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NON LINEAR SCHRÖDINGER LIMIT OF BOSONIC GROUND STATES, AGAIN

NICOLAS ROUGERIE

Abstract. I review an information-theoretic variant of the quantum de Finetti theorem due to Brandão and Harrow and discuss its applications to the topic of bosonic mean-field limits. This leads to slightly improved methods for the derivation of the local non-linear Schrödinger energy functional from many-body quantum mechanics.

CONTENTS

1. INTRODUCTION

The present paper is an addendum to the "quantum de Finetti-based" approach to the mean-field limit of bosonic ground states developed over the past few years. It has two main motivations:

(1) Review an interesting variant of the quantum de Finetti theorem derived in [6, 28].
(2) Couple this variant to the approach of bosonic mean-field limits described in [25], in order to remove unaesthetic restrictions on its range of validity.

Both motivations are mostly pedagogical. Let me briefly discuss the second one.

We consider the ground state(s) of a many-body Hamiltonian of the form

$$H_N = \sum_{j=1}^{N} \left(\left(-\mathrm{i}\nabla_{x_j} + A(x_j) \right)^2 + V(x_j) \right) + \frac{1}{N-1} \sum_{1 \leqslant j < k \leqslant N} N^{d\beta} w(N^{\beta}(x_j - x_k))$$

(1.1)

acting on $L^2_{\mathrm{sym}}(\mathbb{R}^{dN})$, the space of symmetric N-body wave-functions appropriate for the description of bosonic particles. Here $d = 1, 2, 3$ is the dimension of the physical space, $V : \mathbb{R}^d \mapsto \mathbb{R}$ is an external potential, $A : \mathbb{R}^d \mapsto \mathbb{R}^d$ the vector potential of an external magnetic field $B = \operatorname{curl} A$ and $w : \mathbb{R}^d \mapsto \mathbb{R}$ a pair interaction potential. Our convention is that the length scale of the system is set by the external potential V, that we shall take trapping:

$$V(x) \geqslant c|x|^s - C \text{ for some fixed constants } c, C, s > 0. \tag{1.2}$$

The scaling of the interactions is then designed to impose

$$(\text{range of interactions})^d \times \text{average density} \times \text{interaction strength} = O(1) \tag{1.3}$$

in the limit $N \to \infty$, so that the interaction energy is of the same magnitude as typical one-particle energies. Fixing (1.3) still leaves some freedom, and the fixed parameter $\beta \geqslant 0$ is used to interpolate between two scenarios:

(1) $\beta < 1/d$ is a mean-field regime, interactions are of longer range than the mean inter-particle distance.
(2) $\beta > 1/d$ is a dilute regime, interactions are of shorter range than the mean inter-particle distance.

Maximum physical relevance demands rather large values of β: in 3D $\beta = 1$ is, for reasons explained at length elsewhere, e.g. in [34, Chapters 2 and 6] or [48, 49, Chapter 7], the most relevant case. In 2D one might even consider an exponential-like scaling of the interactions' range (thus $\beta = \infty$ formally), see [34, Chapters 3 and 6]. See [50] for a general perspective on scaling limits of bosonic ground states.

However, the larger β, the harder the analysis. For small values of β it is feasible to deal with the $N \to \infty$ limit of the ground-state problem

$$E(N) := \min \left\{ \langle \Psi_N | H_N | \Psi_N \rangle, \ \Psi_N \in L^2_{\mathrm{sym}}(\mathbb{R}^{dN}) \right\} \tag{1.4}$$

using only general structural facts of many-body quantum mechanics [23, 25], within a totally variational[1] proof.

This paper is concerned with improving the conditions on β (i.e. the rate at which the interactions converge to point-like ones) under which one can treat the $N \to \infty$ limit of Problem (1.4) in a totally variational way. We are able to handle the $N \to \infty$ limit of Problem (1.4) provided one stays reasonably deep within the mean-field regime:

$$\beta < \frac{1}{2d}. \tag{1.5}$$

Our general approach to the mean-field limit is that of [25, 39], but we use as main tools the results of [6, 28] instead of those of [11, 24]. Using the latter in [25] led to the condition $\beta < \beta_0(s)$ for some rather small and s-dependent $\beta_0(s)$ (s being the exponent in (1.2)). This annoying dependence on s gets dispensed with here.

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[1] In the spirit of Γ-convergence one might say.

The value (1.5) is optimal with the method exposed here. Larger values of β are known to be reachable by methods outside of the range of this paper (see the comments after Theorem 2.2). The complexity of the proofs increases rather steeply [4, 37, 38, 35, 36, 32] for $\beta > 1/d$. The proofs are no longer purely variational, as one typically uses the many-body Schrödinger equation to obtain a priori bounds on minimizers [26, 33, 43]. I also mention that similar problems and techniques are useful in the context of the "almost bosonic anyon gas" [39, 15] and the dipolar Bose gas [55]. See also [2, 1, 14, 47, 46, 12, 45, 13, 46, 3, 41, 8, 9, 19] for a selection of works dealing with mean-field and/or dilute limits of the dynamical problem associated with (1.1).

Organization of the paper. In Section 2 I state the main result on the mean-field limit of (1.1). Section 3 explains the adaptations to be made in the proof strategy of [25]. The main one is to use an information-theoretic quantum de Finetti theorem. Its statement and proof are reviewed in Appendix A for the benefit of readers who, like myself, lack familiarity with arguments that are standard in quantum information theory, but much less so in many-body quantum mechanics.

Notation. For a vector ψ in a Hilbert space $\mathfrak{H}$ (usually a function $\psi \in L^2(\mathbb{R}^d)$), we use the bra-ket $|\psi\rangle\langle\psi|$ notation for the corresponding orthogonal projector (pure state).

The symbol Tr stands for the trace. When decorated with subscripts, a partial trace with respect to these subscripts is meant. That is, for an operator acting on $\mathfrak{H}_1 \otimes \ldots \otimes \mathfrak{H}_N$, $\mathrm{Tr}_{i_1,\ldots,i_k}$ means tracing over $\mathfrak{H}_{i_1}, \ldots, \mathfrak{H}_{i_k}$ If the operator one takes the trace of acts on a tensor product $\mathfrak{H}^{\otimes N}$ and is symmetric, I indicate $\mathrm{Tr}_{k+1\to N}$ to mean a partial trace with respect to $N - k$ factors of the N-fold tensor product, no matter which.

The interaction potential in (1.1) is denoted

$$w_{N,\beta}(x) := N^{d\beta} w(N^\beta x). \tag{1.6}$$

2. Results and discussion

2.1. **Statements.** For the easiest case $d = 1$, [25] already covers any value of $\beta > 0$ with a fully variational method. We thus focus on the cases $d = 2, 3$ and work under the following assumptions:

ASSUMPTION 2.1 (Stable interactions). — *The pair interaction potential w : $\mathbb{R}^d \mapsto \mathbb{R}$ is a bounded, integrable even function with $|x|w(x) \in L^1(\mathbb{R}^d)$ and Fourier transform $\widehat{w} \in L^1(\mathbb{R}^d)$. It is stable in the sense that*

- *in 3D, $w \geqslant 0$.*
- *in 2D, $\int_{\mathbb{R}^d} |w_-| < a_*$ with w_- the negative part of w and a_* the optimal constant in the Gagliardo-Nirenberg inequality,*

$$\int_{\mathbb{R}^2} |u|^4 \leqslant a_* \Big(\int_{\mathbb{R}^2} |u|^2 \Big) \Big(\int_{\mathbb{R}^2} |\nabla u|^2 \Big)$$

Equivalently $a_* = \big\| Q \big\|_{L^2(\mathbb{R}^2)}^2$ where Q is the unique (up to translations) solution to

$$-\Delta Q + Q - Q^3 = 0 \text{ on } \mathbb{R}^2.$$

See [25] or [48, Chapter 7] for more comments on the necessity of these assumptions. In 2D one can relax the condition to what we called "Hartree-stability" in [25], but that is a small improvement that I sacrifice here for simplicity. For the other data of the problem we make standard assumptions:

$$A \in L^2_{\mathrm{loc}}(\mathbb{R}^d, \mathbb{R}^d), V \in L^1_{\mathrm{loc}}(\mathbb{R}^d, \mathbb{R})$$

and assume (1.2).

The limiting objects in the $N \to \infty$ limit are as follows. Let the non-linear Schrödinger (NLS) functional be

$$\mathcal{E}^{\mathrm{nls}}[u] := \int_{\mathbb{R}^d} \left| (-\mathrm{i}\nabla + A)u \right|^2 + V|u|^2 + \frac{a}{2} \int_{\mathbb{R}^d} |u|^4 \tag{2.1}$$

with

$$a = \int_{\mathbb{R}^d} w.$$

We also define the associated ground-state energy

$$E^{\mathrm{nls}} = \min \left\{ \mathcal{E}^{\mathrm{nls}}[u], \int_{\mathbb{R}^d} |u|^2 = 1 \right\} \tag{2.2}$$

with $\mathcal{M}^{\mathrm{nls}}$ the set of associated minimizers. Our main result is

THEOREM 2.2 (Mean-field/NLS limit of bosonic ground states). — *Fix a parameter*

$$0 < \beta < \frac{1}{2d}.$$

The following holds in the $N \to \infty$ limit.

(1) *Convergence of the N-body ground state energy*

$$\frac{E(N)}{N} \xrightarrow[N \to \infty]{} E^{\mathrm{nls}}. \tag{2.3}$$

(2) *Convergence of reduced density matrices. Let $(\Psi_N)_N$ be a sequence of quasi minimizers for (1.4), i.e.*

$$\langle \Psi_N | H_N | \Psi_N \rangle \leqslant E(N) + o(N). \tag{2.4}$$

For $k \geqslant 1$ let $\gamma_N^{(k)}$ be the associated k-particles reduced density matrix[2]

$$\gamma_N^{(k)} = \mathrm{Tr}_{k+1 \to N} |\Psi_N\rangle \langle \Psi_N|. \tag{2.5}$$

Then

$$\gamma_N^{(k)} \xrightarrow[N \to \infty]{} \int |u^{\otimes k}\rangle \langle u^{\otimes k}| d\mu(u) \tag{2.6}$$

strongly in the trace-class, where μ is a Borel probability measure supported on $\mathcal{M}^{\mathrm{nls}}$.

Note that

(1) Under the stated assumptions it is standard to see that both (1.4) and (2.2) are well-posed.

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[2] $\mathrm{Tr}_{k+1 \to N}$ means partial trace on $N - k$ particles, cf the Notation paragraph at the end of Section 1.

(2) The result is not new, and is actually weaker than what was known already using more-than-variational proofs. In 3D any $\beta < 1$ can be covered with the methods of [33, 43]. Indeed, these papers deal with the special, harder case $\beta = 1$ (where the result is not stated the same). In 2D [26] can handle any $\beta < (s + 1)/(s + 2)$ (in particular some dilute regimes $\beta > 1/2$ are allowed). The novel aspect is thus methodological, as we discuss next.

(3) Coupling the method of the present paper with refined a-priori estimates allows [42] to reach any value of $\beta < 1$ in 2D.

2.2. **Method of proof.** We pursue along the lines of [25]. The argument is based on the quantum de Finetti theorem, which asserts that (2.6) holds for essentially any sequence of bosonic states Ψ_N, for some general Borel probability measure μ over $L^2(\mathbb{R}^d)$ (not necessarily supported on $\mathcal{M}^{\mathrm{nls}}$). The goal is then to identify the support of the measure associated with sequences of quasi-minimizers.

The difficulty in applying this general idea to NLS-like limits ($\beta > 0$) is that one cannot use soft compactness arguments to pass to the limit in the energy. The idea of [25] is to rely on specific versions of the quantum de Finetti theorem which explicitly quantify the error made in replacing the left side of (2.6) by the right side. Unfortunately, explicit estimates are available only when the one-body Hilbert space $L^2(\mathbb{R}^d)$ is replaced by a finite-dimensional one. Thus the need to

- project the problem to finitely many dimensions, i.e. on one-body states whose one-body energy is below a certain energy cut-off.
- use the quantitative finite dimensional de Finetti theorem in the projected space.
- take the energy cut-off high enough for states in the orthogonal complement to be negligible.

The technical limitations imposed on β in [25] arose because the de Finetti theorem [11, 10, 16, 24] we used had errors depending linearly on the low-energy space's dimension. The latter depends polynomially on the energy cut-off (this can be seen by Cwikel-Lieb-Rosenblum-type bounds). We here relax these limitations by using a finite dimensional quantitative de Finetti theorem whose errors [6] depend only logarithmically[3] on the dimension of the one-body Hilbert space.

The trade-off is that the error in the de Finetti theorem of [6] (see also [28]) is not quantified in the usual trace-class norm, and that the measure constructed there does not charge only bosonic states (i.e. the measure might live on mixed one-body operators γ, not just on pure states $|u\rangle\langle u|$). These are the two aspects we have to circumvent to conclude the proof along the lines of [25].

As a final remark on the method, I stress that it is meant to obtain *variationally* the *full statement* of Theorem 2.2 for the *fully general case* of (1.1). For $\beta < 1/d$ one might still obtain [21, 27, 26] part of the statement under restrictive assumptions (typically one does not obtain the convergence of all density matrices and/or assumes that the limit problem has a unique minimizer and/or does not include the possibility of a magnetic field). See [50] for a review on these aspects.

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[3]Thus, for many practical purposes, the theorem is almost as good as a quantitative de Finetti theorem in infinite dimension.

3. Proof of the mean-field limit theorem

We follow the general strategy of [25] (also presented in [48, 49, Chapter 7]), with the appropriate modifications allowing to insert the main new tool, Theorem A.5 below.

3.1. **Localizing the two-body Hamiltonian.** Our first task is to localize the Hamiltonian to low one-body energy states. Let us denote

$$h = \left(-i\nabla + A \right)^2 + V \tag{3.1}$$

and, for some high-energy cut-off $\Lambda \in \mathbb{R}$,

$$P = \mathbb{1}_{h \leqslant \Lambda}, \quad Q = \mathbb{1} - P. \tag{3.2}$$

Recall that since h has compact resolvent, $PL^2(\mathbb{R}^d)$ is finite dimensional. In fact

$$N_\Lambda := \dim(P) \leqslant C\Lambda^{\frac{d}{s} + \frac{d}{2}} \tag{3.3}$$

with s the exponent in (1.2), see [25, Lemma 3.3] and references therein.

We shall write the many-body energy of a quasi-minimizer Ψ_N in the manner

$$\frac{1}{N}\langle \Psi_N | H_N | \Psi_N \rangle = \frac{1}{2} \operatorname{Tr} \left(H_2 \gamma_N^{(2)} \right) \tag{3.4}$$

using the two-particle reduced density matrix $\gamma_N^{(2)}$ and the two-body Hamiltonian

$$H_2 := h_1 + h_2 + w_{N,\beta}(x_1 - x_2)$$

acting on $\mathfrak{H}^2 = L^2(\mathbb{R}^d)^{\otimes 2}$, with $h_1 = h \otimes \mathbb{1}$ and $h_2 = \mathbb{1} \otimes h$.

We shall need a slightly modified version: for $\varepsilon > 0$ let

$$H_2^\varepsilon = H_2 - \varepsilon N^{d\beta} \left| w \left(N^\beta \left(x - y \right) \right) \right| \tag{3.5}$$

Now we project the two-body Hamiltonian below the high-energy cut-off:

LEMMA 3.1 (Localized two-body Hamiltonian). — *Assume* $\Lambda \geqslant C\varepsilon^{-1}N^{d\beta}$ *for a large enough constant* $C > 0$ *and* $0 < \varepsilon < 1$. *Then we have, as operators on* $L^2(\mathbb{R}^{2d})$,

$$H_2 \geqslant P^{\otimes 2} H_2^\varepsilon P^{\otimes 2} + \frac{\Lambda}{2} \left(Q \otimes \mathbb{1} + \mathbb{1} \otimes Q \right) \tag{3.6}$$

Proof. — This is [25, Lemma 3.6]. For brevity I do not reproduce the proof. $\square$

Remark 3.2 (Dependence on the trap). — The virtue of the quantum de Finetti theorem we use below is that only the logarithm of N_Λ enters the estimate. For a polynomial trap as assumed in (1.2), this gives a logarithmic dependence on Λ as per (3.3). Such a dependence is quite negligible for it will come multiplied by negative powers of N, and Λ depends polynomially on N in the previous lemma. If the trap has a weaker growth (say logarithmic), one can still proceed by using adapted variants of (1.2), but now N_Λ depends exponentially on Λ and the dependence of errors on N_Λ becomes relevant. A bit of fine tuning is required to compute the dependence on the growth of V of the maximal β that the method allows. We do not pursue this for simplicity. $\diamond$

3.2. **Quantum de Finetti.** Now we apply the quantum de Finetti theorem whose proof is recalled in Appendix A below to the localized reduced 2-body density matrix of a quasi-minimizer (or any other state for that matter):

PROPOSITION 3.3 (de Finetti representation of projected density matrices). — *Let $\mathfrak{H}$ be a complex separable Hilbert space, and $\mathfrak{H}_N = \mathfrak{H}^{\otimes_{\mathrm{sym}} N}$ the corresponding bosonic space. Let*

$$\gamma_N^{(2)} = \mathrm{Tr}_{3 \to N} |\Psi_N\rangle\langle\Psi_N|$$

be the 2-body reduced density matrix of a N-body state vector $\Psi_N \in \mathfrak{H}_N$ (or general mixed state).

Let P be a finite dimensional orthogonal projector. There exists a Borel measure $\mu_N^{(2)}$ on the set of one-body mixed states

$$\mathcal{S}_P := \Big\{ \gamma \text{ positive trace-class operator on } P\mathfrak{H}, \, \mathrm{Tr}\,\gamma = 1 \Big\} \tag{3.7}$$

such that

$$\sup_{0 \leqslant A, B \leqslant 1} \mathrm{Tr}\,\Big| A \otimes B\Big(P^{\otimes 2}\gamma_N^{(2)}P^{\otimes 2} - \int \gamma^{\otimes 2} d\mu_N^{(2)}(\gamma)\Big)\Big| \leqslant C\sqrt{\frac{\log(\dim(P))}{N}} \tag{3.8}$$

where the sup is over bounded operators on $P\mathfrak{H}$.

Previous comparable statements in [25, 26] have an error which is proportional to $\dim(P)/N$. The point is that we shall be forced to apply the above with a rather large $\dim(P) \gg N^{1/2}$, so that the much-improved dependence on $\dim(P)$ in (3.8) counter-balances the worst dependence on N.

Proof. — We combine Fock-space localization and the information–theoretic quantum de Finetti theorem recalled in Appendix A.

Step 1, de Finetti. Let Γ_N be a mixed state over $P^{\otimes N}\mathfrak{H}_N$. From Theorem A.5 we know there exists a probability measure $\mu_N^{(2)}$ over $\mathcal{S}_P$ such that

$$\sup_{\Lambda_1, \Lambda_2 \in \mathcal{M}(\mathfrak{H})} \Big\|\Lambda_1 \otimes \Lambda_2\Big(\Gamma_N^{(2)} - \int \gamma^{\otimes 2} d\mu_N^{(2)}(\gamma)\Big)\Big\|_{\mathfrak{S}^1(\mathfrak{H}^2)} \leqslant \sqrt{\frac{2\log(\dim P)}{N-1}} \tag{3.9}$$

where the sup is over quantum measurements (see Definition A.1) and

$$\Big\|A\Big\|_{\mathfrak{S}^1} = \mathrm{Tr}\,|A|$$

is the trace-class norm [54, 51]. We claim that this implies

$$\sup_{0 \leqslant A, B \leqslant 1} \mathrm{Tr}\,\Big| A \otimes B\Big(\Gamma_N^{(2)} - \int \gamma^{\otimes 2} d\mu_N^{(2)}(\gamma)\Big)\Big| \leqslant \sqrt{\frac{\log(\dim(P))}{N}} \tag{3.10}$$

where the sup is now over bounded operators. Indeed, given operators A_1, A_2, define measurements

$$\Lambda_j(\gamma) = \mathrm{Tr}\Big[A_j\gamma\Big]|e_1\rangle\langle e_1| + \mathrm{Tr}\Big[(\mathbb{1} - A_j)\gamma\Big]|e_2\rangle\langle e_2|$$

for orthonormal vectors e_1, e_2 (independent of j). Then, for any 2-particle operator γ_2, we have

$$\Lambda_1 \otimes \Lambda_2\, \gamma_2 = \text{Tr} \left[A_1 \otimes A_2 \gamma_2 \right] |e_1^{\otimes 2}\rangle\langle e_1^{\otimes 2}|$$
$$+ \sum_{(B_j, f_j)_{1 \leqslant j \leqslant 2}} \text{Tr} \left[B_1 \otimes B_2 \gamma_2 \right] |f_1 \otimes f_2\rangle\langle f_1 \otimes f_2|$$

where the last sum is over all possible choices of $B_j = A_j$ or $B_j = \mathbb{1} - A_j$, with $f_j = e_1$ in the former case and $f_j = e_2$ in the second, and we impose that for at least one index j, $B_j = \mathbb{1} - A_j$ (and thus $f_j = e_2$). Since e_1 and e_2 are orthogonal it follows that all projectors appearing in the second line live on spaces orthogonal to $e_1^{\otimes 2}$ and thus

$$\text{Tr} \left| \Lambda_1 \otimes \Lambda_2 \gamma_2 \right| \geqslant \left| \text{Tr} \left[A_1 \otimes A_2 \gamma_2 \right] \right|.$$

Applying this to

$$\gamma_2 = \gamma_N^{(2)} - \int \gamma^{\otimes 2} d\mu_N^{(2)}(\gamma)$$

shows that indeed (3.10) follows from (3.9).

Step 2, localization. From methods discussed e.g. in [22] or [48, 49, Chapter 5] we know there exists a state Γ_N^P on the truncated bosonic Fock space

$$\mathfrak{F}_P = \mathbb{C} \oplus P\mathfrak{H} \oplus P^{\otimes 2}\mathfrak{H}_2 \oplus \ldots \oplus P^{\otimes N}\mathfrak{H}_N$$

of the form

$$\Gamma_N^P = \left(c_{N,0}\Gamma_{N,0}^P \right) \oplus \left(c_{N,1}\Gamma_{N,1}^P \right) \oplus \ldots \oplus \left(c_{N,N}\Gamma_{N,N}^P \right),$$

with $c_{N,j} \geqslant 0$, $\sum_{j=0}^N c_{N,j} = 1$ and $\Gamma_{N,j}$ a j-particles state, such that

$$P^{\otimes k} \gamma_N^{(k)} P^{\otimes k} = \sum_{\ell=k}^N c_{N,\ell} \binom{N}{k}^{-1} \binom{\ell}{k} \left(\Gamma_{N,\ell}^P \right)^{(k)}. \tag{3.11}$$

We apply the previous step to each $\Gamma_{N,\ell}^P$, $\ell \geqslant 2$, obtaining probability measures $\mu_{N,\ell}^{(2)}$ and the estimates

$$\sup_{0 \leqslant A, B \leqslant 1} \text{Tr} \left| A \otimes B \left(\left(\Gamma_{N,\ell}^P \right)^{(2)} - \int \gamma^{\otimes 2} d\mu_{N,\ell}^{(2)}(\gamma) \right) \right| \leqslant C \sqrt{\frac{\log(\dim(P))}{\ell}} \tag{3.12}$$

for $\ell \geqslant 2$. Setting

$$\mu_N^{(2)} = \sum_{\ell=2}^N c_{N,\ell} \binom{N}{2}^{-1} \binom{\ell}{2} \mu_{N,\ell}^{(2)},$$

combining (3.12) with (3.11) we get the statement, because

$$\frac{1}{\sqrt{\ell}} \binom{N}{k}^{-1} \binom{\ell}{k} = \frac{1}{\sqrt{N}} \sqrt{\frac{\ell}{N}} \frac{(\ell-1)\ldots(\ell-k+1)}{(N-1)\ldots(N-k+1)} \leqslant \frac{1}{\sqrt{N}}. \quad \square$$

3.3. **Mean-field functionals.** The previous ingredients will allow to replace the N-body problem by a mean-field one, namely reduce attention to two-body matrices of the form $\gamma^{\otimes 2}$ in (3.4). This leads us to considering mixed Hartree and NLS functionals. First, let

$$a = \int_{\mathbb{R}^d} w$$

and[4]

$$\mathcal{E}^{\mathrm{nls,m}}[\gamma] := \mathrm{Tr}\left(\left(-i\nabla + A\right)^2 + V\right)\gamma\right) + \frac{a}{2}\int_{\mathbb{R}^d}\left|\gamma(x;x)\right|^2 dx \tag{3.13}$$

and

$$E^{\mathrm{nls,m}} = \min\left\{\mathcal{E}^{\mathrm{nls}}[\gamma], \gamma \text{ trace-class operator on } L^2(\mathbb{R}^d), \mathrm{Tr}\,\gamma = 1\right\} \tag{3.14}$$

with $\mathcal{M}^{\mathrm{nls,m}}$ the set of associated minimizers. The superscript m means mixed because we allow mixed states γ as arguments. We recover the objects described in Theorem 2.2 by reducing to pure states $\gamma = |u\rangle\langle u|$. Note that the minimization problems amongst all mixed states and amongst only pure states can differ [52, 53], especially if $A \neq 0$. This is a point we shall deal with later.

For the moment we need to ensure that the Hartree problem, with smeared non-linearity, converges to the above. Let thus

$$\mathcal{E}^{\mathrm{H}}[\gamma] := \mathrm{Tr}\left(\left(-i\nabla + A\right)^2 + V\right)\gamma\right) + \frac{1}{2}\mathrm{Tr}\left(w_{N,\beta}\,\gamma^{\otimes 2}\right) \tag{3.15}$$

where (recall (1.6)) $w_{N,\beta}$ is understood as a multiplication operator on $L^2(\mathbb{R}^{2d})$. Also, let

$$E^{\mathrm{H}} = \min\left\{\mathcal{E}^{\mathrm{H}}[\gamma], \gamma \text{ trace-class operator on } L^2(\mathbb{R}^d), \mathrm{Tr}\,\gamma = 1\right\}. \tag{3.16}$$

These are the objects one obtains by inserting a factorized ansatz in (3.4). We shall need the following.

LEMMA 3.4 (Stability of one-body functionals). — *Under the assumptions of Theorem 2.2, there is a constant $C > 0$ such that, for any mixed one-body state γ*

$$\mathrm{Tr}\left(h\gamma\right) \leqslant C(\mathcal{E}^{\mathrm{H}}[\gamma] + C) \tag{3.17}$$

and

$$\left|\mathcal{E}^{\mathrm{H}}[\gamma] - \mathcal{E}^{\mathrm{nls,m}}[\gamma]\right| \leqslant CN^{-\beta}\left(1 + \mathrm{Tr}\left(h\gamma\right)\right)^2. \tag{3.18}$$

Proof. — This is essentially similar to [25, Lemma 4.1]. To extend the proof of (3.18) to mixed states it is convenient to write the kernel of γ as

$$\gamma(x;y) = \sum_j \lambda_j u_j(x)\overline{u_j(y)}. \tag{3.19}$$

Then

$$\mathrm{Tr}\left(w_{N,\beta}\,\gamma^{\otimes 2}\right) = \sum_{i,j} \lambda_i\lambda_j N^{d\beta} \iint_{\mathbb{R}^d \times \mathbb{R}^d} |u_i(x)|^2 w(N^\beta(x-y))|u_j(y)|^2 dxdy$$

and one may apply the arguments of the proof of [25, Lemma 4.1] to each term of the sum. This is the place where we use that $|x|w(x) \in L^1(\mathbb{R}^d)$. $\qquad\square$

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[4]The definition of $\gamma(x;x)$ is recalled in (3.19) below. Formally it is the integral kernel $\gamma(x;y)$ of γ evaluated at $x = y$.

3.4. **Passage to the limit and conclusion.** We now proceed to the

Proof of Theorem 2.2. — The usual trial state argument (testing the energy with a factorized $\Psi_N = u^{\otimes N}$) and Lemma 3.4 give the energy upper bound

$$E(N) \leqslant N E^{\mathrm{nls}} + o(N). \tag{3.20}$$

We focus on the energy lower bound and associated convergence of reduced density matrices. Let Ψ_N be a sequence of quasi-minimizers as in the statement of the theorem and P the projector on low kinetic energy modes defined above.

First energy estimate. Use the Fourier transform to write a smooth pair potential W as

$$
\begin{aligned}
W(x - y) &= \int_{\mathbb{R}^d} \widehat{W}(p) e^{ip \cdot x} e^{-ip \cdot y} dp \\
&= \int_{\mathbb{R}^d} \widehat{W}(p) \Big(\sum_{(i,j) \in \{+,-\}} c_p^i \otimes c_p^j + s_p^i \otimes s_p^j \Big) dp
\end{aligned} \tag{3.21}
$$

with $c_p^\pm, s_p^\pm$ the bounded operators (with bound 1) of multiplication by the positive and negative parts of $\cos(p \cdot x), \sin(p \cdot x)$.

Proposition 3.3 gives

$$\sup_{0 \leqslant A, B \leqslant \mathbb{1}} \Big| \operatorname{Tr} A \otimes B \Big(P^{\otimes 2} \gamma_N^{(2)} P^{\otimes 2} - \int \gamma^{\otimes 2} d\mu_N^{(2)}(\gamma) \Big) \Big| \leqslant C \sqrt{\frac{\log(\dim(P))}{N}}. \tag{3.22}$$

But the sup in the above is bounded by a constant times the sup over signed operators A, B so we may combine with (3.21) and use the triangle inequality to obtain

$$\Big| \operatorname{Tr} \Big[W(x - y) \Big(P^{\otimes 2} \gamma_N^{(2)} P^{\otimes 2} - \int \gamma^{\otimes 2} d\mu_N^{(2)}(\gamma) \Big) \Big] \Big| \leqslant C \sqrt{\frac{\log(\dim(P))}{N}} \int_{\mathbb{R}^d} |\widehat{W}(p)| dp.$$

Applying this with $W(x) = N^{d\beta} w(N^\beta x)$ and P as in (3.2) we get

$$\operatorname{Tr} \Big(P^{\otimes 2} H_2^\varepsilon P^{\otimes 2} \gamma_N^{(2)} \Big) \geqslant \int_{\mathcal{S}_P} \operatorname{Tr} \Big(H_2^\varepsilon \gamma^{\otimes 2} \Big) d\mu_N^{(2)}(\gamma) - C(N^{d\beta} + \Lambda) \sqrt{\frac{\log(N_\Lambda)}{N}}$$

where we also used that on $P L^2(\mathbb{R}^d)$, $h \leqslant \Lambda$ by definition to apply (3.22) to the one-body term. Combining with Lemma 3.1 yields our first energy lower bound

$$
\begin{aligned}
\frac{E(N)}{N} + o(1) &\geqslant \frac{1}{2} \operatorname{Tr} \Big(H_2 \gamma_N^{(2)} \Big) \\
&\geqslant \int_{\mathcal{S}_P} \mathcal{E}_\varepsilon^{\mathrm{H}}[\gamma] d\mu_N^{(2)}(\gamma) + C\Lambda \operatorname{Tr} \Big(Q \gamma_N^{(1)} \Big) - C(N^{d\beta} + \Lambda) \sqrt{\frac{\log(N_\Lambda)}{N}}
\end{aligned} \tag{3.23}
$$

with

$$\mathcal{E}_\varepsilon^{\mathrm{H}}[\gamma] := \operatorname{Tr} \Big(\Big(-i\nabla + A \Big)^2 + V \Big) \gamma \Big) + \frac{1}{2} \operatorname{Tr} \Big(w_{N,\beta} \gamma^{\otimes 2} \Big) - \frac{\varepsilon}{2} \operatorname{Tr} \Big(|w_{N,\beta}| \gamma^{\otimes 2} \Big).$$

It is easy to see that the latter functional is bounded below uniformly in N if we choose ε small enough (but independent of N), which we henceforth do. We may now set

$$\Lambda = C N^{d\beta} \varepsilon^{-1} \tag{3.24}$$

for a large constant C. Then, inserting (3.3) and the uniform lower bound on $\mathcal{E}_\varepsilon^{\mathrm{H}}[\gamma]$ in (3.23) we obtain

$$C \geqslant \Lambda \operatorname{Tr}\left(Q\gamma_N^{(1)}\right) - C_\varepsilon o_N(1) \tag{3.25}$$

under the assumption that

$$\beta < \frac{1}{2d}.$$

The constant C_ε depends only on ε. We deduce that

$$\operatorname{Tr}\left(Q\gamma_N^{(1)}\right) \to 0 \tag{3.26}$$

when $N \to \infty$.

The de Finetti measures converge. Returning to the proof of Proposition 3.3 we have that (recall that $\sum_\ell c_{N,\ell} = 1$)

$$\begin{aligned}
\int_{\mathcal{S}_P} d\mu_N^{(2)}(\gamma) = \operatorname{Tr}\left(P^{\otimes 2}\gamma_N^{(2)}P^{\otimes 2}\right) &= \sum_{\ell=2}^N c_{N,\ell}\frac{\ell(\ell-1)}{N(N-1)} \\
&\geqslant \sum_{\ell=0}^N c_{N,\ell}\frac{\ell^2}{N^2} - \frac{C}{N} \geqslant \left(\sum_{\ell=0}^N c_{N,\ell}\frac{\ell}{N}\right)^2 - \frac{C}{N} \\
&= \left(\operatorname{Tr}\left(P\gamma_N^{(1)}P\right)\right)^2 - \frac{C}{N}
\end{aligned} \tag{3.27}$$

where we used Jensen's inequality. But (3.26) implies

$$\operatorname{Tr}\left(P\gamma_N^{(1)}P\right) \xrightarrow[N\to\infty]{} 1.$$

Returning to (3.27) we have that

$$\int_{\mathcal{S}_P} d\mu_N^{(2)}(\gamma) \xrightarrow[N\to\infty]{} 1.$$

Thus the sequence $(\mu_N^{(2)})_N$ of measures given by Proposition 3.3 is tight on the set of one-body mixed states

$$\mathcal{S} := \left\{\gamma \text{ positive trace-class operator on } L^2(\mathbb{R}^d), \operatorname{Tr}\gamma = 1\right\}.$$

Modulo subsequence $(\mu_N^{(2)})_N$ converges to a measure μ.

Convergence of reduced density matrices. In this step we reproduce for convenience arguments already used repeatedly in [23] and [48, 49]. We may return to (3.23) and derive a similar energy lower bound to

$$\operatorname{Tr}\left(\left(H_2 - \eta h \otimes \mathbb{1} - \eta \mathbb{1} \otimes h\right)\gamma_N^{(2)}\right) \tag{3.28}$$

for some small fixed $\eta > 0$. For η small enough we may use a variant of Lemma 3.4 to deduce that (3.28) is uniformly bounded from below. Hence, combining with (3.4) and the energy upper bound (3.20) we deduce that

$$\frac{\eta}{2}\operatorname{Tr}\left(\left(h \otimes \mathbb{1} + \mathbb{1} \otimes h\right)\gamma_N^{(2)}\right) = \eta\operatorname{Tr}\left(h\gamma_N^{(1)}\right) \leqslant C_{\varepsilon,\eta}.$$

Since h has compact resolvent we deduce (modulo subsequence) that

$$\gamma_N^{(1)} \to \gamma^{(1)}$$

strongly in trace-class, for some limit one-body bosonic density matrix $\gamma^{(1)}$. But we also have (again, modulo subsequences)

$$\gamma_N^{(k)} \underset{\star}{\rightharpoonup} \gamma^{(k)}$$

weakly-$\star$ in the trace-class. Applying the weak quantum de Finetti theorem [23, Theorem 2.2] we deduce that there exists a measure ν on the unit ball of $L^2(\mathbb{R}^d)$ such that

$$\gamma^{(k)} = \int |u^{\otimes k}\rangle\langle u^{\otimes k}| d\nu(u).$$

But since $\gamma^{(1)}$ must have trace 1, the measure ν must actually live on

$$SL^2(\mathbb{R}^d) = \left\{ u \in L^2(\mathbb{R}^d), \int_{\mathbb{R}^d} |u|^2 = 1 \right\},$$

the unit sphere of $L^2(\mathbb{R}^d)$.

Next we claim that the two measures μ and ν just found are related by

$$\int |u^{\otimes 2}\rangle\langle u^{\otimes 2}| d\nu(u) = \int |u^{\otimes 2}\rangle\langle u^{\otimes 2}| d\mu(u). \qquad (3.29)$$

Indeed, let

$$\tilde{P} = \mathbb{1}_{h \leqslant \tilde{\Lambda}}$$

where $\tilde{\Lambda}$ is a fixed cut-off (different from Λ above). Testing (3.8) with A_1, A_2 finite rank operators whose ranges lie within that of $\tilde{P}$ we get

$$\mathrm{Tr}\left(A_1 \otimes A_2 \gamma_N^{(2)}\right) \underset{N \to \infty}{\longrightarrow} \mathrm{Tr}\left(A_1 \otimes A_2 \int_{\mathcal{S}} \gamma^{\otimes 2} d\mu(\gamma)\right)$$

using the convergence of $\mu_N^{(2)}$ to μ. On the other hand, by the convergence of $\gamma_N^{(2)}$ to $\gamma^{(2)}$ we also have

$$\mathrm{Tr}\left(A_1 \otimes A_2 \gamma_N^{(2)}\right) \underset{N \to \infty}{\longrightarrow} \mathrm{Tr}\left(A_1 \otimes A_2 \gamma^{(2)}\right) = \mathrm{Tr}\left(A_1 \otimes A_2 \int_{SL^2(\mathbb{R}^d)} |u^{\otimes 2}\rangle\langle u^{\otimes 2}| d\nu(u)\right).$$

Thus

$$\mathrm{Tr}\left(A_1 \otimes A_2 \int_{\mathcal{S}} \gamma^{\otimes 2} d\mu(\gamma)\right) = \mathrm{Tr}\left(A_1 \otimes A_2 \int_{SL^2(\mathbb{R}^d)} |u^{\otimes 2}\rangle\langle u^{\otimes 2}| d\nu(u)\right) \qquad (3.30)$$

for any A_1, A_2 with range within that of $\tilde{P}$. Letting finally $\tilde{\Lambda} \to \infty$ yields $\tilde{P} \to \mathbb{1}$ and thus (3.30) holds for any compact operators A_1, A_2. This implies (3.29). In particular, since the left-hand side of (3.29) is $\gamma^{(2)}$, a bosonic operator, μ must be supported on pure states $\gamma = |u\rangle\langle u|$, see [18].

Final passage to the liminf. . Let us return to (3.23). We split the integral over one-body states γ between low and high kinetic energy states:

$$\mathtt{Low} = \left\{ \gamma \in \mathcal{S}, \mathrm{Tr}\left(h\gamma\right) \leqslant C_{\mathtt{Kin}} \right\}, \quad \mathtt{High} = \mathcal{S} \setminus \mathtt{Low}$$

with C_{Kin} a constant independent of N (we will take $C_{\text{Kin}} \to \infty$ after $N \to \infty$). Using Lemma 3.4 (or rather an obvious variant applying to $\mathcal{E}_\varepsilon^{\text{H}}$) we obtain

$$\int_{\mathcal{S}_P} \mathcal{E}_\varepsilon^{\text{H}}[\gamma] d\mu_N^{(2)}(\gamma) \geqslant C_\varepsilon C_{\text{Kin}} \int_{\text{High}} N^{\beta/4} d\mu_N^{(2)}(\gamma) + \int_{\text{Low}} \mathcal{E}_\varepsilon^{\text{nls,m}}[\gamma] d\mu_N^{(2)}(\gamma) - C_\varepsilon N^{-\beta}$$

$$\geqslant \int_{\mathcal{S}_P} \min \left(C_\varepsilon C_{\text{Kin}}, \mathcal{E}_\varepsilon^{\text{nls,m}}[\gamma] \right) d\mu_N^{(2)}(\gamma) - C_\varepsilon N^{-\beta}$$

where $\mathcal{E}_\varepsilon^{\text{nls,m}}$ is $\mathcal{E}^{\text{nls,m}}$ with

$$a \rightsquigarrow a - \varepsilon a.$$

Inserting in (3.23) and passing to the liminf in $N \to \infty$ this implies

$$E^{\text{nls}} \geqslant \liminf_{N \to \infty} \frac{E(N)}{N} \geqslant \int_{\mathcal{S}} \min \left(C_\varepsilon C_{\text{Kin}}, \mathcal{E}_{m,\varepsilon}^{\text{nls}}[\gamma] \right) d\mu(\gamma).$$

Finally, we pass to the limit $C_{\text{Kin}} \to \infty$ and then the limit $\varepsilon \to 0$ to deduce

$$E^{\text{nls}} \geqslant \liminf_{N \to \infty} \frac{E(N)}{N} \geqslant \int_{\mathcal{S}} \mathcal{E}_m^{\text{nls}}[\gamma] d\mu(\gamma). \tag{3.31}$$

But as we saw above μ must be supported on pure states $\gamma = |u\rangle\langle u|$, which yields both the energy lower bound concluding the proof of (2.3) and the fact that μ must be supported on $\mathcal{M}^{\text{nls}}$. Because $\mathcal{E}_m^{\text{nls}}[\gamma]$ is a linear function of $\gamma^{\otimes 2}$ we can also combine (3.31) with (3.29) to deduce that also ν must be supported on $\mathcal{M}^{\text{nls}}$, which proves (2.6). $\qquad\square$

Appendix A. An information-theoretic quantum de Finetti theorem

Here we reproduce, for the convenience of the reader, the statement and proof of a Theorem of Brandão and Harrow. No claim of originality is thus made. See also the lecture notes [5] and [28], which contains results related to [6].

A.1. **A local de Finetti theorem.** In [6], Brandão and Harrow proved a quantitative quantum de Finetti theorem, where the quality of the approximation deteriorates only logarithmically with the dimension of the one-body state space, in contrast with previous results [10, 11, 16, 20, 24]. The trade-off is that the control is in a weaker norm than trace-class.

Recall that, for a complex separable Hilbert space $\mathfrak{H}$, the state space is

$$\mathcal{S}(\mathfrak{H}) := \left\{ \gamma \text{ positive trace-class operator on } \mathfrak{H}, \, \text{Tr}\, \gamma = 1 \right\}. \tag{A.1}$$

We shall need a notion of measurement of such states:

DEFINITION A.1 (Quantum measurements). — A quantum measurement Λ on a complex Hilbert space $\mathfrak{H}$ of dimension d is identified with a set $(M_k, e_k)_{k=1\ldots d}$ of bounded operators and vectors such that

- $M_k \geqslant 0$ for all k and $\sum_k M_k = \mathbb{1}$
- (e_k) is an orthonormal basis of $\mathfrak{H}$.

Its action on a state $\rho \in \mathcal{S}(\mathfrak{H})$ is given by

$$\Lambda(\rho) = \sum_k \text{Tr}[M_k \rho] |e_k\rangle\langle e_k|. \tag{A.2}$$

We shall denote $\mathcal{M}(\mathfrak{H})$ the set of quantum measurements on $\mathfrak{H}$.

The definition is usually generalized to a map from states of a Hilbert space $\mathfrak{H}_1$ to states of another Hilbert space $\mathfrak{H}_2$ by taking (e_k) to be an orthonormal basis of the latter.

Given two measurements Λ_1, Λ_2 on $\mathfrak{H}_1, \mathfrak{H}_2$ one can define $\Lambda_1 \otimes \Lambda_2$ on $\mathfrak{H}_1 \otimes \mathfrak{H}_2$ in the natural way: it is associated with the operators $M_{k,1} \otimes M_{k,2}$ and vectors $e_{k,1} \otimes e_{k,2}$. One can also define $\mathbb{1} \otimes \Lambda_2$ as a measurement on $\mathfrak{H}_1 \otimes \mathfrak{H}_2$ by setting

$$\mathbb{1} \otimes \Lambda_2 \Gamma = \sum_k \mathrm{Tr}_2[M_{k,2}\Gamma] \otimes |e_{k,2}\rangle\langle e_{k,2}|. \tag{A.3}$$

The statement we wish to discuss applies to more general states than the bosonic ones encountered in the context of mean-field limits:

DEFINITION A.2 (Symmetric N-body states). — Let $\mathfrak{H}$ be a complex separable Hilbert space. A symmetric N-particles state is a state Γ over $\mathfrak{H}^{\otimes N}$ commuting with label permutations:

$$\Gamma \in \mathcal{S}(\mathfrak{H}^{\otimes N}) \text{ such that } U_\sigma \Gamma = \Gamma U_\sigma$$

for all permutation σ, where U_σ is the unitary operator exchanging labels according to

$$U_\sigma u_1 \otimes \ldots \otimes u_N = u_{\sigma(1)} \otimes \ldots \otimes u_{\sigma(N)}.$$

A bosonic state satisfies the stronger condition

$$U_\sigma \Gamma = \Gamma U_\sigma = \Gamma$$

for all permutation σ, and can thus be restricted to act only on the symmetric subspace $\mathfrak{H}^{\otimes_{\mathrm{sym}} N}$, which is the point of view adopted in the main text. The reduced density matrices of a symmetric N-body state are defined as usual:

$$\mathrm{Tr}\left(B_k \Gamma^{(k)}\right) := \mathrm{Tr}\left(B_k \otimes \mathbb{1}^{\otimes(N-k)}\Gamma\right)$$

for any bounded operator B_k on $\mathfrak{H}^{\otimes k}$. Thus $\Gamma^{(k)}$ is a symmetric state on $\mathfrak{H}^{\otimes k}$.

The rest of the appendix is concerned with exposing the proof (due to [6, 28]) of the following statement:

THEOREM A.3 (Quantum de Finetti under local measurements). — *Let $\mathfrak{H}$ be a finite dimensional complex Hilbert space, with dimension d. Let Γ be a symmetric N-particles state on $\mathfrak{H}^{\otimes N}$. For every $0 \leqslant k \leqslant N$ there exists a probability measure μ_k on one-particle states such that*

$$\sup_{\Lambda_1,\ldots,\Lambda_k \in \mathcal{M}(\mathfrak{H})} \left\| \Lambda_1 \otimes \ldots \otimes \Lambda_k \left(\Gamma^{(k)} - \int \gamma^{\otimes k} d\mu_k(\gamma)\right) \right\|_{\mathfrak{S}^1(\mathfrak{H}^k)} \leqslant \sqrt{\frac{2(k-1)^2 \log d}{N-k+1}}. \tag{A.4}$$

The norm in the above is the trace-class norm $\left\|A\right\|_{\mathfrak{S}^1} := \mathrm{Tr}\,|A|$.

We start by explaining, in Section A.2, how the measure is constructed. Then we state a more "information-theoretic version" of Theorem A.3, and proceed to its proof in Section A.4. Standard tools from quantum information theory are interjected in Section A.3, that the familiarized may want to skip on first reading.

A.2. **Construction.** Denote $\mathcal{S}(\mathfrak{H})$ the space of states over a Hilbert space $\mathfrak{H}$, and $\mathcal{P}(\mathcal{S}(\mathfrak{H}))$ the set of probability measures on it. Theorem A.3 is implied by

$$\inf_{\mu \in \mathcal{P}(\mathcal{S}(\mathfrak{H}))} \sup_{\Lambda_1, \ldots, \Lambda_k \in \mathcal{M}(\mathfrak{H})} \left\| \Lambda_1 \otimes \ldots \otimes \Lambda_k \left(\Gamma^{(k)} - \int \gamma^{\otimes k} d\mu(\gamma) \right) \right\|_{\mathfrak{S}^1(\mathfrak{H}^k)}^2 \leqslant \frac{2k^2 \log d}{N - k}.$$
(A.5)

Let $\mathcal{E}$ be a quantum measurement over $\mathfrak{H}^{\otimes(N-k)}$ acting as

$$\mathcal{E}(\rho) = \sum_{\mu} \mathrm{Tr}[M_\mu \rho] |e_\mu\rangle\langle e_\mu|.$$

Defining, for each μ,

$$\Gamma_\mu := \frac{\mathrm{Tr}_{k+1 \to N} \left[M_\mu \Gamma \right] \otimes |e_\mu\rangle\langle e_\mu|}{p_\mu}, \quad p_\mu := \mathrm{Tr} \left[\mathbb{1}^{\otimes k} \otimes M_\mu \Gamma \right]$$

we have by simple computations the

LEMMA A.4 (Decomposition of the state Γ). — *Let Γ be a N-body state and $\mathcal{E}$ a measurement on $\mathfrak{H}^{\otimes(N-k)}$. For each μ, Γ_μ defined as above is a N-body state. Moreover,*

$$\sum_{\mu} p_\mu \Gamma_\mu = \mathbb{1}^{\otimes k} \otimes \mathcal{E}\, \Gamma$$

and

$$\sum_{\mu} p_\mu \Gamma_\mu^{(k)} = \Gamma^{(k)}.$$

In particular $p_\mu \geqslant 0$ and

$$\sum_{\mu} p_\mu = 1.$$

Notice that Γ being symmetric implies that

$$\Gamma_\mu^{(k)} := \frac{\mathrm{Tr}_{k+1 \to N} \left[M_\mu \Gamma \right]}{p_\mu}$$

also is. Now, the N-body state

$$\tilde{\Gamma}_{\mathcal{E}} := \sum_{\mu} p_\mu \left(\Gamma_\mu^{(1)} \right)^{\otimes N}$$
(A.6)

is certainly of the de Finetti form

$$\tilde{\Gamma}_{\mathcal{E}} = \int \gamma^{\otimes N} dP(\gamma)$$

with P a probability measure on one-body states. Thus

$$\inf_{\mu \in \mathcal{P}(\mathcal{S}(\mathfrak{H}))} \sup_{\Lambda_1, \ldots, \Lambda_k \in \mathcal{M}(\mathfrak{H})} \left\| \Lambda_1 \otimes \ldots \otimes \Lambda_k \left(\Gamma^{(k)} - \int \gamma^{\otimes k} d\mu(\gamma) \right) \right\|_{\mathfrak{S}^1(\mathfrak{H}^k)}^2$$

$$\leqslant \inf_{\mathcal{E} \in \mathcal{M}(\mathfrak{H}^{\otimes N-k})} \sup_{\Lambda_1, \ldots, \Lambda_k \in \mathcal{M}(\mathfrak{H})} \left\| \Lambda_1 \otimes \ldots \otimes \Lambda_k \left(\Gamma^{(k)} - \tilde{\Gamma}_{\mathcal{E}}^{(k)} \right) \right\|_{\mathfrak{S}^1(\mathfrak{H}^k)}^2. \quad \text{(A.7)}$$

This is the first main idea: the measure is constructed by minimizing over measurements as above. The second main idea is to make a detour from the trace-class norm to more information-based measures, such as quantum relative entropies. In

fact Theorem A.3 is implied by an estimate of the error using the von Neumann relative entropy

$$\mathcal{H}(\Gamma, \Gamma') := \mathrm{Tr}\left[\Gamma\left(\log\Gamma - \log\Gamma'\right)\right]. \tag{A.8}$$

THEOREM A.5 (Quantum de Finetti, information-theoretic version). — *Put*

$$\mathbf{L}_k = \Lambda_1 \otimes \ldots \otimes \Lambda_k.$$

We then have

$$\inf_{\mathcal{E}\in\mathcal{M}(\mathfrak{H}^{\otimes(N-k)})} \sup_{\Lambda_1,\ldots,\Lambda_k\in\mathcal{M}(\mathfrak{H})} \sum_\mu p_\mu \mathcal{H}\left(\mathbf{L}_k\Gamma_\mu^{(k)}, \mathbf{L}_k\left(\Gamma_\mu^{(1)}\right)^{\otimes k}\right) \leqslant \frac{(k-1)^2\log d}{N-k+1}. \tag{A.9}$$

In the next subsection we provide more background and tools bearing on the multipartite mutual information of a state (i.e. on the left-hand side of (A.9)). Then we give the proof of Theorem A.5 and conclude that of Theorem A.3 in Section A.4.

A.3. **Quantum information-theoretic tools.** In the sequel,

$$S(\Gamma) = -\mathrm{Tr}\left[\Gamma\log\Gamma\right]$$

and $\mathcal{H}$ as in (A.8) stand for the usual von Neumann entropy and relative entropy. A state over a k-fold tensor product will be denoted $\Gamma^{1\ldots k}$ and for $l \leqslant k$, the reduced states $\Gamma^{1\ldots l}$ over l-fold tensor products are defined as reduced density matrices, taking partial traces.

We start with the simple

LEMMA A.6 (Partial measurements). — *For a three partite state Γ^{123} and a measurement over the third system Λ_3*

$$\left(\mathbb{1}\otimes\mathbb{1}\otimes\Lambda_3\Gamma^{123}\right)^{12} = \Gamma^{12}.$$

Proof. — This is immediately seen from the definition (A.3) □

DEFINITION A.7 (Mutual informations). — *For a quantum state $\Gamma = \Gamma^{1\ldots k}$ over a tensor product $\mathfrak{H}_1\otimes\ldots\otimes\mathfrak{H}_k$, define the bi-partite mutual informations ($l \leqslant k$)*

$$I(\mathfrak{H}_1,\ldots,\mathfrak{H}_l : \mathfrak{H}_{l+1},\ldots,\mathfrak{H}_k)_\Gamma = \mathcal{H}\left(\Gamma^{1\ldots k}, \Gamma^{1\ldots l}\otimes\Gamma^{l+1\ldots k}\right)$$
$$= S\left(\Gamma^{1\ldots l}\right) + S\left(\Gamma^{l+1\ldots k}\right) - S\left(\Gamma^{1\ldots k}\right)$$

and the multipartite mutual information

$$I(\mathfrak{H}_1 : \ldots : \mathfrak{H}_k)_\Gamma = \mathcal{H}\left(\Gamma^{1\ldots k}, \Gamma^1\otimes\ldots\otimes\Gamma^k\right)$$
$$= S\left(\Gamma^1\right) + \ldots + S\left(\Gamma^k\right) - S\left(\Gamma^{1\ldots k}\right).$$

Remark A.8 (Mutual informations). — One can of course define mutual informations over any kind of partition. It follows from their definitions as relative entropies that these are positive quantities. The second equality in each definition comes from the fact that

$$\log(\Gamma^1\otimes\Gamma^2) = \log\left(\Gamma^1\otimes\mathbb{1}\right) + \log\left(\mathbb{1}\otimes\Gamma^2\right)$$

that one uses to prove that the von Neumann entropy is subadditive (which is the same as the bipartite mutual information being positive).   ◇

Mutual informations are positive, as we just saw, but they cannot be too big:

LEMMA A.9 (Bound on bi-partite mutual information). — *Let Γ^{12} be a bipartite state over $\mathfrak{H}_1 \otimes \mathfrak{H}_2$, for two finite-dimensional Hilbert spaces of dimensions d_1 and d_2 respectively. Then*

$$I(\mathfrak{H}_1 : \mathfrak{H}_2)_{\Gamma^{12}} \leqslant 2 \min\left(\log d_1, \log d_2\right).$$

Proof. — Recall the Araki-Lieb inequality (proved by purification, Schmidt decomposition of pure states and subadditivity of entropy [29])

$$S(\Gamma^{12}) \geqslant \left| S(\Gamma^1) - S(\Gamma^2) \right|.$$

Inserting this in the (second) definition given above we have

$$I(\mathfrak{H}_1 : \mathfrak{H}_2)_{\Gamma^{12}} = S(\Gamma^1) + S(\Gamma^2) - S(\Gamma^{12}) \leqslant 2 \min\left(S(\Gamma^1), S(\Gamma^2)\right)$$

and the result follows, for the maximal entropy of a state in dimension d is $\log d$.   □

We also have the useful

LEMMA A.10 (Mutual informations, bipartite to multipartite). — *With the notation of the above definition*

$$I(\mathfrak{H}_1 : \ldots : \mathfrak{H}_k)_{\Gamma^{1\ldots k}} = \sum_{j=2}^{k} I(\mathfrak{H}_1, \ldots, \mathfrak{H}_{j-1} : \mathfrak{H}_j)_{\Gamma^{1\ldots j}}. \qquad (A.10)$$

Proof. — The definitions easily yield

$$I(\mathfrak{H}_1 : \ldots : \mathfrak{H}_k)_{\Gamma^{1\ldots k}} = I(\mathfrak{H}_1, \ldots \mathfrak{H}_{k-1} : \mathfrak{H}_k)_{\Gamma^{1\ldots k}} + I(\mathfrak{H}_1 : \ldots : \mathfrak{H}_{k-1})_{\Gamma^{1\ldots k-1}}$$

and it suffices to iterate this relation.   □

Next we need the

DEFINITION A.11 (Conditional mutual information). — For a quantum state $\Gamma = \Gamma^{123}$ over a three-fold tensor product $\mathfrak{H}_1 \otimes \mathfrak{H}_2 \otimes \mathfrak{H}_3$, define the *conditional mutual information*

$$I(\mathfrak{H}_1 : \mathfrak{H}_2 | \mathfrak{H}_3)_\Gamma = I(\mathfrak{H}_1 : \mathfrak{H}_2, \mathfrak{H}_3)_{\Gamma^{123}} - I(\mathfrak{H}_1 : \mathfrak{H}_3)_{\Gamma^{13}}$$
$$= \mathcal{H}(\Gamma^{123}, \Gamma^1 \otimes \Gamma^{23}) - \mathcal{H}(\Gamma^{13}, \Gamma^1 \otimes \Gamma^3).$$

For a state over a N-fold tensor product we henceforth denote, for $k \leqslant j < N$,

$$I(\mathfrak{H}_1, \ldots, \mathfrak{H}_{k-1} : \mathfrak{H}_j | \mathfrak{H}_{j+1}, \ldots, \mathfrak{H}_N)_{\Gamma^{1\ldots k-1 j \ldots N}}$$
$$:= I(\mathfrak{H}_1 \otimes \ldots \otimes \mathfrak{H}_{k-1} : \mathfrak{H}_j | \mathfrak{H}_{j+1} \otimes \ldots \otimes \mathfrak{H}_N)_{\Gamma^{1\ldots k-1 j \ldots N}}.$$

Remark A.12 (Conditional mutual information). — It turns out that also the conditional mutual information is positive. This is not quite trivial and in fact follows from strong subadditivity of quantum entropy [30, 31].   ◇

A first lemma bearing on the conditional mutual information is

LEMMA A.13 (Conditional mutual information of partly measured states). —
Let Γ^{123} be a tri-partite state of the form

$$\Gamma^{123} = \sum_j p_j \Gamma_j^{12} \otimes |e_j\rangle\langle e_j|$$

*for positive numbers p_j summing to 1, bi-partite states Γ_j^{12} and an orthonormal
basis (e_j). Then*

$$I(\mathfrak{H}_1 : \mathfrak{H}_2 | \mathfrak{H}_3)_\Gamma = \sum_j p_j I(\mathfrak{H}^1 : \mathfrak{H}^2)_{\Gamma_j^{12}}. \qquad (A.11)$$

Proof. — Diagonalize Γ_j^{12} and then Schmidt-decompose its eigenvectors. This
gives

$$\Gamma^{123} = \sum_{j,k,l,m} p_j q_{j,k} \sqrt{r_{j,k,l}} \sqrt{r_{j,k,m}} |a_{j,k,l}\rangle\langle a_{j,k,m}| \otimes |b_{j,k,l}\rangle\langle b_{j,k,m}| \otimes |e_j\rangle\langle e_j|.$$

with orthonormal basis $(a_{j,k,l})_l$ and $(b_{j,k,l})_l$ and positive numbers satisfying

$$\sum_k q_{j,k} = 1, \quad \sum_l r_{j,k,l} = 1.$$

Inserting this in the definitions

$$I(\mathfrak{H}_1 : \mathfrak{H}_2 | \mathfrak{H}_3)_\Gamma = -S(\Gamma^{123}) + S(\Gamma^{23}) - S(\Gamma^3) + S(\Gamma^{13})$$

$$\sum_j p_j I(\mathfrak{H}^1 : \mathfrak{H}^2)_{\Gamma_j^{12}} = \sum_j p_j \Big(S(\Gamma_j^1) + S(\Gamma_j^2) - S(\Gamma_j^{12}) \Big),$$

the proof is a straightforward calculation.   □

The previous lemma morally justifies an extension of Definition A.11:

DEFINITION A.14 (Multi-partite conditional mutual information). — Consider
a $k + 1$-particle state $\Gamma^{1...k+1}$ of the form

$$\Gamma^{1...k+1} = \sum_j p_j \Gamma_j^{1...k} \otimes |e_j\rangle\langle e_j|$$

for positive numbers p_j summing to 1, k-partite states $\Gamma_j^{1...k}$ and an orthonormal
basis (e_j). By definition

$$I(\mathfrak{H}_1 : \ldots : \mathfrak{H}_k | \mathfrak{H}_{k+1})_{\Gamma^{1...k+1}} = \sum_j p_j I(\mathfrak{H}_1 : \ldots : \mathfrak{H}_k)_{\Gamma_j^{1...k}}.$$

Next we state a crucial link between bipartite mutual informations and condi-
tional mutual informations.

LEMMA A.15 (Chain rule for mutual informations). — *Let $\Gamma = \Gamma^{1...N}$ be a
N-partite state.*

$$I(\mathfrak{H}_1, \ldots, \mathfrak{H}_{k-1} : \mathfrak{H}_k, \ldots, \mathfrak{H}_N)_\Gamma = \sum_{j=k}^N I(\mathfrak{H}_1, \ldots, \mathfrak{H}_{k-1} : \mathfrak{H}_j | \mathfrak{H}_{j+1}, \ldots, \mathfrak{H}_N)_{\Gamma^{1...k-1j...N}}$$

$$(A.12)$$

with the conditional mutual information on the right-hand side as in Definition A.11.

Proof. — Call $M = N-k+1$, $A = \mathfrak{H}_1 \otimes \ldots \otimes \mathfrak{H}_{k-1}$, $B_j = \mathfrak{H}_{k+j-1}$. A reformulation is then

$$I(A : B_1, \ldots, B_M) = \sum_{j=1}^{M} I(A : B_j | B_{j+1} \otimes \ldots \otimes B_M).$$

The left-hand side is equal to

$$\text{LHS} = S(\Gamma^A) + S(\Gamma^{B_1 \ldots B_M}) - S(\Gamma^{AB_1 \ldots B_M}).$$

But the $M-$th term of the left-hand side is just a mutual information with no conditioning

$$\text{RHS}_M = S(\Gamma^A) + S(\Gamma^{B_M}) - S(\Gamma^{AB_M}).$$

The other terms of the right-hand side are, for $k < M$,

$$\text{RHS}_k = \mathcal{H}(\Gamma^{AB_k \ldots B_M}, \Gamma^A \otimes \Gamma^{B_k \ldots B_M}) - \mathcal{H}(\Gamma^{AB_{k+1} \ldots B_M}, \Gamma^A \otimes \Gamma^{B_{k+1} \ldots B_M})$$
$$= S(\Gamma^{B_k \ldots B_M}) - S(\Gamma^{AB_k \ldots B_M}) - (S\Gamma^{B_{k+1} \ldots B_M}) - S(\Gamma^{AB_{k+1} \ldots B_M})$$

and the result clearly follows. $\square$

A.4. **Proof of the main estimate.** This is the proof of [6], expanded so as to become more accessible.

Proof of Theorem A.5. — From now on we occasionally label the copies of the one-body Hilbert space, for we will sometimes deal with states that are not fully symmetric. We denote $\mathbf{L}_k = \Lambda_1 \otimes \ldots \otimes \Lambda_k$ a measurement as in the statement. We also let $\mathcal{E}$ be a measurement on $\mathfrak{H}^{\otimes(N-k)}$ and the associated (Γ_μ)'s be defined as in Lemma A.4.

Step 1. We split multipartite informations into bipartite ones using Lemma A.10:

$$I(\mathfrak{H} : \ldots : \mathfrak{H})_{\mathbf{L}_k \Gamma_\mu^{(k)}} = \sum_{j=2}^{k} I(\mathfrak{H}_1, \ldots, \mathfrak{H}_{j-1} : \mathfrak{H}_j)_{\mathbf{L}_j \Gamma_\mu^{(j)}}.$$

Then, by monotony of the relative entropy we know [44] that the mutual information decreases under local measurements, for they are trace-preserving completely positive[5] maps. Thus

$$I(\mathfrak{H} : \ldots : \mathfrak{H})_{\mathbf{L}_k \Gamma_\mu^{(k)}} \leqslant \sum_{j=2}^{k} I(\mathfrak{H}_1, \ldots, \mathfrak{H}_{j-1} : \mathfrak{H}_j)_{\Lambda_j \Gamma_\mu^{(j)}}$$

where we abuse notation by denoting

$$\Lambda_j \Gamma_\mu^{(j)} = \mathbb{1} \otimes \cdots \otimes \Lambda_j \otimes \ldots \otimes \mathbb{1} \, \Gamma_\mu^{(j)}.$$

Next, using symmetry and monotony of the relative entropy under partial traces

$$I(\mathfrak{H} : \ldots : \mathfrak{H})_{\mathbf{L}_k \Gamma_\mu^{(k)}} \leqslant (k-1) I(\mathfrak{H}_1, \ldots, \mathfrak{H}_{k-1} : \mathfrak{H}_k)_{\Lambda_k \Gamma_\mu^{(k)}}.$$

Multiplying by p_μ, summing over μ and using Lemma A.13 this yields

$$\sum_\mu p_\mu I(\mathfrak{H} : \ldots : \mathfrak{H})_{\mathbf{L}_k \Gamma_\mu^{(k)}} \leqslant (k-1) I(\mathfrak{H}_1, \ldots, \mathfrak{H}_{k-1} : \mathfrak{H}_k | \mathfrak{H}_{k+1}, \ldots, \mathfrak{H}_N)_{\Lambda_k \otimes \mathcal{E} \, \Gamma}$$

$$(\text{A.13})$$

with the conditional mutual information as in Definition A.11.

---

[5]Positive suffices actually [40].

Step 2. We claim that

$$(N - k + 1) \min_{\mathcal{E}} \max_{\Lambda_k} I(\mathfrak{H}_1, \ldots, \mathfrak{H}_{k-1} : \mathfrak{H}_k | \mathfrak{H}_{k+1}, \ldots, \mathfrak{H}_N)_{\Lambda_k \otimes \mathcal{E} \, \Gamma}$$

$$\leqslant \max_{\Lambda_k, \ldots, \Lambda_N} I(\mathfrak{H}_1, \ldots, \mathfrak{H}_{k-1} : \mathfrak{H}_k, \ldots, \mathfrak{H}_N)_{\nu} \quad (A.14)$$

where

$$\nu = \mathbb{1}^{\otimes k-1} \otimes \Lambda_k \otimes \Lambda_{k+1} \otimes \ldots \otimes \Lambda_N(\Gamma).$$

This is achieved by a particular choice of the measurements $\Lambda_{k+1}, \ldots, \Lambda_N$ (in particular, the minimum over all measurements on $N - k$ systems is bounded above using tensorized measurements). We start from the right-hand side of (A.14) and use the chain rule, Lemma A.15:

$$I(\mathfrak{H}_1, \ldots, \mathfrak{H}_{k-1} : \mathfrak{H}_k, \ldots, \mathfrak{H}_N)_{\nu} = \sum_{j=k}^{N} I(\mathfrak{H}_1, \ldots, \mathfrak{H}_{k-1} : \mathfrak{H}_j | \mathfrak{H}_{j+1} \ldots, \mathfrak{H}_N)_{\nu_j} \quad (A.15)$$

where in the right-hand side

$$\nu_j = \nu^{1 \ldots k-1 j \ldots N}.$$

Observe that, as per Lemma A.6, the j-th term in the right-hand side of (A.15) does not depend on the measurements $\Lambda_k, \ldots, \Lambda_{j-1}$. We then choose Λ_N to maximize the N-th term, Λ_{N-1} to maximize the $N - 1$-th term given Λ_N, etc ..., Λ_j to maximize the j-th term given the previous choices of $\Lambda_N, \ldots, \Lambda_{j+1}$, and continue this way iteratively. Then we certainly have, for each term,

$$I(\mathfrak{H}_1, \ldots, \mathfrak{H}_{k-1} : \mathfrak{H}_j | \mathfrak{H}_{j+1} \ldots, \mathfrak{H}_N)_{\nu_j}$$

$$\geqslant \min_{\Lambda_{j+1}, \ldots, \Lambda_N} \max_{\Lambda_j} I(\mathfrak{H}_1, \ldots, \mathfrak{H}_{k-1} : \mathfrak{H}_j | \mathfrak{H}_{j+1} \ldots, \mathfrak{H}_N)_{\nu_j}$$

and using Lemma A.6 again we also have

$$I(\mathfrak{H}_1, \ldots, \mathfrak{H}_{k-1} : \mathfrak{H}_j | \mathfrak{H}_{j+1} \ldots, \mathfrak{H}_N)_{\nu_j}$$

$$\geqslant \min_{\Lambda_k, \ldots, \Lambda_{j-1}, \Lambda_{j+1}, \ldots, \Lambda_N} \max_{\Lambda_j} I(\mathfrak{H}_1, \ldots, \mathfrak{H}_{k-1} : \mathfrak{H}_j | \mathfrak{H}_k \ldots \mathfrak{H}_{j-1} \mathfrak{H}_{j+1} \ldots, \mathfrak{H}_N)_{\nu}.$$

By symmetry of Γ then

$$I(\mathfrak{H}_1, \ldots, \mathfrak{H}_{k-1} : \mathfrak{H}_j | \mathfrak{H}_{j+1} \ldots, \mathfrak{H}_N)_{\nu_j}$$

$$\geqslant \min_{\Lambda_{k+1}, \ldots, \Lambda_N} \max_{\Lambda_k} I(\mathfrak{H}_1, \ldots, \mathfrak{H}_{k-1} : \mathfrak{H}_k | \mathfrak{H}_{k+1} \ldots, \mathfrak{H}_N)_{\nu}$$

and since this corresponds to choosing a particular class of measurement $\mathcal{E}$

$$I(\mathfrak{H}_1, \ldots, \mathfrak{H}_{k-1} : \mathfrak{H}_j | \mathfrak{H}_{j+1} \ldots, \mathfrak{H}_N)_{\nu_j}$$

$$\geqslant \min_{\mathcal{E}} \max_{\Lambda_k} I(\mathfrak{H}_1, \ldots, \mathfrak{H}_{k-1} : \mathfrak{H}_k | \mathfrak{H}_{k+1} \ldots, \mathfrak{H}_N)_{\Lambda_k \otimes \mathcal{E} \, \Gamma}.$$

Thus, for the particular choice of measurements we made,

$$(N - k + 1) \min_{\mathcal{E}} \max_{\Lambda_k} I(\mathfrak{H}_1, \ldots, \mathfrak{H}_{k-1} : \mathfrak{H}_k | \mathfrak{H}_{k+1}, \ldots, \mathfrak{H}_N)_{\Lambda_k \otimes \mathcal{E} \, \Gamma}$$

$$\leqslant \sum_{j=k}^{N} I(\mathfrak{H}_1, \ldots, \mathfrak{H}_{k-1} : \mathfrak{H}_j | \mathfrak{H}_{j+1} \ldots, \mathfrak{H}_N)_{\nu_j}$$

and Claim (A.14) is proved upon using (A.15).

Conclusion. Lemma A.9 yields

$$\max_{\Lambda_k,\ldots\Lambda_N} I(\mathfrak{H}_1,\ldots,\mathfrak{H}_{k-1}:\mathfrak{H}_k,\ldots,\mathfrak{H}_N)_\nu \leqslant 2\log\dim(\mathfrak{H}^{\otimes k-1}) = 2(k-1)\log d.$$

Insert this in (A.14), use (A.13) and the result is proved. $\qquad\square$

Finally, we explain how Theorem A.3 follows from Theorem A.5:

Proof. — Denote

$$\mathbf{L}_k = \Lambda_1 \otimes \ldots \otimes \Lambda_k$$

for brevity. Using Lemma A.4, convexity and then Pinsker's inequality (see [7] or [17, Section 5.4])

$$\begin{aligned}
\left\|\mathbf{L}_k\left(\Gamma^{(k)} - \tilde{\Gamma}^{(k)}\right)\right\|_{\mathfrak{S}^1(\mathfrak{H}^k)}^2 &= \left\|\sum_\mu p_\mu \mathbf{L}_k\left(\Gamma_\mu^{(k)} - \left(\Gamma_\mu^{(1)}\right)^{\otimes k}\right)\right\|_{\mathfrak{S}^1(\mathfrak{H}^k)}^2 \\
&\leqslant \sum_\mu p_\mu \left\|\mathbf{L}_k\left(\Gamma_\mu^{(k)} - \left(\Gamma_\mu^{(1)}\right)^{\otimes k}\right)\right\|_{\mathfrak{S}^1(\mathfrak{H}^k)}^2 \\
&\leqslant 2\sum_\mu p_\mu \mathcal{H}\left(\mathbf{L}_k\Gamma_\mu^{(k)}, \mathbf{L}_k\left(\Gamma_\mu^{(1)}\right)^{\otimes k}\right) \qquad \text{(A.16)}
\end{aligned}$$

The last term in (A.16) is nothing but the multipartite mutual information refered to in Theorem A.5, and thus the proof is complete. $\qquad\square$

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