Quantitative estimate of the continuum approximations of interacting particle systems in one dimension

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Abstract

We consider a large class of interacting particle systems in 1D described by an energy whose interaction potential is singular and non-local. This class covers Riesz gases (in particular, log gases) and applications to plasticity and numerical integration. While it is well established that the minimisers of such interaction energies converge to a certain particle density profile as the number of particles tends to infinity, any bound on the rate of this convergence is only known in special cases by means of quantitative estimates. The main result of this paper extends these quantitative estimates to a large class of interaction energies by a different proof. The proof relies on one-dimensional features such as the convexity of the interaction potential and the ordering of the particles. The main novelty of the proof is the treatment of the singularity of the interaction potential by means of a carefully chosen renormalisation.

Keywords: Interacting particle system, calculus of variations, asymptotic analysis

MSC: 82C22, 74Q05, 35A15, 74G10

1 Introduction

We are interested in the quantifying the difference between minimisers of interacting particle energies and the minimisers of the related energies for the particle density. The interacting particle energies are given by

\[ E_n(x) = \frac{1}{n^2} \sum_{i=1}^{n} \sum_{j=0}^{i-1} V(x_i - x_j) + \frac{1}{n} \sum_{i=0}^{n} U(x_i), \]  

where \( n + 1 \) is the number of particles, and

\[ x := (x_0, x_1, \ldots, x_n) \in \Omega := \{ y \in \mathbb{R}^{n+1} : y_0 < y_1 < \ldots < y_n \}. \]

is the list of ordered particle positions. The energies \( E_n \) are the sum of two parts. We interpret the first part as the interaction part, in which \( V \) is the interaction potential, and the second part as a confinement term, in which \( U \) is the confining potential. Typical examples of \( V \) and \( U \) are plotted in Figure 1. We aim to keep the assumptions on \( V \) and \( U \) as weak as possible. These assumptions are as follows.

**Assumption 1.1 (V and U)**. The interaction potential \( V \in L^1_{\text{loc}}(\mathbb{R}) \) splits as \( V = V_a + V_{\text{reg}} \), where

\[ V_a(x) := \begin{cases} 
- \log |x|, & \text{if } a = 0 \\
|x|^{-a}, & \text{if } 0 < a < 1,
\end{cases} \]  

(3)
V(x)
\[x\]

U(x)
\[z_1\]

Figure 1: Typical examples of \(V\) and \(U\).

\[V(\text{even}), \ V \text{ convex on } (0, \infty), \ \lim_{x \to \infty} \frac{V(x)}{x} = 0.\]  

\[\text{The domain of the confining potential } U : \mathbb{R} \to [0, \infty] \text{ is } D(U) := \{x \in \mathbb{R} : U(x) < \infty\} = (z_1, z_2) \]

\[U \in C^2(D(U)), \ U \text{ convex on } \mathbb{R}, \ \min_{\mathbb{R}} U = 0, \ \lim_{|x| \to \infty} U(x) = \infty.\]

We interpret Assumption 1.1 as follows. We consider \(a\) as a fixed parameter which determines the singularity of \(V\) at 0. The part \(V_{\text{reg}}\) is a regular perturbation which determines the bulk and tails of \(V\). Finite values for \(z_i\) correspond to impenetrable barriers for the particle positions.

Given \(E_n\), the related energy for the particle density \(\rho\) is given by

\[E : \mathcal{P}(\mathbb{R}) \to \mathbb{R} \cup \{+\infty\}, \ E(\rho) := \frac{1}{2} \int_{\mathbb{R}} \int_{\mathbb{R}} V(x - y) \, d\rho(y) \, d\rho(x) + \int_{\mathbb{R}} U(x) \, d\rho(x),\]

where \(\mathcal{P}(\mathbb{R})\) is the space of probability measures.

For various choices of \(V\) and \(U\), it is known (see, e.g., [ST97, GPPS13, vM18b, vMMP14]) that \(E_n\) and \(E\) attain their minimal value at some \(x^* \in \Omega\) and \(\bar{\rho} \in \mathcal{P}(\mathbb{R})\) respectively, that \(\bar{\rho} \in \mathcal{P}(\mathbb{R})\) is unique, and that any sequence of minimisers \(x^*\) (parametrised by \(n\)) converges to \(\bar{\rho}\) in a suitable topology as \(n \to \infty\). Yet, any quantitative estimate between \(x^*\) and \(\bar{\rho}\) for finite \(n\) is only available for special choices of \(V\) and \(U\) (see Section 1.3). The aim of this paper is to derive such an estimate for the much larger class of potentials \(V\) and \(U\) characterised in Assumption 1.1.

In order to give meaning to a quantitative estimate between \(x^*\) and \(\bar{\rho}\), we construct from \(x^*\) a probability density function \(\varphi^*\), and seek to bound \(\varphi^* - \bar{\rho}\) in a suitable topology. For any \(x \in \Omega\), we define a related probability density function by

\[\varphi(y) := \begin{cases} \frac{1/n}{x_i - x_{i-1}} & \text{if } x_{i-1} < y < x_i \text{ for some } i \in \{1, \ldots, n\} \\ 0 & \text{otherwise}. \end{cases}\]

Figure 2 illustrates typical examples of \(\varphi^*\) and \(\bar{\rho}\). Especially in the case where \(D(U)\) confines \(\varphi^*\), the graphs of \(\varphi^*\) and \(\bar{\rho}\) are close to each other. This observation is in line with the literature (see, e.g., [GvMPS16, GPPS13, HCO10, HHvM18]). In this paper we wish to finally quantify this observation.
\[ U(x) = 0 \quad U(x) = \gamma_1 x \quad U(x) = \gamma_2(x - \frac{1}{2})^2 \]

Figure 2: Numerical computations of \( x^* \) for \( n = 16, V = V_a \) with \( a = \frac{1}{2} \) and three different choices of \( U \). The points \( x^*_i \) on the horizontal axis are indicated by the vertical edges of each light-gray rectangle (all with area \( \frac{1}{n} \)). The graph of \( \varphi^* \) is given by the top edges of these rectangles. The black curve is the graph of \( \rho \). The region where \( U = \infty \) is indicated in gray. The values of \( \gamma_i \) are chosen such that \( \text{supp} \, \rho = [0, 1] \). The computation of \( x^* \) and \( \rho \) is explained in Section 7.

1.1 Main result

We estimate \( \varphi^* - \rho \) in terms of a fractional Sobolev norm. To introduce this norm, we define the fractional Sobolev space on \( \mathbb{R} \) by

\[ H^{-s}(\mathbb{R}) := \{ \zeta \in S'(\mathbb{R}) : \int_{\mathbb{R}} (1 + \omega^2)^{-s} |\hat{\zeta}(\omega)|^2 d\omega < \infty \}, \quad (8) \]

where \( s > 0 \), \( \hat{\zeta} \) is the Fourier transform of \( \zeta \) and \( S'(\mathbb{R}) \) is the space of tempered distributions, i.e., the dual of the Schwartz space \( S(\mathbb{R}) \).

The main theorem of this paper is Theorem 1.2.

**Theorem 1.2 (The quantitative estimate).** Let \( n \geq 1 \). Let \( E_n \) and \( E \) be as defined in (1) and (6) with potentials \( V \) and \( U \) satisfying Assumption 1.1 for some \( 0 \leq a < 1 \). Then, the minimal values of \( E_n \) and \( E \) are attained, and the minimiser \( \overline{\rho} \) of \( E \) is unique. Moreover, there exists \( C > 0 \) independent of \( n \) such that for any minimiser \( x^* \) of \( E_n \),

\[ \| \varphi^* - \overline{\rho} \|_{H^{-(1-a)/2}(\mathbb{R})} \leq C \left\{ \begin{array}{ll} n^{-1+a} & 0 < a < 1 \\ n^{-1} (\log n)^3 & a = 0, \end{array} \right. \]

where \( \varphi^* \) is constructed from \( x^* \) by (7).

The available tools for the proof of Theorem 1.2 are the monotonicity and convexity of \( V \) and the regularity properties of \( \overline{\rho} \) proven in [KvM19] (see Lemma 3.3 below). The difficulty is that no information on \( x^* \) is available, except for \( x^* \) being a minimiser of \( E_n \).

Next we give an outline of the proof. The proof is divided in 3 parts. Part 1 is a preparatory step; we show that it is not restrictive to assume that

\[ \text{supp} \, V \text{ is compact}. \quad (9) \]

In Part 2, we demonstrate how far we can get with proving Theorem 1.2 without using any information on \( x^* \) except that it is the minimiser of \( E_n \). This part is mainly computational.
Its final result is the desired estimate in Theorem 1.2 with the additional error term $E_n^{nn}(x^*)$ given by

$$E_n^{nn}(x) := \frac{1}{n^2} \sum_{i=1}^{n} V(x_i - x_{i-1}), \quad (10)$$

which is the part of the interaction energy given by all nearest neighbour ('nn') interactions. Finally, in Part 3 we show that $E_n^{nn}(x^*) \leq C n^{-1+a}$ (for $0 < a < 1$). This is the difficult part of the proof of Theorem 1.2; we consider it as the main mathematical novelty of this paper.

Next we give the proof of Theorem 1.2. The proof uses several lemmas which will be established in subsequent sections in the paper.

**Proof of Theorem 1.2.** We first treat the case $0 < a < 1$. In Part 1 (see Section 3), we first prove that the sets of minimisers of both $E_n$ and $E$ are independent of the tails of $V$. This allows us to assume (9). Then, we show that the minimal values of $E_n$ and $E$ are attained, and that the minimiser $\rho$ of $E$ is unique. For this and other properties of $\rho$, we refer to [KvM19]. In particular, $\text{supp} \rho$ is a bounded, closed interval, which by an affine change of variables can be assumed to be $[0,1]$. In addition, the measure $\rho$ has a density in $L^1(0,1) \cap C(0,1)$, which we denote simply by $\rho$ in the remainder of the proof.

In Part 2, we follow [KvM19] by rewriting $E$ as the sum of the square of a norm and a linear term, i.e.,

$$E(\rho) = \frac{1}{2} \|\rho\|_V^2 + \int_{\mathbb{R}} U d\rho, \quad \|\rho\|_V^2 := \int_{\mathbb{R}} (V * \rho) d\rho. \quad (11)$$

We recall from [KvM19] Prop. 3.3 that $\| \cdot \|_V$ is equivalent to the norm on $H^{-(1-a)/2}(\mathbb{R})$. From (11) and the minimality of $\rho$ (see Lemma 3.3(iv)), we obtain

$$\|\varphi^* - \rho\|_{H^{-(1-a)/2}(\mathbb{R})} \lesssim \|\varphi^* - \rho\|_V^2 = 2(\rho, \rho - \varphi^*)_V + \|\varphi^*\|_V^2 - \|\rho\|_V^2 = 2 \int (V * \rho + U) d(\rho - \varphi^*) + 2E(\varphi^*) - 2E(\rho) \leq 0 + 2(E(\varphi^*) - E(\rho)). \quad (12)$$

Then, proving Theorem 1.2 translates into bounding the energy difference in the right-hand side.

To bound this difference, we obtain from the minimality of $x^*$ that

$$E(\varphi^*) - E(\rho) = E(\varphi^*) - E_n(x^*) + E_n(x^*) - E_n(x) + E_n(x) - E(\rho), \quad (13)$$

where $x \in \Omega$ can be chosen freely. We take $x$ such that

$$\rho_0 = 0, \quad \rho_n = 1, \quad \text{and} \quad \int_{\varphi_i}^{\varphi_{i+1}} \rho(x) dx = \frac{1}{n} \quad \text{for all} \ i = 1, \ldots, n. \quad (14)$$

Then, we bound $T_1$ and $T_2$ from above in Section 4. This is easy for the $U$-part of the energy, which can be estimated by $C/n$. For the interaction term, we perform a direct computation in
which we write $\| \cdot \|_V^2$ explicitly as the integral over the square $(0, 1)^2$, which we subdivide into the rectangles $(x_{i-1}, x_i) \times (x_{j-1}, x_j)$; see Figure 3. Then, by the monotonicity and convexity of $V$, we ultimately obtain

$$T_1 \leq C n^{-1+a} + C' E_{nn}^n(x^*) \text{ and } T_2 \leq C n^{-1+a}. \quad (15)$$

This completes Part 2 of the proof of Theorem 1.2.

In Part 3 we bound $E_{nn}^n(x^*)$ from above. Our strategy is to establish the following lower bound on $E_n$:

$$E_n(x) - E(\rho) \geq E_{nn}^n(x) - C n^{-1+a} \text{ for all } x \in \Omega; \quad (16)$$

see Proposition 5.1. Then, taking $x = x^*$, the left-hand side in (16) is bounded from above by $T_2$, and thus (16) gives the desired bound on $E_{nn}^n(x^*)$. Our proof of (16) is inspired by [PS17, Sec. 2]; we also construct a renormalisation of the norm $\| \cdot \|_V$, but we need to construct a different one to allow for $V_{\text{reg}} \neq 0$ and unbounded $\bar{\rho}$.

Finally, we treat the case $a = 0$ in Section 6. The proof is analogous to the case $0 < a < 1$; the only difference is that the factor $\log n$ appears at a few places in the estimates.  

1.2 Remarks on Theorem 1.2

Here we list several remarks on the statement of Theorem 1.2:

Uniform bound on support of $\phi^*$ The proof of Part 1 contains the additional result that $\text{supp } \phi^*$ is bounded uniformly in $n$; see Proposition 3.2. While the proof consists of common arguments in potential theory, we believe that the statement of Proposition 3.2 has merit on its own due to the rather weak assumptions on $V$ and $U$.

Extension of [KvM19] The statement of Part 1 has further merit; the main results in [KvM19] (on the regularity of $\rho$) are stated under the additional assumption that $V \in L^1(\mathbb{R})$. Here, Part 1 extends these results to the larger class of potentials $V$ specified by Assumption 1.1.

Choice of distance/norm Our proof heavily relies on the appropriate choice of norm for $\phi^* - \bar{\rho}$. Indeed, since we know nothing about $x^*$ other than that it is a minimiser of $E_n$, we have chosen our norm such that in the estimate for $\| \phi^* - \bar{\rho} \|$ (see Part 2) we can get rid of the dependence on $x^*$ by using that $E_n(x^*) \leq E_n(x)$ for any $x \in \Omega$. Therefore, our proof does not easily adapt to other commonly used topologies such as $L^p$-norms or the Wasserstein distance.

Other than mathematical convenience, our choice of norm has a further merit; it provides a quantitative estimate for the particle interaction force on $\mathbb{R}$ induced by the particle densities $\phi^*$ and $\bar{\rho}$. These interaction forces are

$$-(V * \phi^*)' - U' \text{ and } -(V * \bar{\rho})' - U'$$

respectively. To obtain a quantitative estimate from Theorem 1.2, we first change $V$ to have \footnote{Changing $V$ changes the interaction forces, but only on a domain which is a certain distance away from $\text{supp } \rho$ and $\text{supp } \phi^*$.} $V' \equiv \nabla \rho$. Then, by [KvM19] Lem. 3.1(iii)] it holds that

$$\exists C > 0 \forall \omega \in \mathbb{R} : \hat{V} (\omega) \leq C (1 + \omega^2)^{-\frac{1-a}{2}}.$$
Hence, writing $\nu := \varphi^* - \rho$ and $s := \frac{1-a}{2}$,
\[
\|\nu\|_{H^{-(1-a)/2}(\mathbb{R})}^2 = \int_{\mathbb{R}} (1 + \omega^2)^{-a} |\tilde{\nu}(\omega)|^2 \, d\omega \geq \frac{1}{C^2} \int_{\mathbb{R}} (1 + \omega^2)^{a} |\tilde{\nu}(\omega)\tilde{V}(\omega)|^2 \, d\omega = \frac{1}{C^2} \|V \ast \nu\|_{H^s(\mathbb{R})}^2.
\]
Thus,
\[
\left\|\left(V \ast \varphi^\prime - (V \ast \bar{\rho})^\prime\right)\right\|_{H^{-(1-a)/2}(\mathbb{R})}^2 \leq C \left\|V \ast (\varphi^* - \bar{\rho})\right\|_{H^{(1-a)/2}(\mathbb{R})}^2 \leq C' \|\varphi^* - \bar{\rho}\|_{H^{-(1-a)/2}(\mathbb{R})}^2,
\]
for which Theorem 1.2 gives an upper bound.

**Choice of $\varphi^*$** We chose the construction for $\varphi^*$ in (7) to ease the computations for the estimate in (15). This choice has been made in the literature before (see, e.g., [HCO10]) to produce plots similar to those in Figure 2. Another commonly used choice in such plots is to construct a one-dimensional Voronoi tessellation from the points $x_i$, and to assign to each Voronoi cell a mass of $1/n$. While Voronoi cells easily extend to higher dimensions, even in one dimension they introduce two complications for proving the corresponding estimates in (15). First, an additional choice for the Voronoi cells at the boundary has to be made. Second, the integral of $\bar{\rho}$ over a Voronoi cell may not equal $1/n$, which complicates our estimate for $T_2$.

### 1.3 Position in the literature

Here we put Theorem 1.2 in the context of the literature. In particular, we show how it applies to problems in plasticity and in numerical integration, and how it compares to recent advances on Riesz gases.

**Plasticity** The paper series started by [GPPS13, Hall11] and continued in [GvMPS16, HHvM18, vM18a, vM18b, vMMP14] studies the connection between models for plasticity of metals and an underlying microscopic model in a one-dimensional setting. This microscopic model is a minimisation problems of a certain $E_n$ of the form (1). In particular, the interaction potential is
\[
V(x) = x \coth x - \log(2|\sinh x|),
\]
which fits to Assumption 1.1 with $a = 0$ and $V_{\text{reg}} \neq 0$. While in this papers series the convergence of $\varphi^*$ to $\bar{\rho}$ as $n \to \infty$ is established, no quantitative estimates between $\varphi^*$ and $\bar{\rho}$ were found which limits the application to plasticity.

The main result of this paper, Theorem 1.2 provides the first quantitative estimate for this microscopic model. The estimate is given by
\[
\|\varphi^* - \bar{\rho}\|_{H^{-1/2}} \leq C(U) \frac{(\log n)^3}{n}. \tag{17}
\]
For the application, a more detailed dependence of the constant $C$ on $U$ is needed. Since the proof of Theorem 1.2 it constructive, it may be possible to use its steps for constructing an explicit expression for $C(U)$.

Our strive for quantitative estimates is also motivated by a problem in plasticity on a larger scope beyond one-dimensional particle systems; see [HvMP20]. On this larger scope, there are on the one hand a few microscopic models for plasticity (depending on a set of

\*An exception is [vM18a], which establishes a quantitative estimate for a special, $n$-dependent choice of $U$. 
parameters) and on the other hand a growing, large number of macroscopic models available. Yet, rigorous connections between them remain elusive, which questions the validity of the macroscopic models. Theorem 1.2 is a step forward in finding such connections in simplified scenarios.

**Numerical integration** In the field of numerical integration, the question on bounding the numerical error can be recast roughly to the question on bounding

\[ E_n(x^*) - E(\bar{\rho}) \]  

from below and above; see [TS19, HT19]. Similar to the application to plasticity, the potentials \( V \) and \( U \) satisfy Assumption 1.1. In particular, the interaction potential is explicitly given by \( V(x) = -\log |\tanh x| \), which satisfies Assumption 1.1 with \( a = 0 \) and \( V_{\text{reg}} \neq 0 \).

The currently available bounds (see [HT19, Thm. 2.3]) on \( E_n(x^*) \) itself. Applying (16) and the estimate on \( T_2 \) in (15) yields

\[ |E_n(x^*) - E(\bar{\rho})| \leq C(U) \frac{(\log n)^3}{n}, \]

which demonstrates that it may be possible to construct a sharper estimate. In this setting, \( U \) depends on \( n \), and thus (similar to the application to plasticity) a more detailed estimate on \( C(U) \) is required.

**Riesz gases** In the paper series by Petrache, Sandier, Serfaty *et al.* ([SS15b, SS15a, PS17] to list a few), it is found ([PS17, Thm. 4]) that

\[ E_n(x^*) - E(\bar{\rho}) = n^{-1+a}(-M + o(1)) \quad \text{as } n \to \infty, \]  

where the constant \( M > 0 \) is explicit in terms of a maximisation problem. In this setting, \( V = V_a \) (i.e., the Riesz potential) and \( D(U) = \mathbb{R} \), but the particle positions can be considered in arbitrary dimension.

Even when (19) is restricted to one dimension, it is a more precise result than our estimates in (15) and (16). The reason for obtaining such a precise result is that for \( V = V_a \) the extension representation of [CSS08] can be used (see [PS17] for details). For our larger class of potential \( V \), we are not aware of a similar extension representation. Moreover, in this paper, \( \bar{\rho} \) need not be bounded, which complicates the estimates (see, e.g., Remark 5.4 below).

The expansion in (19) has the additional merit that it specifies the rate of convergence rather than giving an upper bound for it as in Theorem 1.2. To test the sharpness of the exponent of \( n \) in Theorem 1.2 we perform numerical computations in Section 7. Interestingly, the numerical computations show that

\[ \|\varphi^* - \bar{\rho}\|_{H^{-1+a}/2} \ll n^{-1+a}, \]

which means that the exponent of \( n \) in Theorem 1.2 is not sharp.

To explore where the loss of accuracy in our proof occurs, we first reason in Section 7 that \( \|\varphi^* - \bar{\rho}\|_{H^{-1+a}/2} \) has the same scaling in \( n \) as \( E(\varphi^*) - E(\bar{\rho}) \). Then, by splitting this energy difference as in (13) and estimating the resulting terms independently, the loss of accuracy is guaranteed by (19). In other words, at least for the case in the numerical computations, it should hold that

\[ E(\varphi^*) - E_n(x^*) = n^{-1+a}(M + o(1)). \]

It remains a mystery to us why the same constant \( M \) as in (19) appears.
Organisation of the paper In Section 2 we list our notation. In Sections 3 – 6 we state and prove the lemmas referred to in the proof of Theorem 1.2. In particular, Sections 3, 4 and 5 relate to Parts 1, 2 and 3 respectively of the proof in the case $0 < a < 1$; the case $a = 0$ is treated in Section 6. In Section 7 we describe and discuss our numerical findings for the actual dependence of the left-hand side in Theorem 1.2 on $n$ and $a$.

2 Notation

The following table list the symbols which we use throughout the paper.

| Symbol | Description |
|--------|-------------|
| $\wedge, \vee$ | $\alpha \wedge \beta := \min\{\alpha, \beta\}$ and $\alpha \vee \beta := \max\{\alpha, \beta\}$ |
| $(\cdot, \cdot)_V$ | inner product constructed from $V$; $(f, g)_V = \int (V * g)f$ |
| $\mathbb{1}_A(x)$ | indicator function; $\mathbb{1}_A(x) = 1$ if $x \in A$, and $\mathbb{1}_A(x) = 0$ otherwise |
| $a$ | strength of the singularity of $V$; $0 \leq a < 1$ |
| $C, C', \ldots$ | some $n$-independent constants |
| $E$ | energy for the particle density |
| $E_n$ | interacting particle energy; $E_n : \Omega \to \mathbb{R}$ |
| $E_n^{nn}$ | nearest neighbour interactions; part of $E_n$ |
| $\varphi$ | discrete density (piece-wise constant) constructed from $x \in \Omega$ |
| $\Gamma$ | $\Gamma$-function; $\Gamma(\alpha) := \int_0^\infty x^{\alpha-1} e^{-x} \, dx$ |
| $H^{-s}(\mathbb{R})$ | fractional Sobolev space for $s > 0$ |
| $\ell_i$ | distance between nearest neighbours in $x \in \Omega$; $\ell_i := x_i - x_{i-1}$ |
| $m_i$ | midpoints of nearest neighbours in $x \in \Omega$; $m_i := \frac{1}{2}(x_i + x_{i-1})$ |
| $n$ | $n + 1$ is the number of particles; $n \geq 1$ |
| $\Omega$ | space of admissible particle configurations; $\Omega \subset \mathbb{R}^{n+1}$ |
| $\mathcal{P}(\mathbb{R})$ | space of probability measures on $\mathbb{R}$ |
| $\bar{\rho}$ | the minimiser of $E$ |
| $U$ | confining potential |
| $V$ | interaction potential |
| $V_a$ | singular, homogeneous part of $V$ |
| $V_{\text{reg}}$ | regular part of $V$; $V_{\text{reg}} = V - V_a$ |
| $x^*$ | a minimiser of $E_n$; $x^* \in \Omega$ |
| $\bar{x}$ | particle configuration constructed from $\bar{\rho}$; $\bar{x} \in \Omega$ |

We use the convention that constants denoted by $C$ are independent of $n$ and may change from line to line. In several cases where the estimates are easier to follow when the change in constants is highlighted, we use $C', C'', \ldots$ instead.

3 Proof of Theorem 1.2 Part 1

First, we show that the set of minimisers of $E_n$ and the set of minimisers of $E$ do not depend on the tails of $V$ (see Propositions 3.1 and 3.2 and the conclusion below them). Since we consider these propositions of independent interest, we pose them under weaker conditions of $V$ than Assumption 1.1. Then, we show that the set of minimisers of $E_n$ is not empty. Finally, we prove that the minimiser of $E$ is unique, and list several properties of it.
Minimisers are independent of the tails of $V$. Let $V \in L^1_{\text{loc}}(\mathbb{R})$ satisfy (4) and $U$ satisfy Assumption 1.1. By an affine change of variables, we may assume that $[-1,1] \subset D(U)$. By (5), there exists a constant $M > 0$ such that

$$U(x) \geq \frac{|x|}{M} - M \quad \text{for all } x \in \mathbb{R}.$$  

(20)

By (4), we note that, on $(0,\infty)$, $V$ is non-increasing and $V'$ is non-decreasing. Furthermore, $V'(x) \to 0$ as $x \to \infty$. Hence, there exists a point of differentiability $R \geq 2$ of $V$ for which

$$V'(R) \geq -\frac{1}{4M} \quad \text{and} \quad \frac{V(R)}{R} \geq -\frac{1}{4M}.$$  

(21)

**Proposition 3.1.** Let $V \in L^1_{\text{loc}}(\mathbb{R})$ satisfy (4) and $U$ satisfy Assumption 1.1. Take $M,R > 0$ as in (20) and (21). Then, there exists a constant $S > 0$ independent of $V|_{(R,\infty)}$ such that any minimiser $\rho$ of $E$ satisfies $\text{supp} \rho \subset [-S,S]$.

**Proof.** We start by proving two auxiliary estimates. The first one is given by

$$\inf_{x > 0} \left( V(x) + \frac{x}{4M} \right) \geq \min_{0 < x \leq R} \left( V(x) + \frac{x}{4M} \right) \wedge 0 =: -N.$$  

(22)

To prove it, let $x > R$. Since $V$ is convex, the tangent line of $V$ at $R$ is below the graph of $V$. Then, by (21), we obtain

$$V(x) + \frac{x}{4M} \geq V(R) + (x - R)V'(R) + \frac{x}{4M} \geq -\frac{R}{4M} + \frac{x}{4M} + \frac{x}{4M} = 0.$$  

This proves (22). We note that the constant $N \geq 0$ does not depend on $V|_{(R,\infty)}$. We set

$$S := \left( 2E(\rho_0) + 2 + 2M + N \right) M,$$

where $\rho_0 := \frac{1}{2} \mathbb{1}_{[-1,1]}$ is chosen rather arbitrarily to obtain that the value of $E(\rho_0)$ is finite and independent of $V|_{(R,\infty)}$.

The second auxiliary estimate is given by

$$\frac{V(x - y) + U(x) + U(y)}{2} \geq E(\rho_0) + 1 \quad \text{for all } x,y \text{ such that } |x| \vee |y| \geq S.$$  

(23)

To prove it, we first note from (20) that

$$\frac{U(x) + U(y)}{2} \geq \frac{|x| + |y|}{2M} - M \geq \frac{S}{M} - M = 2E(\rho_0) + 2 + M + N.$$  

Then, using (22),

$$V(x - y) + \frac{U(x) + U(y)}{2} \geq V(x - y) + \frac{|x - y|}{2M} - M \geq -N - M.$$  

(24)

Adding the above two estimates, we obtain (23).

Next, we prove Proposition 3.1. Suppose that $\overline{\rho}$ is a minimiser of $E$ such that $\text{supp} \overline{\rho} \not\subset [-S,S]$. Then, $\overline{m} := \overline{\rho}([-S,S]) < 1$. First, we claim that $\overline{m} > 0$. Indeed, if not, then by (23)

$$E(\overline{\rho}) = \int_{\mathbb{R}} \int_{\mathbb{R}} \frac{V(x - y) + U(x) + U(y)}{2} d\overline{\rho}(y) d\overline{\rho}(x) \geq E(\rho_0) + 1,$$
which contradicts with the minimality of $\bar{\rho}$. Using that $\overline{m} > 0$, we set $\rho := \overline{\rho}|_{[-S,S]} / \overline{m} \in \mathcal{P}(\mathbb{R})$, and rely on (23) to estimate

$$E(\bar{\rho}) = \int_{\mathbb{R}^2 \setminus [-S,S]^2} \frac{V(x-y) + U(x) + U(y)}{2} d\bar{\rho}(y) d\bar{\rho}(x) + \int_{[-S,S]^2} \frac{V(x-y) + U(x) + U(y)}{2} \overline{m}^2 d\rho(y) d\rho(x) \geq (E(\rho_0) + 1)(1 - \overline{m}^2) + \overline{m}^2 E(\rho) \geq (E(\bar{\rho}) + 1)(1 - \overline{m}^2) + \overline{m}^2 E(\rho).$$

Rearranging terms,

$$E(\bar{\rho}) \geq E(\rho) + \frac{1 - \overline{m}^2}{\overline{m}^2} > E(\rho),$$

which contradicts with the minimality of $\bar{\rho}$. □

**Proposition 3.2.** Let $V,U,M,R$ be as in Proposition 3.1 and let $n \geq 1$. Then, there exists a constant $S > 0$ independent of $n$ and $\|V\|_{(R,\infty)}$ such that any minimiser $x^* \in \Omega$ of $E_n$ satisfies $x^*_i \in [-S,S]$ for all $i = 0, \ldots, n$.

**Proof.** The proof is a discrete version of the proof of Proposition 3.1. We rely again on (22) with the same constant $N \geq 0$. Then, we set

$$S := \left(2N + 3M + \int_{-1}^1 (V + U)(x) \, dx\right) M. \quad (25)$$

Since $x^*$ is ordered, it is enough to show that $-S \leq x^*_0$ and $x^*_n \leq S$. Suppose that $x^*_0 < -S$ or $x^*_n > S$. We first treat the case in which both $x^*_0 < -S$ and $x^*_n > S$ hold, and comment on the remaining case afterwards. We may assume that $U(x^*_0) \leq U(x^*_n)$, because otherwise we can obtain this by applying the variable transformation $x \mapsto -x$.

We will reach a contradiction with the minimality of $x^*$ by finding a lower energy state in $\Omega$. We construct this state by replacing $x^*_n$ by a more energetically favourable position $y_n \in [-1,1]$. With this aim, we first compute for any $y \in [-1,1]$

$$n(E_n(x^*) - E_n(x^*_0, \ldots, x^*_n-1, y)) = \frac{1}{n} \sum_{j=0}^{n-1} V(x^*_n - x^*_j) + U(x^*_n) - \left( \frac{1}{n} \sum_{j=0}^{n-1} V(y - x^*_j) + U(y) \right),$$

where, for ease of notation, we have dropped the convention to have the particles positions ordered in the argument of $E_n$.

Since $W_n$ is lower semi-continuous and bounded from below on compact sets, it attains its minimum on $[-1,1]$. We take $y_n$ as a minimiser of $W_n$ over $[-1,1]$. Then, we estimate

$$2W_n(y_n) \leq \int_{-1}^1 W_n(y) \, dy = \frac{1}{n} \sum_{j=0}^{n-1} \int_{-1}^1 V(y - x^*_j) \, dy + \int_{-1}^1 U(y) \, dy \leq \int_{-1}^1 (V + U)(y) \, dy.$$

Next we estimate $W_n(x^*_n)$ from below. Using that $V$ is non-increasing on $(0,\infty)$, we obtain

$$W_n(x^*_n) \geq V(x^*_n - x^*_0) + \frac{U(x^*_n) + U(x^*_0)}{4} + \frac{U(x^*_n) - U(x^*_0)}{4} + \frac{1}{2} U(x^*_n). \quad (27)$$
Then, following the estimates in (24) for the first two terms, and applying (20) to the fourth term, we obtain

\[ W_n(x^*_n) \geq -(N + M) - 0 + \frac{1}{2} \left( \frac{x^*_n}{M} - M \right) > \frac{S}{2M} - N - \frac{3}{2}M. \]  

Collecting our results and substituting them in (26) yields

\[ n(E_n(x^*) - E_n(x^*_0, \ldots, x^*_{n-1}, y_n)) > \frac{S}{2M} - N - \frac{3}{2}M - \frac{1}{2} \int_{-1}^1 (V + U)(y) \, dy, \]

which is non-negative by the choice of \( S \) in (25). This contradicts with the minimality of \( x^* \).

Finally, we treat the case in which either \( x^*_0 < -S \) or \( x^*_n > S \), but not both. Again, by changing variables if needed, we may assume that \( x^*_n > S \), and thus \( -x^*_0 \leq S < x^*_n \). Then, the same proof can be adopted with a minor modification. This modification is to replace (27) with the following:

\[ W_n(x^*_n) \geq V(2x^*_n) + U(x^*_n) + U(x^*_n) + \frac{1}{2} U(x^*_n). \]

This results again in (28).

Next we argue that Propositions 3.1 and Proposition 3.2 imply that the set of minimisers of \( E_n \) and the set of minimisers of \( E \) do not depend on the tails of \( V \). Given \( V \) and \( U \) as in Theorem 1.2, let \( R \) and \( S \) be as in Proposition 3.1. Let \( \tilde{V} \) satisfy (4) such that

\[ \tilde{V} = V \text{ on } (0, \max\{2S, R\}] \quad \text{and} \quad \tilde{V} = C \text{ on } [\max\{2S, R\} + 1, \infty) \]

for some constant \( C \in \mathbb{R} \). Such a \( \tilde{V} \) can be obtained by multiplying \( V' \) with a cut-off function. We further note that \( C = \min_{\mathbb{R}} \tilde{V} \). Then, Proposition 3.1 applies to \( \tilde{V} \) with the same constants \( R \) and \( S \), and thus any minimiser of

\[ \tilde{E}(\rho) := \frac{1}{2} \int_{\mathbb{R}} (\tilde{V} * \rho) \, d\rho + \int_{\mathbb{R}} U \, d\rho \]

is also supported in \([-S, S]\). Since by the choice of \( \tilde{V} \) it holds that \( \tilde{E} = E \) on \( \mathcal{P}([-S, S]) \), any minimiser of \( E \) is a minimiser of \( \tilde{E} \) and vice versa. Analogously, we obtain the same conclusion for \( E_n \). Hence, we may replace \( V \) in Theorem 1.2 by \( \tilde{V} \). In addition, we may further add the constant \( C = \min_{\mathbb{R}} \tilde{V} \) to \( \tilde{E} \) such that the resulting interaction potential has compact support. In the remainder of the paper we assume that this change of potential has been applied.

**\( E_n \) attains its minimum**  The existence of minimisers for \( E_n \) is included in the proofs of Propositions 3.1 and 3.2. Indeed, since \( E_n \) is continuous on \( \Omega \) and \( E_n(x) \to \infty \) as \( \text{dist}(x, \partial \Omega) \to 0 \), it remains to be shown that \( E_n(x) \to \infty \) as \( |x| \to \infty \). To show this, we write

\[ E_n(x) = \frac{1}{2n^2} \sum_{i=0}^n \sum_{j \neq i}^n \left( V(x_i - x_j) + \frac{U(x_i) + U(x_j)}{2} \right) + \frac{1}{2n} \sum_{i=0}^n U(x_i) \]

and obtain from (20) and (24) that

\[ E_n(x) \geq \frac{|x_0| + |x_n|}{2Mn} - C \frac{|x|x \to \infty}{\to \infty}. \]
Properties of $V$ and $\rho$

Since $V$ satisfies Assumption 1.1, there exist constants $b, c > 0$ such that

$$V''(r) \geq cr^{-(2+a)} \quad \text{for all } 0 < r \leq b.$$  

(29)

Since supp $V$ is bounded, it is obvious from the convexity that $V \geq 0$. Moreover, for any $f, g \in L^2(\mathbb{R})$,

$$\int_{\mathbb{R}} (V * f) g =: (f, g)_V$$  

(30)

defines an inner product, which induces the Hilbert space

$$L^2(\mathbb{R}) \cong H^{-1-(a)/2}(\mathbb{R}).$$

(31)

The proof of this is given in [KvM19, Lem. 3.1(iii) and Prop. 3.3]. The following lemma is a simplified version of [KvM19, Thms. 1.4 and 1.5].

**Lemma 3.3** (Properties of $\rho$).

Let $0 \leq a < 1$. $E$ attains its minimal value on $\mathcal{P}(\mathbb{R})$. Its minimiser is unique, and has a density $\rho \in L^1(\mathbb{R})$. Moreover, after applying an appropriate affine change of variables, $\rho$ satisfies

(i) $\text{supp } \rho = [0, 1]$;

(ii) $\rho \in L^1(0, 1) \cap C((0, 1))$;

(iii) $\exists C > 0 \forall 0 < x < 1 : \rho(x) \leq C|x(1-x)|^{-1-a/2}$;

(iv) \( \begin{cases} V * \rho + U - C = 0 & \text{on } [0, 1] \\ V * \rho + U - C \geq 0 & \text{on } \mathbb{R}. \end{cases} \)

where \( C := \int_{\mathbb{R}} (V * \rho) d\rho + \int_{\mathbb{R}} U d\rho > 0. \)

The purpose of changing variables in Lemma 3.3 is to have supp $\rho = [0, 1]$ instead of some other bounded, closed interval. It is easy to see that Assumption 1.1 and (9) are invariant under an affine change of variables. In the remainder of the paper we assume that this change of variables has been applied.

4 Proof of Theorem 1.2: Part 2

In this section we fill in the details of Part 2 of the proof of Theorem 1.2. In fact, the only estimates left to prove are the two inequalities in (15), which we recall and rewrite here as

$$T_1 + T_2 \leq Cn^{-1+a} + C'E_n^\text{nn}(x^*).$$

(32)

where and $C, C' > 0$ are independent of $n$.

The structure of the proof of (32) is as follows. First, we split

$$T_2 = T_3 + T_4,$$

where $\overline{\rho}$ is defined from $\overline{x}$ by (7). We prove that $T_4 \lesssim n^{-1+a}$ in Lemmas 4.2 and 4.3. For $T_1$ and $T_3$, we note that – except for the sign – they are both of the form

$$E(\varphi) - E_n(x),$$
where $x$ and $\varphi$ are related through (7). In Lemma 4.5 we give a precise statement for

$$|E(\varphi) - E_n(x)| \lesssim n^{-1+\alpha} + E_{nn}^n(x),$$

which yields

$$T_1 + T_3 \leq Cn^{-1+\alpha} + C'E_{nn}^n(x^*) + C''E_{nn}^n(x).$$

Finally, in Lemma 4.1(iii) we show that $E_{nn}^n(x) \lesssim n^{-1+\alpha}$, which completes the proof of (32).

**Properties of $x$ and the bound on $E_{nn}^n(x)$** We start by introducing some notation. First, for given $x \in \Omega$, we define

$$m_i := \frac{x_i + x_{i-1}}{2}, \quad \text{and} \quad \ell_i := x_i - x_{i-1}$$

(33)

where $m := (m_1, \ldots, m_n) \in \mathbb{R}^n$ lists the midpoints of neighbouring particles, and $\ell := (\ell_1, \ldots, \ell_n) \in \mathbb{R}^n$ the distances between them. These quantities are illustrated in Figure 3. For the specific choices $x$ and $x^*$, we denote the related midpoints and interdistances as $m_i, \ell_i$ and $m_i^*, \ell_i^*$ respectively.

![Figure 3: The integration domain.](image)

Second, we introduce

$$D_n : \Omega \to [0, \infty), \quad D_n(x) := \frac{1}{2n^2} \sum_{i=1}^n \frac{1}{\ell_i^2} \int_{(0,\ell_i)^2} V(x-y) \, dy \, dx,$$

(34)

where $\ell_i$ depends on $x$ through (33). We note that

$$E_{nn}^n(x) \leq 2D_n(x).$$

(35)

**Lemma 4.1 (Properties of $x$).** There exist constants $C, c > 0$ such that for all $n \geq 1$
(i) \( \bar{\nu}_i \geq c \left( \frac{i}{n} \right)^{-\frac{1}{1+a}} \) and \( \bar{\nu}_{n-i} \leq 1 - c \left( \frac{i}{n} \right)^{-\frac{1}{1+a}} \) for all \( i = 0, \ldots, \left\lfloor \frac{n}{2} \right\rfloor \);

(ii) \( \bar{\ell}_1 \wedge \bar{\ell}_n \geq c \left( \frac{1}{n} \right)^{-\frac{1}{1+a}} \) and \( \bar{\ell}_i \wedge \bar{\ell}_{n+1-i} \geq c \left( \frac{i-1}{n} \right)^{-\frac{1}{1+a}} \) for all \( i = 2, \ldots, \left\lfloor \frac{n}{2} \right\rfloor \);

(iii) \( D_n(\mathbf{x}) + E_{nn}(\mathbf{x}) \leq C n^{-1+a} \).

**Proof.** For convenience we assume that \( n \) is even. Since \( x_0 = 0 \), it is sufficient to consider any \( i \geq 1 \). Using Lemma 3.3.(iii), we find that

\[
\frac{i}{n} = \int_0^{x_i} \bar{\nu} \leq \int_0^{x_i} C x^{-\frac{1-a}{2}} dx = C' \left( \frac{1+a}{2} x_i^2 \right).
\]

This implies the first part of Property (i). The estimate for \( x_{n-i} \) is found analogously.

Next we bound \( \bar{\ell}_i \) from below. For \( i = 1 \), we find

\[
\bar{\ell}_1 = \bar{\nu}_1 \geq c \left( \frac{1}{n} \right)^{-\frac{1}{1+a}}.
\]

For \( i \geq 2 \), we estimate similarly as above

\[
\frac{1}{n} = \int_{x_{i-1}}^{x_i} \bar{\nu} \leq \int_{x_{i-1}}^{x_i} C x^{-\frac{1-a}{2}} dx = C' \left( \frac{1+a}{2} \left( x_i - x_{i-1} \right) \right).
\]

Inserting \( x_i = \bar{\ell}_i - \bar{\ell}_{i-1} \), we obtain

\[
\bar{\ell}_i \geq \left( \frac{1}{C'n} + \frac{1+a}{2} x_{i-1} \right)^{\frac{2}{1+a}} - x_{i-1}.
\]  \hfill (36)

Since \( \frac{2}{1+a} > 1 \), the function \( \psi(t) := t^{2/(1+a)} \) is convex for \( t > 0 \), and thus \( \psi(t+\varepsilon) \geq \psi(t) + \varepsilon \psi'(t) \) for all \( t, \varepsilon > 0 \). Applying this inequality to (36), and then using Property (i) we obtain

\[
\bar{\ell}_i \geq \frac{1}{C'n} \left( \frac{1+a}{2} \right)^{\frac{2}{1+a}} - x_{i-1} \geq \frac{c'}{n} \left( \frac{i-1}{n} \right)^{-\frac{1-a}{1+a}}.
\]

The estimate for \( \bar{\ell}_{i+1} \) is found analogously.

Finally we prove Property (iii). By (35) it is enough to estimate \( D_n(\mathbf{x}) \). From \( V(x) \leq C/|x|^a \) and Property (ii) we obtain

\[
D_n(\mathbf{x}) = \frac{1}{2} \frac{1}{n^2} \sum_{i=1}^{n} \int_{0,1} V(\bar{\ell}_i(x-y)) dy dx \leq \frac{C}{n^2} \left( \bar{\ell}_1^{-a} + \bar{\ell}_n^{-a} + \sum_{i=2}^{n} \bar{\ell}_i^{-a} \right)
\]

\[
\leq C n^{-2+\frac{2a}{1+a}} + C n^{\frac{a}{n} \sum_{i=2}^{n/2} \left( \frac{i-1}{n} \right)^{-\frac{1-a}{1+a}}} \leq C n^{-1+a}.
\]

\( \square \)
Proof. From (7) and (14) we observe that the densities $\varphi$ and $\rho$ have mass 1 on $[\tau_{i-1}, \tau_i]$ for each $i$. We use this to estimate

$$\int_0^1 U(x) (\varphi - \rho)(x) \, dx \leq \frac{U(0) + U(1)}{n}.$$  

Since $U$ is convex with minimiser in $[0, 1]$, we recognize at most two telescopic series. Then, using $\min U = 0$, we obtain the assertion of Lemma 4.2.

Lemma 4.3. There exists a constant $C > 0$ such that for all $n \geq 1$

$$\|\varphi\|^2_V - \|\rho\|^2_V \leq C n^{-1+a}.$$

Proof. We write

$$\|\varphi\|^2_V - \|\rho\|^2_V = \sum_{i=1}^{n} \sum_{j=1}^{n} \int_{\tau_{i-1}}^{\tau_i} \int_{\tau_{j-1}}^{\tau_j} V(x - y) \left( \varphi(x) \varphi(y) - \rho(x) \rho(y) \right) \, dy \, dx =: T_5 + T_6 + T_7,$$

where the terms $T_5$, $T_6$ and $T_7$ correspond to the part of the sum where $i - j = 0$, $|i - j| = 1$ and $|i - j| \geq 2$ respectively. We bound all these three terms separately. With this aim, we set

$$\varphi_i := \varphi|_{(\tau_{i-1}, \tau_i)}$$

for $i = 1, \ldots, n$, and note that, by (34) and Lemma 4.1(iii)

$$\sum_{i=1}^{n} \|\varphi_i\|^2_V = 2D_n(x) \leq C n^{-1+a}.$$

For $T_5$ we simply estimate

$$T_5 = \sum_{i=1}^{n} \int_{\tau_{i-1}}^{\tau_i} \int_{\tau_{i-1}}^{\tau_i} V(x - y) \left( \varphi(x) \varphi(y) - \rho(x) \rho(y) \right) \, dy \, dx \leq \sum_{i=1}^{n} \int_{\tau_{i-1}}^{\tau_i} \int_{\tau_{i-1}}^{\tau_i} V(x - y) \varphi(x) \varphi(y) \, dy \, dx = \sum_{i=1}^{n} \|\varphi_i\|^2_V \leq C n^{-1+a}.$$

For $T_6$, we similarly obtain

$$T_6 = 2 \sum_{i=1}^{n-1} \int_{\tau_{i+1}}^{\tau_i} \int_{\tau_{i-1}}^{\tau_i} V(x - y) \left( \varphi(x) \varphi(y) - \rho(x) \rho(y) \right) \, dy \, dx \leq 2 \sum_{i=1}^{n-1} (\|\varphi_{i+1}\|^2_V + \|\varphi_i\|^2_V) \leq C n^{-1+a}.$$  

The bound on $T_4 = E(\varphi) - E(\rho)$ We recall from (11) that $E$ consists of an interaction part and a confinement part. For $E(\varphi) - E(\rho)$, we bound these terms separately in Lemmas 4.3 and 4.2 respectively.

Lemma 4.2. For all $n \geq 1$

$$\int_0^1 U(x) (\varphi - \rho)(x) \, dx \leq \frac{U(0) + U(1)}{n}.$$
Finally we estimate \( T_7 \). We note that in the integrals in the terms of \( T_7 \), the singularity of \( V \) is avoided. This allows for pointwise evaluation of the integrand. By using that \( V \) is even, and non-increasing on the positive axis, we estimate

\[
T_7 = 2 \sum_{i=3}^{n} \sum_{j=1}^{i-2} \left( \int_{\bar{x}_{i-1}}^{\bar{x}_i} \int_{\bar{x}_{j-1}}^{\bar{x}_j} V(x-y) \left( \varphi(x)\varphi(y) - \varphi(x)\varphi(y) \right) \, dy \, dx \right)
\]

\[
\leq 2 \sum_{i=3}^{n} \sum_{j=1}^{i-2} \left( \int_{\bar{x}_{i-1}}^{\bar{x}_i} \int_{\bar{x}_{j-1}}^{\bar{x}_j} V(\bar{x}_{i-1} - \bar{x}_j) \varphi(x)\varphi(y) \, dy \, dx \right)
\]

\[
- \int_{\bar{x}_{i-1}}^{\bar{x}_i} \int_{\bar{x}_{j-1}}^{\bar{x}_j} V(\bar{x}_i - \bar{x}_{j-1}) \varphi(x)\varphi(y) \, dy \, dx \right)
\]

\[
= \frac{2}{n^2} \sum_{i=3}^{n} \sum_{j=1}^{i-2} \left( V(\bar{x}_{i-1} - \bar{x}_j) - V(\bar{x}_i - \bar{x}_{j-1}) \right).
\]

We recognise a telescopic series after changing the summation index to \( k = i + j - 1 \):

\[
T_7 \leq \frac{2}{n^2} \sum_{i=3}^{n} \sum_{j=1}^{i-2} \left( V(\bar{x}_{i-1} - \bar{x}_j) - V(\bar{x}_i - \bar{x}_{j-1}) \right)
\]

\[
= \frac{2}{n^2} \sum_{i=3}^{n} \sum_{k=i}^{2i-3} \left( V(\bar{x}_{i-1} - \bar{x}_{k-(i-1)}) - V(\bar{x}_i - \bar{x}_{k-i}) \right)
\]

\[
= \frac{2}{n^2} \sum_{k=3}^{2n-3} \sum_{i=\left\lceil \frac{k+1}{2} \right\rceil}^{k \wedge n} \left( V(\bar{x}_{i-1} - \bar{x}_{k-(i-1)}) - V(\bar{x}_i - \bar{x}_{k-i}) \right)
\]

\[
= \frac{2}{n^2} \sum_{k=3}^{2n-3} \left( V(\bar{x}_{\left\lceil \frac{k+1}{2} \right\rceil} - \bar{x}_{\left\lceil \frac{k+1}{2} \right\rceil}) - V(\bar{x}_{k \wedge n} - \bar{x}_0 \wedge (k-n)) \right)
\]

\[
\leq \frac{2}{n^2} \sum_{k=3}^{2n-3} \left( V(\bar{x}_{\left\lceil \frac{k+1}{2} \right\rceil} - \bar{x}_{\left\lceil \frac{k+1}{2} \right\rceil}) \right) \leq \frac{4}{n^2} \sum_{i=2}^{n-1} V(\bar{\Omega}_i) \leq 4E_n^\text{nn}(\bar{\Omega})
\]

which, by Lemma 4.4.iii, is bounded by \( Cn^{-1+a} \).

\[ \square \]

**The upper and lower bound on \( E(\varphi) - E_n(x) \)** First, we state and prove the opposite inequality in (35) as an auxiliary result.

**Lemma 4.4.** There exists constants \( C, C' > 0 \) such that for all \( n \geq 1 \) and all \( \mathbf{x} \in \Omega \)

\[
D_n(\mathbf{x}) \leq CE_n^\text{nn}(\mathbf{x}) + \frac{C'}{n}.
\]

**Proof.** Using \( V = V_a + V_{\text{reg}} \), we split \( D_n(\mathbf{x}) \) in two parts:

\[
D_n(\mathbf{x}) = \frac{1}{2} \sum_{i=1}^{n} \frac{1}{\ell_i^2} \int_{(0,\ell_i)^2} V_a(x-y) \, dy \, dx + \frac{1}{2} \sum_{i=1}^{n} \frac{1}{\ell_i^2} \int_{(0,\ell_i)^2} V_{\text{reg}}(x-y) \, dy \, dx.
\]
The first part can be computed explicitly. This yields

$$\frac{1}{2} \frac{1}{n^2} \sum_{i=1}^{n} \frac{1}{\ell_i^2} \int_{(0,\ell_i)^2} V_a(x-y) \, dy \, dx = \frac{C_a}{n^2} \sum_{i=1}^{n} V_a(\ell_i)$$

for some explicit constant $C_a > 0$. For the second term, we rely on the regularity of $V_{\text{reg}}$ to estimate

$$\frac{1}{2} \frac{1}{n^2} \sum_{i=1}^{n} \frac{1}{\ell_i^2} \int_{(0,\ell_i)^2} V_{\text{reg}}(x-y) \, dy \, dx \leq \frac{1}{n} \left( \frac{1}{2} + C_a \right) \|V_{\text{reg}}\|_{C([-1,1])} + \frac{C_a}{n^2} \sum_{i=1}^{n} V_{\text{reg}}(\ell_i).$$

\[\square\]

**Lemma 4.5** (Energy bounds on the piecewise constant approximation). There exists $C \geq 0$ such that for all $n \geq 1$ and all $x \in \Omega$

$$-E_{nm}(x) - \frac{1}{n} (U(0) + U(1)) \leq E(\varphi) - E_n(x) \leq C \left( E_{nm}(x) + \frac{1}{n} \right),$$

where $\varphi$ is the piece-wise constant function constructed from $x$ by (7).

**Proof.** We divide the proof in four steps. In Step 1 we bound the confinement part of $E(\varphi) - E_n(x)$, and in Steps 2 – 4 we bound the interaction part. Given $x$, we let $m_i$ and $\ell_i$ be defined by (33) (see Figure 3).

**Step 1: bounds on the confinement part.** The confinement part of $E(\varphi) - E_n(x)$ is given by

$$F_n(x) := \int_{0}^{1} U \varphi - \frac{1}{n} \sum_{i=0}^{n} U(x_i) = \frac{1}{n} \sum_{i=1}^{n} \frac{1}{\ell_i} \int_{x_{i-1}}^{x_i} U - \frac{1}{n} \sum_{i=0}^{n} U(x_i).$$

Since $U \geq 0$ is convex, it is easy to see that $-\frac{1}{n} (U(0) + U(1)) \leq F_n(x) \leq 0$.

In the remainder of the proof, we set $U \equiv 0$ to focus on the interaction part.

**Step 2: rewriting $E(\varphi) - E_n(x)$ as a sum of error terms.** We show that

$$E(\varphi) - E_n(x) = D_n(x) + Q_n(x) - C_n(x) - B_n(x), \quad (38)$$

where the four non-negative error terms are given by (34) and

$$Q_n(x) := \frac{1}{n^2} \sum_{i=2}^{n} \sum_{j=1}^{i-1} \left[ \frac{1}{\ell_i \ell_j} \int_{x_{i-1}}^{x_i} \int_{x_{j-1}}^{x_j} V(x-y) \, dy \, dx - V(m_i - m_j) \right],$$

$$C_n(x) := \frac{1}{n^2} \sum_{i=2}^{n} \sum_{j=1}^{i-1} \left( \frac{1}{2} V(x_i - x_j) + \frac{1}{2} V(x_{i-1} - x_{j-1}) - V(m_i - m_j) \right),$$

$$B_n(x) := \frac{1}{2} \frac{1}{n^2} \sum_{i=1}^{n} \left[ V(x_i - x_0) + V(x_n - x_{i-1}) \right].$$
Indeed, (38) follows from

\[ E(\varphi) = \frac{1}{2} \int_0^1 \int_0^1 V(x - y)\varphi(x)\varphi(y) \, dy \, dx \]

\[ = \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \int_{x_{i-1}}^{x_i} \int_{x_{j-1}}^{x_j} V(x - y) \frac{1}{n} \frac{1}{n} \, dy \, dx \]

\[ = \frac{1}{n^2} \sum_{i=1}^n \sum_{j=1}^n \int_{x_{i-1}}^{x_i} \int_{x_{j-1}}^{x_j} V(x - y) \, dy \, dx + D_n(x) \]

\[ = \frac{1}{n^2} \sum_{i=1}^n \sum_{j=1}^n V(m_i - m_j) + (D_n + Q_n)(x) \]

\[ = \frac{1}{2n^2} \sum_{i=2}^n \sum_{j=1}^{i-1} \left( V(x_i - x_j) + V(x_{i-1} - x_{j-1}) \right) + (D_n + Q_n - C_n)(x) \]

\[ = E_n(x) + (D_n + Q_n - C_n - B_n)(x). \]

**Step 3: the lower bound for \( E(\varphi) - E_n(x) \).** Since the error terms \( D_n, Q_n, C_n \) and \( B_n \) are all non-negative, we observe from (38) that it is enough to show that

\[ C_n(x) + B_n(x) \leq E_n^{\text{nn}}(x). \]

By using \( m_i - m_j \leq x_i - x_{j-1} \), we obtain this estimate from

\[ C_n(x) + B_n(x) = \frac{1}{n^2} \sum_{i=1}^n \sum_{j=0}^{i-1} V(x_i - x_j) - \frac{1}{n^2} \sum_{i=2}^n \sum_{j=1}^{i-1} V(m_i - m_j) \]

\[ \leq \frac{1}{n^2} \sum_{i=1}^n \sum_{j=0}^{i-1} V(x_i - x_j) - \frac{1}{n^2} \sum_{i=2}^n \sum_{j=0}^{i-2} V(x_i - x_j) = E_n^{\text{nn}}(x). \]

**Step 4: the upper bound for \( E(\varphi) - E_n(x) \).** Since \( B_n \geq 0 \), it is enough to show that

\[ D_n(x) + Q_n(x) - C_n(x) \leq C \left( E_n^{\text{nn}}(x) + \frac{1}{n} \right). \]

Then, by Lemma 4.4, it suffices to show that \( Q_n - C_n \leq 2D_n \). Writing

\[ Q_n(x) - C_n(x) \]

\[ = \frac{1}{n^2} \sum_{i=2}^n \sum_{j=1}^{i-1} \left[ \frac{1}{\ell_i \ell_j} \int_{x_{i-1}}^{x_i} \int_{x_{j-1}}^{x_j} V(x - y) \, dy \, dx \right] \left( \frac{1}{2} V(x_i - x_j) + \frac{1}{2} V(x_{i-1} - x_{j-1}) \right) \]

we use convexity of \( V \) to bound the integral for \( i \geq j + 2 \) by

\[ \frac{1}{\ell_i \ell_j} \int_{x_{i-1}}^{x_i} \int_{x_{j-1}}^{x_j} V(x - y) \, dy \, dx \leq \frac{1}{2} V(x_{i-1} - x_j) + \frac{1}{2} V(x_i - x_{j-1}). \]
This yields

\begin{equation}
Q_n(x) - C_n(x) \leq \frac{1}{n^2} \sum_{i=1}^{n-1} \frac{1}{\ell_{i+1} \ell_i} \int_{x_i}^{x_{i+1}} \int_{x_{i-1}}^{x_i} V(x - y) \, dy \, dx \\
+ \frac{1}{2n^2} \left( \sum_{i=3}^{n} \sum_{j=1}^{i-2} [V(x_{i-1} - x_j) + V(x_i - x_{j-1})] - \sum_{i=2}^{n} \sum_{j=1}^{i-1} [V(x_i - x_j) + V(x_{i-1} - x_{j-1})] \right).
\end{equation}

For the term within parentheses, a change of index readily reveals that the second summation includes all terms of the first summation. We then use $V \geq 0$ to estimate this term from above by 0. The remaining term in (40) can be estimated similarly as in (37). This yields $Q_n - C_n \leq 2D_n$.

5 Proof of Theorem 1.2: Part 3

In this section we prove (16), which is the crucial step in Part 3 of the proof of Theorem 1.2. More precisely, we prove the following proposition.

Proposition 5.1 (Lower bound on $E_n$). There exists $C > 0$ such that for all $n \geq 1$ and all $x \in \Omega$

\[ E_n(x) - E^\text{nn}_n(x) - E(\rho) \geq -Cn^{-1} \alpha. \]

We give the proof of Proposition 5.1 after some preliminary constructions. In order to renormalise the norm $\| \cdot \|_V$, we introduce

\begin{equation}
V_n(r) := \begin{cases} 
V(\frac{r}{n}) + (\frac{r}{n} - \frac{1}{n})V'(\frac{1}{n}) & \text{if } 0 \leq r \leq \frac{1}{n} \\
V(r) & \text{if } r > \frac{1}{n}
\end{cases}
\end{equation}

with even extension to the negative half-line. Figure 4 illustrates a typical example of $V$ and $V_n$. Lemma 5.2 lists several basic properties of $V_n$.

![Figure 4: The piecewise-affine regularisation $V_n$ of the interaction potential $V$.](image)

Lemma 5.2 (Properties of $V_n$). There exists a constant $C > 0$ such that for all $n \geq 1$:
(i) $V_n$ is non-increasing on $[0, \infty)$;

(ii) $V_n$ and $V - V_n$ are convex on $(0, \infty)$;

(iii) $\text{supp}(V - V_n) \subset [-\frac{1}{n}, \frac{1}{n}]$;

(iv) $V_n(0) \leq Cn^a$;

(v) For $f \in L^2(\mathbb{R})$, \(\|f\|_{V_n} := \sqrt{\int_{\mathbb{R}} (V_n * f) f} \) defines a semi-norm;

(vi) $V_n \uparrow V$ in $L^p(\mathbb{R})$ as $n \to \infty$ for any $1 \leq p < \frac{1}{a}$.

Proof. Except for (v), all properties are a direct consequence of the assumptions and properties of $V$ and the definition of $V_n$ in (41). Property (v) can be proven along the lines of [KvM19, Lem. 3.2]; it relies on the Fourier-transform of $V_n$ being non-negative, which easily follows from the other properties of $V_n$ (see [KvM19, Lem. 3.1] for details).

Next we establish an auxiliary lemma.

**Lemma 5.3.** There exists $C > 0$ such that for all $n \geq 1$ and all $0 \leq x \leq \frac{1}{2}$

\[
((V - V_n) * \bar{p})(x) + ((V - V_n) * \bar{p})(1 - x) \leq Cn^{-\frac{1-a}{2}} \min \left\{ 1, [nx - 1]_+^{\frac{1-a}{2}} \right\}.
\]

Proof. First, we recall the identity

\[
\int_0^x y^{\alpha-1}(x-y)^{\beta-1} \, dy = \frac{\Gamma(\alpha)\Gamma(\beta)}{\Gamma(\alpha + \beta)} x^{\alpha+\beta-1} \quad \text{for all } x, \alpha, \beta > 0,
\]

where $\Gamma(\alpha) = \int_0^{\infty} x^{\alpha-1} e^{-x} \, dx$ is the usual Gamma function.

Take any $0 \leq x \leq \frac{1}{n}$, and set $x_0 := (x - \frac{1}{n}) \lor 0$. Using that $V(r) \leq C/r^a$, and relying on Lemmas 3.3.(iii) and 5.2, we obtain

\[
((V - V_n) * \bar{p})(x) = \int_{\frac{1}{2}}^{x + \frac{1}{n}} (V - V_n)(x-y) \bar{p}(y) \, dy \leq C \int_{\frac{1}{2}}^{x + \frac{1}{n}} |x-y|^{-a} y^{-\frac{1-a}{2}} \, dy
\]

\[
\leq C \int_{\frac{1}{2}}^{x - \frac{1}{n}} (x-x-y)^{-a} y^{-\frac{1-a}{2}} \, dy + C \int_{\frac{1}{2}}^{x + \frac{1}{n}} y^{\frac{1+a}{2}} \, dy \leq C' n^{-\frac{1-a}{2}},
\]

where the last step follows from (42). To sharpen the bound for $\frac{2}{n} \leq x \leq \frac{1}{2}$, we change the estimate above as follows:

\[
((V - V_n) * \bar{p})(x) \leq C \int_{x - \frac{1}{n}}^{x + \frac{1}{n}} |x-y|^{-a} y^{-\frac{1-a}{2}} \, dy
\]

\[
\leq C (x - \frac{1}{n})^{-\frac{1-a}{2}} \int_{x - \frac{1}{n}}^{x + \frac{1}{n}} |x-y|^{-a} \, dy \leq C' n^{-1+a} (x - \frac{1}{n})^{-\frac{1-a}{2}}.
\]

The estimate for $((V - V_n) * \bar{p})(1-x)$ is analogous. □
Proof of Proposition \[5.1\] The assertion of Proposition \[5.1\] is obvious for finite \( n \) (simply take \( C = n^{1-a}E(\bar{\rho}) \)). Therefore, it is not restrictive to assume that \( n \geq 1/b \), where \( b > 0 \) is as in \[29\].

Let \( x \in \Omega \) be given, and set
\[
\mu_n := \frac{1}{n} \sum_{i=0}^{n} \delta_{x_i} \quad \text{and} \quad \nu_n := \mu_n - \bar{\rho}.
\]

Let
\[
\Delta_1 := \{(x_i, x_j) : |i - j| \leq 1\} \subset \mathbb{R}^2
\]
be the particle pairs that are left out in the interaction term of \( E_n(x) - E_{\text{nn}}(x) \), i.e.
\[
E_n(x) - E_{\text{nn}}(x) = \frac{1}{2} \int \int_{\Delta_1^c} V(x - y) \, d\nu_n(y) \, d\mu_n(x) + \int U \, d\mu_n.
\]

Then, we use Lemma \[3.3\] to estimate
\[
E_n(x) - E_{\text{nn}}(x) - E(\bar{\rho})
\]
\[
= \frac{1}{2} \int \int_{\Delta_1^c} V(x - y) \, d\nu_n(y) \, d\mu_n(x) + \int (V * \bar{\rho}) \, d\nu_n + \int U \, d\nu_n
\]
\[
\geq \frac{1}{2} \int \int_{\Delta_1^c} V(x - y) \, d\nu_n(y) \, d\mu_n(x)
\]
\[
= \frac{1}{2} \int\int_{\Delta_1^c} V_n(x - y) \, d\nu_n(y) \, d\mu_n(x) + \frac{1}{2} \int\int_{\Delta_1^c} (V - V_n)(x - y) \, d\nu_n(y) \, d\nu_n(x),
\]
where \( V_n \) is the regularisation introduced in \[41\]. By Lemma \[5.2\]
\[
T_8 = \|\nu_n\|_V^2 - \frac{n + 1}{n^2} V_n(0) - \frac{2}{n^2} \sum_{i=1}^{n} V_n(x_i - x_{i-1}) \geq -\frac{3n + 1}{n^2} V_n(0) \geq -C n^{1+a}.
\]

It remains to bound \( T_9 \) from below by \(-C n^{1+a}\). We expand \( \nu_n = \mu_n - \bar{\rho} \) to rewrite
\[
T_9 = \frac{2}{n^2} \sum_{i=2}^{n} \sum_{j=0}^{n-i} (V - V_n)(x_{j+i} - x_j) - 2 \int ((V - V_n) * \bar{\rho}) \, d\mu_n + \int_{\mathbb{R}^2} (V - V_n)(x - y) \, d\bar{\rho}(y) \, d\bar{\rho}(x).
\]
\[\tag{43}\]

The third term is non-negative; we bound it from below by 0. For the first two terms, we assume for convenience that \( n \) is a multiple of 4, and partition the interval [0, 1] into the \( n/2 \) closed intervals \( I_k := [\frac{2k-1}{n}, \frac{2k}{n}] \), which only overlap at their endpoints. Then, we remove the contribution from the interaction between any two particles located at different intervals \( I_k \). Finally, we minimise the right-hand side of (43) over each \( I_k \) separately, and relax the constraint that the sum of all particles should be \( n+1 \). This yields
\[
T_9 \geq 2 \frac{n/2}{\min_{k \in \mathbb{N}} \left( \frac{1}{n^2} \sum_{i=2}^{n-i} \frac{y_{j+i} - y_j}{n} \right)} \min_{k \in \mathbb{N}} \left( \int_{\frac{2k-1}{n}}^{\frac{2k}{n}} (V - V_n)(x_{j+i} - x_j) \, dx \right) - \frac{N}{n} \| (V - V_n) * \bar{\rho} \|_{C(I_k)}.
\]
\[\tag{44}\]
We treat both terms within the parentheses separately. For the second term, we apply the bound in Lemma \[5.3\]. Since this bound gives the same estimate for the intervals \[I_k\] and \[I_{n/2-k+1}\], we focus on bounding it for \[k \leq n/4\]. This yields

\[
\frac{N}{n} ||(V - V_n) \ast p||_{C(I_k)} \leq C \frac{N}{n} \min \left\{ n \left( \frac{n-1-a}{2}, \frac{n^{-1+a}(2^{k-1}_n - \frac{1}{n})}{k} \right) \right\} \\
\leq C' \frac{N}{n} \left( \frac{1}{k} \right) + \frac{1}{(k-1)^{-\frac{1-a}{2}}} \quad k = 1, \ldots, \frac{n}{2}.
\]

In particular, if the minimum over \[N\] in (44) is reached below an \[n\]-independent value \(C\) (i.e., \(N \leq C\)), then it suffices to bound the first term in parentheses in (44) from below simply by 0. Therefore, we assume next that the minimiser \(N\) is sufficiently large; in particular \(N \geq 9\). We further assume for simplicity that \(N\) is a multiple of 3.

To bound the first term in parentheses in (44), we rely on the basic arguments in the theory of \(i\)-th neighbour interaction energies with convex interaction potentials. We give a sketch of the argument here. First, we bound the minimum from below by exchanging the sum over \(i\) with the minimisation over \((y_j)_j\). Then, the resulting minimisation problem can be written as a sum over independent minimisation problems, indexed by \(l = 1, \ldots, i\), over

\[
2 \frac{k-1}{n} \leq y_l \leq y_{l+i} \leq y_{l+2i} \leq \cdots \leq y_{l+[(N-l)/i]i} \leq 2 \frac{k}{n}.
\]

Each such minimisation problem involves only nearest neighbour interactions with the convex, repelling interaction potential \(V - V_n\), which is minimised by the equispaced configuration. This yields

\[
\frac{1}{n^2} \frac{n}{2^{\frac{k-1}{n}}} \leq y_l \leq y_{l+i} \leq \cdots \leq y_{l+[(N-l)/i]i} \leq 2 \frac{k}{n}
\]

where in the last step we have recognized the sum as a Riemann upper-sum. To estimate the integrand from below, we integrate twice, use that \((V - V_n)(\frac{x}{n}) = 0\) and rely on \(V''' = 0\) on \((0, \frac{1}{n})\) and the lower bound on \(V''\) on \((0, b) \supset (0, \frac{1}{n})\) in (29) to deduce that

\[
(V - V_n)(\frac{x}{n}) = \int_0^x \int_y^1 V''(z) \, dz \, dy \geq C \int_0^x \int_y^1 z^{-2-a} \, dz \, dy = Cn^a \int_x^1 \int_y^1 z^{-2-a} \, dz \, dy > 0
\]

for all \(0 < x < 1\). In particular, the double integral above is independent of \(n\), and decreasing as a function of \(x\). Hence, using that \(6/N \leq 2/3\), we continue the estimate in (45) by

\[
\frac{N^2}{9n^2} \int_0^1 (V - V_n)(\frac{x}{n}) \, dx \geq C' N^2 n^{-2+a} \int_0^1 \int_y^1 z^{-2-a} \, dz \, dy \geq C' N^2 n^{-2+a}.
\]
Finally, collecting our estimates in (44), we obtain two constants $C, C' > 0$ such that

$$T_y \geq C' \sum_{k=1}^{n/2} \min_{N \in \mathbb{R}} \left( N^2 n^{-2+a} - C k^{-\frac{1-a}{2}} N n^{-1-\frac{1-a}{2}} \right)$$

$$= C' n^{-2+a} \sum_{k=1}^{n/2} \min_{N \in \mathbb{R}} \left( N - C \left( \frac{k}{n} \right)^{-\frac{1-a}{2}} \right)$$

$$= -C' n^{-2+a} c^2 \sum_{k=1}^{n/2} \left( \frac{k}{n} \right)^{-1+a} \geq -C n^{-1+a}.$$

**Remark 5.4** (The case $\rho \leq C$). When $\rho$ is bounded, the proof of Proposition 5.1 simplifies significantly. Indeed, if $\rho$ is bounded, then instead of Lemma 5.3 the rougher estimate $\| (V - V_n) * \rho \|_{C([0,1])} \leq C n^{-1+a}$ is sufficient, because this estimate gives immediately the desired bound on the second term in (43).

### 6 Proof of Theorem 1.2 for $a = 0$

The proof of Theorem 1.2 for the case $a = 0$ is the same as in the case $0 < a < 1$ except for several minor changes in the computations. All these changes are ramifications of the change in the upper bound on $V$, which is

$$V(r) \leq C - \log |r|.$$

In Table 2 and the list below we mention all statements of Sections 3 – 5 which are not literally valid for $a = 0$, and provide the required modification.

| Statement | Updated estimate |
|-----------|------------------|
| Lemma 4.4(iii) | $D_n(\overline{x}) + E_{mn}(\overline{x}) \leq C n^{-1} \log n$ |
| Lemma 4.3 | $\| \rho \|_{V}^2 - \| \rho \|_{V}^2 \leq C n^{-1} \log n$ |
| Lemma 5.2(iv) | $V_n(0) \leq \log n + C$ |
| Lemma 5.2(vi) | $V_n \uparrow V$ in $L^p(\mathbb{R})$ as $n \to \infty$ for any $1 \leq p < \infty$ |
| Lemma 5.3 | $\left\{ ((V - V_n) * \overline{\rho})(x) + ((V - V_n) * \overline{\rho})(1-x) \right\} \leq C n^{-1/2} (\log n) \min \left\{ 1, [nx - 1]^{-1/2} \right\}$ |
| Proposition 5.1 | $E_n(x) - E_{mn}(x) - E(\overline{\rho}) \geq -C n^{-1} (\log n)^3$ |

Table 2: Changes in the estimates for $a = 0$.

The two further changes to the proof of Theorem 1.2 are:

1. The constant $C'$ in Lemma 4.4 also contains a contribution from $V_a$. 

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2. In the proof of Proposition 5.1, the estimate in the final display changes as follows:

\[
T_9 \geq C' \sum_{k=1}^{n/2} \min_{N \in \mathbb{R}} \left( N^2 n^{-2} - C k^{-1/2} N n^{-3/2} \log n \right)
= C' n^{-2} \sum_{k=1}^{n/2} \min_{N \in \mathbb{R}} \left( N - C (\log n) \left( \frac{k}{n} \right)^{-1/2} \right)
= -\frac{C'}{n} (\log n)^2 C^2 \sum_{k=1}^{n/2} \left( \frac{k}{n} \right)^{-1} \geq -C n^{-1} (\log n)^3.
\]

7 Numerical computations on the rate in Theorem 1.2

The aim of this section is to compare the upper bound of the convergence rate in Theorem 1.2 with the actual convergence rate in concrete examples. These concrete examples are given by specific choices for the potentials \(V\) and \(U\) for which all quantities except for \(x^*\) can be computed explicitly. With this aim, we take \(V_{\text{reg}} = 0\) and \(U\) a convex polynomial on \(D(U)\). Given the qualitatively different profiles of \(\rho\) observed in Figure 2, we consider two choices for \(D(U)\); a bounded interval (Case 1) and \(\mathbb{R}\) (Case 2).

For each of these two cases, the method to test Theorem 1.2 numerically is as follows. First, we compute \(x^*\) by minimizing \(E_n\) in (1) numerically with Newton’s method for several values of \(n\). One observation we did from this data is that \(x^*_i \in \text{supp } \overline{\rho}\) for all \(i = 0, 1, \ldots, n\) (46).

Then, instead of using the norm in \(H^{-(1-a)/2}\), we use the equivalent norm \(\| \cdot \|_V\) to make the computation easier. Indeed, since by (46) and Lemma 3.3(iv) the inequality in (12) becomes an equality, we obtain that

\[
e_n := \| \overline{\rho} - \phi^* \|^2_V = 2 (E(\phi^*) - E(\overline{\rho})).
\]

Now, \(E(\overline{\rho})\) can be computed explicitly given that \(V_{\text{reg}} = 0\) and \(U\) is a polynomial. To compute \(E(\phi^*)\), we set \(x := x^*\) and \(\ell_i := x_i - x_{i-1}\), and obtain from (39) that

\[
E(\phi^*) = \frac{1}{2n^2} \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{1}{\ell_i \ell_j} \int_{x_{i-1}}^{x_i} \int_{x_{j-1}}^{x_j} V_a(x - y) dy dx + \frac{1}{n} \sum_{i=1}^{n} \frac{1}{\ell_i} \int_{x_{i-1}}^{x_i} U(x) dx.
\]

Since \(U\) is a polynomial, both integrals above can be computed explicitly as a function of \(x\). Hence, once \(x^*\) is computed numerically, \(e_n\) can be computed without any further numerical error.

Finally, to compare the numerically computed values for \(e_n\) with Theorem 1.2, we make the ansatz

\[
e_n = C n^{-p}.
\]

Then, \(e_n/e_{2n} = 2^p\), and thus

\[
p = \frac{\log e_n - \log e_{2n}}{\log 2}.
\]

Hence, by taking \(n\) as subsequent powers of 2, we can compute \(p\) for each pair of subsequent values of \(e_n\), and compare the values of \(p\) with the theoretically obtained power \(1 - a\).
Case 1: the bounded domain $D(U) = [0, 1]$  We take $D(U) = [0, 1]$ and $U = 0$ on $[0, 1]$. Following the computations in, e.g., [KvM19], we obtain

$$\rho(x) = \begin{cases} \frac{1}{\pi} [x(1-x)]^{-\frac{1}{2}} & \text{if } a = 0 \\ \frac{a\Gamma(a)}{\Gamma\left(\frac{1+a}{2}\right)} [x(1-x)]^{-\frac{1-a}{2}} & \text{if } 0 < a < 1 \end{cases}$$

and

$$E(\rho) = \begin{cases} \log 2 & \text{if } a = 0 \\ \frac{\pi a\Gamma(a)}{2\Gamma\left(\frac{1+a}{2}\right)^2 \cos\left(\frac{a\pi}{2}\right)} & \text{if } 0 < a < 1. \end{cases}$$

With $E(\rho)$ specified, we compute $e_n$ and $p$ in (47) and (48) with the method described above. The results are shown in Table 3 and Figures 5 and 6. We note that $-p$ is the slope of the graphs of $e_n$ in Figure 5. For all four values of $a$, $e_n$ seems to converge to 0 as $n \to \infty$. Also, $p$ decreases as $a$ increases. These observations are in line with Theorem 1.2. However, for all four values of $a$, the computed value of $p$ is significantly larger than the theoretical prediction $1 - a$ from Theorem 1.2.

![Figure 5](image)

Figure 5: The numerically computed values for $e_n$ (see (47)) in Cases 1 and 2 for the values $a = 0$ (●), $a = \frac{1}{4}$ (■), $a = \frac{1}{2}$ (▲) and $a = \frac{3}{4}$ (▲).

Case 2: the infinite domain $D(U) = \mathbb{R}$  We take $D(U) = \mathbb{R}$ and

$$U(x) = \gamma_a \left(x - \frac{1}{2}\right)^2, \quad \gamma_a := \begin{cases} 4 & \text{if } a = 0 \\ \frac{2\pi a^2(2 + a)\Gamma(a)}{\Gamma\left(\frac{1+a}{2}\right)^2 \cos\left(\frac{a\pi}{2}\right)} & \text{if } 0 < a < 1. \end{cases}$$

The constant $F_a$ is chosen such that $\text{supp} \rho = [0, 1]$. Following the computations in, e.g., [KvM19] and [ST97 Chap. IV, Thm. 5.1], we obtain

$$\rho(x) = \begin{cases} \frac{8}{\pi} [x(1-x)]^{\frac{1}{2}} & \text{if } a = 0 \\ \frac{4(2 + a)a\Gamma(a)}{(1 + a)\Gamma\left(\frac{1+a}{2}\right)^2} [x(1-x)]^{\frac{1+a}{2}} & \text{if } 0 < a < 1 \end{cases}$$

and

$$E(\rho) = \begin{cases} \log 2 & \text{if } a = 0 \\ \frac{\pi a\Gamma(a)}{2\Gamma\left(\frac{1+a}{2}\right)^2 \cos\left(\frac{a\pi}{2}\right)} & \text{if } 0 < a < 1. \end{cases}$$
Case 1

Case 2

Figure 6: Values of $p$ as a function of $a$ in Cases 1 and 2 compared with the theoretical prediction from Theorem 1.2. The $n$-dependence is removed by taking the average of $p$ over the last four values of $n$ in Table 3.

and

$$E(p) = \begin{cases} \log 2 & \text{if } a = 0 \\ \frac{\pi(2 + a)^2a\Gamma(a)}{2(4 + a)\Gamma\left(\frac{1+a}{2}\right)^2\cos\left(\frac{a\pi}{2}\right)} & \text{if } 0 < a < 1. \end{cases}$$

Similar to Case 1, we compute $e_n$ and $p$. The results are shown in Figure 5 and Table 3. The similarities with Case 1 are that $e_n$ seems to converge to 0 as $n \to \infty$, that $p$ decreases as $a$ increases, and that the computed value of $p$ is significantly larger than the theoretical prediction $1 - a$ from Theorem 1.2.

We end this section with three quantitative comparisons between Cases 1 and 2:

- For $a = 0$, the values of $e_n$ and $p$ are similar.

- When $a$ increases, the values of $e_n$ are larger in Case 2 than in Case 1 (at least when $n$ is not too large). This is consistent with Figure 2, where the graph of $\varphi^*$ seems a better match with the graph of $\varphi$ in Case 1 than in Case 2.

- Yet, the values of $p$ are larger in Case 2, which would imply that for $n$ large enough, the values of $e_n$ in Case 2 are smaller than those in Case 1. A possible reason for this could be the singularities of $\varphi$ at $x = 0$ and $x = 1$ in Case 1.

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Values of $p$ in Case 1

| $n$ | $a = 0$ | $a = \frac{1}{4}$ | $a = \frac{1}{2}$ | $a = \frac{3}{4}$ |
|-----|---------|------------------|------------------|------------------|
| $2^2$ | 1.60 | 1.42 | 1.24 | 0.23 |
| $2^3$ | 1.72 | 1.54 | 1.17 | 0.02 |
| $2^4$ | 1.78 | 1.59 | 0.98 | 0.10 |
| $2^5$ | 1.82 | 1.60 | 0.80 | 0.24 |
| $2^6$ | 1.84 | 1.57 | 0.72 | 0.35 |
| $2^7$ | 1.86 | 1.52 | 0.72 | 0.43 |
| $2^8$ | 1.87 | 1.47 | 0.75 | 0.48 |
| $2^9$ | 1.88 | 1.41 | 0.79 | 0.52 |
| $2^{10}$ | 1.89 | 1.37 | 0.83 | 0.54 |
| $2^{11}$ | 1.90 | 1.34 | 0.86 | 0.55 |

Thm. $\approx 1$ 0.75 0.50 0.25

Values of $p$ in Case 2

| $n$ | $a = 0$ | $a = \frac{1}{4}$ | $a = \frac{1}{2}$ | $a = \frac{3}{4}$ |
|-----|---------|------------------|------------------|------------------|
| $2^2$ | 1.40 | 1.26 | 1.07 | 0.83 |
| $2^3$ | 1.52 | 1.36 | 1.13 | 0.82 |
| $2^4$ | 1.61 | 1.43 | 1.16 | 0.79 |
| $2^5$ | 1.68 | 1.48 | 1.17 | 0.75 |
| $2^6$ | 1.73 | 1.52 | 1.17 | 0.70 |
| $2^7$ | 1.77 | 1.55 | 1.15 | 0.66 |
| $2^8$ | 1.80 | 1.56 | 1.14 | 0.62 |
| $2^9$ | 1.82 | 1.57 | 1.12 | 0.59 |
| $2^{10}$ | 1.84 | 1.58 | 1.09 | 0.57 |
| $2^{11}$ | 1.86 | 1.59 | 1.07 | 0.55 |

Thm. $\approx 1$ 0.75 0.50 0.25

Table 3: The numerically computed values for $p$ (see (48)) in Cases 1 and 2. The bottom row is the prediction from Theorem 1.2.

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