HARTREE PROBLEM IN A DOUBLE WELL

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ABSTRACT. We consider a non-linear Hartree energy for bosonic particles in a symmetric double-well potential. In the limit where the wells are far apart and the potential barrier is high, we prove that the ground state and first excited state are given to leading order by an even, respectively odd, superposition of ground states in single wells. We evaluate the resulting tunneling term splitting the corresponding energies precisely.

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1. INTRODUCTION

Both as a non-linear analysis problem in its own right, and as a basic input to a companion paper [18], we are interested in the low energy states of the bosonic Hartree energy functional

$$\mathcal{E}_{DW}[u] = \int_{\mathbb{R}^d} |\nabla u(x)|^2 dx + \int_{\mathbb{R}^d} V_{DW}(x)|u(x)|^2 dx + \frac{\lambda}{2} \iint_{\mathbb{R}^d \times \mathbb{R}^d} |u(x)|^2 u(x-y)|u(y)|^2 dxdy$$

\hspace{0.5cm} (1.1)
with \( \lambda, w \geq 0 \) a coupling constant and a repulsive pair interaction potential. The crucial feature we tackle is that we take \( V_{\text{DW}} \) to be a double-well potential defined as (\( \ell \) and \( r \) stand for left and right)

\[
V_{\text{DW}}(x) = \min \left\{ V_\ell(x), V_r(x) \right\}
\]  

(1.2)

where for some \( s > 0 \)

\[
V_\ell(x) = |x + x|^s \quad \text{and} \quad V_r(x) = |x - x|^s.
\]  

(1.3)

Here \( x \in \mathbb{R}^d \) is of the form

\[
x = \left( \frac{L}{2}, 0, \ldots, 0 \right)
\]  

(1.4)

for a large \( L \to +\infty \). Hence \( V_{\text{DW}} \) models a potential landscape with two wells, both the distance and the energy bareer between them being large, and becoming infinitely so in the limit.

In [21, 18] we are primarily concerned with the mean-field limit of the many-bosons problem in such a potential double-well. As input to the second paper [18] we use crucially several properties of the ground state problem

\[
E_{\text{DW}} = \inf \left\{ E_{\text{DW}}[u] \mid u \in H^1(\mathbb{R}^d) \cap L^2(\mathbb{R}^d, V_{\text{DW}}(x)dx), \int_{\mathbb{R}^d} |u|^2 = 1 \right\},
\]  

(1.5)

and of the associated low energy states. Namely, let \( u_+ \) be the (unique modulo a constant phase, fixed so as to have \( u_+ > 0 \)) minimizer for (1.5) and

\[
h_{\text{DW}} := -\Delta + V_{\text{DW}} + \lambda w * |u_+|^2
\]  

(1.6)

the associated mean-field Hamiltonian (functional derivative of \( E_{\text{DW}} \) at \( u_+ \)). One easily shows that \( h_{\text{DW}} \) has compact resolvent, and we study its eigenvalues and eigenfunctions. The lowest eigenvalue is

\[
\mu_+ = E_{\text{DW}} + \frac{\lambda}{2} \iint_{\mathbb{R}^d \times \mathbb{R}^d} |u_+(x)|^2 w(x-y)|u_+(y)|^2 dx dy
\]  

(1.7)

with associated eigenfunction \( u_+ \). This follows from the fact that \( h_{\text{DW}} \) has a positive ground state (unique up to phase) [Section XIII.12][20], and of \( u_+ \) being a positive eigenfunction of \( h_{\text{DW}} \).

We denote \( \mu_- \) and \( u_- \) the next smallest eigenvalue and associated eigenfunction, and \( \mu_{\text{ex}} \) the third eigenvalue. We aim at proving

- that \( E_{\text{DW}}, \mu_+ \) and \( \mu_- \) are given at leading order in terms of the ground state problem in a single well (left or right).
- asymptotics for the first spectral gap:

\[
\mu_- - \mu_+ \xrightarrow{L \to \infty} 0.
\]  

(1.8)

with a precise rate (both as an upper and lower bound).

\footnote{Chosen in dependence of a particle number \( N \) in [18].}
asymptotics for the associated eigenfunctions: that they both converge to superpositions of eigenfunctions of the single wells and that
\[ \| u_+ \| - \| u_- \| \to 0 \quad \text{as} \quad L \to \infty \]
in suitable norms, and with a precise optimal rate.

- a $L$ independent lower bound to the second spectral gap:
\[ \mu_{ex} \geq C, \quad \text{independently of} \quad L \]

The spectral theory of Hamiltonians with multiple wells has a long and rich history, selected references most relevant to the following being [17, 8, 4, 3, 11, 12, 14, 15, 22]. See also [9, 13] for reviews. Corresponding non-linear results are also available [5, 6, 7], but we have not found proofs of the aforementioned bounds for the setting just described (dictated by the model of interest in [21, 18]).

Typically, and in particular as regards results with the level of precision we aim at, the analysis in the aforementioned references is carried in a semi-classical regime, namely one studies the spectral properties of
\[ - \hbar^2 \Delta + V \]
as $\hbar \to 0$, with $V$ a fixed multi-well potential. Say the above, symmetric, $V_{DW}$ but with $L$ fixed. One obtains that at leading order the eigenvalues are grouped in pairs around the eigenvalues corresponding to a single well (with appropriate modifications for more than two wells or asymmetric wells). This corresponds to eigenfunctions being strongly suppressed in the classically forbidden region far from the wells. The (small) splitting between pairs of eigenvalues can be estimated with some precision, and corresponds to the tunnel effect, due to quantum eigenfunctions being small but non-zero in the classically forbidden region. That is, quantum mechanically, there is a flux of particles through potential barriers, that is manifested in a lifting of classical energy degeneracies.

In fact, if $u_{j,+}$ and $u_{j,-}$ are the eigenfunctions corresponding respectively to the smallest and largest eigenvalue in the $j$-th pair, one has
\[ u_{j,+} \simeq \frac{u_{j,\ell} + u_{j,r}}{\sqrt{2}} \]
and
\[ u_{j,-} \simeq \frac{u_{j,\ell} - u_{j,r}}{\sqrt{2}} \]
with $u_{j,\ell}$ and $u_{j,r}$ the $j$-th eigenfunction of (respectively) the left and right well. The results on eigenvalues are a reflection of this fact.

Our main results (1.8)-(1.9)-(1.10) (stated more precisely below) are adaptations of this well-known findings to the case at hand, namely $\hbar$ fixed and $L \to \infty$. For the applications in [18] we need the optimal rates in (1.8) and (1.9), i.e. identify the order of magnitude of the tunneling term exactly. To a large extent, the sequel is an adaptation of known techniques, but we face two main new difficulties:

- the fact that we start from the non-linear Hartree problem.
the lack of semi-classical WKB expansions for single-well eigenfunctions, that are essentially fixed in our setting.

The second point is particularly relevant to the derivation of the optimal rates in (1.8) and (1.9).

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2. Main results

We carry on with the previous notation, and also denote

\[ V(x) = |x|^s \]  

(2.1)

with \( s \geq 2 \), our single-well potential, appropriately translated in (1.3), recalling that \( x = (L/2, 0, \ldots, 0) \in \mathbb{R}^d \).

As regards interactions, we consider them repulsive, i.e. assume \( \lambda \geq 0 \) and let \( w \in L^\infty(\mathbb{R}^d) \) with compact support such that \( \hat{w} \) stands for the Fourier transform

\[ w \geq 0, \quad \hat{w} \geq 0. \]  

(2.2)

Regularity assumptions could be relaxed to some extent, but we do not pursue this.

We consider the Hartree functional in the double-well (1.1) The existence of a minimizer for (1.5) follows from standard techniques [16, Theorem 11.8], combined with the fact that \( V_{DW} \) prevents mass losses at infinity. The uniqueness of the minimizer \( u_+ \) up to a constant phase factor follows from the assumption \( \hat{w} \geq 0 \). Let \( u_+ \) be the unique minimizer. With the mean-field double-well Hamiltonian (1.6) we have that \( u_+ \) is the unique ground state of \( h_{DW} \) with energy \( \mu_+ \), i.e.,

\[ h_{DW}u_+ = \mu_+u_+. \]

Due to the growth of \( V_{DW} \) the Hamiltonian \( h_{DW} \) has compact resolvent. We call \( u_- \) and \( u_{ex} \) the eigenvectors whose corresponding energies \( \mu_- \) and \( \mu_{ex} \) are, respectively, the first and second eigenvalue of \( h_{DW} \) above \( \mu_+ \). In other words

\[ h_{DW} = \mu_+|u_+\rangle\langle u_+| + \mu_-|u_-\rangle\langle u_-| + \mu_{ex}|u_{ex}\rangle\langle u_{ex}| + \sum_{n \geq 4} \mu_n|u_n\rangle\langle u_n| \]  

(2.3)

where

\[ \mu_+ < \mu_- \leq \mu_{ex} \leq \mu_n, \quad \forall n, \quad \text{and } \{u_+, u_-, u_{ex}, u_4, u_5, \ldots \} \text{ form an o.n. basis.} \]

Moreover, since the Hamiltonian \( h_{DW} \) commutes with reflections across the \( x_1 = 0 \) hyperplane, we can choose each eigenvector \( u_-, u_{ex}, u_4, u_5, \ldots \) to be either symmetric or anti-symmetric with respect to such a reflection. In particular, \( u_+ \) being positive, it must be symmetric.
We will also consider Hartree functionals with external potential $V_\epsilon$ or $V_r$, that is,

$$E_\epsilon[u] = \int_{\mathbb{R}^d} |\nabla u(x)|^2 dx + \int_{\mathbb{R}^d} V_\epsilon(x)|u(x)|^2 dx + \frac{\lambda}{2} \int_{\mathbb{R}^d \times \mathbb{R}^d} w(x - y)|u(x)|^2 |u(y)|^2 dxdy,$$

$$E_r[u] = \int_{\mathbb{R}^d} |\nabla u(x)|^2 dx + \int_{\mathbb{R}^d} V_r(x)|u(x)|^2 dx + \frac{\lambda}{2} \int_{\mathbb{R}^d \times \mathbb{R}^d} w(x - y)|u(x)|^2 |u(y)|^2 dxdy.$$  

We will use combinations of the minimizers of $E_\epsilon$ and $E_r$ to approximate the function $u_+$. To this end, we define minimal energies at mass $1/2$

$$E_\epsilon = \inf \left\{ E_\epsilon[u] \mid u \in H^1(\mathbb{R}^d) \cap L^2(\mathbb{R}^d, V_\epsilon(x)dx), \int_{\mathbb{R}^d} |u|^2 = \frac{1}{2} \right\} \quad (2.4)$$

$$E_r = \inf \left\{ E_r[u] \mid u \in H^1(\mathbb{R}^d) \cap L^2(\mathbb{R}^d, V_r(x)dx), \int_{\mathbb{R}^d} |u|^2 = \frac{1}{2} \right\}.$$

As for the full double-well problem, our assumptions on $V$ and $w$ are sufficient to deduce the existence and uniqueness of a minimizer using standard methods in the calculus of variations. Since the functionals $E_\epsilon$ and $E_r$ coincide up to a space translation of the external potential,

$$E_\epsilon = E_r = E_\epsilon[u_\epsilon] = E_r[u_r]$$

where $u_\epsilon$ and $u_r$ are, respectively, the unique positive ground states of

$$h_\epsilon = -\Delta + V_\epsilon + \lambda w * |u_\epsilon|^2, \quad h_r = -\Delta + V_r + \lambda w * |u_r|^2 \quad (2.5)$$

with ground state energies $\mu_\epsilon = \mu_r$. Again, since the functionals coincide up to a translation, the minimizers coincide up to a translation, i.e.,

$$u_\epsilon(x) = u_r(x + 2x).$$

Notice that since the mass is $1/2$, we have

$$\langle u_\epsilon, h_\epsilon u_\epsilon \rangle = \frac{\mu_\epsilon}{2}, \quad \langle u_r, h_r u_r \rangle = \frac{\mu_r}{2}.$$

Next we define the main small parameter (in the limit $L \to \infty$) entering our analysis. Associated to (2.1) is a semi-classical Agmon distance [2, 9, 13]

$$A(x) = \int_0^{[x]} \sqrt{V(r')}dr' = \frac{1}{1 + s/2} |x|^{1+s/2}. \quad (2.6)$$

The above governs optimally the decay at infinity of eigenfunctions of the single-well Hamiltonians (2.5). Accordingly it sets the $L$-dependence of the tunneling term (splitting between eigenvalue pairs)

$$T := e^{-2A(\frac{s}{2})} \to 0 \quad (2.7)$$

This is the energetic contribution of classically forbidden regions: $e^{-A(\frac{s}{2})}$ is the order of magnitude of double-well wave-functions close to the potential barrier at $x_1 = 0$ (i.e. at
distances $L/2$ from the potential wells). It has to be squared for the tunneling term is essentially an overlap of two such wave functions. We will express all our estimates in terms of the above parameter.

Similarly one can associate a distance to the double-well potential (1.2)

$$A_{DW}(x) = \begin{cases} A(x - x) & x_1 \geq 0 \\ A(x + x) & x_1 \leq 0. \end{cases}$$

(2.8)

The value $A_{DW}(x)$ represents the Agmon distance $A$ between the point $x$ and the closest of the two bottoms of the wells, namely, either $x$ or $-x$. In Section 5 we will need to introduce a further refinement of $A_{DW}$, namely the distance within the potential landscape $V_{DW}$ between any two points.

We shall prove the following result, for space dimensions $1 \leq d \leq 3$ (the upper restriction is used only for the proof of (2.13)).

**Theorem 2.1 (Hartree problem in a double-well).**

We take $\varepsilon > 0$ to stand for an arbitrarily small number, fixed in the limit $L \to \infty$. Generic constants $c_\varepsilon, C_\varepsilon > 0$ only depend on this number. We have

(i) **Bounds on the fist spectral gap.**

$$c_\varepsilon T^{1+\varepsilon} \leq \mu_- - \mu_+ \leq C_\varepsilon T^{1-\varepsilon}$$

(2.9)

(ii) **Bounds on the second spectral gap.**

$$\mu_{ex} - \mu_- \geq C$$

(2.10)

independently of $L$.

(iii) **Lower eigenvectors convergence.**

$$\left\| |u_+|^2 - |u_-|^2 \right\|_{L^1} \leq C_\varepsilon T^{1-\varepsilon}$$

(2.11)

$$\left\| |u_+| - |u_-| \right\|_{L^2} \leq C_\varepsilon T^{1/2-\varepsilon}$$

(2.12)

$$\left\| |u_+| - |u_-| \right\|_{L^\infty} \leq C_\varepsilon T^{1/2-\varepsilon}$$

(2.13)

A few comments:

(1) As mentioned above, corresponding results for the semi-classical setting have a long history [9, 13]. Obtaining the (almost) sharp lower bound in (2.9) in this case usually relies on WKB expansions, unavailable in the present context. We however need this sharp bound in [18] and have to come up with an alternative method.

(2) The relevance of the definition (2.7) is vindicated by (2.9). With extra effort one should be able to show that $T$ gives the order of magnitude of the first spectral gap up to at most logarithmic corrections.

(3) Item (iii) is also crucial in [18], in particular (2.11). It reflects the expectation (1.12)-(1.13), i.e. that $u_+$ and $u_-$ mostly differ by a sign change in a half-space. This will be put on a rigorous basis later, following [14, 15]. With a suitable choice of $u_j^\varepsilon, u_j, u$ we indeed vindicate (1.12)-(1.13), with remainders $O(T^{1+\varepsilon})$. Then (2.11) follows,
using also decay estimates for the product \( u_{j,c} u_{j,e} \). The less sharp estimates (2.12)-(2.13) are mostly stated for illustration (and will serve as steps in the proof).

The following statement on higher eigenvalues/eigenfunctions follows easily from suitable variants of the arguments below. We do not provide details because we need them only for a side remark in [18]:

**Theorem 2.2 (Higher spectrum).**

Let \( \mu_{2j+1}, \mu_{2j+2}, j \geq 1 \) be the \((2j+1)\)-th and \((2j+2)\)-th eigenvalues of the mean-field Hamiltonian (1.6), with associated eigenfunctions \( u_{2j+1}, u_{2j+2} \). We have

(i) **Bounds on small spectral gaps.**

\[
|\mu_{2j+1} - \mu_{2j+2}| \xrightarrow{L \to \infty} 0
\]

(ii) **Bounds on large spectral gaps.**

\[
\mu_{2j+3} - \mu_{2j+2} \geq C_j
\]

for some constant \( C_j > 0 \) independent of \( L \).

(iii) **Lower eigenvectors convergence.**

\[
\left\| u_{2j+1} - u_{2j+2} \right\|_{L^2} \xrightarrow{L \to \infty} 0
\]

\[
\left\| u_{2j+1} - u_{2j+2} \right\|_{L^\infty} \xrightarrow{L \to \infty} 0
\]

We do not state convergence rates here, but believe the same rates as in Theorem 2.1 can be achieved, for \( j \) fixed in the limit \( L \to \infty \) (or, better said, for convergence rates whose \( j \)-dependence is left unspecified). We do not pursue the details, nor the dependence on \( j \), for we do not need it in our applications [18]. Certainly, if the eigenvalues are taken high enough in the spectrum \((j \to \infty \text{ fast enough as } L \to \infty)\) the two-modes approximation (1.12)-(1.13), on which the result relies, breaks down.

The rest of the paper contains the proof of Theorem 2.1 organized as follows:

- Section 3: optimal bounds on the decay of eigenfunctions far from the potential wells, and first consequences thereof.
- Section 4: proof of Items (i) and (ii) in Theorem 2.1. The hardest part is the lower bound on the first gap in Item (i).
- Section 5: adaptation of techniques of Helffer-Sjöstrand [15] to deduce Item (iii) from the previous bounds.
- Appendix A: a collection of straightforward consequences of the decay estimates of Section 3.

3. Preliminary estimates

3.1. **Pointwise decay estimates.** The first main result of this Section is the following provides precise decay estimates for the eigenfunctions defined in Section 2. We always denote by \( B_x(R) \) the ball of radius \( R \) centered at \( x \).
Proposition 3.1 (Decay estimates for the Hartree minimizers).
Let
\[ \alpha_s = \begin{cases} \frac{2d-2+s}{4s} \frac{2d^s}{2d} & s > 2 \\ \frac{4}{2d} - \frac{s}{2d} & s = 2 \end{cases} \]
with \( * \in \{ +, -, \text{ex}, \ell, r \} \). Then there exists \( R > 0 \) such that, for every \( 0 < \varepsilon < 1 \), there exist constants \( c_\varepsilon, C_\varepsilon > 0 \) such that the following hold.

(i) Estimates for eigenvectors of \( h_{DW} \).
\[
\begin{align*}
c_\varepsilon \frac{e^{-A_{DW}(x)}}{V_{DW}(x)^{\alpha_+ + \varepsilon}} & \leq u_+(x) \leq C_\varepsilon \frac{e^{-A_{DW}(x)}}{V_{DW}(x)^{\alpha_+ \varepsilon}} \\
|u_-(x)| & \leq C_\varepsilon \frac{e^{-A_{DW}(x)}}{V_{DW}(x)^{\alpha_- \varepsilon}} \\
|u_{\text{ex}}(x)| & \leq C_\varepsilon \frac{e^{-A_{DW}(x)}}{V_{DW}(x)^{\alpha_{\text{ex}} \varepsilon}}
\end{align*}
\]
for \( x \not\in B_\varepsilon(R) \cup B_{-\varepsilon}(R) \), i.e., for \( x \) far enough from \( x \) and \(-x\).

(ii) Estimate for \( u_\varepsilon \).
\[
u_\varepsilon(x) \leq C_\varepsilon \frac{e^{-A(x-\varepsilon)}}{V_\varepsilon(x)^{\alpha_\varepsilon \varepsilon}}
\]
for \( x \not\in B_\varepsilon(R) \).

(iii) Estimate for \( u_\varepsilon \).
\[
u_\varepsilon(x) \leq C_\varepsilon \frac{e^{-A(x+\varepsilon)}}{V_\varepsilon(x)^{\alpha_\varepsilon \varepsilon}}
\]
for \( x \not\in B_{-\varepsilon}(R) \).

As we recall during the proof, a pointwise lower bound for \( u_- \) and \( u_{\text{ex}} \) is not to be expected, since excited eigenfunctions are not, in general, strictly positive. A lower bound for \( u_\varepsilon \) and \( u_{\varepsilon} \), in turn, was obtained in [21, Proposition 3.1], but we do not state it because it will not play any role in the sequel. Before proving Proposition 3.1 we state and prove the following Lemma, to which we will refer in what follows.

Lemma 3.2 (Regularity).
The functions \( u_+, u_-, u_{\text{ex}}, u_\varepsilon, u_{\varepsilon} \) belong to \( C^\infty(\mathbb{R}^d) \).

Proof. Define
\[
W := V_{DW} + \lambda w * |u_+|^2 - \mu_+.
\]
The function \( u_+ \) then solves the elliptic equation with locally Lipschitz coefficients
\[
- \Delta u_+ + W u_+ = 0.
\]
This means that we can apply [10, Theorem 8.8] and deduce that \( u_+ \in H^2(K) \) for every compact set \( K \subset \mathbb{R}^d \). In order to prove higher regularity we will use a bootstrap argument.
Recall that, for a sufficiently regular $K$,
\[ \| f g \|_{H^s(K)} \leq C \| f \|_{H^{s_1}(K)} \| g \|_{H^{s_2}(K)} \]
for $s < s_1 + s_2 - d/2$. The validity of the above formula if $K$ is replaced by $\mathbb{R}^d$ is well known, and to deduce it for compact domains one uses Stein’s extension Theorem [II Theorem 5.24]. Now, since $u_+ \in H^2(K)$ and $W \in H^1(K)$, the above inequality proves in particular that $W u_+ \in H^1(K)$. Due to (3.6), this means $\Delta u_+ \in H^1(K)$, and therefore $u_+ \in H^3(K)$. We can now iterate the procedure, because $u_+ \in H^3(K)$ and $W \in H^1(K)$ imply $W u \in H^2(K)$. In this way we deduce that $u_+ \in H^s(K)$ for any $s > 0$. This implies that $u_+$ is $C^\infty$ in every sufficiently regular compact set, which means it is $C^\infty$ on the whole of $\mathbb{R}^d$. The same argument can be repeated for all the other functions.

We are now able to prove Proposition [3.7]

**Proof of Proposition [3.7]** For a number $\beta \in \mathbb{R}$, define the function
\[ f(x) = e^{-A_{DW}(x)} V_{DW}(x)^{-\beta / s} = \begin{cases} e^{-(1+s/2)^{-1} |x-x|^s / 2} |x-x|^{-\beta} & x_1 \geq 0 \\ e^{-(1+s/2)^{-1} |x+x|^s / 2} |x+x|^{-\beta} & x_1 \leq 0 \end{cases} \]

Using that $f$ only depends on $|x-x|$ for $x_1 \geq 0$ or $|x+x|$ for $x_1 \leq 0$, we can compute $\Delta f(x)$
\[ \Delta f(x) = \begin{cases} \left[ |x-x|^s + (2\beta - \frac{s}{2} - d + 1) |x-x|^s / 2 - 1 + \left( \beta^2 + 2\beta - d \right) |x-x|^2 \right] f(x) & x_1 \geq 0 \\ \left[ |x+x|^s + (2\beta - \frac{s}{2} - d + 1) |x+x|^s / 2 - 1 + \left( \beta^2 + 2\beta - d \right) |x+x|^2 \right] f(x) & x_1 \leq 0 \end{cases} \]

Since $w \ast |u_+|^2$ decays at infinity, picking $\beta = s\alpha_+ - \varepsilon$ (respectively $\beta = s\alpha_+ + \varepsilon$) we deduce
\[ \left( -\Delta + V_{DW}(x) + \lambda w \ast |u_+|^2(x) - \mu_+ \right) f(x) \geq 0 \quad \text{(respectively} \leq 0) \quad (3.7) \]
for $|x-x|$ and $|x+x|$ large enough.

In order to prove the upper bound in (3.1), let us assume $\beta = s\alpha_+ - \varepsilon$. Let $R$ be a radius large enough for both (3.7) and (3.8)
\[ V_{DW}(x) > \mu_+ - \lambda w \ast |u_+|^2(x) \quad \text{(3.8)} \]

for $|x-x| \geq R$ and $|x+x| \geq R$. Consider a function $f_{up}^{(+)}$ which is equal to $f$ outside of $B_{\varepsilon}(R) \cup B_{-\varepsilon}(R)$ and smoothly extended to a function bounded away from zero inside $B_{\varepsilon}(R) \cup B_{-\varepsilon}(R)$. Define the constant
\[ C_\varepsilon = \max_{\substack{|x-x|<R \\ |x+x|<R}} \frac{u_+(x)}{f_{up}^{(+)}(x)} \]
Notice that, since $u_+ > 0$, we have $C_\varepsilon > 0$. Let us consider the function
\[ g_{up}^{(+)}(x) = u_+(x) - C_\varepsilon f_{up}^{(+)}(x). \]
By Lemma 3.2 we know that $u_+$ is continuous. Since $f_{up}^{(+)}$ is also continuous by construction, we have that $g_{up}^{(+)}$ is a continuous function. We want to show that $g_{up}^{(+)}$ is negative, which would complete the proof of the upper bound in (3.1). Let us assume for contradiction that $g_{up}^{(+)}$ is strictly positive on a set $\Omega$ of positive measure. Since $g_{up}^{(+)}$ is by definition negative inside $B_\chi(R) \cup B_{-\chi}(R)$, we have that $\Omega \cap (B_\chi(R) \cup B_{-\chi}(R)) = \emptyset$, and that the boundary $\partial \Omega$ must be non-empty. Moreover, by continuity of $g_{up}^{(+)}$ we can assume that $\Omega$ is open and that $g_{up}^{(+)} = 0$ on $\partial \Omega$.

Using $(h_{DW} - \mu_+)u_+ = 0$ and (3.7), we have
\[
\left(-\Delta + V_{DW} + \lambda w \ast |u_+|^2 - \mu_+\right)g_{up}^{(+)} = -C_\varepsilon \left(-\Delta + V_{DW} + \lambda w \ast |u_+|^2 - \mu_+\right)f_{up}^{(+)} \leq 0
\]
on $\Omega$. Since $g_{up}^{(+)} > 0$ on $\Omega$, (3.8) and the above inequality imply
\[
\Delta g_{up}^{(+)} \geq 0 \quad \text{on } \Omega.
\]
By the maximum principle [10, Theorem 8.1], $g_{up}^{(+)}$ satisfies the following inequality
\[
\sup_{\Omega} g_{up}^{(+)} \leq \sup_{\partial \Omega} g.
\]
By construction, the quantity on the left is strictly positive, and the quantity on the right is zero, yielding the desired contradiction and thus proving the upper bound in (3.1).

To prove the lower bound in (3.1) we go back to (3.7) and pick $\beta = s\alpha_+ + \varepsilon$. Hence we have that
\[
\left(-\Delta + V_{DW}(x) + \lambda w \ast |u_+|^2(x) - \mu_+\right)f(x) \leq 0 \quad (3.9)
\]
and
\[
V_{DW}(x) > \mu_+ - \lambda w \ast |u_+|^2(x) \quad (3.10)
\]
for $|x - \chi| \geq R$ and $|x + \chi| \geq R$ with $R$ large enough. Consider now a function $f_{low}^{(+)}$ which is equal to $f$ (with $\beta = s\alpha_+ + \varepsilon$) outside of $B_\chi(R) \cup B_{-\chi}(R)$ and smoothly extended to a function bounded away from zero inside $B_\chi(R) \cup B_{-\chi}(R)$. Define the constant
\[
c_\varepsilon = \min_{|x-\chi| < R} \frac{u_+(x)}{f_{low}^{(+)}(x)}.
\]
Once again\(^2\) since $u_+ > 0$, we have $c_\varepsilon > 0$. Let us consider the function
\[
\tilde{g}_{low}^{(+)} = u_+ - c_\varepsilon f_{low}^{(+)}.
\]
\(^2\)This is the place where the argument ceases to apply to $u_-$ or $u_{ex}$.
As above, $g_{\text{low}}^{(+)}$ is a continuous function, and we now want to prove that it is positive. Let us assume by contradiction that $g_{\text{low}}^{(+)}$ is strictly negative on an open set $\Omega$ with $g_{\text{low}}^{(+)} = 0$ on $\partial \Omega$. Using $(h_{DW} - \mu_+)u_+ = 0$ and (3.9), we have

$$
\left( -\Delta + V_{DW} + \lambda w * |u_+|^2 - \mu_+ \right) g_{\text{low}}^{(+)} = -c_\epsilon \left( -\Delta + V_{DW} + \lambda w * |u_+|^2 - \mu_+ \right) f_{\text{low}}^{(+)} \geq 0
$$
on $\Omega$. Since $g_{\text{low}}^{(+)} < 0$ on $\Omega$, (3.10) and the above inequality imply

$$
\Delta g_{\text{low}}^{(+)} \leq 0 \quad \text{on} \quad \Omega.
$$

By the maximum principle [10, Theorem 8.1], $g_{\text{low}}^{(+)}$ now satisfies the inequality

$$
\inf_{\Omega} g_{\text{low}}^{(+)} \geq \inf_{\partial \Omega} g_{\text{low}}^{(+)}.
$$

The quantity on the left is strictly negative, because $g_{\text{low}}^{(+)}$ is strictly negative on $\Omega$, while the quantity on the right is zero. We have the same contradiction as above, and this proves (3.2).

Let us now show how to obtain the bound (3.2) for $|u_-|$. By picking $\beta = s\alpha_- - \epsilon$ in the definition of $f$, and repeating the arguments that led us to (3.7) and (3.8) we deduce

$$
\left( -\Delta + V_{DW}(x) + \lambda w * |u_+|^2(x) - \mu_- \right) f(x) \geq 0 \quad (3.11)
$$

and

$$
V_{DW}(x) > \mu_- - \lambda w * |u_+|^2(x) \quad (3.12)
$$

for $|x-x| \geq R$ and $|x+x| \geq R$ with $R$ large enough. Consider now a function $f^{(-)}$ which is equal to $f$ (with the choice $\beta = s\alpha_- - \epsilon$) outside of $B_\epsilon(R) \cup B_{-\epsilon}(R)$ and smoothly extended to a function bounded away from zero inside $B_\epsilon(R) \cup B_{-\epsilon}(R)$. Define the constant

$$
C_\epsilon = \min_{|x-x| \leq R} \frac{|u_-|}{f^{(-)}(x)}
$$

and the function

$$
g_{\text{up}}^{(-)} = u_- - C_\epsilon f^{(-)}.
$$

Notice that, for $R$ large enough, $C_\epsilon > 0$, since otherwise we would have $u_- = 0$ everywhere. By Lemma [3.2], $u_-$ is continuous, which makes $g_{\text{up}}^{(-)}$ continuous. Let us show that $g_{\text{up}}^{(-)}$ is negative.

We know that for $x \in B_\epsilon(R) \cup B_{-\epsilon}(R)$ we have, by definition of $C_\epsilon$,

$$
g_{\text{up}}^{(-)}(x) \leq u_-(x) - |u_-(x)| \leq 0.
$$
Assume by contradiction that \( g_{\text{up}}^{(-)} \) is strictly positive on an open set \( \Omega \) with \( g_{\text{up}}^{(-)} = 0 \) on \( \partial \Omega \). Using \( (h_{DW} - \mu_-)u_- = 0 \) and (3.11), we have
\[
\left( -\Delta + V_{DW} + \lambda w * |u_+|^2 - \mu_- \right) g_{\text{up}}^{(-)} = -C_\epsilon \left( -\Delta + V_{DW} + \lambda w * |u_+|^2 - \mu_- \right) f^{(-)} \leq 0
\]
on \( \Omega \). Since \( g_{\text{up}}^{(-)} > 0 \) on \( \Omega \), (3.12) and the above inequality imply
\[
\Delta g_{\text{up}}^{(-)} \geq 0 \quad \text{on} \quad \Omega.
\]
By the maximum principle [10, Theorem 8.1], \( g_{\text{up}}^{(-)} \) now satisfies the inequality
\[
\sup_{\Omega} g_{\text{low}}^{(+)} \leq \sup_{\partial \Omega} g_{\text{low}}^{(+)}.
\]
The quantity on the left is strictly positive, while the quantity on the right is zero. This would prove that \( g_{\text{up}}^{(-)} \geq 0 \) everywhere, but this is not possible since we proved above that \( g_{\text{up}}^{(-)} \) is negative inside \( B_x(R) \cup B_{-x}(R) \). Hence we deduce
\[
u_-(x) \leq C_\epsilon \frac{e^{-A_{DW}(x)}}{V_{DW}(x)^{a_+ - \epsilon}}.
\]
To complete the proof of (3.2) we need to show
\[
u_-(x) \geq -C_\epsilon \frac{e^{-A_{DW}(x)}}{V_{DW}(x)^{a_+ - \epsilon}}.
\]
This is achieved by defining
\[
g_{\text{low}}^{(-)} = u_- + C_\epsilon f^{(-)}
\]
and arguing as we did for \( g_{\text{up}}^{(-)} \) but reversing the inequalities.

The estimates for \( u_\epsilon \) are proven in the same way as those for \( u_- \). The estimates for \( u_\epsilon \) and \( u_- \) are analogously proven as well, and they were already obtained in [21] Proposition 3.1.

The above allows to efficiently bound most terms that have to do with the tunneling effect in the sequel. A list of such is provided in Appendix [A].

3.2. First approximations. An important ingredient for the sequel is a first approximation of \( u_+ \) in terms of functions localized in the left or right wells:

**Proposition 3.3 (First properties of \( u_+ \) and \( u_- \)).**

Let \( \chi_{x_1 \geq 0}, \chi_{x_1 \leq 0} \) be a smooth partition of unity such that
\[
\chi_{x_1 \geq 0}^2 + \chi_{x_1 \leq 0}^2 = 1, \quad \chi_{x_1 \geq 0}(x) = \chi_{x_1 \leq 0}(-x_1, x_2, \ldots, x_d), \quad \| \nabla \chi_{x_1 \geq 0} \|_\infty \leq C.
\]

Then, with \( u_- \) and \( u_+ \), the left and right Hartree minimizers solving (2.4)

\[
\begin{align*}
\| X_{x_1 \geq 0} u_+ - u_+ \|_{L^2} &\leq C_\varepsilon T^{1/2-\varepsilon} \\
\| X_{x_1 \leq 0} u_+ - u_+ \|_{L^2} &\leq C_\varepsilon T^{1/2-\varepsilon}
\end{align*}
\]  
\tag{3.13} 

and for an appropriate choice of the phase of \( u_- \),

\[
\begin{align*}
\| X_{x_1 \geq 0} u_- - u_- \|_{L^2} &\leq C_\varepsilon T^{1/4-\varepsilon} \\
\| X_{x_1 \leq 0} u_- + u_- \|_{L^2} &\leq C_\varepsilon T^{1/4-\varepsilon} 
\end{align*}
\]  
\tag{3.14} 

Notice that the approximation (3.14) has a worse rate than (3.13), and therefore it does not allow to directly deduce (2.12) with the desired rate. Since we will prove Proposition 3.3 using energy inequalities, we will need the following two lemmas.

**Lemma 3.4. Stability inequality for gapped Hamiltonians.**

Let \( h \) be a compact-resolvent self-adjoint Hamiltonian on a Hilbert space \( \mathcal{H} \). Let \( \lambda_0 \) be the ground state energy with ground state \( u_0 \), and let \( G \) be the gap between ground state and first excited state. Then, for any \( u \in D(h) \),

\[
\langle u, hu \rangle_\mathcal{H} \geq \lambda_0 + \frac{G}{2} \min_{\theta \in [0,2\pi]} \| e^{i\theta} u - u_0 \|_{\mathcal{H}}^2. 
\]  
\tag{3.15} 

*Proof.* By the assumptions we have the decomposition

\[
h = \lambda_0 |u_0\rangle \langle u_0| + \sum_n \lambda_n |u_n\rangle \langle u_n|
\]

with \( \lambda_n \geq \lambda_1 + G \) for every \( n \). Then

\[
\langle u, hu \rangle_\mathcal{H} \geq \lambda_0 \left( \langle u_0, u \rangle_\mathcal{H} \right)^2 + (\lambda_0 + G) \left( 1 - \left| \langle u_0, u \rangle_\mathcal{H} \right|^2 \right) = \lambda_0 + G \left( 1 - \left| \langle u_0, u \rangle_\mathcal{H} \right|^2 \right).
\]

On the other hand we have

\[
\min_{\theta \in [0,2\pi]} \| e^{i\theta} u - u_0 \|_{\mathcal{H}}^2 = 2 - 2 \max_{\theta \in [0,2\pi]} \Re \left( e^{i\theta} \langle u_0, u \rangle_\mathcal{H} \right) = 2 - 2 \left| \langle u_0, u \rangle_\mathcal{H} \right|.
\]

Since \( 1 - \left| \langle u_0, u \rangle_\mathcal{H} \right| \leq 1 - \left| \langle u_0, u \rangle_\mathcal{H} \right|^2 \), the last two equations yield the desired estimate. \( \square \)

**Lemma 3.5 (Stability inequality for the one-well Hartree functionals.)**

For a generic \( u \in H^2(\mathbb{R}^d) \cap L^2(\mathbb{R}^d, V_\ell(x) dx) \) with \( \| u \|_{L^2}^2 = \frac{1}{2} \), the following stability inequality holds:

\[
\mathcal{E}_\ell[u] \geq \mathcal{E}_\ell[u_+] + C \min_{\theta \in [0,2\pi]} \| e^{i\theta} u - u_+ \|_{L^2}^2
\]  
\tag{3.16} 

\(^3\)This assumption is clearly not crucial for this Lemma, a unique ground state separated from the rest of the spectrum being enough. We anyway keep it since we only deal with compact-resolvent Hamiltonians.
Proof. First, let us notice that an application of Lemma 3.4 for \( h = h_r \) yields
\[
\langle u, h, u \rangle \geq \langle u_r, h, u_r \rangle + C \min_{\theta \in [0,2\pi]} \|e^{i\theta} u - u_r \|_{L^2}.
\] (3.17)

Indeed, \( h_r \) is obtained from a \( L \)-independent Hamiltonian by a translation of \( x \), and therefore its spectrum does not depend on \( L \). By the properties on \( V \) and \( w \) it then follows that \( h_r \) must have a gap uniform in \( L \) (see, e.g., [20, Theorem XIII.47]), and therefore we can apply Lemma 3.4.

To deduce (3.16), a simple computation gives
\[
\mathcal{E}_r[u] - \mathcal{E}_r[u_r] = \langle u, h, u \rangle - \langle u_r, h, u_r \rangle + \frac{\lambda}{2} \int_{\mathbb{R}^d} (w * |u_r|^2)|u| - \langle u, h_r, u \rangle - \langle u_r, h_r, u_r \rangle + \frac{\lambda}{2} \int_{\mathbb{R}^d} (w * (|u_r|^2 - |u|^2))(|u_r|^2 - |u|^2).
\]

Since \( \hat{w} \geq 0 \), the last integral on the right hand side is non-negative. We discard it for a lower bound and get
\[
\mathcal{E}_r[u] - \mathcal{E}_r[u_r] \geq \langle u, h, u \rangle - \langle u_r, h, u_r \rangle,
\] (3.18)
which proves (3.16) thanks to (3.17).

We are now ready to give the

Proof of Proposition 3.3 Let us first show the upper bound
\[
\mathcal{E}_{DW}[u_+] \leq 2\mathcal{E}_r[u_r] + C_2 T^{1-\varepsilon}
\] (3.19)
The normalized state \( (u_r + u_\varepsilon)/\|u_r + u_\varepsilon\|_{L^2} \) is an admissible trial function for the minimization of \( \mathcal{E}_{DW} \) at unit mass. Notice that, by positivity of \( u_r \) and \( u_\varepsilon \),
\[
\|u_r + u_\varepsilon\|_{L^2}^2 = 1 + 2\Re(u_r, u_\varepsilon) \geq 1,
\]
and hence we can ignore the norms in the denominator for an upper bound. We have
\[
\mathcal{E}_{DW}[u_+] \leq \mathcal{E}_{DW}\left[\frac{u_r + u_\varepsilon}{\|u_r + u_\varepsilon\|_{L^2}}\right]
\]
\[
\leq \int_{\mathbb{R}^d} |\nabla u_r|^2 + \int_{\mathbb{R}^d} V_{DW}|u_r|^2 + \frac{\lambda}{2} \int_{\mathbb{R}^d} |u_r|^2(w * |u_r|^2)
\]
\[
+ \int_{\mathbb{R}^d} |\nabla u_\varepsilon|^2 + \int_{\mathbb{R}^d} V_{DW}|u_\varepsilon|^2 + \frac{\lambda}{2} \int_{\mathbb{R}^d} |u_\varepsilon|^2(w * |u_\varepsilon|^2)
\]
\[
+ 2\int_{\mathbb{R}^d} \nabla u_\varepsilon \cdot \nabla u_r + 2\int_{\mathbb{R}^d} V_{DW}u_\varepsilon u_r
\]
\[
+ \frac{\lambda}{2} \int_{\mathbb{R}^d \times \mathbb{R}^d} w(x-y)\left[2u_\varepsilon(x)u_r(x)|u_r(y) + u_\varepsilon(y)|^2
\]
\[
+ 2|u_\varepsilon(x)|^2(|u_r(y)|^2 + 2u_\varepsilon(y)u_r(y))\right]dxdy.
\] (3.20)
In the first two lines in the right hand side we can use, respectively, $V_{DW} \leq V_\epsilon$ and $V_{DW} \leq V_\epsilon$. In this way the first line equals $E_\epsilon[u_\epsilon]$ and the second one equals $E_\epsilon[u_\epsilon]$, which actually coincide by translation invariance. The terms in the third line are remainders as follows from (A.4) and (A.7). We then deduce

$$E_{DW}[u_\epsilon] \leq 2E_\epsilon[u_\epsilon] + C_\epsilon T^{1-\epsilon}$$

$$+ \frac{\lambda}{2} \int_{\mathbb{R}^d \times \mathbb{R}^d} w(x - y)[2u_\epsilon(x)u_\epsilon(x)u_\epsilon(y) + u_\epsilon(y)]^2$$

$$+ 2|u_\epsilon(x)|^2(2u_\epsilon(y)u_\epsilon(y) + |u_\epsilon(y)|^2) \, dx \, dy.$$

To get rid of the last terms, involving $w$, we notice that by the Cauchy-Schwarz and Young inequalities we have

$$\left| \int_{\mathbb{R}^d \times \mathbb{R}^d} w(x - y)u_\epsilon(x)u_\epsilon(x)g(y) \right| \leq \|w\|_{L^1} \|g\|_{L^1} \int_{\mathbb{R}^d} u_\epsilon u_r,$$

and the scalar product on the right is estimated using (A.1). The only remaining term to estimate is

$$\lambda \int_{\mathbb{R}^d \times \mathbb{R}^d} w(x - y)|u_\epsilon(x)|^2|u_\epsilon(y)|^2 \, dx \, dy,$$

which we bound using (A.14). We thus precisely obtain (3.19).

Let us now prove the lower bound

$$E_{DW}[u_\epsilon] \geq 2E_\epsilon[\chi_{x_1 \geq 0} u_\epsilon] - C_\epsilon T^{1-\epsilon}.$$  \hspace{1cm} (3.21)

Using the IMS localization formula we have

$$-\Delta + V_{DW} = -\chi_{x_1 \geq 0} \Delta \chi_{x_1 \geq 0} + \chi_{x_1 \leq 0} \Delta \chi_{x_1 \leq 0} + \nabla \chi_{x_1 \geq 0}^2 + \nabla \chi_{x_1 \leq 0}^2 - \nabla \chi_{x_1 \geq 0}^2 - \nabla \chi_{x_1 \leq 0}^2.$$

Moreover,

$$\int_{\mathbb{R}^d} (w * |u_\epsilon|^2)|u_\epsilon|^2 = \int_{\mathbb{R}^d} (w * |\chi_{x_1 \geq 0} u_\epsilon|^2)|\chi_{x_1 \geq 0} u_\epsilon|^2 + \int_{\mathbb{R}^d} (w * |\chi_{x_1 \leq 0} u_\epsilon|^2)|\chi_{x_1 \leq 0} u_\epsilon|^2$$

$$+ 2 \int_{\mathbb{R}^d} (w * |\chi_{x_1 \leq 0} u_\epsilon|^2)|\chi_{x_1 \geq 0} u_\epsilon|^2.$$

The last summand in the right hand side of the last equation is positive and we will simply discard it for a lower bound. We thus have

$$E_{DW}[u_\epsilon] \geq 2E_\epsilon[\chi_{x_1 \geq 0} u_\epsilon] + \int_{\mathbb{R}^d} (V_{DW} - V_\epsilon) \chi_{x_1 \geq 0}^2 |u_\epsilon|^2 + \int_{\mathbb{R}^d} (V_{DW} - V_\epsilon) \chi_{x_1 \leq 0}^2 |u_\epsilon|^2$$

$$- \int_{\mathbb{R}^d} (\nabla \chi_{x_1 \geq 0}^2)^2 |u_\epsilon|^2 - \int_{\mathbb{R}^d} (\nabla \chi_{x_1 \leq 0}^2)^2 |u_\epsilon|^2.$$

The first two integrals in the right hand side are estimated in (A.9). The integrals in the second line are smaller or equal than the quantities estimated in (A.2), because $|\nabla \chi_{x_1 \geq 0}|$ and $|\nabla \chi_{x_1 \leq 0}|$ are by construction bounded by a constant and localized in $\{-R \leq x_1 \leq R\}$. This proves (3.21).
Comparing (3.19) and (3.21) we deduce
\[ \mathcal{E}_r[\chi_{x_1 \geq 0} u_+] \leq \mathcal{E}_r[u_r] + C \varepsilon T^{1-\varepsilon}. \]

On the other hand, a direct application of Lemma 3.5 with \( u = \chi_{x_1 \geq 0} u_+ \) yields
\[ \mathcal{E}_r[\chi_{x_1 \geq 0} u_+] \geq \mathcal{E}_r[u_r] + C \min_{\theta \in [0, 2\pi]} \| e^{i\theta} \chi_{x_1 \geq 0} u_+ - u_r \|_{L^2}^2 = \mathcal{E}_r[u_r] + C \| \chi_{x_1 \geq 0} u_+ - u_r \|_{L^2}^2, \]
having noticed that the minimum is attained at \( \theta = 0 \) since \( \chi_{x_1 \geq 0} u_+ \) and \( u_r \) are positive. The last two formulae imply the first estimate in (3.13). The second one immediately follows since \( u_+ \) is symmetric under reflection across the \( x_1 = 0 \) axis, while \( u_r \) is mapped into \( u_\varepsilon \) by such a reflection.

Let us now prove (3.14). As a first ingredient, let us show the following inequality:
\[ \left| \iint_{\mathbb{R}^d \times \mathbb{R}^d} w(x-y) |u_r(x)|^2 \left( |u_+(y)|^2 - |u_r(y)|^2 \right) dx dy \right| \leq C \varepsilon T^{1/2-\varepsilon}. \quad (3.22) \]

Clearly, an analogous inequality holds if \( u_r \) is replaced by \( u_\varepsilon \). To prove it, let us decompose
\[
\iint_{\mathbb{R}^d \times \mathbb{R}^d} w(x-y) |u_r(x)|^2 \left( |u_+(y)|^2 - |u_r(y)|^2 \right) dx dy
\]
\[
= \iint_{\mathbb{R}^d \times \mathbb{R}^d} w(x-y) |u_r(x)|^2 \left( |\chi_{x_1 \geq 0}(y) u_+(y)|^2 - |u_r(y)|^2 \right) dx dy + \iint_{\mathbb{R}^d \times \mathbb{R}^d} w(x-y) |u_r(x)|^2 \left( |\chi_{x_1 < 0}(y) u_+(y)|^2 \right) dx dy
\]
\[
= \iint_{\mathbb{R}^d \times \mathbb{R}^d} w(x-y) |u_r(x)|^2 \left( \chi_{x_1 \geq 0}(y) u_+(y) - u_r(y) \right) \left( \chi_{\varepsilon}(y) u_+(y) + u_r(y) \right) dx dy + \iint_{\mathbb{R}^d \times \mathbb{R}^d} w(x-y) |u_r(x)|^2 \left( \chi_{x_1 < 0}(y) u_+(y) \right) dx dy.
\]
The first term is estimated using Hölder’s inequality and (3.13). The second term is estimated by recognizing that
\[
\iint_{\mathbb{R}^d \times \mathbb{R}^d} w(x-y) |u_r(x)|^2 |\chi_{x_1 < 0}(y) u_+(y)|^2 dx dy \leq C \int_{x_1 \leq 0} |u_r(x)|^2 dx \leq C \varepsilon T^{1/2-\varepsilon}
\]
thanks to (A.8). This shows (3.22). Notice that the error estimate in the right hand side of (3.22) is worse than the one in (3.13). This is the reason why we will obtain a similarly worse error estimate in (3.14).

Let us now proceed to the actual proof of (3.14). We aim at first proving an upper bound of the form
\[ \mu_- \leq \mu_r + C \varepsilon T^{1/2-\varepsilon}. \quad (3.23) \]
Recall that we have
\[ \mu_- = \langle u_-, h_{DW} u_- \rangle = \inf \left\{ \langle u, h_{DW} u \rangle \mid \|u\|_{L^2} = 1, \ u \perp u_+ \right\}. \]
The function \( (u_r - u_\varepsilon)/\|u_r - u_\varepsilon\|_{L^2} \) is then a trial state for this minimization since, by the even parity of \( u_+ \),
\[
\langle u_\varepsilon, u_+ \rangle = \langle u_r, u_+ \rangle.
\]
Moreover, using (A.1) we deduce
\[
\|u_r - u_\varepsilon\|_{L^2}^2 = 1 - 2\text{Re}\langle u_\varepsilon, u_r \rangle \geq 1 - C_\varepsilon T^{1-\varepsilon}.
\]
Hence by the variational principle we have
\[
\mu_- \leq \frac{1}{\|u_r - u_\varepsilon\|_{L^2}^2} \langle u_r - u_\varepsilon, h_{DW}(u_r - u_\varepsilon) \rangle
\leq \langle u_r, h u_\varepsilon \rangle + \langle u_r, h u_r \rangle
- 2 \int \mathbb{R}^d \nabla u_\varepsilon \nabla u_r + \int \varepsilon |u_r|^2 + \int \varepsilon |u_\varepsilon|^2
- 2 \int \mathbb{R}^d V_{DW}u_\varepsilon u_r - \int \varepsilon |u_\varepsilon|^2 - \int \varepsilon |u_r|^2
- \lambda \int \mathbb{R}^d \times \mathbb{R}^d w(x - y)u_\varepsilon(x)u_\varepsilon(y)i\partial_x + \lambda \int \mathbb{R}^d \times \mathbb{R}^d w(x - y)|u_\varepsilon(x)|^2(|u_+(y)|^2 - |u_\varepsilon(y)|^2) dxdy
+ \frac{\lambda}{2} \int \mathbb{R}^d \times \mathbb{R}^d w(x - y)|u_\varepsilon(x)|^2(|u_+(y)|^2 - |u_\varepsilon(y)|^2) dxdy
+ C_\varepsilon T^{1-\varepsilon}.
\]
In the right hand side of (3.24), the first line equals \(2\langle u_+, h u_\varepsilon \rangle \). The second line contains reminders that can be estimated using (A.4) and (A.12). The third and fourth lines are negative and we can safely discard them for an upper bound. The fifth and sixth lines account for the presence of \( w \ast |u_r|^2 \) and \( w \ast |u_\varepsilon|^2 \) in \( h_r \) and \( h_\varepsilon \), and their estimate was provided in (3.22). The only further term in the right hand side of (3.24) is the last line, which comes from the estimate of \( \|u_r - u_\varepsilon\|_{L^2}^2 \). We therefore proved (3.23).

The lower bound
\[
\mu_- = \langle u_-, h_{DW}u_- \rangle \geq 2\langle \chi_{x_1 \geq 0}u_-, h_r \chi_{x_1 \geq 0}u_- \rangle + C_\varepsilon T^{1/2-\varepsilon}
\]
(3.25)
is easily obtained using IMS formula and proceeding as in the proof of (3.21), using also (3.22), (A.2), and (A.5). Comparing (3.17), in which we choose \( u = \chi_{x_1 \geq 0}u_- \), with (3.23) and (3.25) we deduce
\[
\min_{\theta \in [0,2\pi]} \left\| \chi_{x_1 \geq 0}u_- - e^{i\theta} u_- \right\|_{L^2}^2 \leq C_\varepsilon T^{1/2-\varepsilon}.
\]
Repeating the arguments for the function \( \chi_{x_1 \leq 0}u_- \) we also deduce
\[
\min_{\theta \in [0,2\pi]} \left\| \chi_{x_1 \leq 0}u_- - e^{i\theta} u_- \right\|_{L^2}^2 \leq C_\varepsilon T^{1/2-\varepsilon}.
\]
We can fix the overall phase of \( u_- \) so that the first minimization occurs for \( \theta = 0 \). We then have that there exists \( \theta_{\text{min}} \in [0, 2\pi] \) such that

\[
\begin{align*}
\| \chi_{x_1 > 0} u_- - u_+ \|_{L^2}^2 &\leq C_\varepsilon T^{1/2 - \varepsilon} \\
\| \chi_{x_1 \leq 0} u_- - e^{i\theta_{\text{min}}} u_\varepsilon \|_{L^2}^2 &\leq C_\varepsilon T^{1/2 - \varepsilon}.
\end{align*}
\] (3.26)

Now, by orthogonality of \( u_- \) and \( u_+ \), we have

\[
0 = \langle u_-, u_+ \rangle = \langle \chi_\varepsilon u_-, \chi_\varepsilon u_+ \rangle + \langle \chi_{\varepsilon'} u_-, \chi_{\varepsilon'} u_+ \rangle
= e^{i\theta_{\text{min}}} \langle \chi_\varepsilon u_-, \chi_\varepsilon u_+ \rangle + \langle \chi_{\varepsilon'} u_+ - \chi_{\varepsilon'} u_- \rangle.
\]

We know that \( \langle \chi_\varepsilon u_+, \chi_\varepsilon u_+ \rangle \) and \( \langle \chi_{\varepsilon'} u_+, \chi_{\varepsilon'} u_+ \rangle \) are positive sequences that converge to 1 due to (3.13). The last two terms converge to zero by (3.26). We then deduce \( \theta_{\text{min}} = \pi \).

\[\square\]

4. Estimates on spectral gaps

In the present section we prove the claims (2.9) and (2.10) from our main result. The proof of the lower bound in (2.9), being the most involved, requires an extra amount of sharp information on the function \( u_- \), well beyond the preliminary estimates of Proposition 3.1. We discuss this in Subsection 4.2.

4.1. Upper bound on the first gap. To deduce the upper bound in (2.9) we consider the function

\[
u := \frac{\left( \chi_{x_1 > 0} - \chi_{x_1 \leq 0} \right) u_+}{\left\| \left( \chi_{x_1 > 0} - \chi_{x_1 \leq 0} \right) u_+ \right\|_{L^2}}
\]
as a trial function for the minimization

\[
\mu_- = \min \left\{ \langle u, h_{\text{DW}} u \rangle, \| u \|_{L^2} = 1, \ u \perp u_+ \right\}.
\]

Here \( \chi_{x_1 > 0} \) and \( \chi_{x_1 \leq 0} \) are localization functions as in Proposition 3.3 and this ensures

\[
\left\| \left( \chi_{x_1 > 0} - \chi_{x_1 \leq 0} \right) u_+ \right\|_{L^2}^2 = 1 - 2 \int_{\mathbb{R}^d} \chi_{x_1 > 0} \chi_{x_1 \leq 0} |u_+|^2 \geq 1 - C_\varepsilon T^{1-\varepsilon}
\]
(4.1)

thanks to (A.2). By the variational principle we have

\[
\mu_- \leq \langle v, h_{\text{DW}} v \rangle = \frac{2 \langle \chi_{x_1 > 0} u_+, h_{\text{DW}} \chi_{x_1 > 0} u_+ \rangle - 2 \langle \chi_{x_1 > 0} u_+, h_{\text{DW}} \chi_{x_1 \leq 0} u_+ \rangle}{\left\| \left( \chi_{x_1 > 0} - \chi_{x_1 \leq 0} \right) u_+ \right\|_{L^2}^2}.
\]

The second term in the numerator is bounded in absolute value by \( C_\varepsilon T^{1-\varepsilon} \) as can be seen using (A.5), (A.11), and (A.13). For the first term we use IMS formula which implies

\[
\langle u_+, h_{\text{DW}} u_+ \rangle \geq 2 \langle \chi_{x_1 > 0} u_+, h_{\text{DW}} \chi_{x_1 > 0} u_+ \rangle - C_\varepsilon T^{1-\varepsilon}
\]
(4.2)
as can be seen using once again (A.5), (A.11), and (A.13). This, together with (4.1) gives

\[
\mu_- \leq \langle u_+, h_{\text{DW}} u_+ \rangle + C_\varepsilon T^{1-\varepsilon} = \mu_+ + C T^{1-\varepsilon}.
\]
4.2. **Further properties of \( u_- \).** In order to prove the lower bound for the first gap in (2.9) we will need a lower estimate for the \( x_1 \)-directional derivative of \( u_- \) in the region between \(-x\) and \( x\). Recall that we defined \( |x| = L/2 \).

**Proposition 4.1 (Derivative of \( u_- \)).**

*Pick for \( u_- \) the same phase as in Proposition 3.3* For any \( 0 < \varepsilon < 1 \) we have the pointwise bound

\[
\partial_{x_1} u_-(x) \geq c_\varepsilon \frac{e^{-A_{DW}(x)}}{V_{DW}(x)} \quad \text{on} \quad \{ -L/2 + R \leq x_1 \leq L/2 - R \}
\]

(4.3)

for \( R \) large enough and with a constant \( c_\varepsilon \) that depends only on \( \varepsilon \).

The first key ingredients for the proof of Proposition 4.1 are provided in the next Lemma.

**Lemma 4.2 (Symmetry and sign of \( u_- \)).**

The function \( u_- \) is odd with respect to reflections across the \( x_1 = 0 \) plane, i.e.,

\[
u_-(x_1, x_2, \ldots, x_d) = -u_-(x_1, x_2, \ldots, x_d).
\]

Moreover, assume that we pick for \( u_- \) the same phase as in Proposition 3.3. Then \( u_-(x) > 0 \) almost everywhere for \( x_1 > 0 \).

The proof of the positivity of \( u_-(x) \) for \( x_1 > 0 \) will follow from the following abstract result that we directly import, without proof, from [20, Theorem XIII.44].

**Theorem 4.3 (Ground states of Schrödinger operators).**

Assume that \( H \) is a bounded from below, self-adjoint operator on a Hilbert space and that \( e^{-tH} \) is positivity preserving for all \( t > 0 \). Assume further that \( E = \inf \sigma(H) \) is an eigenvalue. Then \( E \) is a simple eigenvalue with (almost everywhere) strictly positive eigenvector if and only if \( e^{-tH} \) is positivity improving \( \forall t > 0 \).

**Proof of Lemma 4.2** Since \( u_- \) must be either odd or even, the fact that it is odd is a trivial consequence of (3.14). To prove that \( u_-(x) > 0 \) for \( x_1 > 0 \), let us first notice that by the odd symmetry

\[
\mu_- = \min \left\{ \langle u, h_{DW} u \rangle, \ |u| \|_{L^2} = 1, \ u \perp u_+ \right\}
\]

\[
= \min \left\{ \langle u, h_{DW} u \rangle, \ |u| \|_{L^2} = 1, \ u \text{ odd} \right\}.
\]

Thus, \( \mu_- \) must coincide with the ground state energy of the Dirichlet Hamiltonian

\[
\hat{h}_{DW,x_1 \geq 0}^{(D)} = -\Delta_{x_1 \geq 0}^{(D)} + V_{DW} + \lambda w \ast |u_+|^2,
\]

where \( \Delta_{x_1 \geq 0}^{(D)} \) is the Dirichlet Laplacian in the half-space \( \{ x_1 \geq 0 \} \). We now want to apply Theorem 4.3 with \( H = \hat{h}_{DW,x_1 \geq 0}^{(D)} \). Using the Trotter product formula [19, Theorem VII.31] and the fact that \( V_{DW} + \lambda w \ast |u_+|^2 \geq 0 \), it is easy to see that \( e^{-tH} \) is positivity improving \( \forall t > 0 \). Notice also that \( H \) has compact resolvent, and hence the bottom of its spectrum is an eigenvalue. Hence we can use Theorem 4.3 and the proof is complete. \( \square \)

We will also need the following result.
Lemma 4.4 (Monotonicity of $u_-$).
Assume we pick for $u_-$ the same phase as in Proposition 3.3. Then, for some fixed constant $R > 0$ large enough,

$$
\partial_{x_1} u_-(x) \geq 0 \quad \text{for} \quad -L/2 \leq x_1 \leq L/2 \quad \text{with} \quad |x \pm x| \geq R.
$$

(4.5)

Proof. Since $u_-$ is odd under reflection across the $x_1 = 0$ hyperplane, $\partial_{x_1} u_-$ must be even. Moreover, by Lemma 3.2, $\partial_{x_1} u_-$ is continuous. This means that if $\partial_{x_1} u_-$ is negative on a set of non-zero measure, then such a set must be open. Assume then that $\partial_{x_1} u_-$ is negative on some open subset of $\{-L/2 \leq x_1 \leq L/2\}$. By even symmetry of $\partial_{x_1} u_-$ this set must be invariant under reflections across the $x_1 = 0$ hyperplane. This in particular means that there is a region in $\{0 \leq x_1 \leq L/2\}$ where $u_-$ decreases when moving in the $x_1$ direction.

We will define a trial state for the $\mu_-$-minimization problem which differs from $u_-$ by a displacement of mass towards larger $x_1$'s. Since $V_{DW}$ strictly decreases as $x_1$ increases, this will cause a net decrease in the energy, thus leading to a contradiction.

Without loss of generality, we can reduce ourselves to the following case: there exists two positive functions $s_1, s_2 : \mathbb{R}^{d-1} \to \mathbb{R}$ and two fixed real numbers $A, B$ such that

$$
\begin{align*}
\partial_{x_1} u_1(s_1(x_2, \ldots, x_d), x_2, \ldots, x_d) &= 0 \\
\partial_{x_1} u_1(s_2(x_2, \ldots, x_d), x_2, \ldots, x_d) &= 0 \\
\partial_{x_1} u_-(x) &< 0, \quad \forall x \text{ s.t. } s_1(x_2, \ldots, x_d) < x_1 < s_2(x_2, \ldots, x_d)
\end{align*}
$$

(4.6)

The hypersurfaces $\{x_1 = s_1(x_2, \ldots, x_d)\}$ and $\{x_1 = s_2(x_2, \ldots, x_d)\}$ delimit in the $x_1$-direction the region where $\partial_{x_1} u_-$ is negative, while all other coordinates are constrained between $A$ and $B$. Hence, for every $x_2, \ldots, x_d$ in the considered region, $u_-$ has a $x_1$-directional maximum at $(s_1, x_2, \ldots, x_d)$ and a $x_1$-directional minimum at $(s_2, x_2, \ldots, x_d)$. By the even symmetry of $\partial_{x_1} u_-$ the requirement $s_1, s_2 > 0$ is not restrictive, and indeed a behavior identical to (4.6) (with reversed inequalities in the third line) happens for negative $x_1$'s.

Define, for some $c > 0$, the set

$$
I_\epsilon = \left\{ x \mid A \leq x_2, \ldots, x_d \leq B, \ s_1(x_2, \ldots, x_d) - c < x_1 < s_2(x_2, \ldots, x_d), \max_{A \leq x_2, \ldots, x_d \leq B} |u_-(s_1(x_2, \ldots, x_d), x_2, \ldots, x_d)|^2 - \epsilon \leq |u_-(x)|^2 \right\},
$$

The parameter $c$ is intended to be picked small enough in order to make sure that $I_\epsilon$ is connected, but it will play no other role. Define the function

$$
\Phi(\epsilon) = \int_{I_\epsilon} \left( |u_-(x)|^2 - \max_{A \leq x_2, \ldots, x_d \leq B} |u_-(s_1(x_2, \ldots, x_d), x_2, \ldots, x_d)|^2 + \epsilon \right) dx_1, \ldots dx_d.
$$
Define the following trial function for the minimization problem: for \( u \leq x_2, \ldots, x_d \leq B, \ s_1(x_2, \ldots, x_d) < x_1 < s_2(x_2, \ldots, x_d) + \epsilon \),

\[
J_\delta = \left\{ x \mid A \leq x_2, \ldots, x_d \leq B, \ s_1(x_2, \ldots, x_d) < x_1 < s_2(x_2, \ldots, x_d) + \epsilon, \right. \\
\min_{A \leq x_2, \ldots, x_d \leq B} |u_-(s_2(x_2, \ldots, x_d), x_2, \ldots, x_d)|^2 \leq |u_-(x)|^2 \\
\leq \min_{A \leq x_2, \ldots, x_d \leq B} |u_-(s_2(x_2, \ldots, x_d), x_2, \ldots, x_d)|^2 + \delta \left\}
\]

and

\[
\Gamma(\delta) = \int_{J_\delta} \left( -|u_-(x)|^2 + \min_{A \leq x_2, \ldots, x_d \leq B} |u_{x}(s_2(x_2, \ldots, x_d), x_2, \ldots, x_d)|^2 + \delta \right) dx_1 \ldots dx_d.
\]

As above, a choice of \( \epsilon \) small enough makes \( J_\delta \) connected. By definition \( \Phi(\epsilon) \) and \( \Gamma(\delta) \) are continuous positive functions such that

\[
\lim_{\epsilon \to 0} \Phi(\epsilon) = 0, \quad \text{and} \quad \lim_{\delta \to 0} \Gamma(\delta) = 0.
\]

This means that for \( \bar{\delta} \) small enough there exists \( \bar{\epsilon} \) such that

\[
\max_{A \leq x_2, \ldots, x_d \leq B} |u_-(s_2(x_2, \ldots, x_d), x_2, \ldots, x_d)|^2 + \bar{\delta} < \min_{A \leq x_2, \ldots, x_d \leq B} |u_-(s_1(x_2, \ldots, x_d), x_2, \ldots, x_d)|^2 - \bar{\epsilon}
\]

and, at the same time,

\[
\Phi(\bar{\epsilon}) = \Gamma(\bar{\delta}). \tag{4.7}
\]

We will consider \( \bar{\epsilon} \to 0 \) as \( \bar{\delta} \to 0 \) while satisfying the two above properties.

Now, recall that

\[
\langle u_-, h_{DW} u_- \rangle = \min \left\{ \langle u, h_{DW} u \rangle, \ |u|_{L^2} = 1, \ u \text{ odd} \right\}.
\]

Define the following trial function for the minimization problem: for \( x_1 \geq 0 \),

\[
u(x) := \begin{cases} 
\sqrt{\max_{A \leq x_2, \ldots, x_d \leq B} |u_-(s_1(x_2, \ldots, x_d), x_2, \ldots, x_d)|^2 - \epsilon} & \text{on } I_\delta \\
\sqrt{\min_{A \leq x_2, \ldots, x_d \leq B} |u_-(s_2(x_2, \ldots, x_d), x_2, \ldots, x_d)|^2 + \delta} & \text{on } J_\delta \\
u_-(x) & \text{elsewhere},
\end{cases}
\]

and, for \( x_1 \leq 0 \),

\[
u(x) = -\nu(-x_1, x_2, \ldots, x_d).
\]

By construction \( \nu \) is odd, and \( \int |\nu|^2 = 1 \) thanks to (4.7), whence it is an admissible trial function. We will show that, having moved mass from \( I_\delta \) to \( J_\delta \), where the external potential is strictly smaller, the energy \( \langle v, h_{DW} v \rangle \) of \( v \) is strictly lower than that of \( u_- \), contradicting the definition of \( u_- \). First, we have

\[
\int_{\mathbb{R}^d} |\nabla u|^2 \leq \int_{\mathbb{R}^d} |\nabla u_-|^2
\]
because the integrands coincide outside of $I_\delta$ and $J_\delta$ and $|v|^2$ is flat on $I_\delta$ and on $J_\delta$. Notice that we are using here Lemma 4.2 to ensure that $u_-$ doesn’t change sign on $\{x_1 > 0\}$, which could make the kinetic energy of $v$ ill-defined. Regarding the potential term, we notice that, for $0 \leq x_1 \leq R$ and $|x - x| \geq R$ with $R$ large enough,

$$\partial_{x_1} V_r(x) < -sR^{s-1} < 0.$$ 

Moreover,

$$\left\| \partial_{x_1} \lambda w * |u_+|^2 \right\|_{L_\infty} \leq C \|\nabla w\|_{L_\infty}.$$ 

These two inequalities imply that

$$\int_{\mathbb{R}^d} \left(V_{DW} + \lambda w * |u_+|^2\right) |v|^2 < \int_{\mathbb{R}^d} \left(V_{DW} + \lambda w * |u_+|^2\right) |u_-|^2$$

because, for $R$ large enough, the decrease in energy given by $V_{DW}$ dominates the contribution coming from $w$. We have then shown $\langle v, h_{DW} v \rangle < \langle u, h_{DW} u \rangle$, which is absurd. The proof is complete. \hfill \Box

We are now in condition to provide the

**Proof of Proposition 4.1** The proof is similar to the one of Proposition 3.1. Define the function

$$f(x) = e^{-A_{DW}(x)} V_{DW}(x)^{-\beta/s},$$

and let us consider the region $\{x_1 \geq 0\}$ first. Similarly to the proof of Proposition 3.1 we pick $\beta = s\alpha_+ + \epsilon$ and $R$ a radius large enough for both

$$W(x) := |x - x|^2 + \lambda w * |u_+|^2(x) - \mu_+ > 0$$

and

$$\left(-\Delta + W(x)\right) f(x) \leq 0$$

(4.8)

(4.9)

to hold for $|x - x| \geq R$ and $x_1 \geq 0$. We also modify $f$ inside the region $|x - x| \leq R$ into a smooth $\tilde{f}$ which is bounded away from zero uniformly in $L$.

Let us first consider the region $\{0 \leq x_1 \leq L/2 - R\}$. Using Item (i) of Theorem 2.1 it is easy to see that there must exists a set $\Sigma$ of positive measure contained in $\{0 < x_1 \leq L/2 - R\}$ where $\partial_{x_1} u_- \geq C > 0$ uniformly in $L \to \infty$. Moreover, the set $\Sigma$ can be chosen at a fixed (independent of $L$) distance from $x$. Indeed, if this were not the case, we would have, by Lemma 4.4 $\partial_{x_1} u_- \to 0$ as $L \to \infty$ almost everywhere at any finite distance from $x$ within $\{0 \leq x_1 \leq L/2 - R\}$. By the convergence (3.14) this would mean that $u_-$ is constant at any finite distance from $x$ within $\{0 \leq x_1 \leq L/2 - R\}$, which is false. Define, for such a $\Sigma$,

$$C_\Sigma = \min_{x \in \Sigma} \frac{\partial_{x_1} u_- (x)}{\tilde{f}(x)},$$

and

$$g = \partial_{x_1} u_- - C_\Sigma \tilde{f}.$$ 

Notice that, by construction, $C_\Sigma \geq C > 0$ uniformly as $L \to \infty$. We will prove that $g \geq 0$ in $\{0 \leq x_1 \leq L/2 - R\}$, hence concluding the proof.
Assume for contradiction that $\mu$ is negative on a set $\Omega$ of positive measure contained in $\{0 \leq x_1 \leq L/2 - R\}$. By continuity of $g$ we can assume that $g = 0$ on the boundary $\partial \Omega$. By direct computation we know that

$$(-\Delta + W) \partial_{x_1} u_- = -(\partial_{x_1} W) u_-.$$ 

Since, for $0 \leq x_1 \leq L/2 - R$, 

$$\partial_{x_1} W(x) \geq -sR^{s-1} - C$$

and $u_-$ is positive on the whole $\{x_1 \geq 0\}$ by Lemma 4.2, we have that 

$$(-\Delta + W) \partial_{x_1} u_- \geq 0 \quad \text{on } \{0 \leq x_1 \leq L/2 - R\}. 
\tag{4.10}$$

Putting together (4.10) and (4.9), we deduce 

$$(-\Delta + W) g \geq 0 \quad \text{on } \Omega.$$ 

Now, since $g < 0$ on $\Omega$, then (4.8) implies also $Wg < 0$ on $\Omega$. This, by the above inequality implies 

$$\Delta g \leq 0$$

on $\Omega$. By the maximum principle [10, Theorem 8.1] $g$ satisfies the following inequality 

$$\inf_{\Omega} g \geq \inf_{\partial \Omega} g.$$ 

However, the quantity on the left is strictly smaller than zero by the contradiction hypothesis, while the quantity on the right is exactly zero, and this is a contradiction. Hence $\Omega$, if non-empty, must occupy the whole $\{0 \leq x_1 \leq L/2 - R\}$. This is absurd since $g > 0$ on $\Sigma$ by construction, and therefore $\Omega$ must be the empty set. This proves (4.3) in the region $\{0 \leq x_1 \leq L/2 - R\}$. However, as we already said, $\partial_{x_1} u_-$ is even with respect to reflections across $\{x_1 = 0\}$. This implies that (4.3) holds also for $\{-L/2 + R \leq x_1 \leq 0\}$, completing the proof. \qed

4.3. **Lower bound for the first gap.** Now we provide the lower bound in (2.9). We use a result due to Harrell. While a more general version can be found in [12, Theorem 2.1], we report it here already adapted to our notation, and recall the proof for self-containedness.

**Theorem 4.5 (The spectral gap as a flux).**

Define 

$$\widetilde{u}_-(x) = \begin{cases} 
  u_-(x) & x_1 \geq 0 \\
  -u_-(x) & x_1 \leq 0.
\end{cases}$$

If $\langle \widetilde{u}_-, u_+ \rangle \neq 0$, then 

$$\mu_- - \mu_+ = \frac{2}{\langle \widetilde{u}_-, u_+ \rangle} \int_{x_1=0} u_+(0, x_2, \ldots, x_d) \frac{\partial}{\partial x_1} u_-(x_1, x_2, \ldots, x_d) |_{x_1=0} \, dx_2 \ldots \, dx_d.$$
Proof. Since 
\[(\mu_- - h_{\text{DW}})u_+ = (\mu_- - \mu_+)u_+\],
we deduce
\[\langle \tilde{u}_- , (\mu_- - h_{\text{DW}})u_+ \rangle = (\mu_- - \mu_+) \langle \tilde{u}_- , u_+ \rangle. \tag{4.11}\]

On the other hand, using the fact that $u_+$ is even and $u_-$ is odd, and then Green’s identity (recall that $u_+$ and $u_-$ are smooth by Lemma 3.2), we have
\[\langle \tilde{u}_- , (\mu_- - h_{\text{DW}})u_+ \rangle = 2 \int_{x_1 > 0} u_-( (\mu_- - h_{\text{DW}})u_+) \]
\[= 2 \int_{x_1 > 0} (\mu_- - h_{\text{DW}})u_+ \]
\[+ 2 \int_{x_1 = 0} (u_+ \frac{\partial u_-}{\partial x_1} |_{x_1 = 0} - u_- \frac{\partial u_+}{\partial x_1} |_{x_1 = 0}) \, dx_2 \ldots dx_d. \]

If we now use $h_{\text{DW}}u_+ = \mu_- u_+$ and the fact that $\partial_{x_1} u_+$ must vanish at $x_1 = 0$ because $u_+$ is smooth and symmetric around the $x_1 = 0$ hyperplane, we see that the above formula reduces to
\[\langle \tilde{u}_- , (\mu_- - h_{\text{DW}})u_+ \rangle = 2 \int_{x_1 = 0} u_+ \frac{\partial u_-}{\partial x_1} |_{x_1 = 0} \, dx_2 \ldots dx_d. \]

The proof is completed by comparing this with (4.11). \hfill \square

Since, by Lemma 4.2, $u_-$ is strictly positive almost everywhere on \(\{x_1 > 0\}\), we deduce that the scalar product $\langle \tilde{u}_- , u_+ \rangle$ is strictly positive, and this allows us to apply Theorem 4.5. By Cauchy-Schwartz $\langle \tilde{u}_- , u_+ \rangle$ is also bounded by one, so we will ignore it for a lower bound. We then use the pointwise lower bounds for $u_+$ and $\partial_{x_1} u_-$ from, respectively, Proposition 3.1 and Proposition 4.1, and evaluate them at $x_1 = 0$. We obtain
\[\mu_- - \mu_+ \geq c_\epsilon \int_{\mathbb{R}^{d-1}} \exp \left[ - \left( \frac{1}{1 + s/2} + \epsilon \right) (L^2/4 + |x_2|^2 + \ldots + |x_d|^2)^{1/2+s/4} \right] \, dx_2 \ldots dx_d \]
\[\geq c_\epsilon \int_{|x| \leq L'} \exp \left[ - \left( \frac{1}{1 + s/2} + \epsilon \right) (L^2/4 + |x_2|^2 + \ldots + |x_d|^2)^{1/2+s/4} \right] \, dx_2 \ldots dx_d. \]

Notice that we omitted the $V_{\text{DW}}$-dependence by adding a small enough $\epsilon$ to the exponent. In the second step we restricted the domain of integration to vectors in $\mathbb{R}^{d-1}$ whose length does not exceed $L'$ for some fixed $\gamma > 0$. In particular, by picking $\gamma < 1$ we can then neglect the dependence on $x_2, \ldots, x_d$ in the exponent thanks to
\[(L^2/4 + |x_2|^2 + \ldots + |x_d|^2)^{1/2+s/4} \leq |L/2|^{1+s/2}(1 + o(1)), \]
and deduce
\[\mu_- - \mu_+ \geq c_\epsilon L^{dy} T^{1+\epsilon}. \]

The factor $L^{dy}$ can be absorbed in the exponential by once again slightly modifying $\epsilon$. This completes the proof of (2.9) thanks to (2.7).
4.4. **Lower bound on the second gap.** To prove (2.10), recall that $u_{\text{ex}}$ is the first excited state above $u_-$, i.e., $\mu_{\text{ex}} = \langle u_{\text{ex}}, h_{\text{DW}} u_{\text{ex}} \rangle$. A lower bound for $\mu_{\text{ex}}$ follows from the IMS formula and reads

$$
\mu_{\text{ex}} \geq 2 \langle \chi \cdot 0 u_{\text{ex}}, h_{\text{DW}} \chi \cdot 0 u_{\text{ex}} \rangle - C \varepsilon T^{1-\varepsilon},
$$

having used (A.6) and (A.3). Here $\chi \cdot 0$ and $\chi \cdot 0$ are localization functions as in Proposition 3.3. We further argue that (A.10) and (3.22) allow to replace $h_{\text{DW}}$ with $h_r$, i.e.,

$$
\mu_{\text{ex}} \geq 2 \langle \chi \cdot 0 u_{\text{ex}}, h_r \chi \cdot 0 u_{\text{ex}} \rangle - C \varepsilon T^{1/2-\varepsilon}.
$$

(4.12)

We now want to bound from below the right hand side using (a suitable modification of) $\chi \cdot 0 u_{\text{ex}}$ as a trial state for the minimization problem

$$
\mu_{r, \text{ex}} := \inf \left\{ \langle u, h_r u \rangle \mid \|u\|_{L^2} = 1, \ u \perp u_r \right\}.
$$

Define then

$$
\nu := \frac{\chi \cdot 0 u_{\text{ex}} - 2 \langle u_r, \chi \cdot 0 u_{\text{ex}} \rangle u_r}{\| \chi \cdot 0 u_{\text{ex}} - 2 \langle u_r, \chi \cdot 0 u_{\text{ex}} \rangle u_r \|_{L^2}}.
$$

By construction $\nu$ is orthogonal to $u_r$ (since $\|u_r\|_{L^2} = 1/2$), which makes it a trial function for the $\mu_{r, \text{ex}}$ minimization. We want to estimate the norm in the denominator. Recall that $u_{\text{ex}}$ must be either even or odd under reflection across the $\{x_1 = 0\}$ hyperplane. Assume it is even. Then

$$
0 = \langle u_+, u_{\text{ex}} \rangle = \langle \chi \cdot 0 u_+, \chi \cdot 0 u_{\text{ex}} \rangle + \langle \chi \cdot 0 u_+, \chi \cdot 0 u_{\text{ex}} \rangle = 2 \langle \chi \cdot 0 u_+, \chi \cdot 0 u_{\text{ex}} \rangle,
$$

which implies

$$
\left\| \chi \cdot 0 u_{\text{ex}} - 2 \langle u_r, \chi \cdot 0 u_{\text{ex}} \rangle u_r \right\|_{L^2}^2 = \frac{1}{2} - 2 \left| \langle u_r, \chi \cdot 0 u_{\text{ex}} \rangle \right|^2
$$

$$
= \frac{1}{2} - 2 \left| \left( u_r - \chi \cdot 0 u_+ \right) \cdot \chi \cdot 0 u_{\text{ex}} \right|^2
$$

$$
\geq \frac{1}{2} - C \varepsilon T^{1-\varepsilon},
$$

where the inequality follows by Cauchy-Schwartz and by approximation of $u_+$ that we deduced in (3.13). If, on the other hand, $u_{\text{ex}}$ is odd, then we can repeat the same calculation with $u_+$ replaced by $u_-$. The variational principle then implies

$$
\mu_{r, \text{ex}} \leq \frac{\langle \chi \cdot 0 u_{\text{ex}}, h_r \chi \cdot 0 u_{\text{ex}} \rangle - 2 \mu_r \left| \langle u_r, \chi \cdot 0 u_{\text{ex}} \rangle \right|^2}{\left\| \chi \cdot 0 u_{\text{ex}} - 2 \langle u_r, \chi \cdot 0 u_{\text{ex}} \rangle u_r \right\|_{L^2}^2}
$$

$$
\leq 2 \langle \chi \cdot 0 u_{\text{ex}}, h_r \chi \cdot 0 u_{\text{ex}} \rangle + C \varepsilon T^{1/2-\varepsilon},
$$

having ignored the second term in the numerator because it is negative. Comparing this with (4.12) we find

$$
\mu_{\text{ex}} \geq \mu_{r, \text{ex}} - C \varepsilon T^{1/2-\varepsilon}.
$$
Now, we know that the spectrum of $h$, does not depend on $N$, since $h$ coincides with the translation of a fixed Hamiltonian. Hence, the gap between $\mu_r$ and $\mu_{r,\text{ex}}$ is a fixed constant. Moreover, by (3.23), we have

$$\mu_r \geq \mu_- - C_\varepsilon T^{1/2-\varepsilon}.$$ 

This gives

$$\mu_{\text{ex}} \geq \mu_{r,\text{ex}} - C_\varepsilon T^{1/2-\varepsilon} \geq \mu_r + C - C_\varepsilon T^{1/2-\varepsilon} \geq \mu_- + C - C_\varepsilon T^{1/2-\varepsilon},$$

which proves (2.10).

### 5. Refined estimates, following Helffer-Sjöstrand

The aim of this section is to prove (2.11), (2.12), and (2.13). The optimal rate in (2.11) will follow from a careful choice of approximating quasi-modes inspired by [14, 15].

Let us denote by $u_r^{(D)}$ the (normalized) ground state of the Dirichlet problem

$$\begin{cases}
-\Delta + V_{\text{DW}} + \lambda w * |u_\varepsilon|^2 u = \mu u \\
u(x) = 0, \quad \text{for } x_1 \leq -\frac{L}{2} + c
\end{cases} \quad (5.1)$$

with eigenvalue $\mu^{(D)}$. Let us, in turn, denote by $u_\varepsilon^{(D)}$ the (normalized) ground state of the Dirichlet problem

$$\begin{cases}
-\Delta + V_{\text{DW}} + \lambda w * |u_\varepsilon|^2 u = \mu u \\
u(x) = 0, \quad \text{for } x_1 \geq -\frac{L}{2} + c
\end{cases} \quad (5.2)$$

By symmetry across the $\{x_1 = 0\}$ hyperplane we have $u_\varepsilon^{(D)}(-x_1, x_2, \ldots, x_d) = u_\varepsilon^{(D)}(x)$ and therefore the eigenvalue corresponding to $u_\varepsilon^{(D)}$ coincides with $\mu^{(D)}$.

The cutoff distance $c > 0$ will eventually be chosen to depend (non-uniformly) on the parameter $\varepsilon$ appearing in the right hand side of (2.11), which we will take arbitrarily small. As a consequence, since most quantities depends on $c$, they will implicitly depend on $\varepsilon$. We will however not keep track of such a dependence.

#### 5.1. Agmon decay estimates

The first step in the proof of (2.11) is to show suitable decay estimates for $u_r^{(D)}$ and $u_\varepsilon^{(D)}$. These will be more refined that what we have proved so far.

We start by defining the double-well Agmon distance between two points $x, y \in \mathbb{R}^d$

$$d_{\text{DW}}(x, y) = \inf_{\gamma \text{ piecewise } C^1 \text{ curve}} \left\{ \int_0^1 \sqrt{V_{\text{DW}}(\gamma(t))} |\gamma'(t)| dt, \quad |\gamma(0) = x, \gamma(1) = y| \right\}. \quad (5.3)$$

The exponentials of the functions $d_{\text{DW}}(\cdot, x)$ and $d_{\text{DW}}(\cdot, -x)$ will model the decay of, respectively, $u_r^{(D)}$ and $u_\varepsilon^{(D)}$. The following general properties are well-known (see, e.g., [13 Equations (3.2.1) and (3.2.2)])

$$d_{\text{DW}}(x, y) \leq d_{\text{DW}}(x, z) + d_{\text{DW}}(z, y), \quad \forall x, y, z \quad \text{(triangular inequality)} \quad (5.4)$$

$$|\nabla_x d_{\text{DW}}(x, y)|^2 \leq V_{\text{DW}}(x), \quad \forall x, y. \quad (5.5)$$

Furthermore, we have the following Lemma.
Lemma 5.1 (Properties of the double-well Agmon distance).

The function $d_{\text{DW}}(\cdot, x)$ satisfies the three following properties, with $A$ the single-well Agmon distance (2.6) and $c$ the constant in (5.1) - (5.2):

(i) **First estimate in the half-space:**

$$d_{\text{DW}}(x, x) \geq A(|x - x|) \quad x_1 \geq 0,$$
$$d_{\text{DW}}(x, -x) \geq A(|x + x|) \quad x_1 \leq 0.$$  \hfill (5.6)

(ii) **Estimate at $(x_2, \ldots, x_d) = 0$:**

$$d_{\text{DW}}((x_1, 0, \ldots, 0), x) \geq \begin{cases} A(|x_1 - \frac{L}{2}|), & x_1 \geq 0 \\ 2A(\frac{L}{2}) - A\left(|\frac{L}{2} + x_1|\right), & -L/2 + c \leq x_1 \leq 0. \end{cases}$$

$$d_{\text{DW}}((x_1, 0, \ldots, 0), -x) \geq \begin{cases} A\left(|x_1 + \frac{L}{2}|\right), & x_1 \leq 0 \\ 2A(\frac{L}{2}) - A\left(|\frac{L}{2} - x_1|\right), & 0 \leq x_1 \leq L/2 - c. \end{cases}$$  \hfill (5.7)

(iii) **Second estimate in the half space:**

$$d_{\text{DW}}((x_1, x_2, \ldots, x_d), x) \geq 2A\left(\frac{L}{2}\right) - A\left(|\frac{L}{2} + x_1|\right), \quad -L/2 + c \leq x_1 \leq 0.$$  \hfill (5.8)

$$d_{\text{DW}}((x_1, x_2, \ldots, x_d), -x) \geq 2A\left(\frac{L}{2}\right) - A\left(|\frac{L}{2} - x_1|\right), \quad 0 \leq x_1 \leq L/2 - c.$$  \hfill (5.8)

**Proof.** For each of the three points we will only prove the property for $d_{\text{DW}}(\cdot, x)$, since the one for $d_{\text{DW}}(\cdot, -x)$ can be then deduced by reflection symmetry.

Let us prove (i). First, notice that, in the $x_1 \geq 0$ region, $V_{\text{DW}}$ only depends on the radial coordinate $|x - x|$. Hence, the same must be true for $d_{\text{DW}}(\cdot, x)$, and thus, without loss of generality, we can assume $x = (x_1, 0, \ldots, 0)$, the general case being then deduced from

$$d_{\text{DW}}(x, x) = d_{\text{DW}}\left(||x - x| - L/2|, 0, \ldots, 0, x\right).$$

Let us now prove that, in order to compute $d_{\text{DW}}((x_1, 0, \ldots, 0), x)$ for $x_1 \geq 0$ we can reduce ourselves, in the definition of $d_{\text{DW}}(\cdot, x)$, to curves supported on the line $x_2, \ldots, x_d = 0$ only. Indeed, for any piecewise $C^1$ curve $\gamma : [0, 1] \to \mathbb{R}^d$ such that $\gamma(0) = x$ and $\gamma(1) = (x_1, 0, \ldots, 0)$, let us define the curve projected onto the $x_2, \ldots, x_d = 0$ line

$$\gamma_1(t) := (\gamma(t), 0, \ldots, 0).$$

Then, by definition,

$$|\gamma_1'(t)| \leq |\gamma'(t)|.$$  

Since $V_{\text{DW}}(\gamma) \geq V_{\text{DW}}((\gamma_1, 0, \ldots, 0))$ for any $\gamma \in \mathbb{R}^d$, we find

$$\int_0^1 \sqrt{V_{\text{DW}}(\gamma(t))}|\gamma'(t)|dt \geq \int_0^1 \sqrt{V_{\text{DW}}(\gamma_1(t))}|\gamma_1'(t)|dt,$$
This shows that it is always favorable to only consider paths restricted to the line. Let then \( \tilde{\gamma} : [0, 1] \to \mathbb{R} \) be a piecewise \( C^1 \) curve such that \( \tilde{\gamma}(0) = L/2 \) and \( \tilde{\gamma}(1) = x_1 \). We have

\[
A(|x - x_0|) = \frac{1}{1 + \frac{|x - x_0|}{2}} |x_1 - \frac{L}{2}|^{1 + \frac{\epsilon}{2}}
\]

\[
= \frac{1}{1 + \frac{|x - x_0|}{2}} \int_0^1 \frac{d}{dt} |\tilde{\gamma}(t) - \frac{L}{2}|^{1 + \frac{\epsilon}{2}} dt
\]

\[
\leq \int_0^1 |\tilde{\gamma}(t) - \frac{L}{2}|^{1/2} |\tilde{\gamma}'(t)| dt
\]

\[
= \int_0^1 \sqrt{V_{DW}(\tilde{\gamma}(t), 0, \ldots, 0)} |\tilde{\gamma}'(t)| dt.
\]

Considering the infimum over all such curves \( \tilde{\gamma} \) (which we proved above to coincide with the infimum over all curves), we deduce (5.6).

Let us now prove (ii). The claim for \( x_1 \geq 0 \) already follows from (5.6). We concentrate on \( x_1 \leq 0 \). By repeating the arguments used above, one easily sees that in order to compute \( d_{DW}(x_1, 0, \ldots, 0, x) \) for \( x_1 \leq 0 \) it is again convenient to restrict to curves supported on \( x_2, \ldots, x_d = 0 \). Let then \( \tilde{\gamma} : [0, 1] \to \mathbb{R} \) be any piecewise \( C^1 \) curve such that \( \tilde{\gamma}(0) = L/2 \) and \( \tilde{\gamma}(1) = x_1 \). Since \( x_1 \leq 0 \), there exists a time \( t_\tilde{\gamma} \), depending on the choice of the curve, such that \( \tilde{\gamma}(t_\tilde{\gamma}) = 0 \). We then write

\[
2A\left(\frac{L}{2}\right) - A\left(\left|\frac{L}{2} + x_1\right|\right) = \int_{t_\tilde{\gamma}}^1 \frac{d}{dt} A\left(\left|\tilde{\gamma}(t) - \frac{L}{2}\right|\right) dt
\]

\[
+ \int_{t_\tilde{\gamma}}^1 \frac{d}{dt} \left[2A\left(\frac{L}{2}\right) - A\left(\left|\frac{L}{2} + \tilde{\gamma}(t)\right|\right)\right] dt
\]

\[
\leq \int_{t_\tilde{\gamma}}^1 \left|\tilde{\gamma}(t) - \frac{L}{2}\right|^{1/2} |\tilde{\gamma}'(t)| dt + \int_{t_\tilde{\gamma}}^1 \left|\tilde{\gamma}(t) + \frac{L}{2}\right|^{1/2} |\tilde{\gamma}'(t)| dt
\]

\[
= \int_{t_\tilde{\gamma}}^1 \sqrt{V_{DW}(\tilde{\gamma}(t), 0, \ldots, 0)} |\tilde{\gamma}'(t)| dt.
\]

Taking the infimum over all such curves \( \tilde{\gamma} \) yields the result.

Finally, (iii) is deduced by arguing, as done above, that projecting a curve onto the \( x_2, \ldots, x_d = 0 \) line cannot increase \( d_{DW}(\cdot, x) \). \( \square \)

The following proposition gives decay estimates for \( u^{(D)}_\epsilon \) and \( u^{(D)}_\epsilon \).

**Proposition 5.2 (Decay estimates for the Dirichlet modes).**

*For every \( \epsilon \geq 0 \) there exist \( C_\epsilon > 0 \) and \( c_\epsilon > 0 \) such that*

\[
\left\| e^{(1-\epsilon)d_{DW}(\cdot, x)} u^{(D)}_\epsilon \right\|_{H^1} = \left\| e^{(1-\epsilon)d_{DW}(\cdot, -x)} u^{(D)}_\epsilon \right\|_{H^1} \leq C_\epsilon, \quad (5.9)
\]

*and*

\[
\left\| e^{(1-\epsilon)d_{DW}(\cdot, x)} \nabla u^{(D)}_\epsilon \right\|_{L^2} = \left\| e^{(1-\epsilon)d_{DW}(\cdot, -x)} \nabla u^{(D)}_\epsilon \right\|_{L^2} \leq C_\epsilon, \quad (5.10)
\]
where $u_r^{(D)}$, respectively $u_r^{(D)}$, is the ground state of (5.1), respectively (5.2), (extended to zero outside of its domain of definition) for $c = c_r$.

The importance of this result is the following: even though in a region at distance of order 1 from $-x$ the total potential $V_{DW} + \lambda w \ast |u_+|^2$ is of order 1, nonetheless $u_r^{(D)}$ is as small as the exponential of minus the Agmon distance from $x$. Compared to the estimates proved previously, it confirms that $u_r^{(D)}$ does not see the left well at all. This is the key to prove (2.11) with such a good rate.

We need the following well-known lemma, which vindicates the importance of (5.5):

**Lemma 5.3 (Computing with the Agmon distance).**

Let $\Omega \subset \mathbb{R}^d$ be open with regular boundary, $v \in C^0(\overline{\Omega}, \mathbb{R})$, $\Phi : \overline{\Omega} \to \mathbb{R}$ locally Lipschitz and $u \in C^2(\overline{\Omega}, \mathbb{R})$ with $u|_{\partial \Omega} = 0$ (including $\lim_{|x| \to \infty} u(x) = 0$ if $\Omega$ is unbounded). Let $\nabla \Phi$ be defined in $L^\infty$ as the limit of a mollified sequence $\nabla \Phi_\epsilon$. Define also

$$h := -\Delta + v.$$

Then

$$\int_\Omega |\nabla (e^\Phi u)|^2 + \int_\Omega (v - |\nabla \Phi|^2) e^{2\Phi} |u|^2 = \int_\Omega e^{2\Phi} (hu).$$

Moreover, assume $v - |\nabla \Phi|^2 = F_+^2 - F_-^2$ with $F_+, F_- \geq 0$, and define $F := F_+ + F_-$. Then

$$\int_\Omega |\nabla (e^\Phi u)|^2 + \frac{1}{2} \int_\Omega |F_+ e^\Phi u|^2 \leq \int_\Omega |F^{-1} e^\Phi hu|^2 + \frac{3}{2} \int_\Omega |F_- e^\Phi u|^2. \quad (5.11)$$

The proof can be found in [15, Lemma 2.3] or [13, Theorem 3.1.1]. We are now ready to prove Proposition 5.2.

**Proof of Proposition 5.2** We will estimate the norms containing $u_r^{(D)}$ only, since, by reflection symmetry, the identities in (5.9) and (5.10) are trivial. We will apply (5.11) with the following choices (recall that $c$ is the constant that appears in (5.1), its choice will be specified later on):

$$\begin{align*}
\Omega &= \left\{ x \mid x_1 \geq -\frac{L}{2} + c \right\} \\
v &= V_{DW} + \lambda w \ast |u_+|^2 - \mu^{(D)} \\
\Phi &= (1 - \varepsilon)d_{DW}(\cdot, x) \\
u &= u_r^{(D)}.
\end{align*}$$

We now explain how to choose the functions $F_+, F_-$ and the constant $c$. The main idea is to define $F_+$ to be equal to the function $v - |\nabla \Phi|^2$ on the set where $v - |\nabla \Phi|^2$ is larger than some fixed arbitrary positive constant $\kappa$, and to be identically equal to the same $\kappa$ on the set where $v - |\nabla \Phi|^2 \leq \kappa$. To this end, notice first that

$$\begin{align*}
v(x) - |\nabla \Phi(x)|^2 &= V_{DW}(x) + \lambda w \ast |u_+|^2(x) - \mu^{(D)} - (1 - \varepsilon)^2 |\nabla d_{DW}(x, x)|^2 \\
&\geq (2\varepsilon - \varepsilon^2)V_{DW}(x) - \mu^{(D)},
\end{align*}$$
having used (5.5) and \( u \geq 0 \) in the second step. This shows that \( v - |\nabla \Phi|^2 \) can be smaller than a fixed constant only in the regions close to \( x \) and \( -x \). As a consequence, for every \( \varepsilon > 0 \), there exists \( c_\varepsilon > 0 \) such that \( v(x) - |\nabla \Phi(x)|^2 \geq \kappa \) for \(-L/2 + c_\varepsilon \leq x_1 \leq 0\). We pick \( c \) equal to such a \( c_\varepsilon \) in the definition (5.11) of \( u_r^{(D)} \). The only other region in which \( v - |\nabla \Phi|^2 \) can be small is the region of small \( |x - x| \). We take care of this by defining

\[
F^2_+(x) := \begin{cases} 
|v(x) - |\nabla \Phi(x)|^2|, & |x - x| \geq \left(\frac{\kappa + \mu^{(D)}}{2\varepsilon - \varepsilon^2}\right)^{1/s} \quad \text{and} \quad x_1 \geq -\frac{L}{2} + c_\varepsilon \\
\kappa, & |x - x| \leq \left(\frac{\kappa + \mu^{(D)}}{2\varepsilon - \varepsilon^2}\right)^{1/s}.
\end{cases}
\]

Correspondingly, we define

\[
F^2_-(x) = F^2_+(x) - v(x) + |\nabla \Phi(x)|^2 \begin{cases} \quad = 0, & |x - x| \geq \left(\frac{\kappa + \mu^{(D)}}{2\varepsilon - \varepsilon^2}\right)^{1/s} \quad \text{and} \quad x_1 \geq -\frac{L}{2} + c_\varepsilon \\
\leq \kappa, & |x - x| \leq \left(\frac{\kappa + \mu^{(D)}}{2\varepsilon - \varepsilon^2}\right)^{1/s}.
\end{cases}
\]

It is then straightforward to verify that, by construction,

\[
F^2_+ \geq \kappa, \quad F^2_- \leq \kappa, \quad \text{supp}(F_-) \subset \left\{ x \mid |x - x| \leq \left(\frac{\kappa + \mu^{(D)}}{2\varepsilon - \varepsilon^2}\right)^{1/s} \right\}. 
\]

We are then ready to apply (5.11), which yields (recall that \( hu = 0 \))

\[
\int_{\{x_1 \geq -L/2 + c_\varepsilon\}} \left| \nabla \left( e^{(1-\varepsilon)d_{DW}(\cdot, x)} u_r^{(D)} \right) \right|^2 + \frac{\kappa}{2} \int_{\{x_1 \geq -L/2 + c_\varepsilon\}} \left| e^{(1-\varepsilon)d_{DW}(\cdot, x)} u_r^{(D)} \right|^2 \leq \frac{3\kappa}{2} \int_{\left\{ |x - x| \leq \left(\frac{\kappa + \mu^{(D)}}{2\varepsilon - \varepsilon^2}\right)^{1/s} \right\}} \left| e^{(1-\varepsilon)d_{DW}(\cdot, x)} u_r^{(D)} \right|^2.
\]

As proven in Lemma 5.1, the function \( d_{DW}(x, x) \) for \( x_1 \geq 0 \) depends on the radial coordinate \( |x - x| \) only. As a consequence, the integral in the right hand side does not depend on \( L \), and therefore it is estimated by a \( (\varepsilon\text{-dependent}) \) constant. This completes the proof of (5.9).

In order to prove (5.10) we write

\[
\left\| e^{(1-\varepsilon)d_{DW}(\cdot, x)} \nabla u_r^{(D)} \right\|_{L^2}^2 \leq \left\| e^{(1-\varepsilon)d_{DW}(\cdot, x)} u_r^{(D)} \right\|_{H^1}^2 + \left\| (\nabla d_{DW}(\cdot, x)) e^{(1-\varepsilon)d_{DW}(\cdot, x)} u_r^{(D)} \right\|_{L^2}^2 \leq \left\| \sqrt{V_{DW}} e^{(1-\varepsilon)d_{DW}(\cdot, x)} u_r^{(D)} \right\|_{L^2}^2 + C_\varepsilon,
\]

where the second inequality follows from (5.4) and (5.9). Using Lemma 5.1, \( d_{DM}(\cdot, x) \) has at least polynomial growth, and therefore one deduces that, for every \( \delta > 0 \), there exists \( K_\delta > 0 \) such that

\[
\sqrt{V_{DW}} \leq K_\delta e^{\delta d_{DW}(\cdot, x)}.
\]

We then deduce,

\[
\left\| e^{(1-\varepsilon)d_{DW}(\cdot, x)} \nabla u_r^{(D)} \right\|_{L^2}^2 \leq K_\delta \left\| e^{(1-\varepsilon+\delta)d_{DW}(\cdot, x)} u_r^{(D)} \right\|_{L^2}^2 + C_\varepsilon \leq K_\delta C_\varepsilon + C_\varepsilon,
\]
which proves \((5.10)\) if we fix \(\delta < \varepsilon\).

5.2. **Quasi-modes construction and proof of \(L^1\) and \(L^2\) estimates.** Now we use linear combinations of \(u_{1}(D)\) and \(u_{2}(D)\) as quasi-modes for the mean-field Hamiltonian \(h_{DW}\). A proper smoothing (around respectively \(x_1 = -L/2 + \varepsilon\) and \(x_1 = L/2 - \varepsilon\)) is required. To this end, define a smooth localization function \(\chi_\varepsilon\) such that

\[
\chi_\varepsilon(x) = \begin{cases} 
0 & x_1 \leq -\frac{L}{2} + 2\varepsilon \\
1 & x_1 \geq -\frac{L}{2} + 3\varepsilon \\
0 \leq \chi_\varepsilon(x) \leq 1,
\end{cases}
\]

and the corresponding \(\chi_\varepsilon(x) = \chi_\varepsilon(-x_1, x_2, \ldots, x_d)\). Define then

\[
\psi_\varepsilon := \chi_\varepsilon u_{1}(D), \quad \psi_\varepsilon := \chi_\varepsilon u_{2}(D)
\]

and

\[
\psi_\varepsilon := (h_{DW} - \mu(D))\psi_\varepsilon, \quad \psi_\varepsilon := (h_{DW} - \mu(D))\psi_\varepsilon.
\]

A direct calculation gives

\[
r_\varepsilon = -2\nabla \chi_\varepsilon \cdot \nabla u_{1}(D) - (\Delta \chi_\varepsilon)u_{1}(D),
\]

and therefore

\[
\text{supp } (r_\varepsilon) \subset \{ x \mid 2\varepsilon \leq |x + x| \leq 3\varepsilon \}.
\]

This means that \(\psi_\varepsilon\) and \(\psi_\varepsilon\) are quasi-modes for \(h_{DW}\), the only error coming from the region where, respectively, \(\chi_\varepsilon\) and \(\chi_\varepsilon\) differ from zero and one.

**Lemma 5.4 (Estimates for quasi-modes).**

*We have, with \(T\) the tunneling parameter \((2.7)\)*

\[
\|r_\varepsilon\|_L^2 = \|r_\varepsilon\|_L^2 \leq C_\varepsilon T^{1-\varepsilon} \tag{5.15}
\]

\[
|\langle \psi_\varepsilon, \psi_\varepsilon \rangle - 1| = |\langle \psi_\varepsilon, \psi_\varepsilon \rangle - 1| \leq C_\varepsilon T^{2-\varepsilon} \tag{5.16}
\]

\[
|\langle \psi_\varepsilon, r_\varepsilon \rangle| = |\langle \psi_\varepsilon, r_\varepsilon \rangle| \leq C_\varepsilon T^{2-\varepsilon} \tag{5.17}
\]

\[
0 \leq \langle \psi_\varepsilon, \psi_\varepsilon \rangle \leq C_\varepsilon T^{1-\varepsilon}. \tag{5.18}
\]

**Proof.** As usual, we can consider only the right functions. To prove \((5.15)\), let us start from \((5.14)\). Multiplying and dividing by \(e^{|-1|d_{DW}(\cdot, x)}\) we find

\[
\|r_\varepsilon\|_L^2 \leq \left\| e^{-|1|d_{DW}(\cdot, x)}(\Delta \chi_\varepsilon)e^{|-1|d_{DW}(\cdot, x)}u_{1}(D) \right\|_L^2 \\
+ 2\left\| e^{-|1|d_{DW}(\cdot, x)}(\nabla \chi_\varepsilon)e^{|-1|d_{DW}(\cdot, x)}\nabla u_{1}(D) \right\|_L^2 \\
\leq C\left( \left\| e^{-|1|d_{DW}(\cdot, x)}u_{1}(D) \right\|_L^2 + \left\| e^{-|1|d_{DW}(\cdot, x)}\nabla u_{1}(D) \right\|_L^2 \right) \\
\times \sup_{2\varepsilon \leq x_1 \leq L/2 \leq 3\varepsilon} e^{-|1|d_{DW}(x, x)}.
\]
The two norms inside the parenthesis were estimated in Proposition 5.2. To estimate the supremum, we deduce from (5.8) that
\[
\sup_{2c_x \leq x_1 + L / 2 \leq 3c_x} e^{-(1-\epsilon)d_{dW}(x,x)} \leq e^{-(1-\epsilon)(2A(\frac{L}{2}) - A(\frac{L}{2} + x_1))} \leq C e^{-2(1-\epsilon)A(\frac{L}{2})},
\]
and this proves (5.15).

To prove (5.16) let us notice that
\[
\langle \psi_r, \psi_r \rangle - 1 = \int_{\mathbb{R}^d} (1 - \chi_r^2) |\mu_r^{(D)}|^2 \leq \int_{2c_x \leq x_1 + L / 2 \leq 3c_x} |\mu_r^{(D)}|^2.
\]
We then argue as above by multiplying and dividing by \(e^{(1-\epsilon)d_{dW}(\cdot,x)}\). The same can be done to prove (5.17).

Finally, let us prove (5.18) (notice that the positivity of the scalar product is trivial). We write
\[
\langle \psi_r, \psi_r \rangle = \int_{\mathbb{R}^d} \chi_x \chi_x u_r^{(D)} u_r^{(D)} \leq \sup_{-L / 2 + 2c_x, \leq x_1 \leq L / 2 - 2c_x} \left( e^{-(1-\epsilon)d_{dW}(x,x) - (1-\epsilon)d_{dW}(x,-x)} \right) \times \int_{\mathbb{R}^d} \chi_x \chi_x u_r^{(D)} e^{-(1-\epsilon)d_{dW}(\cdot,x)} u_r^{(D)} e^{-(1-\epsilon)d_{dW}(\cdot,x)} u_r^{(D)}.
\]
Using Cauchy-Schwartz and then (5.9) we see that the integral in the right hand side is estimated by an \( \epsilon \)-dependent constant. To estimate the supremum we write
\[
\sup_{-L / 2 + 2c_x \leq x_1 \leq L / 2 - 2c_x} \left( e^{-(1-\epsilon)d_{dW}(x,x) - (1-\epsilon)d_{dW}(x,-x)} \right) \leq \sup_{-L / 2 + 2c_x, \leq x_1 \leq 0} \left( e^{-(1-\epsilon)d_{dW}(x,x) - (1-\epsilon)d_{dW}(x,-x)} \right) + \sup_{0 \leq x_1 \leq L / 2 - 2c_x} \left( e^{-(1-\epsilon)d_{dW}(x,x) - (1-\epsilon)d_{dW}(x,-x)} \right) \leq e^{-(1-\epsilon)(2A(\frac{L}{2} - A(|L / 2 + x_1| + A(|x + x|))) + \sup_{0 \leq x_1 \leq L / 2 - 2c_x} e^{-(1-\epsilon)(2A(\frac{L}{2} - x_1) + A(|x - x|))},
\]
where the last inequality follows from (5.6) and (5.8). However, since the function \( A \) is monotone increasing, we have
\[
A(|L / 2 + x_1|) \leq A(|x + x|) \quad \text{and} \quad A(|L / 2 - x_1|) \leq A(|x - x|),
\]
and therefore we find
\[ \sup_{-L/2+2\epsilon \leq x \leq L/2-2\epsilon} \left( e^{-\epsilon d_{DW}(x,x)} - e^{-\epsilon d_{DW}(x,-x)} \right) \leq e^{-2(1-\epsilon)A \left( \frac{1}{2} \right)} , \]
which completes the proof. \( \square \)

Let us now define the orthogonal projections
\[ P_{\pm} := |u_+\rangle \langle u_+| + |u_-\rangle \langle u_-| \quad \text{and} \quad P_{\pm}^{0} = 1 - P_{\pm} , \]
Our aim is an estimate for the norm of \( P_{\pm}^{0} \Psi_{r} \) and \( P_{\pm}^{0} \Psi_{e} \). Let us start with the following

**Lemma 5.5 (Further bounds on \( \mu_{\pm} \)).**

We have
\[ |\mu_{+} - \mu_{\pm}(D)| \leq C_{\epsilon} T^{1-\epsilon} . \]

**Proof.** An upper bound is deduced by taking \( \psi_{r} \) as trial function for the \( \mu_{\pm} \)-minimization problem:
\[ \mu_{+} \leq \frac{1}{\langle \psi_{r}, \psi_{r} \rangle} \langle \psi_{r}, h_{DW} \psi_{r} \rangle = \mu_{\pm}(D) + \frac{\langle \psi_{r}, r_{e} \rangle}{\langle \psi_{r}, \psi_{r} \rangle} \leq \mu_{\pm}(D) + C_{\epsilon} T^{2-\epsilon} , \]
where the second inequality follows from (5.17) and (5.16). A suitable lower bound, in turn,
\[ \mu_{+} \geq 2 \langle \chi_{x_{1} \geq 0} u_{+}, h_{DW} \chi_{x_{1} \geq 0} u_{+} \rangle - C_{\epsilon} T^{1-\epsilon} \geq \mu_{\pm}(D) - C_{\epsilon} T^{1-\epsilon} , \]
where the second inequality follows once again by the variational principle for the Dirichlet minimization. \( \square \)

As a consequence of Lemma 5.5 and of our main results on the gaps (2.9) and (2.10), we see that \( \mu_{\pm}(D) \) is asymptotically close to \( \mu_{+} \) (and therefore to \( \mu_{-} \)), and hence it is separated from the rest of the spectrum of \( h_{DW} \) by a gap of order one. We can then write
\[ P_{\pm}^{0} \psi_{r} = - \frac{1}{2\pi i} \oint_{\Gamma} \left( \frac{1}{\mu_{\pm}(D) - z} - \frac{1}{h_{DW} - z} \right) d z \psi_{r} , \]
where \( \Gamma \) is a closed contour in the complex plane that encircles \( \mu_{+} \), \( \mu_{-} \), and \( \mu_{\pm}(D) \), staying at a finite distance both from them and from the rest of the spectrum. A simple calculation yields
\[ P_{\pm}^{0} \psi_{r} = - \frac{1}{2\pi i} \oint_{\Gamma} \frac{1}{(\mu_{\pm}(D) - z)(h_{DW} - z)} d z r_{e} , \quad (5.20) \]
By our choice of the contour we have
\[ |\mu_{\pm}(D) - z|^{-1} \leq C , \quad \text{and} \quad \left\| (h_{DW} - z)^{-1} \right\|_{op} \leq C , \]
uniformly for \( z \in \Gamma \). Hence, recalling (5.15), we find
\[ \left\| P_{\pm}^{0} \psi_{r} \right\|_{L^{2}} \leq C_{\epsilon} T^{1-\epsilon} \]
\[ \left\| P_{\pm}^{0} \psi_{e} \right\|_{L^{2}} \leq C_{\epsilon} T^{1-\epsilon} . \quad (5.21) \]
Now, define
\[
\psi_+ := \frac{\psi_r + \psi_\ell}{\|\psi_r + \psi_\ell\|_{L^2}} \quad \text{and} \quad \psi_- := \frac{\psi_r - \psi_\ell}{\|\psi_r - \psi_\ell\|_{L^2}}.
\] (5.22)
We have
\[
\left|\|\psi_r + \psi_\ell\|_{L^2}^2 - 2\right| \leq \left|\|\psi_r\|_{L^2}^2 + \|\psi_\ell\|_{L^2}^2 - 2 + 2\langle\psi_r, \psi_\ell\rangle\right| \leq C_\varepsilon T^{1-\varepsilon},
\]
where the last inequality follows from (5.16) and (5.18). Similarly,
\[
\left|\|\psi_r - \psi_\ell\|_{L^2}^2 - 2\right| \leq C_\varepsilon T^{1-\varepsilon}.
\]
Hence the norms in the denominators of (5.22) satisfy
\[
\|\psi_r + \psi_\ell\|_{L^2} = \sqrt{2} + O(T^{1-\varepsilon})
\]
and
\[
\|\psi_r - \psi_\ell\|_{L^2} = \sqrt{2} + O(T^{1-\varepsilon})
\]
and combining with (5.21) we deduce
\[
\psi_+ = au_+ + bu_- + O_{L^2}(T^{1-\varepsilon})
\]
for complex numbers \(a, b\). But since \(\psi_+, u_+\) are even under reflections across \(x_1 = 0\) and \(u_-\) is odd, this must reduce to
\[
\psi_+ = u_+ + O_{L^2}(T^{1-\varepsilon}).
\]
Similarly
\[
\psi_- = u_- + O_{L^2}(T^{1-\varepsilon}).
\]
These are our vindications of (1.12)-(1.13), as in [15]. We deduce from the above that
\[
|u_+|^2 - |u_-|^2 = 2\psi_r \psi_\ell + O_{L^1}(T^{1-\varepsilon})
\]
and (2.11) then follows from (5.18).
To deduce (2.12) let us first recall that, if \(x_1 \geq 0\), then \(u_-(x)\) is positive by Lemma 4.2 and \(u_+(x)\) is positive by general arguments. This allows to write
\[
\int_{\mathbb{R}^d} \left|u_+ - u_-\right|^2 = 2 \int_{x_1 \geq 0} \left|u_+ - u_-\right|^2
\]
\[
\leq 6 \int_{x_1 \geq 0} \left|u_+ - \psi_+\right|^2 + 6 \int_{x_1 \geq 0} \left|\psi_+ - \psi_-\right|^2 + 6 \int_{x_1 \geq 0} \left|\psi_- - u_-\right|^2.
\]
The estimates for the first and third summand follow already from what we discussed above. For the second summand we write
\[
\int_{x_1 \geq 0} \left|\psi_+ - \psi_-\right|^2 \leq \left[\|\psi_r + \psi_\ell\|_{L^2}^{-1} - \|\psi_r - \psi_\ell\|_{L^2}^{-1}\right]^2 \int_{x_1 \geq 0} |\psi_r|^2
\]
\[
+ \left[\|\psi_r + \psi_\ell\|_{L^2}^{-1} + \|\psi_r - \psi_\ell\|_{L^2}^{-1}\right]^2 \int_{x_1 \geq 0} |\psi_\ell|^2.
\]
The first square bracket in the right hand side is smaller than $C_T T^{1-\varepsilon}$ by the estimates above. For the integral of $\psi\varepsilon$ we write

$$\int_{x_1 \geq 0} |\psi\varepsilon|^2 \leq \int_{x_1 \geq 0} |u^{(D)}\varepsilon|^2 \leq \sup_{0 \leq x_1 \leq L/2-c_\varepsilon} e^{-2(1-\varepsilon)d_{\text{HW}}(x,-x)} \|e^{(1-\varepsilon)d_{\text{HW}}(-x)} u^{(D)}\varepsilon\|_{L^2}^2 \leq C_T T^{1-\varepsilon},$$

where the last inequality follows from Lemma 5.1 and Proposition 5.2. This proves (2.12).

### 5.3. Proof of the $L^\infty$ estimate.

In order to prove the $L^\infty$ proximity in (2.13) we will improve the $L^2$ result (2.12) to an estimate for the $H^2$ norms. Notice that, in the notations of Proposition 5.3 the $L^2$ convergence (2.12) implies

$$\left\| \chi_{x_1 \geq 0} (u_+ - u_-) \right\|_{L^2}^2 \leq C_T T^{1-\varepsilon},$$

$$\left\| \chi_{x_1 \leq 0} (u_+ + u_-) \right\|_{L^2}^2 \leq C_T T^{1-\varepsilon},$$

which also means that (3.14) holds with an improved rate. We will improve this result to a higher Sobolev norm.

**Proposition 5.6 ($H^2$ convergence).**

$$\left\| \chi_{x_1 \geq 0} (u_+ - u_-) \right\|_{H^2}^2 \leq C_T T^{1-\varepsilon}$$

$$\left\| \chi_{x_1 \leq 0} (u_+ + u_-) \right\|_{H^2}^2 \leq C_T T^{1-\varepsilon}.$$  

The $L^\infty$ estimate (2.13) is an immediate consequence of Proposition 5.6 thanks to the Sobolev embedding.

$$\|f\|_{L^\infty(\mathbb{R}^d)} \leq C \|f\|_{H^2(\mathbb{R}^d)}$$

that holds for $d = 1, 2, 3$. In order to prove Proposition 5.6 we start with two Lemmas.

**Lemma 5.7 (Estimate on $h^2_{\text{DW}}$).**

$$\frac{1}{2} (-\Delta)^2 \leq h^2_{\text{DW}} + C$$

**Proof.** Let $W = V_{\text{DW}} + \lambda w * |u_\pm|^2$. For $\psi \in D[h^2_{\text{DW}}]$ with $\|\psi\|_{L^2} = 1$ we have, after expanding the square and integrating by parts,

$$\langle \psi, h^2_{\text{DW}} \psi \rangle = \langle \psi, \Delta^2 \psi \rangle + \langle \psi, W^2 \psi \rangle + \langle \nabla \psi, (\nabla W)\psi \rangle + 2 \langle \nabla \psi, W \nabla \psi \rangle + \langle \psi, (\nabla W) \nabla \psi \rangle \geq \langle \psi, \Delta^2 \psi \rangle + \langle \psi, W^2 \psi \rangle + \langle \nabla \psi, (\nabla W)\psi \rangle + \langle \psi, (\nabla W) \nabla \psi \rangle,$$

where for a lower bound we used $W \geq 0$. By Cauchy-Schwarz we have

$$\langle \nabla \psi, (\nabla W)\psi \rangle + \langle \psi, (\nabla W) \nabla \psi \rangle \geq -\langle \psi, (-\Delta) \psi \rangle - \langle \psi, |\nabla W|^2 \psi \rangle,$$

and the further inequality $-\Delta \leq \frac{1}{2} \Delta^2 + 2$ yields

$$\langle \psi, h^2_{\text{DW}} \psi \rangle \geq \frac{1}{2} \langle \psi, \Delta^2 \psi \rangle + \langle \psi, (W^2 - |\nabla W|^2 - 2) \psi \rangle.$$
The lemma is proven once we show $W^2 - |\nabla W|^2 \geq -C$. Let us consider the half-space \( \{x_1 \geq 0\} \). Here,

\[
W^2(x) = |x - x|^2 + (\lambda w \ast |u_+|^2)^2 + 2\lambda |x - x|^2 w \ast |u_+|^2
\]
and

\[
|\nabla W(x)|^2 = s^2|x - x|^{2s - 2} + (\lambda \nabla w \ast |u_+|^2)^2 + 2\lambda s|x - x_N|^{s - 1}\nabla w \ast |u_+|^2.
\]
Let us consider the difference $W^2 - |\nabla W|^2$. For $W^2$ we will use the estimate

\[
W^2(x) \geq |x - x|^{2s}.
\]
For the $\lambda^2$-term in $|\nabla W|^2$ we have, by Young inequality,

\[
-(\lambda \nabla w \ast |u_+|^2)^2 \geq -\lambda^2 \|w\|_{W^{1,\infty}}^2.
\]
For the $\lambda$-term in $|\nabla W|^2$ we use Cauchy-Schwarz followed by Young inequality to get

\[
-2\lambda s|x - x_N|^{s - 1}\nabla w \ast |u_+|^2 \geq -\delta|x - x|^{2s - 2} - C_\delta.
\]
The three last inequalities imply

\[
W^2(x) - |\nabla W(x)|^2 \geq |x - x|^{2s} - (s^2 + \delta)|x - x|^{2s - 2} - C_\delta - 2\lambda^2 \|w\|_{W^{1,\infty}}^2 \geq -C
\]
This concludes the proof. \(\blacksquare\)

**Lemma 5.8 (Commuting $h_{DW}$ and $\chi_{x,\geq 0}$).**

\[
\left\| h_{DW} \chi_{x,\geq 0}(u_+ - u_-) \right\|_{L^2}^2 \leq \left\| \chi_{x,\geq 0} h_{DW}(u_+ - u_-) \right\|_{L^2}^2 + C \varepsilon T^{1-\varepsilon}
\]

**Proof.** We have

\[
\left\langle \chi_{x,\geq 0}(u_+ - u_-), h_{DW}^2 \chi_{x,\geq 0}(u_+ - u_-) \right\rangle = \left\langle \chi_{x,\geq 0} h_{DW}(u_+ - u_-), \chi_{x,\geq 0} h_{DW}(u_+ - u_-) \right\rangle
+ \left\langle [h_{DW}, \chi_{x,\geq 0}] (u_+ - u_-), [h_{DW}, \chi_{x,\geq 0}] (u_+ - u_-) \right\rangle
+ 2\left\langle [h_{DW}, \chi_{x,\geq 0}] (u_+ - u_-), h_{DW} \chi_{x,\geq 0}(u_+ - u_-) \right\rangle
= \left\langle \chi_{x,\geq 0} h_{DW}(u_+ - u_-), \chi_{x,\geq 0} h_{DW}(u_+ - u_-) \right\rangle
+ 3\left\langle [h_{DW}, \chi_{x,\geq 0}] (u_+ - u_-), [h_{DW}, \chi_{x,\geq 0}] (u_+ - u_-) \right\rangle
+ 2\left\langle [h_{DW}, \chi_{x,\geq 0}] (u_+ - u_-), \chi_{x,\geq 0}(\mu_+ u_+ - \mu_- u_-) \right\rangle.
\]

We then have to estimate

\[
\text{Err}_1 = 3\left\langle [h_{DW}, \chi_{x,\geq 0}] (u_+ - u_-), [h_{DW}, \chi_{x,\geq 0}] (u_+ - u_-) \right\rangle
\]
\[
\text{Err}_2 = 2\left\langle [h_{DW}, \chi_{x,\geq 0}] (u_+ - u_-), \chi_{x,\geq 0}(\mu_+ u_+ - \mu_- u_-) \right\rangle.
\]
Since

\[
[h_{DW}, \chi_{x,\geq 0}] = \Delta \chi_{x,\geq 0} + 2(\nabla \chi_{x,\geq 0}) \cdot \nabla,
\]

we deduce, using (A.2) and (A.5),
\[
|\text{Err}_1| \leq \int \left| (\Delta \chi_{x_1 \geq 0} + 2(\nabla \chi_{x_1 = 0} \cdot \nabla)(u_+ - u_-) \right|^2 \\
\leq 2 \int |\Delta \chi_{x_1 \geq 0}|^2 |u_+ - u_-|^2 \\
+ 4 \int |\nabla \chi_{x_1 \geq 0}|^2 |\nabla (u_+ - u_-)|^2 \\
\leq C \epsilon T^{1-\epsilon}.
\]

The estimate of \text{Err}_2 is similar, and this completes the proof. \qed

**Proof of Proposition 5.6** Using Lemma 5.7 and then Lemma 5.8 we have
\[
\left\| \Delta \chi_{x_1 \geq 0}(u_+ - u_-) \right\|^2_{L^2} \leq \left\| h_{DW} \chi_{x_1 \geq 0}(u_+ - u_-) \right\|^2_{L^2} + C \left\| \chi_{x_1 \geq 0}(u_+ - u_-) \right\|^2_{L^2} \\
\leq \left\| \chi_{x_1 \geq 0} h_{DW}(u_+ - u_-) \right\|^2_{L^2} + C \left\| \chi_{x_1 \geq 0}(u_+ - u_-) \right\|^2_{L^2} + C \epsilon T^{1-\epsilon} \\
= \left\| \chi_{x_1 \geq 0}(\mu_+ u_+ - \mu_- u_-) \right\|^2_{L^2} + C \left\| \chi_{x_1 \geq 0}(u_+ - u_-) \right\|^2_{L^2} + C \epsilon T^{1-\epsilon}.
\]

The norm \( \left\| \chi_{x_1 \geq 0}(u_+ - u_-) \right\|^2_{L^2} \) was already estimated in (5.23). To estimate the first term in the right hand side, we expand
\[
\left\| \chi_{x_1 \geq 0}(\mu_+ u_+ - \mu_- u_-) \right\|^2_{L^2} = \frac{\mu_+ + \mu_-}{2} - 2 \mu_+ \mu_- \langle \chi_{x_1 \geq 0} u_+, \chi_{x_1 \geq 0} u_- \rangle.
\]

Since (5.23) implies
\[
-2 \langle \chi_{x_1 \geq 0} u_+, \chi_{x_1 \geq 0} u_- \rangle \leq -1 + C \epsilon T^{1-\epsilon},
\]
we deduce
\[
\left\| \chi_{x_1 \geq 0}(\mu_+ u_+ - \mu_- u_-) \right\|^2_{L^2} \leq \frac{\mu_+ + \mu_-}{2} - \mu_+ \mu_- + C \epsilon T^{1-\epsilon} \\
= \frac{1}{2}(\mu_+ - \mu_-)^2 + C \epsilon T^{1-\epsilon} \\
\leq C \epsilon T^{1-\epsilon},
\]

where the last step follows from the upper bound in (2.9). This proves (5.24). A reflection across the \( \{ x_1 = 0 \} \) hyperplane sends \( \chi_{x_1 \geq 0}(u_+ - u_-) \) into \( \chi_{x_1 < 0}(u_+ + u_-) \) and thus (5.25) also follows. \qed

**Appendix A. Tunneling terms**

Here we deduce a variety of useful bounds from the decay estimates of Section 3.1.
Proposition A.1 (Bounds on tunneling terms).
Let $R \geq 0$ be a fixed number. For any $\varepsilon > 0$ there exist $c_\varepsilon$, $C_\varepsilon$ such that, for $L$ large enough,

$$\int_{\mathbb{R}^d} u_x u_r \leq C_\varepsilon T^{1-\varepsilon} \quad \text{(A.1)}$$

$$\int_{-R \leq x_1 \leq R} |u_\pm(x)|^2 dx \leq C_\varepsilon T^{1-\varepsilon} \quad \text{(A.2)}$$

$$\int_{-R \leq x_1 \leq R} |u_{ex}(x)|^2 dx \leq C_\varepsilon T^{1-\varepsilon} \quad \text{(A.3)}$$

$$\int_{\mathbb{R}^d} \nabla u_\varepsilon \cdot \nabla u_r \leq C_\varepsilon T^{1-\varepsilon} \quad \text{(A.4)}$$

$$\int_{-R \leq x_1 \leq R} |\nabla u_\varepsilon(x)|^2 dx \leq C_\varepsilon T^{1-\varepsilon} \quad \text{(A.5)}$$

$$\int_{-R \leq x_1 \leq R} |\nabla u_{ex}|^2 \leq C_\varepsilon T^{1-\varepsilon} \quad \text{(A.6)}$$

$$\int_{\mathbb{R}^d} V_{DW} u_x u_r \leq C_\varepsilon T^{1-\varepsilon} \quad \text{(A.7)}$$

$$\int_{x_1 \geq -R} |u_\varepsilon(x)|^2 dx = \int_{x_1 \leq R} |u_r(x)|^2 dx \leq C_\varepsilon T^{1-\varepsilon} \quad \text{(A.8)}$$

$$\int_{-R \leq x_1 \leq R} |u_{ex}(x)|^2 (V_\varepsilon(x) - V_{DW}(x)) = \int_{-R \leq x_1 \leq R} |u_\pm|^2 (V_\varepsilon(x) - V_{DW}(x)) \leq C_\varepsilon T^{1-\varepsilon} \quad \text{(A.9)}$$

$$\int_{-R \leq x_1 \leq R} |u_{ex}(x)|^2 (V_\varepsilon(x) - V_{DW}(x)) \leq C_\varepsilon T^{1-\varepsilon} \quad \text{(A.10)}$$

$$\int_{-R \leq x_1 \leq R} V_{DW}(x) |u_\varepsilon(x)|^2 \leq C_\varepsilon T^{1-\varepsilon} \quad \text{(A.11)}$$

$$\int_{x_1 \geq -R} V_\varepsilon |u_\varepsilon|^2 = \int_{x_1 \leq R} V_\varepsilon |u_r|^2 \leq C_\varepsilon T^{1-\varepsilon} \quad \text{(A.12)}$$

$$\int_{-R \leq x_1 \leq R} |u_\varepsilon(x)|^2 (w \ast |u_\varepsilon|^2(x)) \leq C_\varepsilon T^{1-\varepsilon} \quad \text{(A.13)}$$

$$\int_{\mathbb{R}^d \times \mathbb{R}^d} w(x - y)|u_\varepsilon(x)|^2|u_r(y)|^2 dxdy \leq C_\varepsilon T^{1-\varepsilon} \quad \text{(A.14)}$$

Proof. (A.1) was already proven in [21 Proposition (3.3)]. The main point is to use the upper bounds in (3.4) and (3.5) in order to reduce the aim to estimating an integral of the form

$$I_a = \int_{\mathbb{R}^d} e^{-a|x-x_1|^2/a}e^{-a|x-x_1|^2} dx \quad \text{(A.15)}$$
with \( a = (1+s/2)^{-1} - \varepsilon \), the \( \varepsilon \) being used to absorb any polynomial correction due to \( V \).

As said, the estimate of \( I_a \) can then be found in [21 Proposition (3.3)]. The integrals in (A.2) and (A.3) can in the same way be bounded by an integral of the type \( I_a \).

To prove (A.4) we write

\[
\int_{\mathbb{R}^d} \nabla u_\varepsilon \nabla u_\varepsilon = - \int_{\mathbb{R}^d} u_\varepsilon \Delta u_\varepsilon = \int_{\mathbb{R}^d} u_\varepsilon (\mu_\varepsilon - V_\varepsilon - \lambda w * |u_\varepsilon|^2) u_\varepsilon.
\]

We can then reduce ourselves to an integral of the form (A.15) by slightly changing the value of \( \varepsilon \) in order to absorb the corrections coming from \( V_\varepsilon \) and \( \lambda w * |u_\varepsilon|^2 \). The same holds for every other term from (A.5) to (A.13).

To prove (A.14) we use the fact that \( w \) is bounded with compact support to write

\[
\iint_{\mathbb{R}^d \times \mathbb{R}^d} w(x-y) |u_\varepsilon(x)|^2 |u_\varepsilon(y)|^2 \, dx \, dy \leq C \iint_{\{ |x-y| \leq C \}} |u_\varepsilon(x)|^2 |u_\varepsilon(y)|^2 \, dx \, dy
\]

\[
= C \iint_{\{ |x-y| \leq C \} \cap \{ x_1 \leq 0 \}} |u_\varepsilon(x)|^2 |u_\varepsilon(y)|^2 \, dx \, dy
\]

\[
+ C \iint_{\{ |x-y| \leq C \} \cap \{ x_1 \geq 0 \}} |u_\varepsilon(x)|^2 |u_\varepsilon(y)|^2 \, dx \, dy.
\]

The second summand is bounded by \( C \int_{x_1 \geq 0} |u_\varepsilon|^2 \), and hence a bound for it follows from (A.8). For the first summand we write

\[
\iint_{\{ |x-y| \leq C \} \cap \{ x_1 \leq 0 \}} |u_\varepsilon(x)|^2 |u_\varepsilon(y)|^2 \, dx \, dy \leq \iint_{\{ |x-y| \leq C \} \cap \{ x_1 \leq 0 \} \cap \{ y_1 \leq C \}} |u_\varepsilon(x)|^2 |u_\varepsilon(y)|^2 \, dx \, dy.
\]

The right hand side is estimate by \( C \int_{x_1 \leq 0} |u_\varepsilon|^2 \), for which we can again use (A.8) \( \square \)

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