f : \mathbb{R}^d \to \mathbb{R}$ be a bounded Lipschitz function and take $\varphi = e^{2f}\psi \in D[h]$ as a trial function in the quadratic form version of the equation $(-\Delta + V)\psi = E\psi$ to obtain, after an integration by parts,

$$E \int_{\mathbb{R}^d} e^{2f} |\psi|^2 \, dx = \int_{\mathbb{R}^d} \left(|\nabla(e^f \psi)|^2 + (V - |\nabla f|^2)|e^f \psi|^2 \right) dx . \tag{B.4}$$

Thus, in view of the IMS formula (see, e.g., [5, Theorem 3.2]),

$$\begin{aligned} E \int_{\mathbb{R}^d} |e^f \chi_< \psi|^2 \, dx + E \int_{\mathbb{R}^d} |e^f \chi_> \psi|^2 \, dx &= \int_{\mathbb{R}^d} \left(|\nabla(e^f \chi_< \psi)|^2 + \tilde{V} |e^f \chi_< \psi|^2 \right) dx \\ &\quad + \int_{\mathbb{R}^d} \left(|\nabla(e^f \chi_> \psi)|^2 + \tilde{V} |e^f \chi_> \psi|^2 \right) dx \end{aligned}$$

with $\tilde{V} := V - |\nabla f|^2 - |\nabla \chi_<|^2 - |\nabla \chi_>|^2$. For $R \geq R'$ we bound the terms on the right side from below by

$$\int_{\mathbb{R}^d} \left(|\nabla(e^f \chi_< \psi)|^2 + \tilde{V}|e^f \chi_< \psi|^2\right) dx \geq \left(E_1 - \|\nabla f\|_\infty^2 - \epsilon\right) \int_{\mathbb{R}^d} |e^f \chi_< \psi|^2 \, dx$$

with $E_1 := \inf \sigma(-\Delta + V)$, and

$$\int_{\mathbb{R}^d} \left(|\nabla(e^f \chi_> \psi)|^2 + \tilde{V}|e^f \chi_> \psi|^2\right) dx \geq \left(E'' - \|\nabla f\|_\infty^2 - \epsilon\right) \int_{\mathbb{R}^d} |e^f \chi_> \psi|^2 \, dx \,.$$

Thus,

$$\left(E'' - E - \|\nabla f\|_\infty^2 - \epsilon\right) \int_{\mathbb{R}^d} |e^f \chi_> \psi|^2 \, dx \leq \left(E - E_1 + \|\nabla f\|_\infty^2 + \epsilon\right) \int_{\mathbb{R}^d} |e^f \chi_< \psi|^2 \, dx \,,$$

and therefore

$$\begin{aligned}\left(E'' - E - \|\nabla f\|_\infty^2 - \epsilon\right) \int_{\mathbb{R}^d} |e^f \psi|^2 \, dx &\leq (E'' - E_1) \int_{\mathbb{R}^d} |e^f \chi_< \psi|^2 \, dx \\ &\leq (E'' - E_1) \, \|\psi\|^2 \, \sup_{B_R} e^{2f} \,.\end{aligned}$$

Ideally, we would want to choose $f(x) = \kappa|x|$ with κ as large as possible. The wish to have a positive constant (ϵ, say) in front of the integral on the left side then dictates our choice $\kappa = \sqrt{E'' - E - 2\epsilon} = \sqrt{E' - E}$. The problem with this 'ideal' choice of f is that the function $|x|$ is Lipschitz, but not bounded. We remedy this by taking $|x|/(1 + \delta|x|)$ instead and proving bounds which are uniform in the parameter $\delta > 0$, which we will let tend to zero at the end. Thus, let us choose

$$f(x) := \sqrt{E' - E} \, \frac{|x|}{1 + \delta|x|}$$

with a (small) parameter $\delta > 0$. This is a Lipschitz function satisfying $\|\nabla f\|_\infty = \sqrt{E' - E}$. Thus, the previous inequality with $R = R'$ becomes

$$\epsilon \int_{\mathbb{R}^d} |e^f \psi|^2 \, dx \leq (E'' - E_1) \, \|\psi\|^2 \; e^{2R'\sqrt{E'-E}} \,.$$

Since the right side is independent of δ, we can take the limit $\delta \to 0$ and obtain by monotone convergence

$$\epsilon \int_{\mathbb{R}^d} |e^{\sqrt{E'-E}|x|} \psi|^2 \, dx \leq (E'' - E_1) \, \|\psi\|^2 \; e^{2R'\sqrt{E'-E}} \,.$$

This is already one of the inequalities claimed in the theorem.

To prove boundedness of the terms involving the gradient term and V_+ we recall that, by form boundedness,

$$h[e^f\psi] \geq (1-\alpha)\int_{\mathbb{R}^d} |\nabla(e^f\psi)|^2\,dx + \int_{\mathbb{R}^d} V_+|e^f\psi|^2\,dx - C_\alpha \int_{\mathbb{R}^d} |e^f\psi|^2\,dx\,.$$

This, together with identity (B.4), implies

$$\big(E + \|\nabla f\|_\infty^2 + C_\alpha\big)\int_{\mathbb{R}^d} |e^f\psi|^2\,dx \geq (1-\alpha)\int_{\mathbb{R}^d} |\nabla(e^f\psi)|^2\,dx + \int_{\mathbb{R}^d} V_+|e^f\psi|^2\,dx\,.$$

Using

$$\begin{aligned}|\nabla(e^f\psi)|^2 &= e^{2f}|\nabla\psi + \psi\nabla f|^2 = e^{2f}\left(|\nabla\psi|^2 + 2\,\mathrm{Re}\,\overline{\psi}\nabla\psi\cdot\nabla f + |\psi|^2|\nabla f|^2\right)\\ &\geq e^{2f}\left(\frac{1}{2}|\nabla\psi|^2 - |\psi|^2|\nabla f|^2\right),\end{aligned}$$

we obtain

$$\big(E + (2-\alpha)\|\nabla f\|_\infty^2 + C_\alpha\big)\int_{\mathbb{R}^d} |e^f\psi|^2\,dx \geq \frac{1-\alpha}{2}\int_{\mathbb{R}^d} |e^f\nabla\psi|^2\,dx + \int_{\mathbb{R}^d} V_+|e^f\psi|^2\,dx\,.$$

Since we have already shown an upper bound on the left side, this completes the proof of the theorem. □

Thus, we are left with proving Theorem B.2. We use the following abstract characterization of the essential spectrum.

Lemma B.3. *Let a be a lower semibounded, closed quadratic form in a Hilbert space and A the corresponding self-adjoint operator. Then*

$$\inf\sigma_{\mathrm{ess}}(A) = \inf\left\{\liminf_{j\to\infty} a[\xi_j]:\ \xi_j \rightharpoonup 0\,,\ \|\psi_j\| = 1\right\}$$

(with the convention that $\inf\emptyset = +\infty$). Moreover, if both sides are finite, then there is a sequence (ξ_j) with $\|\xi_j\| = 1$, $a[\xi_j] \to \inf\sigma_{\mathrm{ess}}(A)$ and $\xi_j \rightharpoonup 0$ in $D[a]$.

This lemma is classical. The proof in [8, Lemma 1.20] shows the first assertion and, in the case of finiteness, the existence of a normalized sequence with $a[\xi_j] \to \inf\sigma_{\mathrm{ess}}(A)$ and $\xi_j \rightharpoonup 0$. Since this sequence is bounded in $D[a]$, a subsequence converges weakly in $D[a]$ and, since $D[a]$ is continuously embedded into the Hilbert space, the weak limit is necessarily zero, as claimed.

Proof of Theorem B.2. We abbreviate $E'_\infty := \sup_{K \text{ compact}} E_1(-\Delta + V|_{\mathbb{R}^d\setminus K})$.

We begin by proving $E_\infty \geq E'_\infty$. We may assume that $E_\infty < \infty$ and we shall show that for all $R > 0$,

$$E_1(-\Delta + V|_{B_R^c}) \leq E_\infty \,, \tag{B.5}$$

for then the claimed inequality follows as $R \to \infty$. Fix $R > 0$ and let $\chi_<$ and $\chi_>$ be as in the proof of Theorem B.1. By Lemma B.3, there is a sequence $(\xi_j) \subset D[h]$ with $\|\xi_j\| = 1$ such that $\xi_j \rightharpoonup 0$ in $D[h]$ and $h[\xi_j] \to E_\infty$. Then

$$E_1(-\Delta + V|_{B_R^c}) \leq h\left[\frac{\chi_>\xi_j}{\|\chi_>\xi_j\|}\right] \tag{B.6}$$

and our goal is to estimate the right side as $j \to \infty$.

By Rellich's compactness theorem, $\xi_j \to 0$ in $L^2_{\mathrm{loc}}(\mathbb{R}^d)$, so $\chi_<\xi_j \to 0$ in $L^2(\mathbb{R}^d)$ and

$$\|\chi_>\xi_j\|^2 = \|\xi_j\|^2 - \|\chi_<\xi_j\|^2 \to 1 \qquad \text{as } j \to \infty \,. \tag{B.7}$$

Moreover, by the IMS formula,

$$h\left[\chi_>\xi_j\right] = h\left[\xi_j\right] - h\left[\chi_<\xi_j\right] + \left\| \left(|\nabla\chi_<|^2 + |\nabla\chi_>|^2\right)^{1/2} \xi_j \right\|^2 . \tag{B.8}$$

The last term vanishes as $j \to \infty$ again by Rellich's theorem. Moreover,

$$h\left[\chi_<\xi_j\right] \geq E_1\|\chi_<\xi_j\|^2$$

and therefore

$$\liminf_{j\to\infty} h\left[\chi_<\xi_j\right] \geq \liminf_{j\to\infty} E_1\|\chi_<\xi_j\|^2 = 0 \,.$$

Putting this into (B.8), we learn that

$$\limsup_{j\to\infty} h\left[\chi_>\xi_j\right] \leq \limsup_{j\to\infty} h\left[\xi_j\right] = E_\infty \,.$$

This, together with (B.6) and (B.7), yields (B.5).

We now prove the converse inequality $E_\infty \leq E'_\infty$. Let $(R_j) \subset (0, \infty)$ be a sequence with $R_j \to \infty$ and let $(\psi_j) \subset D[h]$ be a sequence with $\|\psi_j\| = 1$, $\psi_j \equiv 0$ in $\{|x| < R_j\}$ and $h[\psi_j] - E_1(-\Delta + V|_{B_{R_j}^c}) \to 0$. The support condition implies that $\psi_j \rightharpoonup 0$ in $L^2(\mathbb{R}^d)$ and therefore, by Lemma B.3,

$$E_\infty \leq \liminf_{j\to\infty} h[\psi_j] = \liminf_{j\to\infty} E_1(-\Delta + V|_{B_{R_j}^c}) \leq E'_\infty \,,$$

which proves the theorem. $\square$

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