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CLASSICAL FIELD THEORY LIMIT OF 2D MANY-BODY QUANTUM GIBBS STATES

MATHIEU LEWIN, PHAN THÀNH NAM, AND NICOLAS ROUGERIE

ABSTRACT. We prove that the grand-canonical Gibbs states of a large 2D bosonic system converges to the Gibbs measure of an interacting classical field theory, in a mean-field-type limit. Reduced density matrices of the quantum Gibbs state converge to their classical analogues, given by a nonlinear Schrödinger-Gibbs measure supported on distributions with low regularity. Tuning the chemical potential of the grand-canonical ensemble provides a counter-term for the diverging repulsive interactions, analogue to the Wick ordering of the limit classical theory.

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1. INTRODUCTION

The mean-field (and related) limit(s) of large bosonic systems is a research topic almost as old as quantum mechanics itself. It has been spectacularly rejuvenated by the birth of cold atoms physics in the 1990's, most notably by the landmark experimental observation of Bose-Einstein condensates in alkali gases [35, 72]. On the mathematical side this gave a new impetus to the general enterprise of rigorously deriving, from first principles (the many-body Schrödinger Hamiltonian), the effective models used for the discussion and interpretation of experimental data.

Following pioneer contributions [65, 49, 50, 125, 43, 12, 94, 103, 106, 131], the last two decades have seen a great deal of progress on the derivation of effective non-linear Schrödinger (NLS) type models:

- for the ground state of interacting Bose gases, see [78, 91, 109, 112] for reviews;
- for the time-evolution of such ground states after an initial perturbation, see [11, 53, 114] for reviews.

Refinements of the mean-field non-linear Schrödinger description have also been derived, i.e. the so-called Bogoliubov approximation [133], which can be seen as a second quantization of the Hessian of the NLS energy functional. Recent results bear both on the low-lying eigenfunctions of the many-body Hamiltonian [117, 56, 88, 99, 40, 17, 18] and on the time-evolution thereof after an initial perturbation [57, 58, 87, 98, 97, 95, 19, 26].

All of this work is of relevance mainly for very low temperature states of the Bose gas, well below the Bose-Einstein critical temperature. Rigorous mathematical works including the effect of temperature seem much scarcer in the literature, a few references being [14, 115, 116, 118, 132, 41]. In particular, the rigorous derivation of the Bose-Einstein phase transition in interacting Bose gases still seems way out of reach, except for the trapped case in the Gross-Pitaevskii limit [41] and for special lattice models [91, Chapter 11].

Recently, a study of the positive temperature case has been initiated [83, 80, 85, 47, 48, 111], whose main feature is the derivation, from positive temperature equilibria (Gibbs states) of the many-body Bose gas, of nonlinear Gibbs measures based on the mean-field NLS energy functional. This works in a certain mean-field limit where a transition from

quantum to classical fields occurs. On the physics side we note that such approaches have been successful around the BEC phase transition, to obtain the leading order corrections due to interaction effects [6, 9, 10, 67, 71].

So far, the mean-field/semi-classical limit we mentioned has been fully controlled only in one spatial dimension. The purpose of the present contribution is to give the first solution for the 2D problem (we announced some of our main results in the note [86]). This involves a very significant jump in difficulty, both from a conceptual and technical point of view, as we now briefly explain (see also the introduction to [47]). We suggest readers unfamiliar with the vocabulary below to jump back and forth between this discussion and the main definitions, given in Section 2.

The general goal is to connect quantum objects (positive self-adjoint operators with unit trace on a Hilbert space) to classical ones (probability measures on a function space). In [47, 48] this is accomplished by comparing term by term perturbative expansions of both objects, and controlling the remainders. Here we shall continue in the direction of [83, 85], using the so-called de Finetti measure (or Wigner measure, depending on the point of view) [2, 109, 112], a very general tool to associate classical states to essentially generic many-particles bosonic quantum states. The main difficulty consists in controlling the error made when introducing the de Finetti measure.

The classical measure we aim at deriving is of the form

$$(\text{exponential of } (- \text{interaction})) \times \text{Gaussian measure.}$$

The reference measure, according to which typical classical fields are drawn at random, is a Gaussian measure with a covariance containing the inverse of the Laplacian. An important fact is that, in spatial dimensions larger than one, this Gaussian measure is supported on distributions rather than functions. The mean-field interaction being a nonlinear object involving products, it is ill-defined on the support of the reference Gaussian measure. This is a well-know issue in several fields of research, including:

- *Constructive quantum field theory* (CQFT, see [39, 52, 119, 127] for reviews). Here the divergence of the interaction energy reflects small-scale/high-momentum/high-energy physics not taken into account in the models constructed. It is in this field that the techniques appropriate to the rigorous definition of the nonlinear Gibbs measure (Euclidean field theory in this context) have been first invented.
- *Probabilistic Cauchy theory for nonlinear dispersive equations*. It is tempting to expect that the nonlinear Gibbs measure is invariant under the appropriate NLS flow (and in particular that one can make sense of the latter on the support of the measure). A rigorous proof of this (and extensions to other nonlinear dispersive PDEs) has motivated a lot of works [77, 21, 22, 27, 28, 29, 101]. In particular, this approach allows to prove global well-posedness at regularity levels out of reach of deterministic methods.
- *Stochastic nonlinear partial differential equations*. The Gibbs measure is the long-time asymptote of the nonlinear heat equation driven by space-time white noise (see [37, 36, 62, 76, 96, 108, 129] and references therein). The lack of regularity of typical fields drawn from the measure is related to that of the noise, which is inherited by solutions to the equation and makes the interpretation of nonlinear terms problematic.

In the above fields, the solution to the measure's indefiniteness is well-known: **renormalization**. One subtracts infinite counter-terms to the interaction energy to actually

construct a measure of the form

$$(\text{exponential of } (- \text{ interaction } + \text{ counter-terms })) \times \text{Gaussian measure.} \quad (1.1)$$

More precisely, one starts from a measure with a ultra-violet/high-frequency cut-off, and the counter-terms diverge when the latter is removed, so as to compensate the divergence of the interaction.

This ‘compensating infinities’ scenario is what we need to understand, but for a quantum problem, with non-commutative fields. The divergences of the classical theory indeed have quantum analogues that are very difficult to control in the mean-field approximation. The difficulties we face are (almost) purely of a quantum nature, for the estimates we shall derive are rather easy in the classical theory, when fields commute.

The quantum problem we start from is the grand-canonical ensemble of the interacting Bose gas. In this paper we study the case where the gas is essentially trapped to a unit volume. Infinities occur when the temperature T tends to infinity, which makes the average density diverge. The counter-term allowing to control the limit is provided by tuning the chemical potential of the theory, thus penalizing too large particle numbers. Note that, by scaling, it is possible to reformulate this large- T limit in a fixed box to the more conventional thermodynamic limit where the size of the box is sent to infinity and T stays fixed.

In this paper, we first deal with the homogeneous case (an interacting Bose gas on the unit torus). The reference Gaussian measure appearing in (1.1) is then nothing but that obtained in the non-interacting case, with an appropriately chosen chemical potential. This is the renormalization we alluded to: tuning the (divergent) chemical potential appropriately in the quantum problem gives in the limit the classical measure with any prescribed chemical potential. This is however very specific to the translation-invariant case.

Then we turn to the more complicated case of a gas trapped by an external potential, or to a finite domain with any chosen boundary conditions. The absence of translation-invariance requires to compensate infinities by introducing x -dependent counter-terms. In this case, the reference Gaussian measure to be used in (1.1) *cannot* be a non-interacting Gaussian and finding it is already a nontrivial task. The procedure is to first identify the optimal quantum state in a special subclass of Gaussian-type states called *quasi-free states*. This optimal quasi-free state solves a nonlinear equation. Passing to the mean-field limit provides a corresponding classical Gaussian measure, whose covariance also solves a nonlinear equation, that was first considered in [47]. It is this Gaussian measure which must be used in (1.1) to construct the limiting interacting classical measure. We will indeed prove that the total free energy of the quantum system behaves as

$$\begin{aligned} \text{quantum free energy} &= \text{quantum free energy of reference quasi-free state} \\ &\quad + \lambda^{-1} \times \text{classical free energy} + o(\lambda^{-1}) \end{aligned}$$

where $\lambda = 1/T \rightarrow 0$ is the parameter used to place the system in a mean-field regime, and where the quasi-free quantum energy diverges much faster than λ^{-1} .

Our control of the quantum renormalization procedure is based on the rationale that on high momenta, the interacting and quasi-free Gibbs states almost coincide: particles going too fast are hardly affected by interactions. The main difficulty we face is to put this intuition in a rigorous form allowing to get the machinery started. In brief, we approach this problem as follows.

We first use a classical argument and express the two-body interaction as a sum of squares of one-body terms. Then we observe that, after subtracting the counter-term, the expectation of the two-body interaction can be seen as a sum of **variances** of one-body terms. We control each such term separately by a fluctuation-dissipation-type argument, inspired by linear response theory¹. More precisely we relate the variance (fluctuation) of a one-body observable \mathbb{A} to its **linear response** (dissipation), calculated by perturbing the Gibbs state's Hamiltonian by $-\varepsilon\mathbb{A}$ for a small parameter ε , measuring the expectation of \mathbb{A} in the new Gibbs state and differentiating the result with respect to ε . For a classical Gibbs state the relation between variance and linear response is an identity. The main semi-classical insight of our proof is that such an identity almost holds in the mean-field limit.

What this method (referred to as a variance estimate² in the sequel) accomplishes is to reduce estimates of two-body terms (variances) to estimates of one-body terms (linear responses). Now that the detailed structure of correlations has thus been by-passed, an estimate of one-body density matrices will be enough to achieve the desired control. This we obtain via a Feynman-Hellmann-type argument (perturbing the one-body Hamiltonian) whose upshot is a new inequality of possible independent interest. It relates the difference between one-body density matrices of the free and interacting states, to the relative entropy³ of the states themselves. The latter is easily controlled by independent, variational, arguments for it is related to the difference in free energies.

This is as much as we can say of the control of high momentum divergences without entering the details. For the low-momentum part of our problem, we use our previous technique [81, 82, 83, 85] based on the *de Finetti measure* to relate quantum and classical free-energies/partition functions. Our proof being variational (Gibbs states minimize the free-energy functional), we then deduce convergence of the states themselves (or rather, their reduced density matrices) by controls on various relative entropies, byproducts of our free-energy bounds.

The paper is organized as follows. In the next section we properly define the quantum and classical models and we give some hints on the relation between the two. Then, in Section 3 we state all our results. Section 4 contains a detailed explanation of the strategy of proof, which is then carried over in the rest of the paper, starting from Section 6. Section 5 contains some known properties of classical measures, useful for the proof.

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¹There is no time-dependence in our problem, the static part of the response is meant throughout.

²Other types of correlation estimates have been used in the literature previously [7, 55, 115].

³This has a flavor of Pinsker's inequality, but it is important for us that we handle directly the difference between density matrices, not the difference between the states themselves.

2. SETTING AND DEFINITIONS

We recap here all the standard and less-standard notions needed to state and discuss our main results. Perhaps the acquainted reader will want to jump directly to Section 3, and come back to this one if some notation is unclear later.

2.1. Fock space formalism. Our basic one-body Hilbert space is

$$\mathfrak{H} = L^2(\Omega) \quad (2.1)$$

with Ω an open domain in \mathbb{R}^2 . The reader might think of the two model cases, when Ω is either the 2D unit cube (to which we add periodic boundary conditions, which is then the same as taking $\Omega = \mathbb{T}^2$, the torus) or the full plane \mathbb{R}^2 .

For the many-body problem we work grand-canonically, i.e. with fluctuating particle number. The many-body Hilbert space is thus the *bosonic Fock space*

$$\mathfrak{F} = \mathbb{C} \oplus \mathfrak{H} \oplus \dots \oplus \mathfrak{H}^{\otimes_s n} \oplus \dots \quad (2.2)$$

The symbol $\otimes_s n$ stands for the n -fold symmetric tensor product, as appropriate for the n -body configuration space of bosons. Operators acting on finitely many particles are lifted to the Fock space in the usual way:

Definition 2.1 (Second quantization).

Let A_k be a self-adjoint operator on $\mathfrak{H}^{\otimes_s k}$. We define its action on the Fock space as

$$\mathbb{A}_k := 0 \oplus \dots \oplus \bigoplus_{n=k}^{\infty} \left(\sum_{1 \leq i_1 < \dots < i_k \leq n} (A_k)_{i_1, \dots, i_k} \right) \quad (2.3)$$

where $(A_k)_{i_1, \dots, i_k}$ denotes the operator A_k acting on the variables labeled i_1, \dots, i_k in $\mathfrak{H}^{\otimes_s n}$. \diamond

When $k = 1$, it is customary to use the notation

$$d\Gamma(A) := \mathbb{A} = 0 \oplus \bigoplus_{n=1}^{\infty} \left(\sum_{1 \leq i \leq n} A_i \right) \quad (2.4)$$

for one-body operators, a tradition that we will also follow throughout. For example, the *particle number operator* is

$$\mathcal{N} = d\Gamma(\mathbb{1}_{\mathfrak{H}}) = \bigoplus_{n=0}^{\infty} n.$$

Next, quantum states are as usual:

Definition 2.2 (Quantum states and reduced density matrices).

A pure state is an orthogonal projection $|\Psi\rangle\langle\Psi|$ on some normalized vector Ψ of the Fock space \mathfrak{F} . A mixed state Γ is a convex superposition of pure states, i.e. a positive trace-class operator on \mathfrak{F} with unit trace. We denote

$$\mathcal{S}(\mathfrak{F}) := \{\Gamma \text{ self-adjoint operator on } \mathfrak{F}, \Gamma \geq 0, \text{Tr}_{\mathfrak{F}}[\Gamma] = 1\} \quad (2.5)$$

the set of all mixed states.

The reduced k -body density matrix $\Gamma^{(k)}$ of a state Γ is the operator on $\mathfrak{H}^{\otimes_s k}$ defined by setting

$$\mathrm{Tr}_{\mathfrak{H}^{\otimes_s k}} [A_k \Gamma^{(k)}] := \mathrm{Tr}_{\mathfrak{H}} [\mathbb{A}_k \Gamma] \quad (2.6)$$

for any self-adjoint operator A_k on $\mathfrak{H}^{\otimes_s k}$, with \mathbb{A}_k the second-quantization (2.3) of A_k . \diamond

If Γ is of the diagonal form

$$\Gamma = \Gamma_0 \oplus \Gamma_1 \oplus \dots \oplus \Gamma_n \oplus \dots$$

then the reduced density matrices are equivalently given via partial traces as

$$\Gamma^{(k)} = \sum_{n \geq k} \binom{n}{k} \mathrm{Tr}_{k+1 \rightarrow n} [\Gamma_n].$$

Also recall that the expected particle number of a state is given as

$$\mathrm{Tr}_{\mathfrak{H}} [\mathcal{N} \Gamma] = \mathrm{Tr}_{\mathfrak{H}} [\Gamma^{(1)}].$$

We shall use standard bosonic creation/annihilation operator:

Definition 2.3 (Creation/annihilation operators).

Let $f \in \mathfrak{H}$. The associated annihilation operator acts on the Fock space as specified by

$$a(f) u_1 \otimes_s \dots \otimes_s u_n = n^{-1/2} \sum_{j=1}^n \langle f | u_j \rangle u_1 \otimes_s \dots \otimes_s u_{j-1} \otimes_s u_{j+1} \otimes_s \dots \otimes_s u_n$$

and then extended by linearity. Its formal adjoint, the creation operator $a^\dagger(f)$ acts as

$$a^\dagger(f) u_1 \otimes_s \dots \otimes_s u_n = (n+1)^{1/2} f \otimes_s u_1 \otimes_s \dots \otimes_s u_n.$$

The canonical commutation relations (CCR) hold: for all $f, g \in \mathfrak{H}$

$$[a(f), a(g)] = [a^\dagger(f), a^\dagger(g)] = 0, \quad [a(f), a^\dagger(g)] = \langle f, g \rangle. \quad (2.7)$$

\diamond

The reduced density matrices of a state Γ can alternatively be defined by the relations

$$\left\langle g_1 \otimes_s \dots \otimes_s g_k, \Gamma^{(k)} f_1 \otimes_s \dots \otimes_s f_k \right\rangle = \mathrm{Tr} \left[a^\dagger(f_1) \dots a^\dagger(f_k) a(g_1) \dots a(g_k) \Gamma \right]. \quad (2.8)$$

2.2. Quantum model. The many-body Hamiltonians we shall study are of the form

$$\boxed{\mathbb{H}_\lambda = d\Gamma(h) + \lambda \mathbb{W} - \nu \mathcal{N} + E_0.} \quad (2.9)$$

Here $h > 0$ is an operator on \mathfrak{H} with compact resolvent. The reader might think of the case when

$$h = -\Delta + \mathrm{const}$$

on \mathbb{T}^2 or

$$h = -\Delta + V$$

for some confining potential V on \mathbb{R}^2 . The interaction term \mathbb{W} is the second quantization of the multiplication operator by $w(x - y)$ on the two-body space $\mathfrak{H}^{\otimes_s 2}$:

$$\mathbb{W} := 0 \oplus 0 \oplus \bigoplus_{n=2}^{\infty} \left(\sum_{1 \leq i < j \leq n} w(x_i - x_j) \right). \quad (2.10)$$

The coupling constant $\lambda > 0$ models the interaction strength and the chemical potential ν will be tuned to serve as a counter-term. The constant E_0 is just an energy shift, which we use in order that the renormalized interaction

$$\boxed{\lambda \mathbb{W}^{\text{ren}} = \lambda \mathbb{W} - \nu \mathcal{N} + E_0} \quad (2.11)$$

stays positive.

The quantum *Gibbs state* associated with the above Hamiltonian is the minimizer of the free-energy functional (energy minus temperature times entropy)

$$\mathcal{F}_{\lambda, T}[\Gamma] = \text{Tr} [\mathbb{H}_\lambda \Gamma] + T \text{Tr} [\Gamma \log \Gamma] \quad (2.12)$$

over all quantum states Γ on the Fock space. Explicitly

$$\boxed{\Gamma_\lambda = \frac{1}{\mathcal{Z}_\lambda} \exp \left(-\frac{1}{T} \mathbb{H}_\lambda \right)} \quad (2.13)$$

where the *partition function* \mathcal{Z}_λ normalizes the state,

$$\mathcal{Z}_\lambda = \text{Tr} \left[\exp \left(-\frac{1}{T} \mathbb{H}_\lambda \right) \right],$$

and satisfies

$$\boxed{F_\lambda := \min_{\Gamma \in \mathcal{S}(\mathfrak{F})} \mathcal{F}_{\lambda, T}[\Gamma] = -T \log \mathcal{Z}_\lambda.} \quad (2.14)$$

In the sequel we work in the limit $T \rightarrow \infty$ with λ, ν, E_0 appropriately tuned. It turns out that the appropriate scaling has λ proportional to T^{-1} and $\nu \rightarrow \infty$ faster than T . Note that the energy shift E_0 does not modify the Gibbs state.

2.3. Classical model. Let us briefly recap the definitions related to the nonlinear Gibbs measure. More details are in Section 5.1.

We shall denote by μ_0 the Gaussian measure with covariance h^{-1} . To be precise, from the spectral decomposition of the one-body operator

$$h = \sum_{j=1}^{\infty} \lambda_j |u_j\rangle \langle u_j| \quad (2.15)$$

we introduce the scale of Sobolev-like spaces

$$\mathfrak{H}^s = \left\{ u = \sum_{j=1}^{\infty} \alpha_j u_j, \quad \sum_{j=1}^{\infty} |\alpha_j|^2 \lambda_j^{s/2} < \infty \right\}.$$

The Gaussian probability measure is

$$d\mu_0(u) := \bigotimes_{i=1}^{\infty} \left(\frac{\lambda_i}{\pi} e^{-\lambda_i |\alpha_i|^2} d\alpha_i \right) \quad (2.16)$$

with $\alpha_i = \langle u_i, u \rangle$ and $d\alpha = d\Re(\alpha) d\Im(\alpha)$ the Lebesgue measure on $\mathbb{C} \simeq \mathbb{R}^2$. The formula (2.16) must be interpreted in the sense that the cylindrical projection of μ_0 onto the finite-dimensional space

$$V_K = \text{Span}\{u_1, \dots, u_K\}$$

is given by

$$d\mu_{0,K}(\alpha_1, \dots, \alpha_K) := \prod_{i=1}^K \left(\frac{\lambda_i}{\pi} e^{-\lambda_i |\alpha_i|^2} d\alpha_i \right) \quad (2.17)$$

for every $K \geq 1$. Assuming that for some $p > 0$

$$\text{Tr}[h^{-p}] < \infty, \quad (2.18)$$

the limit measure μ_0 is supported on \mathfrak{H}^{1-p} [83, Section 3.1]. In the cases of interest to this paper we have $p > 1$ and thus μ_0 is supported on negative Sobolev spaces, whence the need for renormalization in the definition of the interacting measure.

Let P_K be the orthogonal projector on V_K . Consider the interaction energy with local mass renormalization

$$\mathcal{D}_K[u] = \frac{1}{2} \iint_{\Omega \times \Omega} \left(|P_K u(x)|^2 - \langle |P_K u(x)|^2 \rangle_{\mu_0} \right) w(x-y) \left(|P_K u(y)|^2 - \langle |P_K u(y)|^2 \rangle_{\mu_0} \right) dx dy. \quad (2.19)$$

Here, for any $f \in L^1(d\mu_0)$,

$$\langle f(u) \rangle_{\mu_0} := \int f(u) d\mu_0(u) \quad (2.20)$$

denotes the expectation in the measure μ_0 . We shall assume that

$$w(x) = \int_{\Omega^*} \widehat{w}(k) e^{ik \cdot x} dk \quad (2.21)$$

where the Fourier transform \widehat{w} satisfies

$$0 \leq \widehat{w}(k) \in L^1(\Omega^*). \quad (2.22)$$

Here by convention $\Omega^* = \mathbb{R}^2$, except if $\Omega = \mathbb{T}^2$ then $\Omega^* = (2\pi\mathbb{Z})^2$ (and the integral in (2.21) becomes a sum). Then, as recalled in Lemma 5.3 below, when $\widehat{w} \geq 0$ the sequence $\mathcal{D}_K[u]$ converges to a limit $\mathcal{D}[u]$ in $L^1(d\mu_0)$, hence we may define the renormalized interacting probability measure by

$$\boxed{d\mu(u) := \frac{1}{z} \exp(-\mathcal{D}[u]) d\mu_0(u)} \quad (2.23)$$

with $0 < z < \infty$ a normalization constant (to make μ a probability measure).

Note that the reduced one-body density matrix

$$\gamma_\mu^{(1)} := \int |u\rangle \langle u| d\mu(u) \quad (2.24)$$

is a priori an operator from \mathfrak{H}^{p-1} to \mathfrak{H}^{1-p} (since $|u\rangle \langle u|$ is not any better, μ -almost surely). However, averaging with respect to μ has a regularizing effect, so that $\gamma_\mu^{(1)}$ turns out to be a compact operator from \mathfrak{H} to \mathfrak{H} . In fact, one can show that

$$\gamma_\mu^{(1)} = h^{-1}. \quad (2.25)$$

Similarly, the reduced k -body density matrix

$$\gamma_\mu^{(k)} := \int |u^{\otimes k}\rangle \langle u^{\otimes k}| d\mu(u) = k! P_s^k (h^{-1})^{\otimes k} P_s^k \quad (2.26)$$

belongs to the p -th Schatten class $\mathfrak{S}^p(\mathfrak{H}^{\otimes_s k})$, see [83, Lemma 3.3]. In the right-hand side of (2.26), P_s^k denotes the orthogonal projector on the symmetric subspace.

2.4. Formal quantum/classical correspondence. Our aim is to relate the quantum Gibbs state (2.13) to the classical Gibbs measure (2.23).

If we ignore the renormalizing terms for the moment (in particular, think of $\nu = E_0 = 0$), the formal correspondence between the two objects can be seen as follows. First, the Gibbs measure can be interpreted as a rigorous version of the formal

$$d\mu(u) = z^{-1} e^{-\mathcal{E}_H[u]} du \quad (2.27)$$

with $\mathcal{E}_H[u]$ the nonlinear Hartree energy functional

$$\mathcal{E}_H[u] = \int_\Omega \overline{u(x)} (hu)(x) dx + \frac{1}{2} \iint_{\Omega \times \Omega} |u(x)|^2 w(x-y) |u(y)|^2 dx dy.$$

Define the quantum fields (operator-valued distributions) $a^\dagger(x), a(x)$, creating/annihilating a particle at position x by the formulae

$$a(f) = \int a(x) f(x) dx, \quad a^\dagger(f) = \int a^\dagger(x) f(x) dx \quad (2.28)$$

for all $f \in \mathfrak{H}$. Inherited from (2.7) we have the canonical commutation relations

$$[a(x), a(y)] = [a^\dagger(x), a^\dagger(y)] = 0, \quad [a(x), a^\dagger(y)] = \delta_{x=y}. \quad (2.29)$$

These operator-valued distributions allow to rewrite the many-body Hamiltonian as

$$\frac{\mathbb{H}_\lambda}{T} = \frac{1}{T} \int_\Omega a^\dagger(x) h_x a(x) dx + \frac{\lambda}{2T} \iint_{\Omega \times \Omega} a^\dagger(x) a^\dagger(y) w(x-y) a(x) a(y) dx dy. \quad (2.30)$$

The formal manipulation relating (2.13) and (2.27) is then to replace the quantum fields $a^\dagger(x), a(x)$ by classical fields, i.e. operators by functions. This involves in particular that the commutation relations (2.29) become trivial in some limit, all fields commuting at any position. How this can come about is further explained in [83, Section 5.2] and the introduction to [47] (in these works the link between the classical and quantum problems has been made rigorous in 1D). Basically, the order of magnitude of commutators stays fixed by definition, but the typical value of the fields $a(x)$ and $a^\dagger(x)$ is of order \sqrt{T} when computing expectations against the quantum Gibbs state. This suggests to introduce new fields $b(x) = a(x)/\sqrt{T}$ and $b^\dagger(x) = a^\dagger(x)/\sqrt{T}$ and to choose

$$\boxed{\lambda \sim \frac{1}{T}}.$$

This is now a clean semi-classical limit, since the commutators of the new fields is of order $1/T \rightarrow 0$.

Let us discuss now the inclusion of counter-terms. It is useful to write the mean-field interaction, using Fourier variables,

$$\iint_{\Omega \times \Omega} |u(x)|^2 w(x-y) |u(y)|^2 dx dy = \int \widehat{w}(k) \left| \widehat{|u|^2}(k) \right|^2 dk = \int \widehat{w}(k) \left| \int |u(x)|^2 e^{ik \cdot x} dx \right|^2 dk. \tag{2.31}$$

On the other hand, the quantum interaction can be expressed as

$$\mathbb{W} = \frac{1}{2} \int \widehat{w}(k) \left| d\Gamma(e^{ik \cdot x}) \right|^2 dk - \frac{w(0)}{2} \mathcal{N} \tag{2.32}$$

where the second term is typically of lower order and may be ignored. Thus, one formally obtains the quantum interaction by replacing

$$\int |u(x)|^2 f(x) dx \rightsquigarrow d\Gamma(f)$$

with $f(x) = e^{ik \cdot x}$, identified with the corresponding multiplication operator on \mathfrak{H} .

To see how to include the renormalization, observe that (2.19) formally leads to

$$\mathcal{D}[u] = \frac{1}{2} \int \widehat{w}(k) \left| \widehat{|u|^2}(k) - \left\langle \widehat{|u|^2}(k) \right\rangle_{\mu_0} \right|^2 dk.$$

Thus the appropriate renormalized quantum interaction should be

$$\mathbb{W}^{\text{ren}} = \frac{1}{2} \int \widehat{w}(k) \left| d\Gamma(e^{ik \cdot x}) - \left\langle d\Gamma(e^{ik \cdot x}) \right\rangle_{\Gamma_0} \right|^2 dk. \tag{2.33}$$

After expanding the square, this suggests a natural choice for the chemical potential ν and the energy shift E_0 , as we will see. Making the above formal quantum/classical correspondence rigorous is the goal of our paper.

Note that here we use Fourier variables mostly for convenience. What they help accomplish is rewriting interactions (two-body terms) as sums of products of one-body terms. Other methods to accomplish this, such as Fefferman-de la Llave type decompositions [45, 61] could replace the Fourier transform.

2.5. Rigorous results. The nonlinear, classical, Gibbs state is a natural candidate for an invariant measure under the NLS flow

$$i\partial_t u = -\Delta u + Vu + (w * |u|^2) u, \tag{2.34}$$

or rather, under a suitable renormalization thereof. This idea has been made rigorous in [29, 20, 21, 22, 23, 24, 28, 77, 101, 128, 130]. In particular, in [21, 22, 101], cases where renormalizations related to that we use are dealt with.

On the other hand, it is known in rather large generality [11, 53, 114] that the NLS flow is the mean-field limit of the many-body Schrödinger flow defined by Hamiltonians akin to those defined in Section 2.2. But the quantum Gibbs state is obviously invariant under the many-body Schrödinger flow. Putting these observations together begs for a rigorous proof that the nonlinear Gibbs measure is in some sense the mean-field limit of the many-body Gibbs state.

This has been accomplished in 1D in [83, 85], and in [47] by a different method. The time-dependent problem in 1D is investigated in [48], yielding in particular an alternative

proof of the measure's invariance under the NLS flow. The 2D and 3D cases are approached in [47], but the Gibbs state defined above is replaced by the modified

$$\Gamma_\lambda^\eta = \frac{1}{\mathcal{Z}_\lambda^\eta} \exp\left(-\frac{\eta}{2T} d\Gamma(h)\right) \exp\left(-\frac{1-\eta}{T} d\Gamma(h) - \frac{\lambda}{T} \mathbb{W}^{\text{ren}}\right) \exp\left(-\frac{\eta}{2T} d\Gamma(h)\right) \quad (2.35)$$

where $0 < \eta < 1$ is a parameter held fixed in the mean-field limit. If operators would commute, the above would coincide with the true Gibbs state. The modification brought by η is a significant gain of commutativity used to control some particularly delicate remainder terms in a perturbative expansion. Note that the modification does not affect the limiting measure, since all classical objects commute.

In our approach, some commutativity will be gained using the new correlation estimates of Section 7. This allows us to treat the proper Gibbs state, instead of the modified one in (2.35). However, we may control the limit only in 2D so far.

In the next section we present our main results in the following order:

- *Homogeneous case.* We consider the emblematic case where $\Omega = \mathbb{T}^2$ and $h = -\Delta + \text{const.}$ Modulo an appropriate choice of parameters ν, E_0 , the many-body interaction in (2.11) can be made to coincide with (2.33), and we prove a rigorous connection between the classical renormalized and quantum problems. We announced this part in [86].
- *Inhomogeneous case.* We consider here the case

$$h = -\Delta + V(x)$$

where $V(x) \rightarrow +\infty$ when $|x| \rightarrow \infty$. The reference Gaussian measure to be found in the limit and the non-interacting Gaussian measure are in general mutually singular, for every chemical potential. The correct reference Gaussian measure solves a nonlinear equation. First we reinterpret the results of [47] on this Gaussian measure, in light of the quasi-free approximation at the quantum level. Then we state our main result on the mean-field limit, using the optimal quasi-free quantum energy as a reference.

- *Inhomogeneous case, inverse statement.* It is also possible to start with a one-particle Hamiltonian h and modify the interaction as in (2.33). We then do not have to solve any nonlinear equation and in the limit we end up with the interacting measure based on the Gaussian measure associated with h . This we call an *inverse statement* because we have to modify the initial quantum model such as to find the desired measure in the limit. This is less natural from a physical point of view. Nevertheless, it turns out that the previous *direct statement* where one starts with h and identifies what the limiting measure is, follows from our proof of the inverse statement and the results of [47] on the nonlinear equation. So the inverse statement is indeed our main result and its proof occupies most of the article. We are able to prove an abstract statement which covers a very large class of one-particle Hamiltonians, including $h = -\Delta + V(x)$ in \mathbb{R}^2 for a potential V growing sufficiently fast at infinity, and $h = -\Delta + \text{const}$ on a bounded domain.

3. MAIN RESULTS

3.1. Homogeneous gas. Let us consider the case where

$$\boxed{\Omega = \mathbb{T}^2, \quad h = -\Delta + \kappa}$$

with $-\Delta$ the usual Laplace-Beltrami operator on the torus and $\kappa > 0$ a constant.

Let

$$\Gamma_0 = \mathcal{Z}_0^{-1} e^{-d\Gamma(h)/T}, \quad \mathcal{Z}_0 = \text{Tr} \left(e^{-d\Gamma(h)/T} \right)$$

be the non-interacting quantum Gibbs state, namely the state as in (2.13) with $\lambda = \nu = E_0 = 0$. Its expected particle number is

$$N_0(T) := \text{Tr}_{\mathfrak{F}} [\mathcal{N}\Gamma_0] = \langle \mathcal{N} \rangle_{\Gamma_0} = \sum_{k \in (2\pi\mathbb{Z})^2} \frac{1}{e^{\frac{|k|^2 + \kappa}{T}} - 1}.$$

This is proportional to $T \log T$ as $T \rightarrow \infty$, for fixed positive chemical potential κ , see below.

Let

$$\Gamma_\lambda = \mathcal{Z}_\lambda^{-1} e^{-\mathbb{H}_\lambda/T}, \quad \mathcal{Z}_\lambda = \text{Tr} \left(e^{-\mathbb{H}_\lambda/T} \right)$$

be the interacting Gibbs state with coupling constant $\lambda \sim T^{-1}$ and the choice of chemical potential and energy reference as

$$\nu = \lambda \widehat{w}(0) N_0(T) - \lambda \frac{w(0)}{2}, \quad E_0 := \lambda \frac{\widehat{w}(0)}{2} N_0(T)^2. \quad (3.1)$$

This choice makes the physical Hamiltonian \mathbb{H}_λ in (2.9) coincide with $d\Gamma(h) + \lambda \mathbb{W}^{\text{ren}}$ with \mathbb{W}^{ren} being of the desired form in (2.33), namely

$$\begin{aligned} \mathbb{H}_\lambda &= d\Gamma(h) + \lambda \mathbb{W} - \nu \mathcal{N} + E_0 \\ &= d\Gamma(h) + \underbrace{\frac{\lambda}{2} \sum_{k \in (2\pi\mathbb{Z})^2} \widehat{w}(k) \left| d\Gamma(e^{ik \cdot x}) - \langle d\Gamma(e^{ik \cdot x}) \rangle_{\Gamma_0} \right|^2}_{=: \lambda \mathbb{W}^{\text{ren}}}. \end{aligned} \quad (3.2)$$

This follows from the fact that, by translation invariance,

$$\langle d\Gamma(e^{ik \cdot x}) \rangle_{\Gamma_0} = \delta_{k=0} N_0(T),$$

Here $\langle \cdot \rangle_{\Gamma_0}$ denotes expectation against the free Gibbs state Γ_0 .

We will require that the interaction potential decays a bit more than stated in (2.22). To be precise, we assume that

$$\begin{cases} \widehat{w}(k) \geq 0 \text{ for all } k \in 2\pi\mathbb{Z}^2, \\ \sum_{k \in (2\pi\mathbb{Z})^2} \widehat{w}(k) (1 + |k|^\alpha) < \infty \text{ for some } \alpha > 0, \end{cases} \quad (3.3)$$

with the Fourier expansion

$$w(x) = \sum_{k \in (2\pi\mathbb{Z})^2} \widehat{w}(k) e^{ik \cdot x}.$$

Our first result is

Theorem 3.1 (Homogeneous gas).

Let $h = -\Delta + \kappa$ on the torus \mathbb{T}^2 with a constant $\kappa > 0$. Let $w : \mathbb{T}^2 \rightarrow \mathbb{R}$ be an even function satisfying (3.3). Let μ_0 be the Gaussian measure with covariance h^{-1} and let μ be the associated interacting Gibbs measure as in (2.23). We have, in the limit $T \rightarrow +\infty$, $\lambda T \rightarrow 1$,

$$\frac{F_\lambda - F_0}{T} \longrightarrow -\log z = -\log \left(\int e^{-\mathcal{D}[u]} d\mu_0(u) \right), \quad (3.4)$$

with F_λ the free-energy in (2.14) for the Hamiltonian \mathbb{H}_λ as in (3.2), and z the classical relative partition function in (2.23).

Moreover, the reduced density matrices of the quantum Gibbs state Γ_λ of \mathbb{H}_λ satisfy

$$\mathrm{Tr} \left| \frac{k!}{T^k} \Gamma_\lambda^{(k)} - \int |u^{\otimes k}\rangle \langle u^{\otimes k}| d\mu(u) \right|^p \rightarrow 0 \quad (3.5)$$

for every $k \geq 1$ and $p > 1$. For $k = 1$ we have the more precise convergence in trace-class

$$\mathrm{Tr} \left| \frac{1}{T} \left(\Gamma_\lambda^{(1)} - \Gamma_0^{(1)} \right) - \int |u\rangle \langle u| \left(d\mu(u) - d\mu_0(u) \right) \right| \rightarrow 0. \quad (3.6)$$

Here are some immediate comments on the homogeneous gas.

1. In this case, we have $\mathrm{Tr}(h^{-p})$ for all $p > 1$, and μ_0 is supported on all negative Sobolev spaces $\bigcap_{t < 0} \mathfrak{H}^t$ (but not on $\mathfrak{H} = L^2(\mathbb{T}^2)$). This already leads to a big jump in difficulty in comparison to our previous treatment in 1D [83, 85].

2. The main part of the chemical potential ν in (3.1) is a counter-term compensating the divergence of the interactions. Physically, the theorem means that classical field theory becomes exact for chemical potentials in the vicinity of $\lambda \widehat{w}(0) N_0(T)$, if λ is appropriately tuned. The term $\lambda w(0)/2$ is not important and can be removed in the definition of ν without changing our results. The constant E_0 has no effect on the Gibbs state itself.

3. Since $N_0(T)$ itself depends on κ , the relationship between the total physical chemical potential

$$\tilde{\nu} = \nu - \kappa \sim \lambda \widehat{w}(0) N_0(T) - \kappa$$

and its renormalization κ is still somewhat implicit. It is in fact desirable to deduce κ from $\tilde{\nu}$ rather than the other way around. In that regard, observe that for large T and fixed κ

$$N_0(T) = T \log T - T \log \kappa + TK_0 + o(T) \quad (3.7)$$

with

$$K_0 = \log(e-1) + \int_1^\infty \frac{1}{e^x - 1} dx + 1.$$

It follows that, if the physical chemical potential is chosen as

$$\tilde{\nu} = \widehat{w}(0) \log T - \nu_0 \quad (3.8)$$

with ν_0 fixed, then the limit classical field theory is based on the Gaussian measure with variance $(-\Delta + \kappa)^{-1}$ with κ solving the nonlinear equation

$$\kappa + \widehat{w}(0) \log \kappa = \nu_0 + \widehat{w}(0) K_0. \quad (3.9)$$

This defines κ implicitly but uniquely, for the function on the left-hand side is increasing on \mathbb{R}^+ . We shall see below that the correspondence between the quantum and classical parameters is much more involved in the inhomogeneous case.

4. Our proof also shows that, for every $k \geq 2$, the difference $T^{-k}(\Gamma_\lambda^{(k)} - \Gamma_0^{(k)})$ is *not* bounded in trace class, see Remark 10.4. When $k \geq 2$ there is in fact no simple replacement for (3.6) where one would remove from $\Gamma_\lambda^{(k)}$ combinations of $\Gamma_0^{(\ell)}$ for $\ell \leq k$ to obtain an operator converging in trace-class.

5. The corresponding theorem should be true on the 3D torus, but this remains an open problem. In this case the particle number of the free Gibbs state diverges as

$$\frac{N_0(T)}{T} \sim T^{1/2}$$

and our proof cannot handle such a strong divergence. In fact, one of our key tools is the variance estimate in Theorem 7.1, which requires that the one-body operator satisfies $\text{Tr}[h^{-p}] < \infty$ for some $p < 3/2$. The latter condition just barely fails for $h = -\Delta + \kappa$ in \mathbb{T}^3 .

6. In the physics literature, classical field theories [134] are used as effective descriptions at criticality, i.e. around the Bose-Einstein [6, 9, 10, 67, 71] or Berezinskii-Kosterlitz-Thouless [16, 51, 68, 69, 105, 104, 123] transition, to obtain the leading order corrections due to interaction effects. These works argue that the critical densities are related as

$$\rho_\lambda^{\text{quant}}(T) - \rho_0^{\text{quant}}(T) \sim \rho_\lambda^{\text{clas}}(T) - \rho_0^{\text{clas}}(T).$$

Note that it is only the *difference* in critical densities (interacting minus non interacting) that one can obtain using classical field theory. This is related to our result (3.6). The latter implies the convergence of the relative number of particles

$$\frac{\langle \mathcal{N} \rangle_{\Gamma_\lambda} - \langle \mathcal{N} \rangle_{\Gamma_0}}{T} \rightarrow \int \mathcal{M}(u) d\mu(u),$$

with $\mathcal{M}(u)$ the renormalized mass defined in Lemma 5.2. This is rather non-trivial, for the two terms on the left-hand side diverge when taken separately. We note that estimates on relative one-particle density matrices related to (3.6) are recently obtained in [41], in a different setting however.

7. In our setting, the Bose gas occupies a volume of order 1 and the Gibbs measure emerges in the large temperature limit. It is possible to reformulate our setting in the more conventional thermodynamic limit where the system is in the large torus $L\mathbb{T}^d \subset \mathbb{R}^d$ with $L \rightarrow \infty$. By scaling we see that a Bose gas with temperature T' , total chemical potential ν' and interaction w' in the large box corresponds in our setting to choosing

$$T = L^2 T', \quad \nu - \kappa = \tilde{\nu} = L^2 \nu', \quad w(x) = L^4 T' w'(Lx) \tag{3.10}$$

if we take $\lambda = 1/T$ as before. In the non-interacting case where $\nu = \lambda = 0$ (hence the chemical potential equals $-\kappa$) and T' stay fixed, we obtain $\nu' = -\kappa/L^2 \rightarrow 0^-$, that is, we are approaching the critical density of the Bose gas *from below*,

$$\rho_0(L) = \frac{\text{Tr}[\mathcal{N}\Gamma_0]}{L^d} = \frac{1}{L^d} \sum_{k \in 2\pi\mathbb{Z}^d} \frac{1}{e^{\frac{k^2 + \kappa}{L^2 T'}} - 1} \rightarrow \rho_c(T') = \begin{cases} +\infty & \text{in } d = 1, 2 \\ (T')^{d/2} \int_{\mathbb{R}^3} \frac{1}{e^{|2\pi k|^2} - 1} dk & \text{in } d = 3, \end{cases} \tag{3.11}$$

simultaneously with $L \rightarrow \infty$. For the usual thermodynamic limit, this is the regime in which the quantum problem converges to the effective classical Gaussian measure with covariance $(-\Delta + \kappa)^{-1}$, in any dimension. One can equivalently fix the density and take the temperature to its critical value *from above*.

In the interacting case the situation is more involved. In 2D, we obtain from (3.8) that the chemical potential in the box of size L must behave as

$$\nu'(L) = \hat{w}(0) \frac{\log(L^2 T')}{L^2} - \frac{\nu_0}{L^2}$$

hence still converges to 0, but more slowly. The constant ν_0 determines the final value of κ through the nonlinear equation (3.9). The result therefore allows to quantify the effect of the interactions at the transition to the Bose-Einstein condensate (i.e. at large densities), in the coupled limit $L \rightarrow \infty$ with $\nu' \rightarrow 0$. The system is described by the classical Gibbs measure, with a renormalized chemical potential κ . In 3D we expect similar results, with however $\log(L^2 T')$ replaced by $L\sqrt{T'}$ and $\rho(L)$ converging to the (non-interacting) finite critical density $\rho_c(T')$.

Note that the rescaled interaction potential in (3.10),

$$w'(x) = \frac{w(x/L)}{L^A T'}$$

with a fixed potential w , is very long range such as to correlate particles over the whole box $L\mathbb{T}^d$, but it has a very small intensity. More physical interactions are much bigger and have a much shorter range (they should be described by a dilute, rather than mean-field, limit), but this case is still out of reach of our methods.

3.2. Inhomogeneous gas: the reference quasi-free state. Here we focus on the case

$$\boxed{\Omega = \mathbb{R}^2, \quad h = -\Delta + V(x)}$$

where $V(x) \rightarrow +\infty$ when $|x| \rightarrow \infty$. We are typically thinking of $V(x) = |x|^s + 1$.

If we take as reference state $\Gamma_0 = (\mathcal{Z}_0)^{-1} \exp(-d\Gamma(h/T))$ and start with a renormalized Hamiltonian in the same form as (3.2), then we perturb the original physical Hamiltonian by an x -dependent counter term. This is physically questionable since it does not correspond to adjusting the two constants ν and E_0 . This means that Γ_0 is not the right reference state to study the limit of \mathbb{H}_λ .

Let V_T be a general one-body potential (which will be specified later and can depend on T). Let $\tilde{\Gamma}_0$ be the free Gibbs state associated with $-\Delta + V_T(x)$, namely

$$\tilde{\Gamma}_0 := \frac{1}{\tilde{\mathcal{Z}}_0} \exp\left(\frac{d\Gamma(-\Delta + V_T)}{T}\right), \quad (3.12)$$

and let $\varrho_0^{V_T}(x)$ be its one-body density defined by

$$\varrho_0^{V_T}(x) := \tilde{\Gamma}_0^{(1)}(x; x) = \left[\frac{1}{e^{\frac{-\Delta + V_T}{T}} - 1} \right] (x; x). \quad (3.13)$$

where $\tilde{\Gamma}_0^{(1)}(x; y)$ is the integral kernel of the one-body density matrix $\tilde{\Gamma}_0^{(1)}$ (the diagonal part $\tilde{\Gamma}_0^{(1)}(x; x)$ can be defined properly for instance by the spectral decomposition). Note that in general $\varrho_0^{V_T}(x)$ depends on x (except of course in the periodic case studied previously).

Following the discussion in Section 2.4, we consider the renormalized Hamiltonian as in (2.33), but with the reference state $\tilde{\Gamma}_0$. This results in

$$\begin{aligned} \mathbb{H}_\lambda &= d\Gamma(-\Delta + V_T) + \frac{\lambda}{2} \int_{\mathbb{R}^2} \hat{w}(k) \left| d\Gamma(e^{ik \cdot x}) - \left\langle d\Gamma(e^{ik \cdot x}) \right\rangle_{\tilde{\Gamma}_0} \right|^2 dk \\ &= d\Gamma\left(-\Delta + V_T - \lambda w * \varrho_0^{V_T} - \lambda w(0)/2\right) + \lambda \mathbb{W} + E_T \end{aligned} \quad (3.14)$$

where E_T is given by

$$E_T := \frac{\lambda}{2} \iint_{\mathbb{R}^2 \times \mathbb{R}^2} \varrho_0^{V_T}(x) w(x-y) \varrho_0^{V_T}(y) dx dy. \quad (3.15)$$

This Hamiltonian coincides with the physical Hamiltonian in (2.9) with chemical potential ν and energy reference $E_0 = E_T$ if V_T solves the nonlinear equation (*counter-term problem*)

$$\boxed{V_T - \lambda w * \varrho_0^{V_T} = V - \nu.} \quad (3.16)$$

This is an equation of the same spirit as (3.9) seen before for κ , but where the unknown is now a function. It turns out that the equation (3.16) arises naturally when restricting the problem to a special class of Gaussian-type quantum states, also called quasi-free states. This is what we discuss next.

We recall that to any one-body density matrix $\gamma \geq 0$ one can associate a unique state Γ_γ on the Fock space, called a quasi-free state, which is entirely characterized by γ via Wick's theorem [8, 124]. Then its energy terms and entropy can be expressed as

$$\begin{aligned} -\operatorname{Tr} [\Gamma_\gamma \log \Gamma_\gamma] &= \operatorname{Tr} [(1 + \gamma) \log(1 + \gamma) - \gamma \log \gamma], \\ \operatorname{Tr} [d\Gamma (-\Delta + V - \nu) \Gamma_\gamma] &= \operatorname{Tr} [(-\Delta + V - \nu) \gamma], \\ \operatorname{Tr} [\mathbb{W}\Gamma_\gamma] &= \frac{1}{2} \iint \gamma(x; x) w(x-y) \gamma(y; y) dx dy \\ &\quad + \frac{1}{2} \iint w(x-y) |\gamma(x; y)|^2 dx dy. \end{aligned} \quad (3.17)$$

If we are interested in equilibrium states minimizing the free energy, in the quasi-free class this leads to the following variational problem

$$F_\lambda^H = \inf_{\gamma = \gamma^* \geq 0} \mathcal{F}^H[\gamma] \quad (3.18)$$

where

$$\begin{aligned} \mathcal{F}^H[\gamma] &:= \operatorname{Tr} [(-\Delta + V - \nu) \gamma] + \frac{\lambda}{2} \iint \gamma(x; x) w(x-y) \gamma(y; y) dx dy \\ &\quad + \frac{\lambda}{2} \iint w(x-y) |\gamma(x; y)|^2 dx dy - T \operatorname{Tr} [(1 + \gamma) \log(1 + \gamma) - \gamma \log \gamma] \end{aligned}$$

is called the *Hartree free energy*. When $\hat{w} \geq 0$, the functional $\mathcal{F}^H[\gamma]$ turns out to be strictly convex. Hence, with the confining potential V it admits a unique minimizer γ^H , that defines a unique corresponding quasi-free state in Fock space Γ^H (see Lemma 3.2 below for a related result). The optimal density matrix solves the nonlinear equation

$$\gamma^H = \left\{ \exp \left(\frac{-\Delta + V - \nu + \lambda \rho^H * w + \lambda X^H}{T} \right) - 1 \right\}^{-1}$$

where $\rho^H(x) = \gamma^H(x; x)$ is the density and X^H is the exchange operator with integral kernel $X^H(x; y) = w(x-y) \gamma^H(x; y)$.

In the limit $T \rightarrow \infty$ with $\lambda T \rightarrow 1$, the quasi-free state Γ^H is rather badly behaved. Its density ρ^H diverges very fast. However, it turns out that, although $\rho^H(x)$ depends on x , its

growth as $T \rightarrow \infty$ is more or less uniform in x and can be captured by

$$\rho^{\text{H}}(x) \sim \varrho_0^\kappa = \left[\frac{1}{e^{\frac{-\Delta+\kappa}{T}} - 1} \right] (x; x), \quad (3.19)$$

provided that

$$\nu = \lambda \widehat{w}(0) \varrho_0^\kappa - \kappa.$$

Recall from the homogeneous case studied in the previous section that ϱ_0^κ diverges like $T \log T$ but it does not depend on x by translation invariance of $-\Delta + \kappa$. On the other hand, λX^{H} typically stays bounded, for instance in the Hilbert-Schmidt norm.

This suggests to simplify things a little bit by removing the exchange term from the beginning, that is, to consider the simplified minimization problem

$$F_\lambda^{\text{rH}} = \inf_{\gamma=\gamma^* \geq 0} \mathcal{F}^{\text{rH}}[\gamma] \quad (3.20)$$

where

$$\begin{aligned} \mathcal{F}^{\text{rH}}[\gamma] := \text{Tr} [(-\Delta + V - \nu)\gamma] + \frac{\lambda}{2} \iint \gamma(x; x) w(x - y) \gamma(y; y) dx dy \\ - T \text{Tr} [(1 + \gamma) \log(1 + \gamma) - \gamma \log \gamma] \end{aligned} \quad (3.21)$$

is now called the *reduced Hartree free energy*. By doing so we will pick as reference state a quasi-free state which is not the absolute minimizer of the true quantum free energy in the quasi-free class. However, manipulating states depending only on a potential simplifies the analysis.

The following lemma is a simple consequence of the convexity of the functional \mathcal{F}^{rH} . For completeness we state it in any dimension $d \geq 1$. The proof is given in Appendix A.

Lemma 3.2 (Existence and uniqueness of the reference quasi-free state).

Let $T, \lambda > 0$ and $d \geq 1$. Assume that $0 \leq V \in L^1_{\text{loc}}(\mathbb{R}^d)$ is a positive function tending to $+\infty$ at infinity, such that $\int_{\mathbb{R}^d} e^{-V(x)/T} dx < \infty$. Assume also that $w \in L^1(\mathbb{R}^d)$ has a positive Fourier transform $0 \leq \widehat{w} \in L^1(\mathbb{R}^d)$ and is such that $w \neq 0$. Then, for every $\nu \in \mathbb{R}$, the infimum in (3.20) is finite and admits a unique minimizer. This minimizer solves the nonlinear equation

$$\gamma^{\text{rH}} = \left\{ \exp \left(\frac{-\Delta + V - \nu + \lambda \rho_{\gamma^{\text{rH}}} * w}{T} \right) - 1 \right\}^{-1},$$

and hence its potential $V_T := \lambda \rho_{\gamma^{\text{rH}}} * w + V - \nu$ solves the nonlinear equation (3.16).

Solutions V_T of the nonlinear equation (3.16) have been studied for a particular class of potentials $V(x)$ in [47, Section 5] where it is proved that the corresponding density satisfies the homogeneous divergence mentioned previously in (3.19). The limit object $V_\infty = \lim_{T \rightarrow \infty} V_T$ will play the role of a renormalized potential.

Theorem 3.3 (Limit renormalized potential [47, Section 5]).

In dimension $d \leq 3$, let $V(x) \in L^\infty_{\text{loc}}(\mathbb{R}^d)$ be a positive function such that

$$\begin{cases} \lim_{|x| \rightarrow \infty} V(x) = +\infty, \\ V(x+y) \leq CV(x)V(y), \\ |\nabla V(x)| \leq CV(x), \\ \iint_{\mathbb{R}^d \times \mathbb{R}^d} \frac{dx dk}{(|k|^2 + V(x) + 1)^p} < \infty \end{cases} \quad (3.22)$$

for some $1 < p \leq 2$. Let $w \in L^1(\mathbb{R}^d) \cap L^\infty(\mathbb{R}^d)$ be a real-valued, even function satisfying

$$\int_{\mathbb{R}^d} |w(x)| |V(x)|^2 dx < \infty. \quad (3.23)$$

Take a constant $\kappa > 0$ and set

$$\varrho_0^\kappa := \int_{k \in \mathbb{R}^d} \frac{1}{e^{\frac{|k|^2 + \kappa}{T}} - 1} dk, \quad \nu := \lambda \widehat{w}(0) \varrho_0^\kappa - \kappa. \quad (3.24)$$

Then, if κ is large enough (independently of $T = 1/\lambda \geq 1$), we have the following statements.

(1) The unique solution V_T obtained in Lemma 3.2 satisfies

$$\frac{V}{2} \leq V_T - \kappa \leq \frac{3V}{2}. \quad (3.25)$$

(2) There exists some V_∞ satisfying

$$\frac{V}{2} \leq V_\infty - \kappa \leq \frac{3V}{2}$$

such that

$$\lim_{T \rightarrow \infty} \left\| \frac{V_T - V_\infty}{V} \right\|_{L^\infty(\mathbb{R}^d)} = 0$$

and

$$\lim_{T \rightarrow \infty} \text{Tr} \left| (-\Delta + V_T)^{-1} - (-\Delta + V_\infty)^{-1} \right|^p = 0. \quad (3.26)$$

(3) The limiting potential V_∞ solves the nonlinear equation

$$\begin{cases} V_\infty = V + w * \rho_\infty + \kappa, \\ \rho_\infty(x) = \left(\frac{1}{-\Delta + V_\infty} - \frac{1}{-\Delta + \kappa} \right) (x; x). \end{cases} \quad (3.27)$$

Theorem 3.3 is not stated exactly as in [47, Section 5], where the limiting nonlinear equation (3.27) for V_∞ was indeed not mentioned. We quickly discuss the link with [47] and the proof of (3.27) in Appendix A. Note that the limiting equation (3.27) is formally obtained by replacing the Bose-Einstein entropy $\text{Tr}(-\gamma \log \gamma + (1+\gamma) \log(1+\gamma))$ by $\text{Tr}(\log \gamma)$ (which is its leading behavior at large γ) in the variational principle (3.21) and then writing the associated variational equation.

We remark that the assumptions of Theorem 3.3 are satisfied for

$$V(x) = |x|^s + 1 \quad \text{for } s > \frac{2}{p-1}.$$

The Lieb-Thirring inequality in [42, Theorem 1] implies that

$$\mathrm{Tr}[(-\Delta + V)^{-p}] \leq \frac{1}{(2\pi)^2} \iint_{\mathbb{R}^2 \times \mathbb{R}^2} \frac{dx dk}{(|k|^2 + V(x))^p}. \quad (3.28)$$

Hence the last condition in (3.22) implies that $\mathrm{Tr}[(-\Delta + V)^{-p}] < \infty$. If $V(x) = |x|^s + 1$, the integral on the right-hand side is finite if and only if $p > 1 + 2/s$.

Although in principle it should be possible to derive a result similar to Theorem 3.3 for the true quasi-free minimizer Γ^H with exchange term, handling states depending only on a potential is much easier technically. The main theorem of the next section will prove that using the quasi-free reference state minimizing the reduced-Hartree energy without exchange is sufficient in the mean-field limit. That the minimizing quasi-free state gives an appropriate reference in renormalization procedures has been used before in several contexts, for instance in quantum electrodynamics [92, 59].

3.3. Inhomogeneous gas: limit of the quantum problem. Now we can finally state the result relating the physical inhomogeneous Hamiltonian to nonlinear Gibbs measure. The method is to

- solve the counter-term problem for the original external potential V and a suitably scaled chemical potential;
- use the so-obtained potential V_T to rewrite the physical Hamiltonian as in (3.14). Modulo the fact that the one-body potential and the counter-term now depend on T , this form is the same as that described in Section 2.4.

This leads to

Theorem 3.4 (Inhomogeneous gas).

Let $\Omega = \mathbb{R}^2$ and let $h = -\Delta + V$ with V satisfying all the assumptions of Theorem 3.3, for

$$p < \frac{\sqrt{673} - 1}{24} \simeq 1.039. \quad (3.29)$$

Let $w \in L^1(\mathbb{R}^2)$ be an even function satisfying

$$\widehat{w}(k) \geq 0, \quad \int_{\mathbb{R}^2} \widehat{w}(k) (1 + |k|^{1/2}) dk < \infty, \quad \int_{\mathbb{R}^2} |w(x)| V(x)^2 dx < \infty. \quad (3.30)$$

Take a large constant $\kappa > 0$ and set

$$\nu = \lambda \widehat{w}(0) \varrho_0^\kappa - \kappa.$$

Let V_T be the counter-term potential defined by Theorem 3.3 and V_∞ be its limit when $T \rightarrow \infty$. Take $E_0 = E_T$ as in (3.15).

With this choice of parameters, let Γ_λ be the interacting Gibbs state associated with the physical Hamiltonian \mathbb{H}_λ in (2.9) and

$$\widetilde{\Gamma}_0 := \frac{1}{\widetilde{\mathcal{Z}}_0} \exp\left(\frac{d\Gamma(-\Delta + V_T)}{T}\right), \quad (3.31)$$

be the quasi-free state associated with the potential V_T . Let μ_0 , μ and $\mathcal{D}[u]$ be the free and interacting Gibbs measures and the renormalized classical interaction associated with $-\Delta + V_\infty > 0$.

Then we have, in the limit $T \rightarrow +\infty$, $\lambda T \rightarrow 1$:

(1) Convergence of the relative free-energy:

$$\frac{F_\lambda + T \log \tilde{Z}_0}{T} \longrightarrow -\log z = -\log \left(\int e^{-\mathcal{D}[u]} d\mu_0(u) \right) \quad (3.32)$$

where

$$-T \log \tilde{Z}_0 = \langle \mathbb{H}_\lambda \rangle_{\tilde{\Gamma}_0} - \frac{\lambda}{2} \iint_{\mathbb{R}^2 \times \mathbb{R}^2} w(x-y) |\tilde{\Gamma}_0^{(1)}(x,y)|^2 dx dy + T \operatorname{Tr} \left(\tilde{\Gamma}_0 \log \tilde{\Gamma}_0 \right) \quad (3.33)$$

is the free-energy associated to (3.31).

(2) Convergence of all density matrices in Hilbert-Schmidt norm: for every $k \geq 1$, we have

$$\operatorname{Tr} \left| \frac{k!}{T^k} \Gamma_\lambda^{(k)} - \int |u^{\otimes k}\rangle \langle u^{\otimes k}| d\mu(u) \right|^2 \longrightarrow 0. \quad (3.34)$$

(3) Convergence of few-particles density matrices in better Schatten norms: if

$$1 \leq k < \frac{14 - 12p^2 - p}{2(p-1)(15p+18)} \quad (3.35)$$

then

$$\operatorname{Tr} \left| \frac{k!}{T^k} \Gamma_\lambda^{(k)} - \int |u^{\otimes k}\rangle \langle u^{\otimes k}| d\mu(u) \right|^p \longrightarrow 0. \quad (3.36)$$

(4) Convergence of the relative one-body density matrix in trace-norm: if (3.35) is satisfied for $k = 1$, namely if

$$p < \frac{\sqrt{8449} - 7}{84} \simeq 1.011, \quad (3.37)$$

then

$$\operatorname{Tr} \left| \frac{1}{T} \left(\Gamma_\lambda^{(1)} - \tilde{\Gamma}_0^{(1)} \right) - \int |u\rangle \langle u| (d\mu(u) - d\mu_0(u)) \right| \longrightarrow 0. \quad (3.38)$$

Here are our comments on this result.

1. The free-energy convergence (3.32) can be more explicitly rewritten as

$$F_\lambda = T \operatorname{Tr} \log \left(1 - e^{-\frac{-\Delta + V_\infty}{T}} \right) - T \log z + o(T) \quad (3.39)$$

where the first energy diverges very fast to $-\infty$ with T . Classical field theory then allows to calculate the remaining part of the interaction energy, minimized jointly with some entropy relative to the mean-field quasi-free state. The first trace can also be expressed as

$$-T \log \tilde{Z}_0 = T \operatorname{Tr} \log \left(1 - e^{-\frac{-\Delta + V_\infty}{T}} \right) = F_\lambda^{\text{rH}} + 3E_T$$

where F_λ^{rH} is the minimum reduced Hartree free-energy in (3.20). The expression (3.33) stated in the theorem follows from Lemma 3.2 and makes it clearer that to leading order the free energy may be computed in the reference quasi-free state.

Note that, although this leading order term is by far the largest in the expansion (3.39), its knowledge is not sufficient to determine the state. Roughly speaking, it only allows to obtain a limit measure absolutely continuous with respect to the appropriate Gaussian. To identify the limit fully, we need to evaluate the second, lower order term.

As we have mentioned, it is known in the physics literature [6, 9, 10, 67, 71] that, at the phase transition, a weakly-interacting Bose gas should be described by mean-field theory at leading order⁴ and a classical nonlinear theory for the next order. This is the spirit of the theorem above. To our knowledge, it is indeed the first mathematically rigorous statement of this kind.

2. If $V(x) = |x|^s + 1$, the last condition in (3.22) holds if and only if $p > 1 + \frac{2}{s}$. Our condition (3.29) on p then translates to

$$s > \frac{48}{\sqrt{673} - 25} \simeq 50.942 \quad (3.40)$$

whereas the more stringent condition (3.37) which gives the trace-class convergence of the relative one-particle density matrix becomes

$$s > 91 + \sqrt{8449} \simeq 182.918.$$

We expect the convergence of the k -particle density matrices in the p th Schatten space for all $p > 1 + 2/s$ and for all k , but are only able to prove it for small k satisfying (3.35). Nevertheless, for larger k we get the Hilbert-Schmidt convergence (3.34) which is still sufficient to determine the measure μ .

3. We certainly do not claim that our restrictions on p and s represent the true state of affairs. Indeed, one should expect the previous theorem to hold as soon as the limiting Gibbs measure makes sense, which only requires $p \leq 2$, i.e. $s > 2$ for $V(x) = |x|^s$ in our two-dimensional setting, see Section 5.1 below and [47]. Obtaining the optimal s remains an open problem, as does the extension to 3D where the condition $p \leq 2$ leads to $s > 6$, cf [83, Example 3.2].

In fact, the values of p we can handle at present are rather far from the expected optimal value 2. Compared to the homogeneous case discussed previously, the above theorem however illustrates that our method (i) does not require translation invariance (ii) can handle small polynomial divergences, not only logarithmic ones as in bounded domains, (iii) can be combined with the analysis of the counter-term problem.

3.4. Inhomogeneous gas: inverse statement. We turn to what can be called the *inverse* problem. Here we study the limit of the quantum model (with an arbitrary one-particle Hamiltonian h), to which we add properly chosen, x -dependent, counter terms so that the limit measure is absolutely continuous with respect to the non-interacting gaussian (instead of the mean-field one as in the previous section). The previous (direct) statement in the case $h = -\Delta + V_T(x)$ will easily follow from the inverse, thanks to Theorem 3.3.

We assume that Ω is an arbitrary domain in \mathbb{R}^2 and h is a positive operator on $L^2(\Omega)$. The reader might think of the typical case $h = -\Delta + V$ on $L^2(\mathbb{R}^2)$ with a trapping potential V diverging fast enough at infinity, as before. However, in order to cover as many practical situations as possible, we will keep h rather arbitrary in this section.

⁴The aforementioned reference deal with the homogeneous case, where the mean-field just amounts to a shift of the chemical potential, as in Section 3.1.

Let Γ_0 be the free Gibbs state, namely the state as in (2.13) with $\lambda = \nu = E_0 = 0$. Its one-body density $\varrho_0(x)$ is as before given by

$$\varrho_0(x) := \Gamma_0^{(1)}(x; x) = \left[\frac{1}{e^{\frac{h}{T}} - 1} \right] (x; x). \quad (3.41)$$

We then consider the renormalized interaction

$$\begin{aligned} \mathbb{W}^{\text{ren}} &= \frac{1}{2} \int_{\mathbb{R}^2} \widehat{w}(k) \left| \text{d}\Gamma(e^{ik \cdot x}) - \left\langle \text{d}\Gamma(e^{ik \cdot x}) \right\rangle_{\Gamma_0} \right|^2 dk \\ &= \mathbb{W} - \text{d}\Gamma(w * \varrho_0) + \frac{1}{2} \int_{\mathbb{R}^2} \varrho_0(x) w(x-y) \varrho_0(y) dx dy + \frac{\mathcal{N}}{2} w(0). \end{aligned} \quad (3.42)$$

We can write the renormalized Hamiltonian as

$$\mathbb{H}_\lambda := \text{d}\Gamma(h) + \lambda \mathbb{W}^{\text{ren}} = \text{d}\Gamma(h - \lambda w * \varrho_0 - \lambda w(0)/2) + \lambda \mathbb{W} + E_0 \quad (3.43)$$

where

$$E_0 := \frac{\lambda}{2} \iint_{\mathbb{R}^2 \times \mathbb{R}^2} \varrho_0(x) w(x-y) \varrho_0(y) dx dy. \quad (3.44)$$

Thus instead of varying the chemical potential (we set $\nu = 0$ here), we have replaced the bare one-body operator h by the dressed operator $h - \lambda w * \varrho_0 - \lambda w(0)/2$.

We will, for the sake of generality, only assume that

$$\text{Tr}[h^{-p}] < \infty \text{ for some } p > 1, \quad (3.45)$$

$$\|[h, e^{ik \cdot x}]\|^2 \leq C(1 + |k|^2)^2 h, \quad \forall k \in \mathbb{R}^2, \quad (3.46)$$

$$e^{-th}(x, y) \geq 0, \quad \forall t > 0. \quad (3.47)$$

Here besides the natural condition (3.45), some technical difficulties in the proof force us to require the bound on the commutator of h with the multiplication operator $x \mapsto e^{ik \cdot x}$ in (3.46). The precise meaning of (3.46) is that we assume $e^{ik \cdot x}$ stabilizes $D(h)$ for all k , and that

$$\|[h, e^{ik \cdot x}]u\|^2 \leq C(1 + |k|^2)^2 \langle u, hu \rangle.$$

for all $u \in D(h)$.

Our assumptions on w are the same as in (3.30):

$$w(x) = \int_{\mathbb{R}^2} \widehat{w}(k) e^{ik \cdot x} dk, \quad \widehat{w}(k) \geq 0, \quad \int_{\mathbb{R}^2} \widehat{w}(k) (1 + |k|^{1/2}) dk < \infty. \quad (3.48)$$

Our main result is as follows.

Theorem 3.5 (Inhomogeneous gas: inverse statement).

Let h be a positive operator on $L^2(\Omega)$ satisfying (3.45)-(3.46)-(3.47) with

$$p < \frac{\sqrt{673} - 1}{24} \simeq 1.039, \quad (3.49)$$

and let $w : \mathbb{R}^2 \rightarrow \mathbb{R}$ satisfy (3.48). Let μ_0 be the free Gibbs measure with variance h^{-1} and let μ be the associated interacting Gibbs measure as in Section 2.3. We consider the Gibbs state Γ_λ at temperature T associated with \mathbb{H}_λ in (3.43). Then, in the limit $T \rightarrow +\infty$, $\lambda T \rightarrow 1$, we have

(1) Convergence of the relative free-energy: With

$$F_\lambda = -T \log \operatorname{Tr}(e^{-\mathbb{H}_\lambda/T}), \quad F_0 = -T \log \operatorname{Tr}(e^{-d\Gamma(h/T)}) = T \operatorname{Tr} \log(1 - e^{-h/T})$$

the free-energies corresponding to interacting and non-interacting states,

$$\frac{F_\lambda - F_0}{T} \rightarrow -\log z = -\log \left(\int e^{-\mathcal{D}[u]} d\mu_0(u) \right). \quad (3.50)$$

(2) Convergence of reduced density matrices: For every $k \geq 1$, we have

$$\operatorname{Tr} \left| \frac{k!}{T^k} \Gamma_\lambda^{(k)} - \int |u^{\otimes k}\rangle \langle u^{\otimes k}| d\mu(u) \right|^q \rightarrow 0 \quad (3.51)$$

with

$$q = \begin{cases} p & \text{if } 1 \leq k < \frac{14 - 12p^2 - p}{2(p-1)(15p+18)}, \\ 2 & \text{otherwise.} \end{cases} \quad (3.52)$$

(3) Convergence of the relative one-particle density matrix: If the first condition in (3.52) is satisfied for $k = 1$, namely if

$$p < (\sqrt{8449} - 7)/84 \simeq 1.011,$$

then we have

$$\operatorname{Tr} \left| \frac{1}{T} \left(\Gamma_\lambda^{(1)} - \Gamma_0^{(1)} \right) - \int |u\rangle \langle u| (d\mu(u) - d\mu_0(u)) \right| \rightarrow 0. \quad (3.53)$$

Here are our comments on Theorem 3.5.

1. Let us go back to the case $h = -\Delta + V$. When V is not a constant, the many-body Hamiltonian (3.43) is different from the physical Hamiltonian (2.9) because we have replaced the bare potential V by the new potential $V - \lambda w * \varrho_0$, with $\varrho_0 = \varrho_0^V$, instead of simply shifting a chemical potential. Thus to obtain the Gibbs measure associated with V , we have started with an ad-hoc, different external potential. In this regard the above is an inverse statement.

2. The commutator condition (3.46) is a technical condition needed for the key variance estimate in Section 7 (more precisely to go from variance to linear response, see Lemma 7.7). For $h = -\Delta + V$ in $\Omega = \mathbb{R}^d$, it follows immediately from the computation

$$[e^{ik \cdot x}, h] = [e^{ik \cdot x}, -\Delta] = -|k|^2 e^{ik \cdot x} + 2ie^{ik \cdot x} k \cdot \nabla \quad (3.54)$$

and the fact that $e^{ik \cdot x}$ stabilizes the domain of the Friedrichs realization of $-\Delta + V$ (the latter being included in $H^1(\mathbb{R}^2)$). The assumption is also satisfied for the Dirichlet Laplacian in a bounded domain.

3. Our other technical assumption (3.47) is well-known to hold for $h = -\Delta + V$ (positivity of the heat kernel). For $-\Delta + V$ on $L^2(\mathbb{R}^2)$ this is a consequence of the Feynmann-Kac formula (see for example [122]). But other models are covered, including fractional Laplacian, and localized versions on bounded domains with various boundary conditions. It is only needed for the Hilbert-Schmidt convergence in (3.51). Without (3.47) the other claims in Theorem 3.5 remain valid. In fact, we will only need this condition at the very end of the proof, Section 10.3, to derive a uniform bound on the Hilbert-Schmidt norm of the density matrices. We conjecture that the limit (3.51) is valid for $q = p$ without any constraint on k .

4. PROOF STRATEGY

In the rest of the paper, we will focus on the proof of Theorem 3.5, from which our other results can be deduced. Indeed, Theorem 3.1 is a particular instance of Theorem 3.5, the only small difference being the weaker decay of $\widehat{w}(k)$ in (3.3) (with $\alpha > 0$ small). We handle this point in Remark 8.3. As regards Theorem 3.4, its proof follows exactly that of Theorem 3.5 replacing V by V_T in the original model and using the results on the counter-term problem recalled in Section 3.2. All estimates in our proof of Theorem 3.5 are quantitative and none of them relies on any special property of V , except its growth at infinity, which is quantified via only $\text{Tr}[h^{-p}]$. The bound (3.25) provided by Theorem 3.3 thus ensures that this does not alter our error estimates.

From now on we use the notation of Section 3.4. We also take $\lambda = T^{-1}$ throughout. Our general method is variational, in the same spirit as our previous works [83, 85]. We shall however rely much more on the Gibbs' state structure, i.e. on the fact that it is the exact minimizer (and not just an approximate one) of the free-energy

$$-T \log \mathcal{Z}_\lambda = \inf_{\Gamma \geq 0, \text{Tr} \Gamma = 1} (\text{Tr} [\mathbb{H}_\lambda \Gamma] + T \text{Tr} [\Gamma \log \Gamma]). \quad (4.1)$$

From (4.1) and a similar formula for the free Gibbs state Γ_0 , we deduce that Γ_λ is also the unique minimizer for the *relative free energy*:

$$\begin{aligned} -\log \frac{\mathcal{Z}_\lambda}{\mathcal{Z}_0} &= \inf_{\Gamma \geq 0, \text{Tr}_{\mathcal{F}} \Gamma = 1} (\mathcal{H}(\Gamma, \Gamma_0) + T^{-1} \text{Tr}[(\mathbb{H}_\lambda - \mathbb{H}_0)\Gamma]) \\ &= \inf_{\Gamma \geq 0, \text{Tr}_{\mathcal{F}} \Gamma = 1} (\mathcal{H}(\Gamma, \Gamma_0) + T^{-2} \text{Tr}[(\mathbb{W} - \text{d}\Gamma(w * \varrho_0^V) + T^{-1}E_0)\Gamma]) \end{aligned} \quad (4.2)$$

Here

$$\mathcal{H}(\Gamma, \Gamma') := \text{Tr}_{\mathcal{F}(\mathfrak{S})} (\Gamma(\log \Gamma - \log \Gamma')) \geq 0$$

is the von Neumann *relative entropy* of two quantum states Γ and Γ' . The simple rewriting (4.2) is particularly useful, for the left-hand side is nothing but the free-energy difference, divided by T . This is the quantity we show converges when $T \rightarrow \infty$ in (3.4) and (3.50). Characterizing the difference directly as an infimum is much more convenient than working on both terms seen as infima separately.

Similarly, the classical Gibbs measure μ defined in Section 2.3 is the unique minimizer for the variational problem

$$-\log z = \inf_{\substack{\nu \text{ proba. meas.} \\ \nu \ll \mu_0}} \left(\mathcal{H}_{\text{cl}}(\nu, \mu_0) + \int \mathcal{D}[u] d\nu(u) \right) \quad (4.3)$$

where

$$\mathcal{H}_{\text{cl}}(\nu, \nu') := \int_{\mathfrak{S}^s} \frac{d\nu}{d\nu'}(u) \log \left(\frac{d\nu}{d\nu'}(u) \right) d\nu'(u) \geq 0$$

is the classical relative entropy of two probability measures ν and ν' .

The variational problems (4.3), (4.2) and their basic properties will be discussed in Section 5.1 and Section 6, respectively. For now, observe that (4.3) begs for being interpreted as a semi-classical version of (4.2). This is the route we follow, using semi-classical-type measures associated with general states on the Fock space. Before discussing this, we point out that deriving the Gaussian measure μ_0 as the limit of the free Gibbs state Γ_0 is a straightforward application of Wick's theorem, see [83, Section 3].

Assume now that for some reason we could reduce trial states to the form

$$\Gamma \approx \int |\xi(\sqrt{T}u)\rangle\langle\xi(\sqrt{T}u)|d\mu(u) \quad (4.4)$$

with $\xi(v)$ the coherent state

$$\xi(v) = e^{-\|v\|^2/2} \bigoplus_{n \geq 0} \frac{1}{\sqrt{n!}} v^{\otimes n}$$

and μ a probability measure over one-body wave-functions. It would follow that

$$\frac{k!}{T^k} \Gamma^{(k)} \approx \int |u^{\otimes k}\rangle\langle u^{\otimes k}|d\mu(u). \quad (4.5)$$

Inserting this in the interaction energy

$$T^{-2} \text{Tr}[\mathbb{W} - d\Gamma(w * \varrho_0^V) + T^{-1}E_0]\Gamma = T^{-2} \left(\text{Tr}[w(x-y)\Gamma^{(2)}] - \text{Tr}[w * \varrho_0^V \Gamma^{(1)}] + \frac{1}{2} \iint_{\mathbb{R}^2 \times \mathbb{R}^2} \varrho_0^V(x)w(x-y)\varrho_0^V(y)dx dy \right)$$

and using the correspondence between the classical and quantum non-interacting states (obtained by Wick's theorem) immediately leads to the energetic part of the classical problem (4.3). The relationship between classical and quantum relative entropies is less straightforward, but it can be deduced from so-called Berezin-Lieb inequalities, see [13, 89, 121] for original references, [109, Appendix B] for review and [83] for the precise version we use.

Thus, the problem is essentially solved if we know how to vindicate (4.4) and/or (4.5). This is a general theory, not particularly linked to the fact that we consider Gibbs states. The measure μ , called de Finetti or Wigner measure, can be constructed for very general states, and the precise sense in which it approximates the quantum state made fairly explicit [3, 4, 81, 82, 83, 109, 112]. However, the sense in which (4.5) is known to hold generally is way too weak to control the errors made by inserting the approximation in the energy. The main source for this difficulty is that, due to the renormalization procedure the Hamiltonian must contain terms depending on the large parameter T . This rules out the compactness arguments we used previously [83, 85].

As regards estimates on the error made in (4.5), the state-of-the-art results [34, 33, 63, 82] in this direction require the one-body Hilbert space \mathfrak{H} to be finite-dimensional, and the error depends linearly on the finite dimension. To be able to use these known bounds we project our states in finite dimensional subspaces using the Fock-space/geometric localization method [79]. The main novelty of this paper is a new way of controlling the projection error, that we have briefly described at the end of the introduction.

Let us elaborate a bit more on the main ideas involved. First we write the renormalized interaction operator as in (2.33):

$$\begin{aligned} \frac{1}{2T^2} \int \widehat{w}(k) \left| d\Gamma(e^{ik \cdot x}) - \langle d\Gamma(e^{ik \cdot x}) \rangle_{\Gamma_0} \right|^2 dk = \\ \frac{1}{2T^2} \int \widehat{w}(k) \left| d\Gamma(\cos(k \cdot x)) - \langle d\Gamma(\cos(k \cdot x)) \rangle_{\Gamma_0} \right|^2 dk \\ + \frac{1}{2T^2} \int \widehat{w}(k) \left| d\Gamma(\sin(k \cdot x)) - \langle d\Gamma(\sin(k \cdot x)) \rangle_{\Gamma_0} \right|^2 dk \end{aligned}$$

and deal with each Fourier mode separately. We obtain the projected part of the Hamiltonian by replacing

$$\cos(k \cdot x) \rightsquigarrow P \cos(k \cdot x)P, \quad \sin(k \cdot x) \rightsquigarrow P \sin(k \cdot x)P$$

where P is a finite-dimensional projector. Here $\cos(k \cdot x)$ and $\sin(k \cdot x)$ are understood as multiplication operators. Let thus

$$e_k^- := P \cos(k \cdot x)P, \quad e_k^+ := \cos(k \cdot x) - P \cos(k \cdot x)P$$

or the corresponding operator with \cos changed to \sin . The natural choice for P is to project on low kinetic⁵ energy modes:

$$P = \mathbb{1}_{h \leq \Lambda}$$

for some finite but large energy cut-off $\Lambda = \Lambda(T)$ to be optimized over. Then, we have to obtain efficient bounds on

$$T^{-2} \left\langle \left| \mathrm{d}\Gamma(e_k^+) - \langle \mathrm{d}\Gamma(e_k^+) \rangle_{\Gamma_0} \right|^2 \right\rangle_{\Gamma_\lambda} \tag{4.6}$$

to ascertain that this term is $o(1)$ when Λ is chosen large enough in dependence on T .

We use two main estimates to this end. The first one is given in Lemma 6.8 below and reads

$$\mathrm{Tr} \left| h^\alpha \frac{\Gamma_\lambda^{(1)} - \Gamma_0^{(1)}}{T} h^\alpha \right| \leq C_\alpha \tag{4.7}$$

for some small $\alpha > 0$ and T -independent C_α . This is a convenient way of confirming the physical intuition that, in the ultraviolet (for large values of h), the free and interacting Gibbs states do not differ much. We can obtain (4.7) by using an inequality for the relative entropy which may be of general interest and is stated in Section 6.1. Roughly speaking, it states that the relative entropy controls the trace-class norm of $h^\alpha (\Gamma_\lambda^{(1)} - \Gamma_0^{(1)}) h^\alpha / T$ for some $\alpha \geq 0$, provided that $\mathrm{Tr}(h^{-p}) < \infty$ for some $p \leq 2$. This is similar to Pinsker's inequality for the usual relative entropy, except that it provides a bit of information on the one-particle density matrices instead of the states themselves. Unfortunately, we have not been able to use the relative entropy to get good bounds of the same kind on the higher density matrices.

This point leads us to our second main estimate. For starters, using (4.7) jointly with (2.6) we can replace the expectation in the free state Γ_0 by that in the interacting state Γ_λ , which reduces the estimate of (4.6) to one on

$$T^{-2} \left\langle \left| \mathrm{d}\Gamma(e_k^+) - \langle \mathrm{d}\Gamma(e_k^+) \rangle_{\Gamma_\lambda} \right|^2 \right\rangle_{\Gamma_\lambda}, \tag{4.8}$$

which now has the form of a variance. The idea we discussed in the introduction, whose implementation occupies all of Section 7, is that for large T and Λ

$$T^{-2} \left\langle \left| \mathrm{d}\Gamma(e_k^+) - \langle \mathrm{d}\Gamma(e_k^+) \rangle_{\Gamma_\lambda} \right|^2 \right\rangle_{\Gamma_\lambda} \approx \frac{1}{T} \partial_\varepsilon \left(\langle \mathrm{d}\Gamma(e_k^+) \rangle_{\Gamma_{\lambda,\varepsilon}} \right) \Big|_{\varepsilon=0} \tag{4.9}$$

⁵Note that in the inhomogeneous case, P does not project on Fourier modes. In the homogenous case it does, but this has nothing to do with our chosen frequency decomposition of the interaction.

where

$$\Gamma_{\lambda,\varepsilon} := \frac{1}{\mathcal{Z}_{\lambda,\varepsilon}} \exp \left(-\frac{1}{T} (\mathbb{H}_\lambda - \varepsilon d\Gamma(e_k^+)) \right). \quad (4.10)$$

We shall refer to the right-hand side of (4.9) as the *linear response* of $d\Gamma(e_k^+)$. It measures how the expectation of an observable in the Gibbs state varies to leading order when the Hamiltonian is perturbed by a small multiple of the observable⁶ itself. Note that the linear response is also the second derivative of the free-energy:

$$\partial_\varepsilon \left(\langle d\Gamma(e_k^+) \rangle_{\Gamma_{\lambda,\varepsilon}} \right)_{|\varepsilon=0} = -T \partial_\varepsilon^2 (\log \mathcal{Z}_{\lambda,\varepsilon})_{|\varepsilon=0}.$$

This is the Feynman-Hellmann principle, which tells us that the expectation value of $d\Gamma(e_k^+)$ is the derivative of the free-energy⁷ with respect to ε .

The main advantage of (4.9) is that it reduces the estimate of a two-body term (left-hand side) to that of the derivative in ε of a one-body term (right-hand side). Modulo the variations in ε , the right-hand side will be controlled by employing (4.7) again.

An estimate such as (4.9) is motivated by the fact that the linear response does seem a sensible way to physically measure the variance of an observable in the Gibbs state. To explain it further, let us return to (4.10) and replace $d\Gamma(e_k^+)$ by \mathbb{A} where \mathbb{A} commutes with \mathbb{H}_λ . Then we have exactly (this is a fluctuation-dissipation-type result [74, 75])

$$T^{-2} \langle |\mathbb{A} - \langle \mathbb{A} \rangle_{\Gamma_{\lambda,0}}|^2 \rangle_{\Gamma_{\lambda,0}} = T^{-1} \partial_\varepsilon \left(\langle \mathbb{A} \rangle_{\Gamma_{\lambda,\varepsilon}} \right)_{|\varepsilon=0}.$$

In the cases of interest to this paper, $\mathbb{A} = d\Gamma(e_k^+)$ certainly does not commute with \mathbb{H}_λ , but since we are dealing with a semi-classical problem, one may hope that the commutators will be small enough in the limit $T \rightarrow \infty$ for some of this structure to survive. Notice that (4.9), unlike our other estimates, is not a variational argument: it deeply relies on the fact that we consider an exact Gibbs state. We postpone a more detailed discussion to Section 7.

This concludes our sketch of the proofs' main ideas. Here is how they shall be articulated in the sequel:

- In Section 5 we discuss classical and semi-classical measures. First we go into more details regarding the construction of the Gibbs measure, then we explain how to introduce de Finetti measures.
- Section 6 contains several preliminary estimates on the free and interacting quantum Gibbs states. In particular we prove our estimate on the relative entropy there and obtain (4.7) as a consequence.
- The technical core of the paper is Section 7 where we discuss correlation estimates of the form (4.9) in more details, and provide their proofs.
- We bound the (relative) free-energy from below in Section 8, using de Finetti measures and controlling the errors as sketched above.
- A matching free-energy upper bound is derived in Section 9, by a trial state argument and some finite dimensional semiclassical analysis. This is much easier than the lower bound.

⁶One could similarly define the linear response of an observable \mathbb{A} to another observable \mathbb{B} , and connect this concept to the covariance of \mathbb{A} and \mathbb{B} .

⁷In other words, taking the derivative in ε and taking the expectation in the Gibbs state are two commuting operations.

- Finally, in Section 10 the convergence of reduced density matrices is deduced from various estimates developed to prove the free-energy convergence, plus Pinsker inequalities.
- An appendix contains some material on the counter-term problem.

5. CLASSICAL MEASURES

In this section, we collect some useful facts on the classical Gibbs measures we derive from the quantum problem, and on the semiclassical de Finetti measures that serve as our main tool.

5.1. Gibbs measures. We do not claim originality for the material below, the methods having been well-known to constructive quantum field theory experts for a long time. A related discussion can be found in [47, Section 3] but for pedagogical purposes we follow a somewhat more pedestrian route.

In this section, we always assume that h satisfies (2.18). Let $\{\lambda_i\}_{i=1}^\infty, \{u_i\}_{i=1}^\infty$ be the eigenvalues and the corresponding eigenfunctions of h , as in (2.15). Let us start by recalling the definition of the free Gibbs measure:

Lemma 5.1 (Free Gibbs measure).

Let $h > 0$ on \mathfrak{H} satisfy

$$\mathrm{Tr}[h^{-p}] < \infty \quad \text{for some } p > 1.$$

The free Gibbs measure μ_0 in (2.16) is the unique probability measure over the negative Sobolev-type space \mathfrak{H}^{1-p} such that for every $K \geq 1$ its cylindrical projection on $V_K = \mathrm{Span}(u_1, \dots, u_K)$ is

$$d\mu_{0,K}(u) = \prod_{i=1}^K \left(\frac{\lambda_i}{\pi} e^{-\lambda_i |\alpha_i|^2} d\alpha_i \right) \tag{5.1}$$

where $\alpha_i = \langle u_i, u \rangle$ and $d\alpha_i = d\Re(\alpha_i) d\Im(\alpha_i)$ is the Lebesgue measure on $\mathbb{C} \simeq \mathbb{R}^2$. Moreover, the corresponding k -particle density matrix

$$\gamma_{\mu_0}^{(k)} := \int |u^{\otimes k}\rangle \langle u^{\otimes k}| d\mu_0(u) = k! (h^{-1})^{\otimes k} \tag{5.2}$$

belongs to the Schatten space $\mathfrak{S}^p(\mathfrak{H}^{\otimes_s k})$.

Our convention in (5.2) is to consider the action of $\gamma_{\mu_0}^{(k)}$ only on the symmetric subspace $\mathfrak{H}^{\otimes_s k}$. On the full space with no symmetry we have

$$\gamma_{\mu_0}^{(k)} = k! P_s^k (h^{-1})^{\otimes k} P_s^k \tag{5.3}$$

with P_s^k the orthogonal projector on the symmetric subspace.

Proof. See [83, Section 3.1]. □

The measure just defined on the space \mathfrak{H}^{1-p} does *not* live on any better behaved subspace if $\mathrm{Tr}[h^{-p'}] = +\infty$ for $p' < p$. This is called Fernique’s theorem and is recalled e.g. in [83, Equation (3.4)]. The need for renormalization arises from this fact.

In particular, when $\mathrm{Tr}[h^{-1}] = +\infty$, μ_0 is supported on a negative Sobolev space and thus the mass $\int_{\mathbb{R}^2} |u|^2$ is equal to infinity μ_0 -a.e. However, it turns out that when $\mathrm{Tr}[h^{-2}] < \infty$, this infinity “is the same” for μ_0 -almost every u . This allows to define a notion of

renormalized mass. The idea goes back to Nelson [100] and has been thoroughly studied in constructive quantum field theory [52, 119].

Lemma 5.2 (Mass renormalization).

Assume that $h > 0$ satisfies $\text{Tr}[h^{-2}] < \infty$. For every $K \geq 1$, define the truncated renormalized mass

$$\mathcal{M}_K[u] := \int_{\Omega} |P_K u(x)|^2 dx - \left\langle \int_{\Omega} |P_K u(x)|^2 dx \right\rangle_{\mu_0} \quad (5.4)$$

where P_K is the orthogonal projection onto $V_K = \text{Span}(u_1, \dots, u_K)$. Then the sequence \mathcal{M}_K converges strongly to a limit \mathcal{M} in $L^2(d\mu_0)$.

More generally, for every operator A with $D(A) \subset D(h)$ and such that Ah^{-1} is Hilbert-Schmidt, the renormalized expectation value

$$\mathcal{M}_K^A[u] := \langle P_K u, AP_K u \rangle - \langle \langle P_K u, AP_K u \rangle \rangle_{\mu_0} \quad (5.5)$$

converges strongly in $L^2(d\mu_0)$ to a limit \mathcal{M}^A , uniformly in the Hilbert-Schmidt norm $\|Ah^{-1}\|_{\mathfrak{S}^2(\mathfrak{H})}$. In fact

$$\left\langle |\mathcal{M}^A[u]|^2 \right\rangle_{\mu_0} := \lim_{K \rightarrow \infty} \left\langle |\mathcal{M}_K^A[u]|^2 \right\rangle_{\mu_0} = \text{Tr} [Ah^{-1}A^*h^{-1}]. \quad (5.6)$$

Proof. Writing $u = \sum_{j=1}^K \alpha_j u_j$, we first recall the simple Gaussian integration formulae (Wick's theorem)

$$\langle \bar{\alpha}_i \alpha_j \rangle_{\mu_0} = \frac{1}{\lambda_j} \delta_{i=j}, \quad \langle \alpha_i \bar{\alpha}_j \bar{\alpha}_k \alpha_\ell \rangle_{\mu_0} = \frac{1}{\lambda_i \lambda_k} \delta_{i=j} \delta_{k=\ell} + \frac{1}{\lambda_i \lambda_\ell} \delta_{i=k} \delta_{j=\ell}. \quad (5.7)$$

Then we compute

$$\mathcal{M}_K[u] = \sum_{j=1}^K |\alpha_j|^2 - \left\langle \sum_{j=1}^K |\alpha_j|^2 \right\rangle_{\mu_0} = \sum_{j=1}^K |\alpha_j|^2 - \sum_{j=1}^K \lambda_j^{-1}.$$

Therefore, for $L \geq K$,

$$\mathcal{M}_L[u] - \mathcal{M}_K[u] = \sum_{j=K+1}^L (|\alpha_j|^2 - \lambda_j^{-1}).$$

From this and (5.7) we find

$$\begin{aligned} \langle (\mathcal{M}_L[u] - \mathcal{M}_K[u])^2 \rangle_{\mu_0} &= \sum_{j=K+1}^L \sum_{\ell=K+1}^L \left\langle (|\alpha_j|^2 - \lambda_j^{-1})(|\alpha_\ell|^2 - \lambda_\ell^{-1}) \right\rangle_{\mu_0} \\ &= \sum_{j=K+1}^L \sum_{\ell=K+1}^L \left(\langle |\alpha_j|^2 |\alpha_\ell|^2 \rangle_{\mu_0} - \lambda_j^{-1} \lambda_\ell^{-1} \right) = \sum_{j=K+1}^L \lambda_j^{-2}. \end{aligned}$$

Since

$$\sum_{j=1}^{\infty} \lambda_j^{-2} = \text{Tr}(h^{-2}) < \infty, \quad (5.8)$$

we conclude that $\{\mathcal{M}_K\}_{K=1}^{\infty}$ is a Cauchy sequence in $L^2(d\mu_0)$ and hence it converges strongly in $L^2(d\mu_0)$.

Now consider an operator A such that Ah^{-1} is Hilbert-Schmidt. We check that (5.5) is in $L^2(d\mu_0)$ uniformly in K and leave to the reader the similar proof that it is a Cauchy sequence. Using (5.7) again we have

$$\begin{aligned}
 \langle \mathcal{M}_K^A[u]^2 \rangle_{\mu_0} &= \sum_{1 \leq i, j, k, \ell \leq K} \langle \alpha_i \bar{\alpha}_j \bar{\alpha}_k \alpha_\ell \rangle_{\mu_0} \langle u_i, Au_j \rangle \overline{\langle u_k, Au_\ell \rangle} \\
 &\quad - \sum_{1 \leq i, j, k \leq K} \langle \alpha_i \bar{\alpha}_j \rangle_{\mu_0} \frac{1}{\lambda_k} \langle u_i, Au_j \rangle \overline{\langle u_k, Au_k \rangle} \\
 &\quad - \sum_{1 \leq i, j, k \leq K} \langle \bar{\alpha}_i \alpha_j \rangle_{\mu_0} \frac{1}{\lambda_k} \overline{\langle u_i, Au_j \rangle} \langle u_k, Au_k \rangle + \sum_{i, j} \frac{1}{\lambda_i \lambda_j} \langle u_j, Au_j \rangle \overline{\langle u_i, Au_i \rangle} \\
 &= \sum_{1 \leq i, k \leq K} \frac{1}{\lambda_i \lambda_k} \langle u_i, Au_k \rangle \overline{\langle u_i, Au_k \rangle} \\
 &= \text{Tr} [A(P_K h^{-1}) A^* (P_K h^{-1})].
 \end{aligned}$$

which is bounded by assumption. □

In particular we may choose A to be the multiplication operator by some bounded function f localized around some point x . Thus (5.5) implies that not only the global mass, but also the smeared local mass density $|u(x)|^2$ around x , is renormalizable. In fact, in this case (5.9) reduces to

$$\left\langle \left| \mathcal{M}^f[u] \right|^2 \right\rangle_{\mu_0} = \text{Tr} [f(x) h^{-1} \bar{f}(x) h^{-1}] = \iint_{\Omega \times \Omega} f(x) \overline{f(y)} |G(x, y)|^2 dx dy \quad (5.9)$$

with G the Green's function of h (i.e. the integral kernel of h^{-1}). This function is certainly square-integrable on $\Omega \times \Omega$, for h^{-1} is a Hilbert-Schmidt operator.

Consider now an interaction potential w as in (3.30). For the same reasons as the mass, the interaction energy is not well-defined on the support of μ_0 and it is necessary to introduce a renormalization. In our context, it is in fact sufficient to insert the local mass renormalization in the interaction's expression. This leads to

Lemma 5.3 (Renormalized interaction and nonlinear measure).

Assume that $h > 0$ satisfies $\text{Tr}[h^{-2}] < \infty$. Let $w \in L^\infty(\Omega)$ be such that its Fourier transform satisfies $0 \leq \hat{w} \in L^1(\Omega^*)$. For every $K \geq 1$, define the truncated renormalized interaction as in (2.19):

$$\mathcal{D}_K[u] := \frac{1}{2} \iint_{\Omega \times \Omega} \left(|P_K u(x)|^2 - \langle |P_K u(x)|^2 \rangle_{\mu_0} \right) w(x-y) \left(|P_K u(y)|^2 - \langle |P_K u(y)|^2 \rangle_{\mu_0} \right) dx dy.$$

Then $\mathcal{D}_K[u] \geq 0$ and $\mathcal{D}_K[u]$ converges strongly to a limit $\mathcal{D}[u] \geq 0$ in $L^1(d\mu_0)$. Consequently, the probability measure

$$d\mu(u) := \frac{1}{z_r} e^{-\mathcal{D}[u]} d\mu_0(u) \quad (5.10)$$

is well-defined. Moreover, the reduced density matrices

$$\gamma_\mu^{(k)} := \int |u^{\otimes k}\rangle \langle u^{\otimes k}| d\mu(u) \quad (5.11)$$

belong to $\mathfrak{S}^p(\mathfrak{H}_k)$ for p as in (2.18). Finally, the relative one-particle density matrix

$$\gamma_\mu^{(1)} - \gamma_{\mu_0}^{(1)} := \lim_{K \rightarrow \infty} \int |u\rangle\langle u| (d\mu(P_K u) - d\mu_0(P_K u)) \quad (5.12)$$

is a trace-class operator, with

$$\mathrm{Tr} \left| \gamma_\mu^{(1)} - \gamma_{\mu_0}^{(1)} \right| \leq (z_r)^{-1} \sqrt{\mathrm{Tr}[h^{-2}]}. \quad (5.13)$$

Proof. We use the Fourier transform

$$w(x - y) = \int \widehat{w}(k) e^{ik \cdot x} e^{-ik \cdot y} dk$$

and denote e_k the multiplication operator by $e^{ik \cdot x}$. Then, using the notation of Lemma 5.2,

$$\mathcal{D}_K[u] = \frac{1}{2} \int \widehat{w}(k) |\mathcal{M}_K^{e_k}[u]|^2 dk$$

Since $\widehat{w} \geq 0$ by assumption, we obtain immediately that $\mathcal{D}_K[u] \geq 0$.

In order to prove that \mathcal{D}_K is a Cauchy sequence in $L^1(d\mu_0)$, we use the Cauchy-Schwarz inequality

$$\begin{aligned} |\mathcal{D}_L[u] - \mathcal{D}_K[u]| &= \frac{1}{2} \left| \int \widehat{w}(k) (|\mathcal{M}_K^{e_k}[u]|^2 - |\mathcal{M}_L^{e_k}[u]|^2) dk \right| \\ &\leq \frac{1}{2} \left| \int \widehat{w}(k) |\mathcal{M}_K^{e_k}[u] - \mathcal{M}_L^{e_k}[u]|^2 dk \right|^{1/2} \\ &\quad \times \left| \int \widehat{w}(k) (|\mathcal{M}_K^{e_k}[u]| + |\mathcal{M}_L^{e_k}[u]|)^2 dk \right|^{1/2}. \end{aligned} \quad (5.14)$$

Averaging over μ_0 , using Lemma 5.2 and recalling that $\widehat{w} \in L^1$, this goes to zero when $L, K \rightarrow \infty$. Thus $\mathcal{D}_K[u]$ is a Cauchy sequence in $L^1(d\mu_0)$ and hence it converges strongly to a limit $\mathcal{D}[u]$. Since $\mathcal{D}_K[u] \geq 0$, we have $\mathcal{D}[u] \geq 0$. It follows that

$$z_r := \int e^{-\mathcal{D}[u]} d\mu_0(u) \quad (5.15)$$

is positive, which ensures that (5.10) is well-defined.

Averaging with respect to μ_0 and using (5.9) we also find after passing to the limit $K \rightarrow \infty$

$$\begin{aligned} 0 \leq \langle \mathcal{D}[u] \rangle_{\mu_0} &= \frac{1}{2} \int \widehat{w}(k) \langle |\mathcal{M}^{e_k}[u]|^2 \rangle_{\mu_0} dk \\ &= \frac{1}{2} \int \widehat{w}(k) \iint_{\Omega \times \Omega} e^{ik \cdot (x-y)} |G(x, y)|^2 dx dy dk \\ &= \frac{1}{2} \iint_{\Omega \times \Omega} w(x - y) |G(x, y)|^2 dx dy. \end{aligned} \quad (5.16)$$

That the density matrices (5.11) are in \mathfrak{S}^p directly follows from the positivity of the renormalized interaction and the corresponding statement for the free density matrices (5.2).

To see that the relative one-particle density matrix (5.12) is trace-class, note that for any finite-rank operator A

$$\mathrm{Tr} \left[A \left(\gamma_\mu^{(1)} - \gamma_{\mu_0}^{(1)} \right) \right] = \int \mathcal{M}^A[u] d\mu(u).$$

Using Cauchy-Schwarz and the fact that $\mu \leq (z_r)^{-1} \mu_0$ we find

$$\begin{aligned} \left| \mathrm{Tr} \left[A \left(\gamma_\mu^{(1)} - \gamma_{\mu_0}^{(1)} \right) \right] \right| &\leq \int |\mathcal{M}^A[u]| d\mu(u) \\ &\leq (z_r)^{-1} \left(\int \mathcal{M}^A[u]^2 d\mu_0(u) \right)^{1/2} \leq (z_r)^{-1} \|A\| \sqrt{\mathrm{Tr}[h^{-2}]}. \end{aligned}$$

By duality, the relative one-particle density matrix is thus trace-class, with

$$\mathrm{Tr} \left| \gamma_\mu^{(1)} - \gamma_{\mu_0}^{(1)} \right| \leq (z_r)^{-1} \sqrt{\mathrm{Tr}[h^{-2}]}.$$

□

Remark 5.4 (The interaction as an exchange term).

Note that, by Gaussian integrations similar to those appearing in the proof of Lemma 5.2, we obtain that, formally

$$\begin{aligned} \left\langle \iint_{\Omega \times \Omega} |u(x)|^2 w(x-y) |u(y)|^2 dx dy \right\rangle_{\mu_0} &= \frac{1}{2} \iint_{\Omega \times \Omega} w(x-y) G(x,x) G(y,y) dx dy \\ &\quad + \frac{1}{2} \iint_{\Omega \times \Omega} w(x-y) |G(x,y)|^2 dx dy \end{aligned}$$

where the first term is called the *direct term* and the second the *exchange term*, see Section 3.2. Here the direct term is infinite because $\lim_{y \rightarrow x} G(x,y) = +\infty$. For instance for the Laplacian on a bounded domain we have (see e.g. [113, Lemma 5.4])

$$G(x,y) \underset{x \sim y}{\sim} -\frac{1}{2\pi} \log |x-y|.$$

From (5.16) we see that renormalizing the mass density to define the interaction is equivalent to dropping the direct term from the bare interaction. In fact (5.16), proves that the renormalized interaction is well defined under the sole condition that w satisfies

$$\iint_{\Omega \times \Omega} |w(x-y)| |G(x,y)|^2 dx dy < \infty$$

with $G(x,y) = h^{-1}(x,y)$ the Green function of h . ◇

◇

5.2. De Finetti measure. Here we review how to associate a semiclassical measure (that we call de Finetti measure) on the one-body Hilbert space to a given sequence of many-particles bosonic states. This idea has a long history, for it is related to the de Finetti-Hewitt-Savage theorem used in classical statistical mechanics to approximate a many-particle state by a statistical mixture of i.i.d. laws. See [110, 109] for review.

The approach we use in this paper is a blend of ideas originating from semi-classical analysis [3, 4, 5, 13, 89, 121] and quantum information theory [25, 34, 33, 63] with many-body localization methods [1, 38, 79, 81, 84, 83].

It will be crucial for us that, once the one-body state-space is projected to finitely many dimensions, quantitative estimates on the error made by approximating a many-body state using a classical measure are available [34, 82]. We thus begin by recalling what Fock-space localization is. Then we continue with the quantitative version of the quantum de Finetti theorem available after finite dimensional localization. To deal with the entropy term it is crucial that the de Finetti measure we use is in fact a lower symbol (associated to a coherent states basis). This allows us to use a Berezin-Lieb-type inequality from [83].

Fock-space localization. In our proof, we will localize the problem to low kinetic energy mode. For this purpose, let us recall the standard *localization method* in Fock space. Let P be an orthogonal projection on \mathfrak{H} and let $Q = 1 - P$. Since $\mathfrak{H} = (P\mathfrak{H}) \oplus (Q\mathfrak{H})$, we have the corresponding factorization of Fock spaces

$$\mathcal{F}(\mathfrak{H}) \simeq \mathcal{F}(P\mathfrak{H}) \otimes \mathcal{F}(Q\mathfrak{H}) \quad (5.17)$$

in the sense of a unitary equivalence. That is, there is a unitary

$$\mathcal{U} : \mathcal{F}(P\mathfrak{H} \oplus Q\mathfrak{H}) \mapsto \mathcal{F}(P\mathfrak{H}) \otimes \mathcal{F}(Q\mathfrak{H}) \quad (5.18)$$

satisfying $\mathcal{U}\mathcal{U}^* = \mathbb{1}$. Its action on creation operators is

$$\mathcal{U}a^*(f)\mathcal{U}^* = a^*(Pf) \otimes \mathbb{1} + \mathbb{1} \otimes a^*(Qf) \quad (5.19)$$

and a similar formula for annihilation operators. We refer to [60, Appendix A] and references therein for precise definitions and properties.

Definition 5.5 (Fock-space localization).

For any state Γ on $\mathcal{F}(\mathfrak{H})$ and any orthogonal projector P , we define its *localization* Γ_P as a state on $\mathcal{F}(\mathfrak{H})$ obtained by taking the partial trace over $\mathcal{F}(Q\mathfrak{H})$:

$$\Gamma_P := \text{Tr}_{\mathcal{F}(Q\mathfrak{H})} [\mathcal{U}\Gamma\mathcal{U}^*].$$

The density matrices of Γ_P can be shown to be equal to

$$(\Gamma_P)^{(k)} = P^{\otimes k} \Gamma^{(k)} P^{\otimes k}, \quad \forall k \geq 1. \quad (5.20)$$

◇

The crucial property (5.20) follows immediately from (2.8) and (5.19), see again [60, Appendix A] and references therein for detailed discussions. An equivalent but more pedestrian definition leading to (5.20) originates in [79] and is reviewed in [109, Chapter 5].

Coherent states and lower symbols. The de Finetti measure is in fact a lower symbol with respect to the over-complete basis of $\mathcal{F}(P\mathfrak{H})$ given by coherent states when P is a finite-dimensional orthogonal projector. Below, the notation

$$|0\rangle = 1 \oplus 0 \oplus 0 \oplus \dots$$

stands for the vacuum of Fock space.

Definition 5.6 (Coherent states).

A *coherent state* is a Weyl-rotation of the vacuum $|0\rangle$ in the Fock space $\mathcal{F}(\mathfrak{H})$: for $u \in \mathfrak{H}$

$$\xi(u) := W(u)|0\rangle := \exp(a^\dagger(u) - a(u))|0\rangle = e^{-\|u\|^2/2} \bigoplus_{n \geq 0} \frac{1}{\sqrt{n!}} u^{\otimes n}. \quad (5.21)$$

◇

The Weyl operator $W(u)$ is a unitary operator satisfying the relations

$$W(f)^* a^\dagger(g) W(f) = a^\dagger(g) + \langle f, g \rangle, \quad W(f)^* a(g) W(f) = a(g) + \langle g, f \rangle. \quad (5.22)$$

The second equality in (5.21) follows from this. So does the fact that the k -particle density matrix of the coherent state $\xi(u)$ is

$$[|\xi(u)\rangle\langle\xi(u)|]^{(k)} = \frac{1}{k!} |u^{\otimes k}\rangle\langle u^{\otimes k}|. \quad (5.23)$$

Definition 5.7 (Lower symbol).

For any state Γ on $\mathcal{F}(\mathfrak{H})$ and any scale $\varepsilon > 0$, we define the *lower symbol* (or *Husimi function*) of Γ on $P\mathfrak{H}$ at scale ε by

$$d\mu_{P,\Gamma}^\varepsilon(u) := (\varepsilon\pi)^{-\text{Tr}(P)} \langle \xi(u/\sqrt{\varepsilon}), \Gamma_P \xi(u/\sqrt{\varepsilon}) \rangle_{\mathcal{F}(P\mathfrak{H})} du. \quad (5.24)$$

Here du is the usual Lebesgue measure on $P\mathfrak{H} \simeq \mathbb{C}^{\text{Tr}(P)}$. \diamond

Thanks to the resolution of the identity/closure relation

$$\pi^{-\text{Tr}(P)} \int_{P\mathfrak{H}} |\xi(u)\rangle\langle\xi(u)| du = \pi^{-\text{Tr}(P)} \left(\int_{P\mathfrak{H}} e^{-|u|^2} du \right) \mathbb{1}_{\mathcal{F}(V)} = \mathbb{1}_{\mathcal{F}(P\mathfrak{H})}, \quad (5.25)$$

the lower symbol $\mu_{P,\Gamma}^\varepsilon(u)$ is a probability measure on $P\mathfrak{H}$. Moreover, it provides a good approximation for the density matrices $\Gamma_P^{(k)}$, as per the following version of the *quantum de Finetti theorem*:

Theorem 5.8 (Lower symbols as de Finetti measures).

We have, for all $k \in \mathbb{N}$,

$$\int_{P\mathfrak{H}} |u^{\otimes k}\rangle\langle u^{\otimes k}| d\mu_{P,\Gamma}^\varepsilon(u) = k! \varepsilon^k \Gamma_P^{(k)} + k! \varepsilon^k \sum_{\ell=0}^{k-1} \binom{k}{\ell} \Gamma^{(\ell)} \otimes_s \mathbb{1}_{\otimes_s^{k-\ell} P\mathfrak{H}}. \quad (5.26)$$

Thus, with $d = \text{Tr}[P]$,

$$\text{Tr} \left| k! \varepsilon^k \Gamma_P^{(k)} - \int_{P\mathfrak{H}} |u^{\otimes k}\rangle\langle u^{\otimes k}| d\mu_{P,\Gamma}^\varepsilon(u) \right| \leq \varepsilon^k \sum_{\ell=0}^{k-1} \binom{k}{\ell}^2 \frac{(k-\ell+d-1)!}{(d-1)!} \text{Tr} \left[\mathcal{N}^\ell \Gamma_P \right]. \quad (5.27)$$

The result is taken from [83, Lemma 6.2 and Remark 6.4]. It is an elaboration on a theorem originating on [34] and a proof thereof later provided in [82]. If k is fixed and $\text{Tr} [(\varepsilon\mathcal{N})^\ell \Gamma_P] = O(1)$, then the upper bound in (5.27) behaves as $Cd\varepsilon$ in the limit $\varepsilon \rightarrow 0$. This is similar to the bound $4kd/N$ obtained for N -particle states in the references just mentioned.

Finally, we recall a Berezin-Lieb type inequality, which links the von Neumann relative entropy of two quantum states to the classical Boltzmann entropy of their lower symbols.

Theorem 5.9 (Relative entropy: quantum to classical).

Let Γ and Γ' be two states on $\mathcal{F}(\mathfrak{H})$. Let $\mu_{P,\Gamma}^\varepsilon$ and $\mu_{P,\Gamma'}^\varepsilon$ be the lower symbols defined in (5.24). Then we have

$$\mathcal{H}(\Gamma, \Gamma') \geq \mathcal{H}(\Gamma_P, \Gamma'_P) \geq \mathcal{H}_{\text{cl}}(\mu_{P,\Gamma}^\varepsilon, \mu_{P,\Gamma'}^\varepsilon). \quad (5.28)$$

The result is taken from [83, Theorem 7.1], whose proof goes back to the techniques in [13, 89, 121]. Note that, to obtain an approximation of density matrices, other constructions than that based on the lower symbol we just discussed are available [25, 32, 70, 126]. Most of those do not give quantitative estimates, but the main reason for us to rely on lower symbols (a.k.a. Husimi functions, covariant symbols, anti-Wick symbols) is that (5.28) is heavily based on their properties.

6. QUANTUM GIBBS STATES: A-PRIORI ESTIMATES

In this section we collect several estimates on the free and interacting quantum Gibbs states that we shall use throughout the paper. The most crucial and novel estimate is that bearing on the relative one-particle density matrix, which we present first in Section 6.1 in an abstract setting. It is the seed for the analysis of correlations and variances in Section 7.

6.1. General estimates on the entropy relative to a quasi-free state. In this section we derive some estimates of general interest on the relative entropy

$$\mathcal{H}(\Gamma, \Gamma_0) = \text{Tr}_{\mathcal{F}(\mathfrak{K})} \Gamma(\log \Gamma - \Gamma_0)$$

of two states over the Fock space $\mathcal{F}(\mathfrak{K})$ of an arbitrary Hilbert space \mathfrak{K} , under the assumption that

$$\Gamma_0 = \frac{e^{-d\Gamma(h)}}{\text{Tr}_{\mathcal{F}(\mathfrak{K})}(e^{-d\Gamma(h)})}$$

is a quasi-free Gibbs state, with $h > 0$ and $\text{Tr}_{\mathfrak{K}}(e^{-h}) < \infty$. We recall (see e.g. [83, Appendix A]) that the partition function of the free Gibbs state satisfies

$$\mathcal{Z}_0 = \text{Tr}_{\mathcal{F}(\mathfrak{K})}(e^{-d\Gamma(h)}) = \text{Tr}_{\mathfrak{K}} \left(\log(1 - e^{-h}) \right) = \exp \left(-\frac{1}{T} F_0 \right) \quad (6.1)$$

where the free-energy

$$F_0 = \mathcal{F}_0[\Gamma_0] = \min \mathcal{F}[\Gamma] = \min \{ \text{Tr}(d\Gamma(h)\Gamma) + T \text{Tr}(\Gamma \log \Gamma) \}$$

is the infimum over all states of the free-energy functional associated with Γ_0 .

We shall use the explicit expression of the one-particle density matrix of Γ_0

$$\Gamma_0^{(1)} = \frac{1}{e^h - 1}$$

and also recall that the entropy of a state Γ relative to Γ_0 is given by

$$\begin{aligned} \mathcal{H}(\Gamma, \Gamma_0) &= \text{Tr}_{\mathcal{F}(\mathfrak{K})} \left(\Gamma(\log \Gamma - \log \Gamma_0) \right) \\ &= \text{Tr}_{\mathcal{F}(\mathfrak{K})} \left(d\Gamma(h)(\Gamma - \Gamma_0) \right) + \text{Tr}_{\mathcal{F}(\mathfrak{K})} (\Gamma \log \Gamma) - \text{Tr}_{\mathcal{F}(\mathfrak{K})} (\Gamma_0 \log \Gamma_0) \\ &= \mathcal{F}_0[\Gamma] - \mathcal{F}_0[\Gamma_0] \end{aligned}$$

It is well known that $\mathcal{H}(\Gamma, \Gamma_0)$ vanishes if and only if $\Gamma = \Gamma_0$. Pinsker's inequality indeed states that

$$\mathcal{H}(\Gamma, \Gamma_0) \geq \frac{1}{2} \left(\text{Tr}_{\mathcal{F}(\mathfrak{K})} |\Gamma - \Gamma_0| \right)^2 \quad (6.2)$$

(see [31] and [64, Section 5.4]). Our goal here is to deduce some bounds on the difference $\Gamma^{(1)} - \Gamma_0^{(1)}$ of the one-particle density matrices, instead of the difference $\Gamma - \Gamma_0$ of the states in Fock space.

Theorem 6.1 (From relative entropy to reduced density matrices).

Let $h > 0$ be a positive self-adjoint operator on a separable Hilbert space \mathfrak{K} , such that $\text{Tr}(e^{-h}) < \infty$ and consider the associated quasi-free state

$$\Gamma_0 = \frac{e^{-d\Gamma(h)}}{\text{Tr}_{\mathcal{F}(\mathfrak{K})}(e^{-d\Gamma(h)})}$$

on the Fock space $\mathcal{F}(\mathfrak{K})$. Let Γ be any other state on $\mathcal{F}(\mathfrak{K})$. Then we have, for the corresponding one-particle density matrices,

$$\left\| h^\alpha (\Gamma^{(1)} - \Gamma_0^{(1)}) h^\alpha \right\|_{\mathfrak{S}^2} \leq 2 \|h^{-1}\|^{1-2\alpha} \left(\sqrt{2} \sqrt{\mathcal{H}(\Gamma, \Gamma_0)} + \mathcal{H}(\Gamma, \Gamma_0) \right) \quad (6.3)$$

for all $0 \leq \alpha \leq 1/2$. If in addition $\text{Tr}(h^{-p}) < \infty$ for some $1 \leq p \leq 2$, then we have

$$\left\| h^\alpha (\Gamma^{(1)} - \Gamma_0^{(1)}) h^\alpha \right\|_{\mathfrak{S}^1} \leq 2\sqrt{2} \sqrt{\text{Tr}(h^{-2+4\alpha})} \sqrt{\mathcal{H}(\Gamma, \Gamma_0)} + 2 \|h^{-1}\|^{1-2\alpha} \mathcal{H}(\Gamma, \Gamma_0) \quad (6.4)$$

for all

$$0 \leq \alpha \leq \frac{2-p}{4}.$$

The constants in the above inequalities are not optimal and are displayed only for concreteness. The trace-class bound (6.4) is one of our most crucial estimate, and the seed for most of the analysis in Section 7. It starts exploiting the fact that quantities calculated relative to the free state are much better behaved than bare ones, provided that $\text{Tr}(h^{-2}) < \infty$.

Remark 6.2 (Bosonic relative entropy of reduced density matrices).

If we take Γ a quasi-free state with one-particle density matrix γ , then Proposition 6.1 furnishes lower bounds on the Bose-Einstein relative entropy

$$\mathcal{H}_{\text{B-E}}(\gamma, \gamma_0) := \text{Tr}_{\mathfrak{K}} \left(\gamma (\log \gamma - \log \gamma_0) - (1 + \gamma) (\log(1 + \gamma) - \log(1 + \gamma_0)) \right) \quad (6.5)$$

which coincides with $\mathcal{H}(\Gamma_\gamma, \Gamma_0)$ when Γ is quasi-free. See [41, Lemma 4.1] for other recent lower bounds on this quantity. \diamond

The proof of Theorem (6.1) is a Feynman-Hellmann-like argument, i.e. a perturbation of the variational principle defining Γ_0 . The following lemma, consequence of Klein's inequality, allows to estimate the effect the perturbation:

Lemma 6.3 (Perturbed free Gibbs state).

Let A be a self-adjoint operator with $A \leq ch$ for a constant $0 < c < 1$. We have

$$0 \leq \text{Tr} \left(A \left(\frac{1}{e^{h-A} - 1} - \frac{1}{e^h - 1} \right) \right) \leq \frac{1}{1-c} \text{Tr} \left(\frac{1}{h} A \frac{1}{h} A \right). \quad (6.6)$$

Proof. The function

$$x \mapsto \frac{1}{e^x - 1} - \frac{1}{x}$$

is increasing on \mathbb{R}^+ , whereas $x \mapsto \frac{1}{e^x - 1}$ is decreasing. Thus, for all $x, y > 0$ we have

$$0 \leq (x - y) \left(\frac{1}{e^y - 1} - \frac{1}{e^x - 1} \right) \leq (x - y) \left(\frac{1}{y} - \frac{1}{x} \right).$$

Using Klein's matrix inequality [102, Proposition 3.16] this implies that, for any positive self-adjoint operators C, D

$$0 \leq \operatorname{Tr} \left[(C - D) \left(\frac{1}{e^D - 1} - \frac{1}{e^C - 1} \right) \right] \leq \operatorname{Tr} \left[(C - D) \left(\frac{1}{D} - \frac{1}{C} \right) \right].$$

Applying this with $D = (h - A)/T$ and $C = h/T$ yields

$$0 \leq \operatorname{Tr} \left[\frac{A}{T} \left(\frac{1}{e^{(h-A)/T} - 1} - \frac{1}{e^{h/T} - 1} \right) \right] \leq \operatorname{Tr} \left[A \left(\frac{1}{h - A} - \frac{1}{h} \right) \right].$$

There remains to use the resolvent expansion

$$\frac{1}{h - A} = \frac{1}{h} + \frac{1}{h} A \frac{1}{h - A}$$

and observe that by the assumption $A \leq ch$,

$$\operatorname{Tr} \left[\frac{1}{h} A \frac{1}{h - A} A \right] = \operatorname{Tr} \left[\frac{1}{h^{1/2}} A \frac{1}{h - A} A \frac{1}{h^{1/2}} \right] \leq \frac{1}{1 - c} \operatorname{Tr} \left[\frac{1}{h^{1/2}} A \frac{1}{h} A \frac{1}{h^{1/2}} \right]$$

to conclude the proof. \square

Proof of Theorem 6.1. Let A be an arbitrary finite rank self-adjoint operator on \mathfrak{K} , such that $A < h$ and let

$$\Gamma_A = \frac{1}{\mathcal{Z}_A} \exp(-d\Gamma(h - A))$$

be the associated quasi-free state, with one-particle density matrix

$$\gamma_A := \frac{1}{e^{h-A} - 1}.$$

Recall that Γ_A minimizes the free-energy

$$\operatorname{Tr} (d\Gamma(h - A)\Gamma) - TS(\Gamma)$$

with the entropy denoted by $S(\Gamma) = -\operatorname{Tr} \Gamma \log \Gamma$. Hence, we find

$$\begin{aligned} \mathcal{H}(\Gamma, \Gamma_0) - \operatorname{Tr} (A\Gamma^{(1)}) &= \operatorname{Tr} (d\Gamma(h - A)\Gamma) - S(\Gamma) - \operatorname{Tr} (d\Gamma(h)\Gamma_0) + S(\Gamma_0) \\ &\geq \operatorname{Tr} (d\Gamma(h - A)\Gamma_A) - S(\Gamma_A) - \operatorname{Tr} (d\Gamma(h)\Gamma_0) + S(\Gamma_0) \\ &\geq -\operatorname{Tr} (d\Gamma(A)\Gamma_A) \\ &= -\operatorname{Tr} \left(A \frac{1}{e^{h-A} - 1} \right). \end{aligned}$$

Therefore we have shown that

$$\operatorname{Tr} (A\Gamma^{(1)}) \leq \mathcal{H}(\Gamma, \Gamma_0) + \operatorname{Tr} \left(A \frac{1}{e^{h-A} - 1} \right) \quad (6.7)$$

for any $A < h$. From this we deduce in particular that

$$\operatorname{Tr} \left(A(\Gamma^{(1)} - \Gamma_0^{(1)}) \right) \leq \mathcal{H}(\Gamma, \Gamma_0) + \operatorname{Tr} \left(A \left(\frac{1}{e^{h-A} - 1} - \frac{1}{e^h - 1} \right) \right). \quad (6.8)$$

Inserting Lemma 6.3 gives

$$\boxed{\operatorname{Tr} \left(A(\Gamma^{(1)} - \Gamma_0^{(1)}) \right) \leq \mathcal{H}(\Gamma, \Gamma_0) + \frac{1}{1 - c} \left\| \frac{1}{\sqrt{h}} A \frac{1}{\sqrt{h}} \right\|_{\mathfrak{S}^2}^2}. \quad (6.9)}$$

for any $A \leq ch$ with $0 < c < 1$. The last term on the right-hand side will appear many times in the following, see for instance Lemma 6.5 below.

Let us now take

$$A = \pm \frac{\varepsilon}{2} \lambda_1^{1-2\alpha} h^\alpha B h^\alpha$$

where $\lambda_1 = \|h^{-1}\|^{-1}$ is the first eigenvalue of h , $0 < \varepsilon < 1$, $0 \leq \alpha \leq 1/2$ and B is a bounded finite rank self-adjoint operator with $\|B\| \leq 1$ and range in $D(A)$. Our choice ensures that $A \leq h/2$ for all $0 \leq \varepsilon \leq 1$. Then we obtain

$$\left| \text{Tr} \left(B h^\alpha (\Gamma^{(1)} - \Gamma_0^{(1)}) h^\alpha \right) \right| \leq \frac{2\mathcal{H}(\Gamma, \Gamma_0)}{\varepsilon \lambda_1^{1-2\alpha}} + \varepsilon \lambda_1^{1-2\alpha} \left\| h^{\alpha-\frac{1}{2}} B h^{\alpha-\frac{1}{2}} \right\|_{\mathfrak{S}^2}^2. \quad (6.10)$$

Proof of (6.3). To prove (6.3), we assume that $\|B\|_{\mathfrak{S}^2} \leq 1$, which implies as required that $\|B\| \leq 1$. We find

$$\begin{aligned} \left\| h^\alpha (\Gamma^{(1)} - \Gamma_0^{(1)}) h^\alpha \right\|_{\mathfrak{S}^2} &= \max_{\|B\|_{\mathfrak{S}^2} \leq 1} \text{Tr} \left(B h^\alpha (\Gamma^{(1)} - \Gamma_0^{(1)}) h^\alpha \right) \\ &\leq 2 \frac{\mathcal{H}(\Gamma, \Gamma_0)}{\varepsilon \lambda_1^{1-2\alpha}} + \varepsilon \lambda_1^{1-2\alpha} \left\| h^{\alpha-1/2} \right\|^4 \\ &\leq \frac{1}{\lambda_1^{1-2\alpha}} \left(2 \frac{\mathcal{H}(\Gamma, \Gamma_0)}{\varepsilon} + \varepsilon \right). \end{aligned}$$

Optimizing over ε gives

$$\left\| h^\alpha (\Gamma^{(1)} - \Gamma_0^{(1)}) h^\alpha \right\| \leq \frac{1}{\lambda_1^{1-2\alpha}} \min \left(2\sqrt{2} \sqrt{\mathcal{H}(\Gamma, \Gamma_0)}, 2\mathcal{H}(\Gamma, \Gamma_0) + 1 \right)$$

which is bounded above by the right-hand side of (6.3).

Proof of (6.4). To prove (6.4), we assume in addition that $\text{Tr}(h^{-p}) < \infty$ for some $p \leq 2$ and obtain, using $\|B\| \leq 1$ and Hölder's inequality in Schatten spaces

$$\begin{aligned} \text{Tr} \left| h^\alpha (\Gamma^{(1)} - \Gamma_0^{(1)}) h^\alpha \right| &= \max_{\|B\| \leq 1} \text{Tr} \left(B h^\alpha (\Gamma^{(1)} - \Gamma_0^{(1)}) h^\alpha \right) \\ &\leq \frac{2\mathcal{H}(\Gamma, \Gamma_0)}{\varepsilon \lambda_1^{1-2\alpha}} + \varepsilon \lambda_1^{1-2\alpha} \left\| h^{\alpha-\frac{1}{2}} \right\|_{\mathfrak{S}^4}^4 \\ &= \frac{2\mathcal{H}(\Gamma, \Gamma_0)}{\varepsilon \lambda_1^{1-2\alpha}} + \varepsilon \lambda_1^{1-2\alpha} \text{Tr}(h^{-2+4\alpha}). \end{aligned}$$

This gives (6.4) and concludes the proof of Theorem 6.1. □

6.2. Free Gibbs state in the limit $T \rightarrow \infty$. Now we introduce the temperature T and study the limit $T \rightarrow \infty$. We start by stating some simple properties of the free Gibbs state. Let $h > 0$ satisfy $\text{Tr}(h^{-p}) < \infty$ for some $p \geq 1$. Then, $\text{Tr}[e^{-\beta h}] < \infty$ for all $\beta > 0$ and we may define the associated free Gibbs state by

$$\Gamma_0 = \frac{1}{\mathcal{Z}_0} \exp \left(-\frac{\mathbb{H}_0}{T} \right), \quad \mathbb{H}_0 = d\Gamma(h), \quad \mathcal{Z}_0 = \text{Tr}_{\mathcal{F}(\mathfrak{S})} \left[\exp \left(-\frac{\mathbb{H}_0}{T} \right) \right].$$

We collect some of its first properties in the

Lemma 6.4 (Free Gibbs state).

Let $h > 0$ satisfy

$$\mathrm{Tr}(h^{-p}) < \infty \quad \text{for some } p \geq 1. \quad (6.11)$$

The k -particle density matrix of the free Gibbs state is given by

$$\Gamma_0^{(k)} = \left(\frac{1}{e^{h/T} - 1} \right)^{\otimes k} \leq T^k (h^{-1})^{\otimes k}. \quad (6.12)$$

Consequently, for every $k \geq 1$,

$$\frac{k!}{T^k} \Gamma_0^{(k)} \rightarrow k! (h^{-1})^{\otimes k} = \int |u^{\otimes k}\rangle \langle u^{\otimes k}| d\mu_0(u) \quad (6.13)$$

strongly in the Schatten space $\mathfrak{S}^p(\mathfrak{H}^k)$. Moreover,

$$\mathrm{Tr} \left[\Gamma_0^{(k)} \right] = \left\langle \binom{\mathcal{N}}{k} \right\rangle_0 \leq C^k T^{pk}. \quad (6.14)$$

and, if in addition $p > 1$,

$$\lim_{T \rightarrow \infty} \frac{1}{T^{pk}} \mathrm{Tr} \left[\Gamma_0^{(k)} \right] = 0. \quad (6.15)$$

Here \mathcal{N} is the particle number operator and $\langle \cdot \rangle_0$ is the expectation against Γ_0 .

Regarding (6.12) we recall the notational convention discussed around Equation (5.3). To illustrate the bounds on the particle number (6.14)-(6.15), recall that in the homogeneous case where $h = -\Delta + \kappa$ on a box with peridodic boundary conditions we have that

$$\begin{cases} \text{in 1D (6.11) holds with } p = 1 \text{ and } \langle \mathcal{N} \rangle_0 \sim T \\ \text{in 2D (6.11) holds with any } p > 1 \text{ and } \langle \mathcal{N} \rangle_0 \sim T \log T \\ \text{in 3D (6.11) holds with any } p > 3/2 \text{ and } \langle \mathcal{N} \rangle_0 \sim T^{3/2} \end{cases}$$

Proof. Formula (6.12) is taken from [83, Lemma 2.1]. Formula (6.13) follows from the monotone convergence of operators and the fact that h^{-1} belongs to the Schatten space $\mathfrak{S}^p(\mathfrak{H})$ by the assumption (2.18). Finally, (6.14) holds true because

$$\mathrm{Tr} \left[\Gamma_0^{(k)} \right] = \left\langle \binom{\mathcal{N}}{k} \right\rangle_0 \leq C_k \langle \mathcal{N} \rangle_0^k = C_k \left(\mathrm{Tr} \left[\frac{1}{e^{h/T} - 1} \right] \right)^k \leq C_k (\mathrm{Tr} [(T/h)^p])^k.$$

We have used here that

$$\frac{1}{e^x - 1} \leq \frac{C_p}{x^p}, \quad \forall p \geq 1. \quad (6.16)$$

Here in the first estimate we have used Wick's formula for the quasi-free state Γ_0 . We then remark that

$$\frac{1}{T^p} \mathrm{Tr} \left[\frac{1}{e^{h/T} - 1} \right] = \sum_{j \geq 1} \frac{1}{T^p (e^{\lambda_j/T} - 1)}$$

so the limit (6.15) follows from the dominated convergence theorem, since

$$\frac{1}{T^p (e^{\lambda_j/T} - 1)} \leq \min \left\{ \frac{1}{T^{p-1} \lambda_j}, \frac{C_p}{(\lambda_j)^p} \right\}$$

by (6.16) and $1/(T^{p-1} \lambda_j) \rightarrow 0$ when $p > 1$. □

The following result is the counterpart of Lemma 5.2. It shows in particular that the renormalized mass is also bounded independently of T for the quantum Gibbs state (take $A = 1$ in the statement).

Lemma 6.5 (Variance estimate for the free Gibbs state).

Assume that $h > 0$ satisfies $\text{Tr}[h^{-2}] < \infty$. For every bounded self-adjoint operator A , we have

$$\lim_{T \rightarrow \infty} T^{-2} \left\langle \left| \text{d}\Gamma(A) - \langle \text{d}\Gamma(A) \rangle_0 \right|^2 \right\rangle_0 = \text{Tr}[Ah^{-1}Ah^{-1}]. \quad (6.17)$$

Proof. Pick an orthonormal basis (u_i) of \mathfrak{H} and denote a_i^*, a_i the associated creation and annihilation operators. Since Γ_0 is a quasi-free state and it commutes with \mathcal{N} , we can compute explicitly, using the CCR and Wick's theorem:

$$\begin{aligned} \left\langle |\text{d}\Gamma(A)|^2 \right\rangle_0 &= \sum_{m,n,p,q=1}^{\infty} \langle u_m, Au_n \rangle \langle u_p, Au_q \rangle \langle a_m^* a_n a_p^* a_q \rangle_0 \\ &= \sum_{m,n,p,q=1}^{\infty} \langle u_m, Au_n \rangle \langle u_p, Au_q \rangle (\langle a_m^* a_n \rangle_0 \langle a_p^* a_q \rangle_0 + \langle a_m^* a_q \rangle_0 \delta_{np} + \langle a_m^* a_q \rangle_0 \langle a_p^* a_n \rangle_0) \\ &= \left\langle \text{d}\Gamma(A) \right\rangle_0^2 + \text{Tr} \left[A^2 \Gamma_0^{(1)} \right] + \text{Tr} \left[A \Gamma_0^{(1)} A \Gamma_0^{(1)} \right]. \end{aligned}$$

Then using (6.13) and (6.14), we conclude that

$$\begin{aligned} T^{-2} \left\langle \left| \text{d}\Gamma(A) - \langle \text{d}\Gamma(A) \rangle_0 \right|^2 \right\rangle_0 &= T^{-2} \left(\left\langle |\text{d}\Gamma(A)|^2 \right\rangle_0 - \langle \text{d}\Gamma(A) \rangle_0^2 \right) \\ &= T^{-2} \text{Tr} \left[A^2 \Gamma_0^{(1)} \right] + T^{-2} \text{Tr} \left[A \Gamma_0^{(1)} A \Gamma_0^{(1)} \right] \\ &\xrightarrow{T \rightarrow \infty} \text{Tr}[Ah^{-1}Ah^{-1}]. \end{aligned} \quad (6.18)$$

In the last line we have used that

$$\frac{1}{T^2} \text{Tr} \left[A^2 \Gamma_0^{(1)} \right] \leq \frac{\|A\|^2}{T^2} \text{Tr} \Gamma_0^{(1)} \xrightarrow{T \rightarrow \infty} 0$$

by (6.14) for $p < 2$ and by (6.15) for $p = 2$. □

An important consequence of the previous lemma is that the quantum Gibbs state has a bounded renormalized interaction energy:

Lemma 6.6 (Interaction energy of the free Gibbs state).

Assume that $h > 0$ satisfies $\text{Tr}[h^{-2}] < \infty$ and that $w \in L^\infty(\Omega)$ has a Fourier transform satisfying $0 \leq \widehat{w} \in L^1(\Omega^*)$. For the interaction operator defined as in (3.42), namely

$$\mathbb{W}^{\text{ren}} = \frac{1}{2} \int \widehat{w}(k) \left| \text{d}\Gamma(e^{ik \cdot x}) - \left\langle \text{d}\Gamma(e^{ik \cdot x}) \right\rangle_{\Gamma_0} \right|^2 dk, \quad (6.19)$$

we have

$$T^{-2} \langle \mathbb{W}^{\text{ren}} \rangle_{\Gamma_0} \leq C \text{Tr}[h^{-2}]. \quad (6.20)$$

Proof. Let us write

$$\begin{aligned} \mathbb{W}^{\text{ren}} &= \frac{1}{2} \int \widehat{w}(k) |\text{d}\Gamma(\cos(k \cdot x)) - \langle \text{d}\Gamma(\cos(k \cdot x)) \rangle_0|^2 dk \\ &\quad + \frac{1}{2} \int \widehat{w}(k) |\text{d}\Gamma(\sin(k \cdot x)) - \langle \text{d}\Gamma(\sin(k \cdot x)) \rangle_0|^2 dk. \end{aligned}$$

Next, we take the expectation against Γ_0 and use (6.17) with $A = \cos(k \cdot x)$ or $\sin(k \cdot x)$ since $\|A\| \leq 1$ in this case (6.20) follows immediately:

$$T^{-2} \langle \mathbb{W}^{\text{ren}} \rangle_0 \leq C \int \widehat{w}(k) \text{Tr}[h^{-2}] dk \leq C \text{Tr}[h^{-2}].$$

□

6.3. Interacting Gibbs state: first bounds. In this section let us consider the interacting Hamiltonian

$$\mathbb{H}_\lambda = \text{d}\Gamma(h) + \lambda \mathbb{W}^{\text{ren}} \quad (6.21)$$

with the interaction \mathbb{W}^{ren} defined in (6.19). Recall that the interacting Gibbs state

$$\Gamma_\lambda := \frac{1}{\mathcal{Z}_\lambda} \exp\left(-\frac{1}{T} \mathbb{H}_\lambda\right), \quad \mathcal{Z}_\lambda = \text{Tr}\left(\exp\left(-\frac{1}{T} \mathbb{H}_\lambda\right)\right), \quad (6.22)$$

is the unique minimizer for the variational problem (4.2):

$$-\log \frac{\mathcal{Z}_\lambda}{\mathcal{Z}_0} = \inf_{\Gamma \geq 0, \text{Tr}_{\mathcal{F}} \Gamma = 1} (\mathcal{H}(\Gamma, \Gamma_0) + T^{-2} \text{Tr}(\mathbb{W}^{\text{ren}} \Gamma_\lambda)).$$

We can first control the relative free energy, or equivalently the ratio of the free and interacting partition functions:

Lemma 6.7 (Bound on relative partition function).

We have

$$0 \leq -\log \frac{\mathcal{Z}_\lambda}{\mathcal{Z}_0} \leq C \text{Tr}[h^{-2}]. \quad (6.23)$$

In particular, we deduce that

$$\mathcal{H}(\Gamma, \Gamma_0) \leq C \text{Tr}[h^{-2}] \quad (6.24)$$

and

$$\text{Tr}[\mathbb{W}^{\text{ren}} \Gamma_\lambda] \leq CT^2 \text{Tr}[h^{-2}], \quad (6.25)$$

uniformly in T .

Proof. For the upper bound in (6.23) we take the trial state $\Gamma = \Gamma_0$ in (4.2) and use (6.20). Then (6.24) and (6.25) follow immediately, and since both these quantities are positive, we also get the lower bound in (6.23). □

The relative entropy bound (6.24) immediately implies a control on the difference of the one-particle density matrices, by Theorem 6.1.

Lemma 6.8 (Bounds on the one-particle density matrix).

Assume that $h > 0$ satisfies $\text{Tr}(h^{-p}) < \infty$ for some $1 < p \leq 2$. We have the operator bound

$$0 \leq \frac{\Gamma_\lambda^{(1)}}{T} \leq \frac{C(\text{Tr}[h^{-2}] + 1)}{h}. \quad (6.26)$$

Moreover, for any $0 \leq \beta \leq 1$

$$\mathrm{Tr} \left[h^\beta \Gamma_\lambda^{(1)} \right] \leq C \left(T \mathrm{Tr}[h^{-2}] + T^{p+\beta} \mathrm{Tr}[h^{-p}] \right). \quad (6.27)$$

Finally, for any $0 \leq \alpha \leq \frac{2-p}{4}$ we have

$$\left\| h^\alpha \left(\frac{\Gamma_\lambda^{(1)} - \Gamma_0^{(1)}}{T} \right) h^\alpha \right\|_{\mathfrak{S}^1} \leq C \left(\sqrt{\|h^{p-2+4\alpha}\| \mathrm{Tr}(h^{-p})} \sqrt{\mathrm{Tr}(h^{-2})} + \|h^{-1}\|^{1-2\alpha} \mathrm{Tr}(h^{-2}) \right). \quad (6.28)$$

Proof. Take $\alpha = 1/2$ in (6.3) and replace h by h/T . Then we deduce that

$$\left\| T^{-1} h^{1/2} \Gamma_\lambda^{(1)} h^{1/2} - 1 \right\| \leq \left\| T^{-1} h^{1/2} \Gamma^{(1)} h^{1/2} - 1 \right\|_{\mathfrak{S}^2} \leq 2\sqrt{2} \sqrt{\mathcal{H}(\Gamma_\lambda, \Gamma_0)} + 2\mathcal{H}(\Gamma_\lambda, \Gamma_0)$$

which is bounded by $C(1 + \mathrm{Tr}[h^{-2}])$ by (6.24). This proves that

$$\frac{h^{1/2} \Gamma_\lambda^{(1)} h^{1/2}}{T} \leq C(1 + \mathrm{Tr}[h^{-2}])$$

which is (6.26). Similarly, (6.28) follows immediately from (6.4).

For (6.27) it is simpler to go back to (6.7), with $A = \lambda_1^{1-\beta} h^\beta / (2T) \leq h/2$, which yields

$$\begin{aligned} \frac{\lambda_1^{1-\beta}}{2T} \mathrm{Tr} (h^\beta \Gamma^{(1)}) &\leq \mathcal{H}(\Gamma, \Gamma_0) + \frac{\lambda_1^{1-\beta}}{2T} \mathrm{Tr} \left(h^\beta \frac{1}{e^{\frac{h-\lambda_1^{1-\beta} h^\beta / 2}{T}} - 1} \right) \\ &\leq \mathcal{H}(\Gamma, \Gamma_0) + \frac{C\lambda_1^{1-\beta}}{2} T^{p+\beta-1} \mathrm{Tr} \left(\frac{h^\beta}{(h - \lambda_1^{1-\beta} h^\beta / 2)^{p+\beta}} \right) \\ &\leq C \mathrm{Tr}(h^{-2}) + C_{\beta,p} T^{p+\beta-1} \frac{\lambda_1^{1-\beta}}{2} \mathrm{Tr}(h^{-p}). \end{aligned} \quad (6.29)$$

This concludes the proof of Lemma 6.8. \square

Accessing higher-order density matrices is not as easy. We however have an immediate consequence of Lemma 6.7:

Lemma 6.9 (Moments of the particle number).

Assume that $h > 0$ satisfies $\mathrm{Tr}(h^{-p}) < \infty$ for some $1 < p \leq 2$. For every $k \geq 1$, we have

$$\mathrm{Tr} \left[\Gamma_\lambda^{(k)} \right] \leq \langle \mathcal{N}^k \rangle_\lambda \leq C_k T^{pk} \exp(C \mathrm{Tr}[h^{-2}]) \quad (6.30)$$

where $\langle \cdot \rangle_\lambda$ is the expectation against Γ_λ .

Proof. Using $\mathbb{H}_\lambda \geq \mathbb{H}_0$ and the fact that \mathcal{N} commutes with the Hamiltonians, we have

$$\mathrm{Tr} \left[\mathcal{N}^k e^{-\mathbb{H}_\lambda / T} \right] = \mathrm{Tr} \left[e^{k \log \mathcal{N} - \mathbb{H}_\lambda / T} \right] \leq \mathrm{Tr} \left[e^{k \log \mathcal{N} - \mathbb{H}_0 / T} \right] = \mathrm{Tr} \left[\mathcal{N}^k e^{-\mathbb{H}_0 / T} \right]$$

because (see e.g. [30, Section 2.2]) for an increasing function $f : \mathbb{R} \rightarrow \mathbb{R}$ and self-adjoint operators A, B

$$A \leq B \Rightarrow \mathrm{Tr} [f(A)] \leq \mathrm{Tr} [f(B)].$$

Therefore,

$$\langle \mathcal{N}^k \rangle_\lambda \leq \frac{\mathcal{Z}_0}{\mathcal{Z}_\lambda} \langle \mathcal{N}^k \rangle_0 \quad (6.31)$$

and the conclusion follows from (6.23) and (6.14). \square

In a slightly more subtle manner, we can combine the arguments of the two previous proofs to obtain

Lemma 6.10 (Joint kinetic and number bounds).

Assume that $h > 0$ satisfies $\text{Tr}(h^{-p}) < \infty$ for some $1 < p \leq 2$. For any $k \geq 1$ and every $0 < \beta \leq 1$, we have

$$\langle \mathcal{N}^k d\Gamma(h^\beta) \rangle_\lambda \leq C_{k,\beta} T^{p(k+1)+\beta} \exp(C \text{Tr}(h^{-p})). \quad (6.32)$$

Proof. We consider an auxiliary normalized Gibbs state

$$\Gamma'_\lambda := \frac{1}{\mathcal{Z}'_\lambda} \exp(-\mathbb{H}_\lambda/T + k \log \mathcal{N}).$$

The convention here is that $\Gamma'_\lambda = 0$ on the Fock space vacuum. Then, since the particle number commutes with all the relevant operators

$$\langle \mathcal{N}^k d\Gamma(h^\beta) \rangle_\lambda = \text{Tr} \left[d\Gamma(h^\beta) \mathcal{N}^k \Gamma'_\lambda \right] = \frac{\mathcal{Z}'_\lambda}{\mathcal{Z}_\lambda} \text{Tr} \left[d\Gamma(h^\beta) \Gamma'_\lambda \right] = \langle \mathcal{N}^k \rangle_\lambda \text{Tr} \left[d\Gamma(h^\beta) \Gamma'_\lambda \right].$$

On the other hand, by a variant of the proof of (6.8),

$$c \text{Tr} \left[d\Gamma(h^\beta) \Gamma'_\lambda \right] \leq \mathcal{H}(\Gamma'_\lambda, \Gamma'_0) + c \text{Tr} \left(d\Gamma(h^\beta) \Gamma''_0 \right)$$

for a small constant $c > 1$ such that $ch^\beta < h/2$ and with

$$\Gamma''_0 = \frac{1}{\mathcal{Z}''_0} \exp \left(-d\Gamma(h - ch^\beta)/T + k \log \mathcal{N} \right).$$

Next, taking Γ'_0 as a trial state in the variational principle defining Γ'_λ and using that

$$0 \leq \mathbb{W}^{\text{ren}} \leq C (\mathcal{N}^2 + \langle \mathcal{N}^2 \rangle_0)$$

yields

$$\mathcal{H}(\Gamma'_\lambda, \Gamma'_0) \leq \text{Tr} \left(\frac{\mathbb{W}^{\text{ren}}}{T^2} \Gamma'_0 \right) = \frac{\langle \mathcal{N}^k \frac{\mathbb{W}^{\text{ren}}}{T^2} \rangle_0}{\langle \mathcal{N}^k \rangle_0} \leq C \frac{\langle \mathcal{N}^{k+2} \rangle_0}{T^2 \langle \mathcal{N}^k \rangle_0} + C \frac{\langle \mathcal{N}^2 \rangle_0}{T^2}.$$

An application of Wick's theorem then shows that

$$\mathcal{H}(\Gamma'_\lambda, \Gamma'_0) \leq C_k T^{-2} \langle \mathcal{N}^2 \rangle_0 = C_k T^{2p-2}.$$

By the same token

$$\begin{aligned} \text{Tr} \left(d\Gamma(h^\beta) \Gamma''_0 \right) &= \frac{\text{Tr} \left(d\Gamma(h^\beta) \mathcal{N}^k \exp \left(-d\Gamma(h - ch^\beta)/T \right) \right)}{\text{Tr} \left(\mathcal{N}^k \exp \left(-d\Gamma(h - ch^\beta)/T \right) \right)} \\ &= \frac{\langle \mathcal{N}^k d\Gamma(h^\beta) \rangle_{0,\beta}}{\langle \mathcal{N}^k \rangle_{0,\beta}} \leq \frac{\langle \mathcal{N}^{2k} \rangle_{0,\beta}^{1/2}}{\langle \mathcal{N}^k \rangle_{0,\beta}} \langle d\Gamma(h^\beta)^2 \rangle_{0,\beta}^{1/2} \end{aligned}$$

with the perturbed quasi-free state

$$\Gamma_{0,h^\beta} := \frac{1}{\mathcal{Z}_{0,h^\beta}} \exp \left(-d\Gamma(h - ch^\beta)/T \right).$$

Another calculation using Wick's theorem and the use of Lemma 6.4 yield

$$\text{Tr} \left(d\Gamma(h^\beta) \Gamma''_0 \right) \leq C_{k,\beta} T^{p+\beta}.$$

In that regard observe that

$$d\Gamma(h^\beta)^2 = d\Gamma(h^{2\beta}) + \bigoplus_{n \geq 2} \sum_{1 \leq i \neq j \leq n} h_i^\beta \otimes h_j^\beta.$$

Collecting all the preceding estimates and using (6.30) gives

$$\langle \mathcal{N}^k d\Gamma(h^\beta) \rangle_\lambda \leq C_{k,\beta} T^{p+pk+\beta} + C_k T^{2p+pk-2}.$$

For $\beta > 0$, $p \leq 2$ and T large, the main term is the first one. □

7. CORRELATION ESTIMATES FOR HIGH MOMENTA

In this section we prove the main estimate allowing us to control errors when localizing to low-momentum modes. We denote by $\langle \cdot \rangle_\lambda$ the expectation against the interacting Gibbs state in (6.22):

$$\Gamma_\lambda := \frac{1}{\mathcal{Z}_\lambda} \exp\left(-\frac{1}{T} \mathbb{H}_\lambda\right), \quad \mathbb{H}_\lambda = d\Gamma(h) + \lambda \mathbb{W}^{\text{ren}}$$

with \mathbb{W}^{ren} as in (6.19). Define the spectral projections associated to the energy cut-off Λ_e

$$P = \mathbb{1}_{h \leq \Lambda_e}, \quad Q = \mathbb{1} - P. \tag{7.1}$$

The cut-off shall be optimized over later, for the moment we only assume that $\Lambda_e \rightarrow \infty$ when $T \rightarrow \infty$. Let e_k denote the multiplication operator either by $\cos(k \cdot x)$ or $\sin(k \cdot x)$ and

$$e_k^+ = e_k - P e_k P = Q e_k Q + P e_k Q + Q e_k P. \tag{7.2}$$

The main result of this section is

Theorem 7.1 (Variance estimates for interactions at high momenta).

Assume that $h > 0$ satisfies $\text{Tr}(h^{-p}) < \infty$ for some $1 < p \leq 3/2$. and let w satisfy (3.30). We have, for any k , for $\lambda^{-1} \sim T$ sufficiently large,

$$T^{-2} \left\langle \left| d\Gamma(e_k^+) - \langle d\Gamma(e_k^+) \rangle_\lambda \right|^2 \right\rangle_\lambda \leq C \left((1 + |k|^2)^2 T^{2p-3} + T^{\frac{3(p-1)}{2}} \Lambda_e^{\frac{p-2}{8}} + \Lambda_e^{\frac{p-2}{2}} \right). \tag{7.3}$$

Here the constant C depends on h only via $\text{Tr}[h^{-p}]$.

Note that the left side involves the expectation $\langle d\Gamma(e_k^+) \rangle_\lambda$ in the interacting state Γ_λ instead of that in the non-interacting state Γ_0 , as in the definition of the renormalized interaction \mathbb{W}^{ren} . However, we will use later that the difference between these two constants is small, by Lemma 6.8.

Our proof relies on the important fact that the left-hand side of (7.3) is the quantum variance of the observable $d\Gamma(e_k^+/T)$ in the state Γ_λ , that we shall relate to a notion of linear response. In order to explain the general strategy, we first need to recall some general properties of quantum variance.

7.1. Quantum variance(s). Here we provide some simple properties of the quantum variance. We work in a general setting, since our observations could be useful in other contexts.

Let Γ be a general quantum (mixed) state on a Hilbert space \mathfrak{K} . For a self-adjoint operator A on \mathfrak{K} , the quantum variance is usually defined [44] by

$$\mathrm{Var}_{\Gamma}^{(0)}(A) := \mathrm{Tr} \left((A - \mathrm{Tr}(A\Gamma))^2 \Gamma \right) = \mathrm{Tr}(A^2\Gamma) - (\mathrm{Tr}(A\Gamma))^2. \quad (7.4)$$

For the formula to make sense it is only required that $\sqrt{\Gamma}A \in \mathfrak{S}^2$, in which case the first term on the right side is understood as $\mathrm{Tr}(A^2\Gamma) = \mathrm{Tr}(\sqrt{\Gamma}A^2\sqrt{\Gamma}) = \|\sqrt{\Gamma}A\|_{\mathfrak{S}^2}^2$. For simplicity of exposition, we will most of the time assume that A is bounded.

When A does not commute with Γ , one might be interested in other, non-equivalent, possibilities for the definition of the variance:

Definition 7.2 (Quantum s -variance, averaged quantum variance).

Let A be a self-adjoint operator and Γ a quantum state. For $0 \leq s \leq 1$ we define the *quantum s -variance* as

$$\begin{aligned} \mathrm{Var}_{\Gamma}^{(s)}(A) &:= \mathrm{Tr} \left((A - \mathrm{Tr}(A\Gamma)) \Gamma^s (A - \mathrm{Tr}(A\Gamma)) \Gamma^{1-s} \right) \\ &= \left\| \Gamma^{\frac{s}{2}} (A - \mathrm{Tr}(A\Gamma)) \Gamma^{\frac{1-s}{2}} \right\|_{\mathfrak{S}^2}^2 \\ &= \mathrm{Tr}(A\Gamma^s A\Gamma^{1-s}) - (\mathrm{Tr}(A\Gamma))^2. \end{aligned} \quad (7.5)$$

We call

$$\mathrm{Var}_{\Gamma}^{\mathrm{av}}(A) := \int_0^1 \mathrm{Var}_{\Gamma}^{(s)}(A) ds = \int_0^1 \mathrm{Tr}(A\Gamma^s A\Gamma^{1-s}) ds - (\mathrm{Tr}(A\Gamma))^2 \quad (7.6)$$

the *averaged quantum s -variance*. \diamond

Since A is assumed to be self-adjoint, we clearly have $\mathrm{Var}_{\Gamma}^{(s)}(A) = \mathrm{Var}_{\Gamma}^{(1-s)}(A)$, with the usual quantum variance (7.4) obtained for $s = 0$ and $s = 1$. The following says that the s -variance in fact attains its maximum at $s = 0$ and $s = 1$, and set bounds on the possible discrepancy at different values of s :

Lemma 7.3 (Quantum s -variance as a function s).

Let $\Gamma > 0$ be a positive state on a separable Hilbert space \mathfrak{K} . For any bounded self-adjoint operator A , we have

$$0 \leq \mathrm{Var}_{\Gamma}^{(s)}(A) \leq \mathrm{Var}_{\Gamma}^{(0)}(A) \quad (7.7)$$

for all $0 \leq s \leq 1$. Also, if $A D(\log \Gamma) \subset D(\log \Gamma)$, we have

$$\mathrm{Var}_{\Gamma}^{(s)}(A) \geq \mathrm{Var}_{\Gamma}^{(0)}(A) - \frac{1}{2} \left\| [A, \log \Gamma] \Gamma^{1/2} \right\|_{\mathfrak{S}^2}^2. \quad (7.8)$$

Note that the two variances coincide if (the proof shows this is actually a “if and only if”) A and $\log \Gamma$ (hence Γ) commute. The bound (7.8) is crucial for the sequel: it allows to make rigorous the intuition that all the s -variances coincide in a semi-classical limit, where commutators ought to disappear.

Proof. The estimate (7.7) follows from Hölder’s inequality in Schatten spaces [120] and the matrix Lieb-Thirring inequality (see [93, Theorem 9] and [90, Theorem 4.5] or [15,

Section IX.2]). We use the polar decomposition $A = |A|U = U|A|$ where $U = \text{sgn}(A)$ and estimate, using that $0 \leq s \leq 1$ for the last inequality,

$$\begin{aligned}
 \text{Tr} [A\Gamma^s A\Gamma^{1-s}] &= \left\| \Gamma^{\frac{s}{2}} |A|^s U |A|^{1-s} \Gamma^{\frac{1-s}{2}} \right\|_{\mathfrak{S}^2}^2 \\
 &\leq \left\| \Gamma^{\frac{s}{2}} |A|^s \right\|_{\mathfrak{S}^{\frac{2}{s}}}^2 \left\| |A|^{1-s} \Gamma^{\frac{1-s}{2}} \right\|_{\mathfrak{S}^{\frac{2}{1-s}}}^2 \\
 &= \left(\text{Tr} \left(\Gamma^{\frac{s}{2}} |A|^{2s} \Gamma^{\frac{s}{2}} \right)^{\frac{1}{s}} \right)^{2s} \left(\text{Tr} \left(\Gamma^{\frac{1-s}{2}} |A|^{2(1-s)} \Gamma^{\frac{1-s}{2}} \right)^{\frac{1}{1-s}} \right)^{2(1-s)} \\
 &\leq \text{Tr} \left(\Gamma^{1/2} A^2 \Gamma^{1/2} \right) = \text{Tr} (A^2 \Gamma). \tag{7.9}
 \end{aligned}$$

Next, we claim that, denoting $H = -\log \Gamma$,

$$\begin{aligned}
 &\text{Var}_{\Gamma}^{(s)}(A) \\
 &= \text{Var}_{\Gamma}^{(0)}(A) - \frac{1}{2} \int_0^1 \int_0^1 \text{Tr} \left([A, H] \Gamma^{st_1 + (1-s)t_2} [A, H] \Gamma^{s(1-t_1) + (1-s)(1-t_2)} \right) dt_1 dt_2 \\
 &= \text{Var}_{\Gamma}^{(0)}(A) - \frac{1}{2} \int_0^1 \int_0^1 \text{Var}_{\Gamma}^{(st_1 + (1-s)t_2)}(i[A, H]) dt_1 dt_2 \tag{7.10}
 \end{aligned}$$

In the right side one should understand

$$\text{Tr} \left([A, H] \Gamma^{\alpha} [A, H] \Gamma^{1-\alpha} \right) = \left\| \Gamma^{\frac{\alpha}{2}} [A, H] \Gamma^{\frac{1-\alpha}{2}} \right\|_{\mathfrak{S}^2}^2,$$

where $\alpha = st_1 + (1-s)t_2$. For $\alpha \in (0, 1)$, $\log \Gamma$ is always multiplied by some Γ^t with $t > 0$, which defines a bounded operator and gives a clear meaning to the commutator. It follows from (7.7) that the integral in the second line of (7.10) is finite. To express it as an s -variance, we have used in the last line of (7.10) that $\text{Tr}([A, \log \Gamma]\Gamma) = 0$.

To obtain the first equality (7.10) we remark that

$$\text{Tr} \left(A e^{-sH} A e^{-(1-s)H} \right) = \text{Tr} (A^2 e^{-H}) + \frac{1}{2} \text{Tr} \left([A, e^{-sH}] [A, e^{-(1-s)H}] \right).$$

Inserting the formula

$$[X, e^Y] = - \int_0^1 \partial_t \left(e^{tY} X e^{(1-t)Y} \right) dt = \int_0^1 e^{tY} [X, Y] e^{(1-t)Y} dt \tag{7.11}$$

in the last term and using the cyclicity of the trace gives (7.10). Finally, applying (7.7) with $A \rightsquigarrow [A, H]$ in the second line of (7.10) and recalling that

$$\text{Tr}([A, H]\Gamma) = -\text{Tr}([A, \log \Gamma]\Gamma) = 0$$

yields the lower bound in (7.8). □

It turns out that $\text{Var}_{\Gamma}^{\text{av}}(A)$ appears naturally when $\Gamma = e^{-H}$ is a Gibbs state and we consider the family of states

$$\Gamma_{\varepsilon} := \frac{e^{-H+\varepsilon A}}{\text{Tr}(e^{-H+\varepsilon A})}$$

obtained by perturbing the underlying Hamiltonian H by $-\varepsilon A$ for a small ε . In that respect, $\text{Var}_{\Gamma}^{\text{av}}(A)$ is a (static) response function, and the following lemma is the form of the fluctuation/dissipation theorem appropriate for quantum systems:

Lemma 7.4 (Averaged quantum s -variance = linear response).

Let H be a self-adjoint operator on a separable Hilbert space \mathfrak{K} such that $\mathrm{Tr}[e^{-sH}] < \infty$ for any $s > 0$. Let A be another self-adjoint operator, which we assume to be H -bounded. Then the function

$$\varepsilon \mapsto \mathrm{Tr}(A\Gamma_\varepsilon) = \frac{\mathrm{Tr}(Ae^{-H+\varepsilon A})}{\mathrm{Tr}(e^{-H+\varepsilon A})} \quad (7.12)$$

is C^1 in a neighborhood of the origin and we have

$$\frac{d}{d\varepsilon} \mathrm{Tr}(A\Gamma_\varepsilon) = \mathrm{Var}_{\Gamma_\varepsilon}^{\mathrm{av}}(A), \quad (7.13)$$

the averaged variance introduced in (7.6). In particular,

$$\frac{d}{d\varepsilon} \mathrm{Tr}(A\Gamma_\varepsilon)|_{\varepsilon=0} = \mathrm{Var}_{\Gamma}^{\mathrm{av}}(A) \quad (7.14)$$

Remark 7.5 (Linear response function).

The result (7.14) is well-known in linear response theory, see [75, Chapter 4] or [74]. Hints in this direction also are in [46, Section 2.10]. Note that what we call ‘‘averaged quantum variance’’ is exactly the ‘‘canonical correlation’’ of [75].

We also have, from the Feynman-Hellmann principle, that $\mathrm{Var}_{\Gamma}^{\mathrm{av}}(A)$ is the second derivative of minus the free-energy:

$$\mathrm{Var}_{\Gamma}^{\mathrm{av}}(A) = \left. \frac{d^2}{d\varepsilon^2} \log \mathrm{Tr}(e^{-H+\varepsilon A}) \right|_{\varepsilon=0}$$

but this is not going to be useful in our proof. Also note that the positivity of $\mathrm{Var}_{\Gamma}^{\mathrm{av}}(A)$ (which we have just derived by other means) is a consequence of the simple fact that (7.12) is an increasing function of ε , as follows from using Gibbs’ variational principle. \diamond

Proof. Under the assumption that A is H -bounded, that is $A^2 \leq aH^2 + b$, we have by the Kato-Rellich theorem $D(H - \varepsilon A) = D(H)$ for ε small enough. In addition, A and H are $(H - \varepsilon A)$ -bounded. In particular, we deduce that $H - \varepsilon A \geq \alpha H - \beta$ for a small constant α . This proves that

$$\mathrm{Tr}\left(e^{-s(H-\varepsilon A)}\right) \leq C \mathrm{Tr}\left(e^{-s\alpha H}\right)$$

is finite for all $s > 0$. Then,

$$\begin{aligned} \mathrm{Tr}(A^2 e^{-H+\varepsilon A}) &\leq \mathrm{Tr}((aH^2 + b)e^{-H+\varepsilon A}) \\ &\leq \mathrm{Tr}((a'(H - \varepsilon A)^2 + b')e^{-H+\varepsilon A}) \\ &\leq C \mathrm{Tr}\left(e^{-\frac{H-\varepsilon A}{2}}\right) \leq C' \mathrm{Tr}\left(e^{-\frac{\alpha}{2}H}\right) \end{aligned}$$

is finite as well. The claim (7.13) is a consequence of Duhamel’s formula

$$\frac{d}{d\varepsilon} e^{X(\varepsilon)} = \int_0^1 e^{sX(\varepsilon)} \frac{dX(\varepsilon)}{d\varepsilon} e^{(1-s)X(\varepsilon)} ds. \quad (7.15)$$

Indeed, we have

$$\frac{d}{d\varepsilon} \mathrm{Tr}(e^{-H+\varepsilon A}) = \int_0^1 \mathrm{Tr}\left(e^{-s(H-\varepsilon A)} A e^{-(1-s)(H-\varepsilon A)}\right) ds = \mathrm{Tr}(Ae^{-H+\varepsilon A})$$

by the cyclicity of the trace and

$$\frac{d}{d\varepsilon} \text{Tr}(Ae^{-H+\varepsilon A}) = \int_0^1 \text{Tr} \left(Ae^{-s(H-\varepsilon A)} A e^{-(1-s)(H-\varepsilon A)} \right) ds.$$

The formula (7.13) follows. □

We can now describe the main ideas of the proof of Theorem 7.1. We introduce the perturbed state

$$\Gamma_{\lambda,\varepsilon} = \frac{1}{\mathcal{Z}_{\lambda,\varepsilon}} \exp \left(-\frac{1}{T} \mathbb{H}_{\lambda,\varepsilon} \right), \quad \mathbb{H}_{\lambda,\varepsilon} = \mathbb{H}_\lambda - \varepsilon d\Gamma(e_k^+) \tag{7.16}$$

where the partition function $\mathcal{Z}_{\lambda,\varepsilon}$ normalizes the trace. This is well-defined when ε is sufficiently small, by Lemma 7.4, because $d\Gamma(e_k^+)$ is \mathcal{N} -bounded, hence \mathbb{H}_λ -bounded. Our idea is to first prove that

$$T^{-2} \left\langle \left| d\Gamma(e_k^+) - \langle d\Gamma(e_k^+) \rangle_\lambda \right|^2 \right\rangle_\lambda = \text{Var}_{\Gamma_\lambda}^0 (d\Gamma(e_k^+/T)) \simeq \text{Var}_{\Gamma_\lambda}^{\text{av}} (d\Gamma(e_k^+/T))$$

namely, to replace $s = 0$ by the uniform average over all $s \in [0, 1]$. This amounts to estimating the remainder in the left side of (7.8). It being small reflects the semi-classical nature of the regime we study: it will carry a prefactor $1/T^4$ and, importantly, it involves a commutator $[d\Gamma(e_k^+), \mathbb{H}_\lambda]$, ensuring that the estimate does not deteriorate too fast with the particle number (see Lemma 7.8).

Now, by Lemma 7.4, the averaged variance $\text{Var}_{\Gamma_\lambda}^{\text{av}} (d\Gamma(e_k^+/T))$ is the ε -derivative of a one-body term, amenable to Feynman-Hellmann-based estimates. Using Lemma 6.8 we can prove that for the observables of interest (living on high momenta), the function that gets differentiated is almost constant. That the function is close to a constant pointwise does not guarantee that its derivative is small, but we can conclude the proof using a rather rough bound bearing on the second derivative.

Remark 7.6. Note that $d\Gamma(e_k^+)$ is not a bounded operator. However, like \mathbb{H}_λ , it commutes with \mathcal{N} and on each n -particle sector, $d\Gamma(e_k^+)_{|\mathfrak{H}^{\otimes n}}$ is indeed bounded. The results of this section are therefore easily applicable to $\mathbb{A} = d\Gamma(e_k^+)$, after summing over n . ◇

7.2. From variance to linear response. Here is the first main ingredient of the proof of Theorem 7.1.

Lemma 7.7 (High momenta variance \sim linear response).

Let e_k^+ be as in Theorem 7.1. Assume that $h > 0$ satisfies $\text{Tr}(h^{-p}) < \infty$ for some $1 < p \leq 2$. Define $\Gamma_{\lambda,\varepsilon}$ as in (7.16) with $\mathbb{A} = d\Gamma(e_k^+)$, and denote by $\langle \cdot \rangle_{\lambda,\varepsilon}$ the corresponding expectation values. Then for $\lambda^{-1} \sim T$ sufficiently large, we have

$$\left| T^{-2} \left\langle \left| \mathbb{A} - \langle \mathbb{A} \rangle_{\lambda,0} \right|^2 \right\rangle_{\lambda,0} - T^{-1} \partial_\varepsilon \left(\langle \mathbb{A} \rangle_{\lambda,\varepsilon} \right) \Big|_{\varepsilon=0} \right| \leq C(1 + |k|^2)^2 \left(T^{2p-3} + T^{2(2p-3)} \right). \tag{7.17}$$

Note that the result also holds for non-zero, small enough ε , but we shall not need it. Also, for $p \leq 3/2$ as in the statement of Theorem 7.1, the term T^{2p-3} is dominant. As anticipated, our main task is to estimate the commutator appearing in the left side of (7.8). This is the only place where we use the commutator condition in (3.46).

Lemma 7.8 (Commutator estimate).

Assume that $h > 0$ satisfies (3.46) and $\text{Tr}(h^{-p}) < \infty$ for some $1 < p \leq 2$. We have

$$|[\text{d}\Gamma(e_k^+), \mathbb{H}_\lambda]|^2 \leq C(1 + |k|^2)^2 \left(\text{d}\Gamma(h)\mathcal{N} + T^{-2}\mathcal{N}^4 + T^{2p-2}\mathcal{N}^2 \right)$$

Proof. By the Cauchy-Schwarz inequality we have

$$\begin{aligned} 0 \leq |[\text{d}\Gamma(e_k^+), \mathbb{H}_\lambda]|^2 &= -[\text{d}\Gamma(e_k^+), \mathbb{H}_\lambda]^2 = -[\text{d}\Gamma(e_k^+), \text{d}\Gamma(h) + \lambda\mathbb{W}^{\text{ren}}]^2 \\ &\leq -2[\text{d}\Gamma(e_k^+), \text{d}\Gamma(h)]^2 - 2\lambda^2[\text{d}\Gamma(e_k^+), \mathbb{W}^{\text{ren}}]^2. \end{aligned}$$

To bound the commutator with \mathbb{W}^{ren} , we use that operators acting on different variables commute: recalling the expression (3.42)-(3.43)

$$\begin{aligned} [\text{d}\Gamma(e_k^+), \mathbb{W}^{\text{ren}}] &= [\text{d}\Gamma(e_k^+), \mathbb{W}] - 2[\text{d}\Gamma(e_k^+), \text{d}\Gamma(w * \varrho_0)] \\ &= \frac{1}{2} \bigoplus_{n \in \mathbb{N}} \sum_{1 \leq i \neq j \leq n} ((e_k^+)_j w(x_i - x_j) - w(x_i - x_j)(e_k^+)_j) \\ &\quad - 2 \bigoplus_{n \in \mathbb{N}} \sum_{j=1}^N ((e_k^+)_j (w * \varrho_0)(x_j) - (w * \varrho_0)(x_j)(e_k^+)_j). \end{aligned}$$

Since w is bounded and

$$\|w * \varrho_0\|_{L^\infty} \leq \|w\|_{L^\infty} \|\varrho_0\|_{L^1} = \|w\|_{L^\infty} \langle \mathcal{N} \rangle_0 \leq CT^p$$

by (6.14), we deduce that

$$\pm i [\text{d}\Gamma(e_k^+), \mathbb{W}^{\text{ren}}] \leq C(\mathcal{N}^2 + T^p \mathcal{N}).$$

Then since \mathcal{N} commutes with $i[\text{d}\Gamma(e_k^+), \mathbb{W}^{\text{ren}}]$, we can square the latter estimate and obtain

$$-\lambda^2[\text{d}\Gamma(e_k^+), \mathbb{W}^{\text{ren}}]^2 \leq C(T^{-2}\mathcal{N}^4 + T^{2p-2}\mathcal{N}^2)$$

Next, observe that for any pair of one-body observables

$$[\text{d}\Gamma(A), \text{d}\Gamma(B)] = \text{d}\Gamma([A, B])$$

and moreover, by Cauchy-Schwarz,

$$\begin{aligned} \text{d}\Gamma(A)^2 &= \text{d}\Gamma(A^2) + \bigoplus_{n \geq 2} \sum_{1 \leq i \neq j \leq n} A_i A_j \\ &\leq \text{d}\Gamma(A^2) + \frac{1}{2} \bigoplus_{n \geq 2} \sum_{1 \leq i \neq j \leq n} (A_i^2 + A_j^2) = \mathcal{N} \text{d}\Gamma(A^2). \end{aligned}$$

Thus

$$0 \leq -[\text{d}\Gamma(e_k^+), \text{d}\Gamma(h)]^2 \leq \mathcal{N} \text{d}\Gamma(-[e_k^+, h]^2).$$

Moreover, from Assumption (3.46) and the fact that h commutes with the projections P, Q , we have the one-body inequality

$$0 \leq -[e_k^+, h]^2 \leq C(1 + |k|^2)^2 h$$

Thus

$$0 \leq -[\text{d}\Gamma(e_k^+), \text{d}\Gamma(h)]^2 \leq (1 + |k|^2)^2 \text{d}\Gamma(h)\mathcal{N}.$$

This ends the proof. \square

We now have all the ingredients to complete the

Proof of Lemma 7.7. By (7.8) we have

$$\left| T^{-2} \left\langle \left| \mathbb{A} - \langle \mathbb{A} \rangle_{\lambda,0} \right|^2 \right\rangle_{\lambda,0} - T^{-1} \partial_\varepsilon \left(\langle \mathbb{A} \rangle_{\lambda,\varepsilon} \right) \Big|_{\varepsilon=0} \right| \leq \frac{1}{2T^4} \langle |[\mathbb{A}, \mathbb{H}_\lambda]|^2 \rangle_\lambda.$$

To be precise, the results of Section 7.1 were for simplicity stated for a bounded observable. Following Remark 7.6, we can however apply the estimate (7.8) in each n -particle sector separately and then sum over n . By Lemma 7.8, we have

$$|[\mathbb{A}, \mathbb{H}_\lambda]|^2 \leq C(1 + |k|^2)^2 (\mathcal{N} d\Gamma(h) + T^{-2} \mathcal{N}^4 + T^{2p-2} \mathcal{N}^2). \quad (7.18)$$

Taking the expectation value in the Gibbs state and inserting the a-priori estimates of Lemma 6.10 give

$$\left| T^{-2} \left\langle \left| \mathbb{A} - \langle \mathbb{A} \rangle_{\lambda,0} \right|^2 \right\rangle_{\lambda,0} - T^{-1} \partial_\varepsilon \left(\langle \mathbb{A} \rangle_{\lambda,\varepsilon} \right) \Big|_{\varepsilon=0} \right| \leq \frac{C(1 + |k|^2)^2}{T^4} (T^{2p+1} + T^{4p-2}).$$

□

7.3. Rough estimates on higher order correlations. Now we turn to the second ingredient of the proof of Theorem 7.1, namely a rough bound on some sort of “higher-order correlation”. In our approach, this will refer (perhaps improperly) to the second derivative⁸ in ε of $\langle d\Gamma(e_k^+) \rangle_{\lambda,\varepsilon}$.

Lemma 7.9 (Bound on a higher-order correlation).

Assume that $h > 0$ satisfies $\text{Tr}(h^{-p}) < \infty$ for some $1 < p \leq 2$. For any $\varepsilon > 0$ small enough (independently of T) and $\lambda^{-1} \sim T$ sufficiently large,

$$\left| T^{-1} \partial_\varepsilon^2 \langle d\Gamma(e_k^+) \rangle_{\lambda,\varepsilon} \right| \leq CT^{3(p-1)}. \quad (7.19)$$

Proof. Recall that

$$\mathcal{Z}_{\lambda,\varepsilon} = \text{Tr} \left[e^{-\frac{1}{T} \mathbb{H}_{\lambda,\varepsilon}} \right], \quad \mathbb{H}_{\lambda,\varepsilon} = \mathbb{H}_\lambda - \varepsilon \mathbb{A}, \quad \mathbb{A} = d\Gamma(e_k^+).$$

From the Feynman-Hellmann principle we get

$$T^{-1} \langle \mathbb{A} \rangle_{\lambda,\varepsilon} = -\partial_\varepsilon \log \mathcal{Z}_{\lambda,\varepsilon}$$

and thus

$$\partial_\varepsilon^2 (T^{-1} \langle \mathbb{A} \rangle_{\lambda,\varepsilon}) = \partial_\varepsilon^2 \left(\frac{\partial_\varepsilon \mathcal{Z}_{\lambda,\varepsilon}}{\mathcal{Z}_{\lambda,\varepsilon}} \right) = \frac{\partial_\varepsilon^3 \mathcal{Z}_{\lambda,\varepsilon}}{\mathcal{Z}_{\lambda,\varepsilon}} - 3 \frac{(\partial_\varepsilon \mathcal{Z}_{\lambda,\varepsilon})(\partial_\varepsilon^2 \mathcal{Z}_{\lambda,\varepsilon})}{\mathcal{Z}_{\lambda,\varepsilon}^2} + 2 \frac{(\partial_\varepsilon \mathcal{Z}_{\lambda,\varepsilon})^3}{\mathcal{Z}_{\lambda,\varepsilon}^3} \quad (7.20)$$

where, by (7.15),

$$\begin{aligned} \partial_\varepsilon \mathcal{Z}_{\lambda,\varepsilon} &= T^{-1} \text{Tr} \left[\mathbb{A} e^{-\frac{s}{T} \mathbb{H}_{\lambda,\varepsilon}} \right], \\ \partial_\varepsilon^2 \mathcal{Z}_{\lambda,\varepsilon} &= T^{-2} \int_0^1 \text{Tr} \left[\mathbb{A} e^{-\frac{s}{T} \mathbb{H}_{\lambda,\varepsilon}} \mathbb{A} e^{-\frac{(1-s)}{T} \mathbb{H}_{\lambda,\varepsilon}} \right] ds, \\ \partial_\varepsilon^3 \mathcal{Z}_{\lambda,\varepsilon} &= 2T^{-3} \int_0^1 \int_0^1 \text{Tr} \left[\mathbb{A} e^{-\frac{st}{T} \mathbb{H}_{\lambda,\varepsilon}} \mathbb{A} e^{-\frac{s(1-t)}{T} \mathbb{H}_{\lambda,\varepsilon}} \mathbb{A} e^{-\frac{(1-s)}{T} \mathbb{H}_{\lambda,\varepsilon}} \right] ds dt. \end{aligned}$$

⁸Thus the third derivative of the free energy.

We shall estimate separately the absolute value of each term on the right side of (7.20). Let us discuss for instance the first one. Since \mathcal{N} commutes with \mathbb{A} and $\mathbb{H}_{\lambda,\varepsilon}$, we can write

$$\begin{aligned} & \text{Tr} \left[\mathbb{A} e^{-\frac{st}{T} \mathbb{H}_{\lambda,\varepsilon}} \mathbb{A} e^{-\frac{s(1-t)}{T} \mathbb{H}_{\lambda,\varepsilon}} \mathbb{A} e^{-\frac{(1-s)}{T} \mathbb{H}_{\lambda,\varepsilon}} \right] \\ &= \text{Tr} \left[(\mathbb{A} \mathcal{N}^{-1}) \mathcal{N}^{3st} e^{-\frac{st}{T} \mathbb{H}_{\lambda,\varepsilon}} (\mathbb{A} \mathcal{N}^{-1}) \mathcal{N}^{3s(1-t)} e^{-\frac{s(1-t)}{T} \mathbb{H}_{\lambda,\varepsilon}} (\mathbb{A} \mathcal{N}^{-1}) \mathcal{N}^{3(1-s)} e^{-\frac{(1-s)}{T} \mathbb{H}_{\lambda,\varepsilon}} \right]. \end{aligned}$$

Here we have used

$$st + s(1-t) + (1-s) = 1.$$

Then using the Hölder inequality in Schatten spaces as in (7.9) we have

$$\begin{aligned} & \left| \text{Tr} \left[\mathbb{A} e^{-\frac{st}{T} \mathbb{H}_{\lambda,\varepsilon}} \mathbb{A} e^{-\frac{s(1-t)}{T} \mathbb{H}_{\lambda,\varepsilon}} \mathbb{A} e^{-\frac{(1-s)}{T} \mathbb{H}_{\lambda,\varepsilon}} \right] \right| \\ & \leq \left\| (\mathbb{A} \mathcal{N}^{-1}) \mathcal{N}^{3st} e^{-\frac{st}{T} \mathbb{H}_{\lambda,\varepsilon}} \right\|_{\mathfrak{S}^{\frac{1}{st}}} \left\| (\mathbb{A} \mathcal{N}^{-1}) \mathcal{N}^{3s(1-t)} e^{-\frac{s(1-t)}{T} \mathbb{H}_{\lambda,\varepsilon}} \right\|_{\mathfrak{S}^{\frac{1}{s(1-t)}}} \times \\ & \quad \times \left\| (\mathbb{A} \mathcal{N}^{-1}) \mathcal{N}^{3(1-s)} e^{-\frac{(1-s)}{T} \mathbb{H}_{\lambda,\varepsilon}} \right\|_{\mathfrak{S}^{\frac{1}{1-s}}} \\ & \leq \|\mathbb{A} \mathcal{N}^{-1}\|^3 \left\| \mathcal{N}^{3st} e^{-\frac{st}{T} \mathbb{H}_{\lambda,\varepsilon}} \right\|_{\mathfrak{S}^{\frac{1}{st}}} \left\| \mathcal{N}^{3s(1-t)} e^{-\frac{s(1-t)}{T} \mathbb{H}_{\lambda,\varepsilon}} \right\|_{\mathfrak{S}^{\frac{1}{s(1-t)}}} \left\| \mathcal{N}^{3(1-s)} e^{-\frac{(1-s)}{T} \mathbb{H}_{\lambda,\varepsilon}} \right\|_{\mathfrak{S}^{\frac{1}{1-s}}} \\ & \leq \text{Tr}[\mathcal{N}^3 e^{-\frac{1}{T} \mathbb{H}_{\lambda,\varepsilon}}]. \end{aligned}$$

We also used that $\|\mathbb{A} \mathcal{N}^{-1}\| \leq 1$ and $[\mathcal{N}, \mathbb{H}_{\lambda,\varepsilon}] = 0$ in the last step. The bounds on moments of the particle number from Lemma 6.9 extend straightforwardly to the perturbed Gibbs state (for ε small enough), and it follows that

$$\left| \frac{\partial_\varepsilon^3 \mathcal{Z}_{\lambda,\varepsilon}}{\mathcal{Z}_{\lambda,\varepsilon}} \right| \leq 2T^{-3} \langle \mathcal{N}^3 \rangle_{\lambda,\varepsilon} \leq CT^{3(p-1)}.$$

This concludes the estimate for the first term of (7.20). Using the same method for the other terms completes the proof of the lemma. \square

7.4. Proof of Theorem 7.1. Let us denote

$$f(\varepsilon) := T^{-1} \langle d\Gamma(e_k^+) \rangle_{\lambda,\varepsilon}.$$

From Lemma 7.7 we have

$$\left| T^{-2} \left\langle \left| d\Gamma(e_k^+) - \langle d\Gamma(e_k^+) \rangle_\lambda \right|^2 \right\rangle_\lambda - f'(0) \right| \leq C(1 + |k|^2)^2 T^{2p-3}.$$

To control $f'(0)$ we will use Taylor's expansion

$$f(\varepsilon) - f(0) = \varepsilon f'(0) + \frac{\varepsilon^2}{2} f''(\theta_\varepsilon), \quad \theta_\varepsilon \in [0, \varepsilon]. \quad (7.21)$$

The second derivative is controlled by Lemma 7.7

$$|f''(\theta_\varepsilon)| \leq CT^{3(p-1)}$$

for $\varepsilon > 0$ sufficiently small. The left side of (7.21) can be bounded using Lemma 6.8. First observe that

$$\|h^{-\alpha} e_k^+ h^{-\alpha}\| \leq C \|Qh^{-\alpha}\| \leq C \Lambda_e^{-\alpha}, \quad (7.22)$$

where Λ_e is the cut-off entering in (7.1). Picking $\alpha = (2 - p)/4$ and using the bound from Lemma 6.8 (which holds uniformly in ε for ε small) we can write

$$\begin{aligned} |f(\varepsilon) - T^{-1} \langle d\Gamma(e_k^+) \rangle_{0,\varepsilon}| &= T^{-1} \left| \text{Tr} \left[e_k^+ (\Gamma_{\lambda,\varepsilon}^{(1)} - \Gamma_{0,\varepsilon}^{(1)}) \right] \right| \\ &\leq \frac{\|h^{-\alpha} e_k^+ h^{-\alpha}\|}{T} \text{Tr} \left| h^\alpha (\Gamma_\lambda^{(1)} - \Gamma_0^{(1)}) h^\alpha \right| \leq C \Lambda_e^{\frac{p-2}{4}} \end{aligned} \quad (7.23)$$

On the other hand, since $\langle d\Gamma(e_k^+) \rangle_{0,\varepsilon}$ is an expectation in a free Gibbs state, we may compute explicitly, then use Lemma 6.3 and (7.22) to obtain

$$\begin{aligned} T^{-1} |\langle d\Gamma(e_k^+) \rangle_{0,\varepsilon} - \langle d\Gamma(e_k^+) \rangle_{0,0}| &= T^{-1} \varepsilon^{-1} \text{Tr} \left(\varepsilon e_k^+ \left(\frac{1}{e^{(h-\varepsilon e_k^+)/T} - 1} - \frac{1}{e^{h/T} - 1} \right) \right) \\ &\leq C \varepsilon \text{Tr} \left(\frac{1}{h} e_k^+ \frac{1}{h} e_k^+ \right) \leq C \varepsilon \Lambda_e^{(p-2)/2}, \end{aligned}$$

using that h^{-1} is Hilbert-Schmidt, $p \leq 2$, and

$$\text{Tr} \left(\frac{Q}{h^2} \right) \leq \Lambda_e^{p-2} \text{Tr} (h^{-p}).$$

Thus

$$|f(\varepsilon) - f(0)| \leq C (\Lambda_e^{(p-2)/4} + \varepsilon \Lambda_e^{(p-2)/2})$$

for $\varepsilon > 0$ sufficiently small. In summary, we conclude from (7.21) that

$$|f'(0)| \leq \varepsilon^{-1} |f(\varepsilon) - f(0)| + \frac{\varepsilon}{2} |f''(\theta_\varepsilon)| \leq C \varepsilon^{-1} \Lambda_e^{(p-2)/4} + C \varepsilon T^{3(p-1)} + C \Lambda_e^{(p-2)/2}.$$

Optimizing over $\varepsilon > 0$ we obtain

$$|f'(0)| \leq C T^{3(p-1)/2} \Lambda_e^{(p-2)/8} + C \Lambda_e^{(p-2)/2}.$$

Thus we conclude that

$$\left| T^{-2} \left\langle \left| d\Gamma(e_k^+) - \langle d\Gamma(e_k^+) \rangle_{\lambda,\varepsilon} \right|^2 \right\rangle_{\lambda,\varepsilon} \right| \leq C(1 + |k|^2)^2 T^{2p-3} + C T^{3(p-1)/2} \Lambda_e^{(p-2)/8} + C \Lambda_e^{(p-2)/2}$$

as desired. □

8. FREE ENERGY LOWER BOUND

We are now ready to prove the free energy lower bound leading to (3.4). As usual in variational approaches, the lower bound on the free energy is the harder part. A matching upper bound will be obtained in the next section by a trial state argument.

Consider $\mathbb{H}_\lambda = \mathbb{H}_0 + \lambda \mathbb{W}^{\text{ren}}$. Recall that we can write directly the relative free-energy as an infimum:

$$\begin{aligned} \frac{F_\lambda - F_0}{T} &= -\log \frac{\mathcal{Z}_\lambda}{\mathcal{Z}_0} = \mathcal{H}(\Gamma_\lambda, \Gamma_0) + T^{-2} \text{Tr}[\mathbb{W}^{\text{ren}} \Gamma_\lambda] \\ &= \inf_{\Gamma \geq 0, \text{Tr}_F \Gamma = 1} (\mathcal{H}(\Gamma, \Gamma_0) + T^{-2} \text{Tr}[\mathbb{W}^{\text{ren}} \Gamma_\lambda]). \end{aligned}$$

where \mathcal{H} is the von Neumann relative entropy. We shall relate this variational principle to its classical analogue (cf. Section 5.1)

$$-\log z_r = \inf \left\{ \int f(u) d\mu_0(u) + \int f(u) \log(f(u)) d\mu_0(u) \mid f \in L^1(d\mu_0), \int f(u) d\mu_0(u) = 1 \right\}.$$

This section is devoted to the proof of the following

Proposition 8.1 (Free-energy lower bound).

Let $h > 0$ satisfy (3.46) and $\text{Tr}(h^{-p}) < \infty$ with p as in (3.49), that is,

$$1 < p < p_c = \frac{\sqrt{673} - 1}{24}.$$

Let z_r be the classical relative partition function defined in Lemma 5.3. In the limit $T \rightarrow \infty, \lambda T \rightarrow 1$ we have

$$\frac{F_\lambda - F_0}{T} = -\log \frac{\mathcal{Z}_\lambda}{\mathcal{Z}_0} \geq -\log z_r - CT^{-\frac{14-12p^2-p}{15p+18}}. \quad (8.1)$$

Note that the last exponent is negative under the stated condition on p .

We split the proof in two parts, occupying a subsection each. The core novelty with respect to our previous papers [83, 85] is to be found in Section 8.1, where the correlation estimates of Section 7 are used. We project the energy (together with counter-terms) on low momentum modes and estimate the error thus made. Combining with the quantitative de Finetti Theorem 5.8 this leads to a quantitative energy lower bound in terms of the projected classical energy of a de Finetti measure. The proof is then concluded in Section 8.2 where we

- rely on Theorem 5.9 to control the relative entropy as in our previous papers, obtaining a projected classical free-energy as a lower bound;
- remove the localization in the so-obtained classical problem.

8.1. Localization and energy lower bound. Recall the projections on low or high kinetic energy modes from Section 7

$$P = \mathbb{1}_{h \leq \Lambda_e}, \quad Q = \mathbb{1} - P. \quad (8.2)$$

Note that we have

$$K := \dim(P\mathfrak{H}) = \text{Tr} P \leq \text{Tr}[(\Lambda_e/h)^p] \leq C\Lambda_e^p. \quad (8.3)$$

Our energy lower bound is as follows:

Lemma 8.2 (Renormalized energy lower bound).

Let $h > 0$ satisfy

$$\text{Tr}(h^{-p}) < \infty, \quad \text{for } 1 < p \leq 3/2$$

and let $1 \leq \Lambda_e \leq T$. Then we have

$$T^{-2} \text{Tr}[\mathbb{W}^{\text{ren}}\Gamma_\lambda] \geq \frac{1}{2} \int_{P\mathfrak{H}} \mathcal{D}_K[u] d\mu_{P,\lambda}(u) - C \left(T^{-1} \Lambda_e^{2p-1} + T^{\frac{61p-65}{32}} \Lambda_e^{\frac{2-p}{128}} + T^{\frac{3(p-1)}{4}} \Lambda_e^{-\frac{2-p}{16}} + T^{-\frac{3(p-1)}{4}} \Lambda_e^{-\frac{7(2-p)}{16}} \right) \quad (8.4)$$

where $\mu_{P,\lambda}$ is the lower symbol/Husimi function of Γ_λ associated with the projection P and the scale $\varepsilon = T^{-1}$ (as in Definition 5.7) as in (5.24), and \mathcal{D}_K is the truncated renormalized interaction from Lemma 5.3.

We have made all error terms in (8.4) explicit for convenience. The worst error term will turn out to be $T^{3(p-1)/4} \Lambda_e^{-(2-p)/16}$.

Proof. We write the renormalized interaction as in (3.42) and estimate each Fourier component separately.

Step 1: Localization. As in Section 7, denote e_k the multiplication operator by either $\cos(k \cdot x)$ or $\sin(k \cdot x)$, and let

$$e_k^- = P e_k P, \quad e_k^+ = e_k - e_k^-.$$

We write

$$d\Gamma(e_k) - \langle d\Gamma(e_k) \rangle_0 = A + A_1 + A_2 \tag{8.5}$$

with

$$A = d\Gamma(e_k^-) - \langle d\Gamma(e_k^-) \rangle_0, \quad A_1 = d\Gamma(e_k^+) - \langle d\Gamma(e_k^+) \rangle_\lambda, \quad A_2 = \langle d\Gamma(e_k^+) \rangle_\lambda - \langle d\Gamma(e_k^+) \rangle_0$$

and use the Cauchy-Schwarz inequality

$$(1 + \varepsilon)(A + A_1 + A_2)^2 \geq A^2 - 2\varepsilon^{-1}A_1^2 - 2\varepsilon^{-1}A_2^2$$

for all $\varepsilon > 0$. Then we take the expectation value in the interacting Gibbs state. We have, using Theorem 7.1,

$$T^{-2} \text{Tr}[A_1^2 \Gamma_\lambda] \leq C(1 + |k|^2)^2 T^{2p-3} + CT^{3(p-1)/2} \Lambda_e^{(p-2)/8}$$

and, by arguing as in (7.23),

$$T^{-2} |A_2|^2 = T^{-2} \left| \text{Tr} \left[e_k^+ (\Gamma_\lambda^{(1)} - \Gamma_0^{(1)}) \right] \right|^2 \leq C \Lambda_e^{(p-2)/2}.$$

Thus

$$(1 + \varepsilon) T^{-2} \left\langle |d\Gamma(e_k) - \langle d\Gamma(e_k) \rangle_0|^2 \right\rangle_\lambda \geq T^{-2} \left\langle |d\Gamma(e_k^-) - \langle d\Gamma(e_k^-) \rangle_0|^2 \right\rangle_\lambda - C\varepsilon^{-1} \left[(1 + |k|^2)^2 T^{2p-3} + T^{3(p-1)/2} \Lambda_e^{(p-2)/8} + \Lambda_e^{(p-2)/2} \right]. \tag{8.6}$$

If we integrate over k and assume that $\int_{\Omega^*} |\widehat{w}(k)| (1 + |k|^2)^2 dk < \infty$, then we get a similar error term for the interaction energy. It turns out that (after optimizing over Λ_e) the coefficient T^{2p-3} is much smaller than the other error terms, so we will use a slightly more convoluted argument and separate low and large momenta with a parameter L . This will allow us to relax a bit the assumption on w to (3.48) used in the main theorem, that is,

$$\int_{\Omega^*} |\widehat{w}(k)| (1 + |k|^{1/2}) dk < \infty.$$

Integrating (8.6) against $\widehat{w}(k)$ for $|k| \leq L$, then using (3.42) for the left side and using the last condition in (3.30) for the right side, we obtain

$$(1 + \varepsilon) T^{-2} \int_{\Omega^*} \widehat{w}(k) \left\langle |d\Gamma(e_k) - \langle d\Gamma(e_k) \rangle_0|^2 \right\rangle dk \geq \frac{1}{2T^2} \int_{|k| \leq L} \widehat{w}(k) \left\langle |d\Gamma(e_k^-) - \langle d\Gamma(e_k^-) \rangle_0|^2 \right\rangle_\lambda dk - C\varepsilon^{-1} \left(L^{7/2} T^{2p-3} + T^{3(p-1)/2} \Lambda_e^{(p-2)/8} + \Lambda_e^{(p-2)/2} \right) \tag{8.7}$$

for

$$\int_{|k| \geq L} |\widehat{w}(k)| (1 + |k|^2)^2 dk \leq CL^{7/2} \int_{\Omega^*} |\widehat{w}(k)| (1 + |k|^{1/2}) dk.$$

On the other hand, by (3.30) again and Lemma 6.9,

$$\begin{aligned} & \frac{1}{2T^2} \int_{|k| \geq L} \widehat{w}(k) \left\langle \left| d\Gamma(e_k^-) - \langle d\Gamma(e_k^-) \rangle_0 \right|^2 \right\rangle_\lambda dk \\ & \leq \frac{1}{2T^2} \int_{\Omega^*} \widehat{w}(k) \left(\frac{(1+|k|)}{L} \right)^{1/2} (\langle \mathcal{N}^2 \rangle_\lambda + \langle \mathcal{N}^2 \rangle_0) dk \leq CT^{2p-2}L^{-1/2}. \end{aligned} \quad (8.8)$$

Putting (8.7) and (8.8) together we get

$$\begin{aligned} (1+\varepsilon)T^{-2} \operatorname{Tr}[\mathbb{W}^{\text{ren}}\Gamma_\lambda] & \geq \frac{1}{2T^2} \int \widehat{w}(k) \left\langle \left| d\Gamma(e_k^-) - \langle d\Gamma(e_k^-) \rangle_0 \right|^2 \right\rangle_\lambda dk \\ & \quad - C\varepsilon^{-1} \left(L^{7/2}T^{2p-3} + T^{3(p-1)/2}\Lambda_e^{(p-2)/8} + \Lambda_e^{(p-2)/2} \right) - CT^{2p-2}L^{-1/2}. \end{aligned} \quad (8.9)$$

Then choosing $L = (T\varepsilon)^{1/4}$ we arrive at

$$\begin{aligned} (1+\varepsilon)T^{-2} \operatorname{Tr}[\mathbb{W}^{\text{ren}}\Gamma_\lambda] & \geq \frac{1}{2T^2} \int \widehat{w}(k) \left\langle \left| d\Gamma(e_k^-) - \langle d\Gamma(e_k^-) \rangle_0 \right|^2 \right\rangle_\lambda dk \\ & \quad - C\varepsilon^{-1} \left(\varepsilon^{7/8}T^{(16p-17)/8} + T^{3(p-1)/2}\Lambda_e^{(p-2)/8} + \Lambda_e^{(p-2)/2} \right) \end{aligned} \quad (8.10)$$

for all $\varepsilon \in (0, 1)$. From (4.2) and (6.23) we see that $T^{-2} \operatorname{Tr}[\mathbb{W}^{\text{ren}}\Gamma_\lambda]$ is bounded. Consequently,

$$\begin{aligned} T^{-2} \operatorname{Tr}[\mathbb{W}^{\text{ren}}\Gamma_\lambda] & \geq \frac{1}{2T^2} \int \widehat{w}(k) \left\langle \left| d\Gamma(e_k^-) - \langle d\Gamma(e_k^-) \rangle_0 \right|^2 \right\rangle_\lambda dk \\ & \quad - C\varepsilon - C\varepsilon^{-1} \left(\varepsilon^{7/8}T^{(16p-17)/8} + T^{3(p-1)/2}\Lambda_e^{(p-2)/8} + \Lambda_e^{(p-2)/2} \right) \end{aligned}$$

for all $\varepsilon \in (0, 1)$. We optimize over ε the sum of the smallest and largest error terms

$$-C\varepsilon - C\varepsilon^{-1}T^{3(p-1)/2}\Lambda_e^{(p-2)/8},$$

finding $\varepsilon = T^{3(p-1)/4}\Lambda_e^{(p-2)/16}$. Hence

$$\begin{aligned} T^{-2} \operatorname{Tr}[\mathbb{W}^{\text{ren}}\Gamma_\lambda] & \geq \frac{1}{2T^2} \int \widehat{w}(k) \left\langle \left| d\Gamma(e_k^-) - \langle d\Gamma(e_k^-) \rangle_0 \right|^2 \right\rangle_\lambda dk \\ & \quad - C \left(T^{\frac{61p-65}{32}}\Lambda_e^{\frac{2-p}{128}} + T^{\frac{3(p-1)}{4}}\Lambda_e^{-\frac{2-p}{16}} + T^{-\frac{3(p-1)}{4}}\Lambda_e^{-\frac{7(2-p)}{16}} \right). \end{aligned} \quad (8.11)$$

The worse error term will be $T^{\frac{3(p-1)}{4}}\Lambda_e^{\frac{p-2}{16}}$. The last error already tends to 0 since $p \leq 2$.

Remark 8.3 (Refinement in the homogeneous case).

In the homogeneous case (Theorem 3.1), we only assumed in (3.3) that

$$\sum_{k \in \Omega^*} |\widehat{w}(k)|(1+|k|)^\alpha dk < \infty$$

for some $\alpha > 0$. In this case, the error terms $L^{4-1/2}T^{2p-3}$ in (8.7) and $T^{2p-2}L^{-1/2}$ in (8.7) will be replaced by $L^{4-\alpha}T^{2p-3}$ and $T^{2p-2}L^{-\alpha}$, respectively. Then optimizing over $L > 0$ gives the error $T^{2p-2-\alpha/4}$ (instead of $T^{(16p-17)/8}$ in (8.10)). This error can still be made small if $\alpha > 0$, for in the homogeneous case $\operatorname{Tr}(h^{-p}) < \infty$ for every $p > 1$ and we are thus at

liberty to insert any such p in the estimate. This is the only difference between the proofs of Theorem 3.5 and Theorem 3.1. \diamond

Step 2: Use of the de Finetti theorem. Now we turn to the low-momentum part of the interaction. For any self-adjoint one-body operator A we have

$$d\Gamma(A)^2 = 2 \bigoplus_{n \geq 2} \sum_{1 \leq i < j \leq n} A_i \otimes A_j + d\Gamma(A^2).$$

Hence

$$\begin{aligned} \left\langle \left| d\Gamma(e_k^-) - \langle d\Gamma(e_k^-) \rangle_0 \right|^2 \right\rangle_\lambda &= 2 \operatorname{Tr} \left((e_k^-)^{\otimes 2} \Gamma_\lambda^{(2)} \right) - 2 \operatorname{Tr} \left(e_k^- \Gamma_\lambda^{(1)} \right) \operatorname{Tr} \left(e_k^- \Gamma_0^{(1)} \right) \\ &\quad + \left(\operatorname{Tr} \left(e_k^- \Gamma_0^{(1)} \right) \right)^2 + \operatorname{Tr} \left((e_k^-)^2 \Gamma_\lambda^{(1)} \right). \end{aligned} \quad (8.12)$$

The last term $\operatorname{Tr} \left((e_k^-)^2 \Gamma_\lambda^{(1)} \right) \geq 0$ can be omitted for a lower bound. From the explicit formulas (6.12) and (5.2), the operator bound

$$\left| \frac{1}{e^{h/T} - 1} - \frac{T}{h} \right| \leq \frac{1}{2}$$

and (8.3), it follows that

$$\begin{aligned} T^{-1} \operatorname{Tr} \left(e_k^- \Gamma_0^{(1)} \right) &= T^{-1} \operatorname{Tr} \left(e_k^- \frac{1}{e^{h/T} - 1} \right) \\ &= \operatorname{Tr} \left(e_k^- h^{-1} \right) + T^{-1} \operatorname{Tr} \left(e_k^- \left(\frac{1}{e^{h/T} - 1} - \frac{T}{h} \right) \right) \\ &= \left\langle \langle u, e_k^- u \rangle \right\rangle_{\mu_0} + O(T^{-1} \Lambda_e^p) \end{aligned} \quad (8.13)$$

On the other hand, using (6.26), (2.18) and Hölder's inequality in Schatten spaces we get

$$T^{-1} \operatorname{Tr} \left(e_k^- \Gamma_\lambda^{(1)} \right) \leq C \operatorname{Tr} \left(P h^{-1} \right) \leq C \Lambda_e^{p-1} \operatorname{Tr} \left(h^{-p} \right) \quad (8.14)$$

Thus (8.12) gives

$$\begin{aligned} T^{-2} \left\langle \left| d\Gamma(e_k^-) - \langle d\Gamma(e_k^-) \rangle_0 \right|^2 \right\rangle_\lambda &\geq 2T^{-2} \operatorname{Tr} \left((e_k^-)^{\otimes 2} \Gamma_\lambda^{(2)} \right) - 2T^{-1} \operatorname{Tr} \left(e_k^- \Gamma_\lambda^{(1)} \right) \left\langle \langle u, e_k^- u \rangle \right\rangle_{\mu_0} \\ &\quad + \left\langle \langle u, e_k^- u \rangle \right\rangle_{\mu_0}^2 - C \left(T^{-1} \Lambda_e^{2p-1} + T^{-2} \Lambda_e^{2p} \right). \end{aligned} \quad (8.15)$$

Note that, for $\Lambda_e \leq T$ the last error term is of lower order.

Next, let $\mu_{P,\lambda}$ be the lower symbol of Γ_λ associated with the projection P and the scale $\varepsilon = T^{-1}$ as in (5.24). We apply (5.26) to obtain the density matrices of the P -projected state $\Gamma_{\lambda,P}$:

$$\begin{aligned} T^{-2} \Gamma_{\lambda,P}^{(2)} &= \frac{1}{2} \int_{P\mathfrak{H}} |u^{\otimes 2}\rangle \langle u^{\otimes 2}| d\mu_{P,\lambda}(u) - 2T^{-2} \Gamma_{\lambda,P}^{(1)} \otimes_s P - 2T^{-2} P \otimes_s P, \\ T^{-1} \Gamma_{\lambda,P}^{(1)} &= \int_{P\mathfrak{H}} |u\rangle \langle u| d\mu_{P,\lambda}(u) - T^{-1} P. \end{aligned}$$

Recalling (5.20) we have

$$\Gamma_{\lambda,P}^{(k)} = P^{\otimes k} \Gamma_\lambda^{(k)} P^{\otimes k}$$

and using (8.14), we deduce that

$$\begin{aligned} T^{-2} \operatorname{Tr} \left[(e_k^-)^{\otimes 2} \Gamma_\lambda^{(2)} \right] &= \frac{1}{2} \int_{P\mathfrak{H}} |\langle u, e_k^- u \rangle|^2 d\mu_{P,\lambda}(u) + O(T^{-1} \Lambda_e^{2p-1}), \\ T^{-1} \operatorname{Tr} \left[e_k^- \Gamma_\lambda^{(1)} \right] &= \int_{P\mathfrak{H}} \langle u, e_k^- u \rangle d\mu_{P,\lambda}(u) + O(T^{-1} \Lambda_e^p). \end{aligned}$$

Inserting the latter formulas in (8.15) and using (8.14) again we obtain

$$\begin{aligned} T^{-2} \left\langle \left| d\Gamma(e_k^-) - \langle d\Gamma(e_k^-) \rangle_0 \right|_\lambda^2 \right\rangle &\geq \int_{P\mathfrak{H}} \left| \langle u, e_k^- u \rangle - \langle \langle u, e_k^- u \rangle \rangle_{\mu_0} \right|^2 d\mu_{P,\lambda}(u) \\ &\quad - CT^{-1} \Lambda_e^{2p-1}. \end{aligned} \quad (8.16)$$

Integrating (8.16) against $\widehat{w}(k)$ and comparing with (8.11) yields our final bound

$$\begin{aligned} T^{-2} \operatorname{Tr}[\mathbb{W}^{\text{ren}} \Gamma_\lambda] &\geq \frac{1}{2} \int_{P\mathfrak{H}} \mathcal{D}_K[u] d\mu_{P,\lambda}(u) \\ &\quad - C \left(T^{-1} \Lambda_e^{2p-1} + T^{\frac{61p-65}{32}} \Lambda_e^{\frac{2-p}{128}} + T^{\frac{3(p-1)}{4}} \Lambda_e^{-\frac{2-p}{16}} + T^{-\frac{3(p-1)}{4}} \Lambda_e^{-\frac{7(2-p)}{16}} \right) \end{aligned} \quad (8.17)$$

where \mathcal{D}_K is the truncated renormalized interaction as in Lemma 5.3. This concludes the proof of Lemma 8.2. \square

8.2. Removing the localization and concluding. Now let us denote by $\mu_{P,0}$ the lower symbol of the free Gibbs state Γ_0 associated with P and the scale $\varepsilon = T^{-1}$ as in (5.24). By the Berezin-Lieb inequality (5.28), we have

$$\mathcal{H}(\Gamma_\lambda, \Gamma_0) \geq \mathcal{H}((\Gamma_\lambda)_P, (\Gamma_0)_P) \geq \mathcal{H}_{\text{cl}}(\mu_{P,\lambda}, \mu_{P,0}). \quad (8.18)$$

Putting (8.4) and (8.18) together, we conclude by the classical variational principle (4.3) that

$$\begin{aligned} -\log \frac{\mathcal{Z}_\lambda}{\mathcal{Z}_0} &= \mathcal{H}(\Gamma_\lambda, \Gamma_0) + T^{-2} \operatorname{Tr}[\mathbb{W}^{\text{ren}} \Gamma_\lambda] \\ &\geq \mathcal{H}_{\text{cl}}(\mu_{P,\lambda}, \mu_{P,0}) + \frac{1}{2} \int_{P\mathfrak{H}} \mathcal{D}_K[u] d\mu_{P,\lambda}(u) - \text{Err} \\ &\geq -\log \left(\int_{P\mathfrak{H}} e^{-\mathcal{D}_K[u]} d\mu_{P,0}(u) \right) - \text{Err} \end{aligned} \quad (8.19)$$

where Err is the error term in (8.4).

In order to estimate further the right side of (8.19) from below, our task is now to compare the lower symbol $\mu_{P,0}$ of Γ_0 with the cylindrical projection $\mu_{0,K}$ of the free Gibbs measure μ_0 on $P\mathfrak{H}$ in Lemma 5.1. In this direction we prove the following lemma. For its statement, recall that both measures we are interested in are absolutely continuous with respect to the Lebesgue measure on $P\mathfrak{H}$.

Lemma 8.4 (Further comparisons for the projected free state).

Assume that $h > 0$ satisfies $\operatorname{Tr}(h^{-p}) < \infty$ for some $p \geq 1$. Then,

$$\|\mu_{P,0} - \mu_{0,K}\|_{L^1(P\mathfrak{H})} \leq 2 \operatorname{Tr}[h^{-p}] T^{-1} \Lambda_e^{p+1}. \quad (8.20)$$

Proof. Recall that

$$d\mu_{0,K}(u) = \prod_{j=1}^K \left(\frac{\lambda_j}{\pi} e^{-\lambda_j |\alpha_j|^2} \right) d\alpha_j, \quad \text{with} \quad u = \sum_{j=1}^K \alpha_j u_j.$$

On the other hand, by Definition 5.7, and the explicit action of Fock-space localization on quasi-free states [79, Example 12]

$$\begin{aligned} d\mu_{P,0}(u) &= (T/\pi)^K \left\langle \xi(\sqrt{T}u) \middle| (\Gamma_0)_P \middle| \xi(\sqrt{T}u) \right\rangle du \\ &= (T/\pi)^K \left[\text{Tr} \left(e^{-d\Gamma(P_h)/T} \right) \right]^{-1} \left\langle \xi(\sqrt{T}u) \middle| e^{-d\Gamma(P_h)/T} \middle| \xi(\sqrt{T}u) \right\rangle du. \end{aligned}$$

Using the Peierls-Bogoliubov inequality $\langle x, e^{Ax} \rangle \geq e^{\langle x, Ax \rangle}$ and the coherent states' definition (5.21), we have

$$\begin{aligned} \left\langle \xi(\sqrt{T}u) \middle| e^{-d\Gamma(P_h)/T} \middle| \xi(\sqrt{T}u) \right\rangle &\geq \exp \left[- \left\langle \xi(\sqrt{T}u) \middle| d\Gamma(P_h/T) \middle| \xi(\sqrt{T}u) \right\rangle \right] \\ &= \exp [-\langle u, Ph u \rangle] = \exp \left[- \sum_{j=1}^K \lambda_j |\alpha_j|^2 \right]. \end{aligned}$$

Combining with the explicit formula for the free partition function (c.f. (6.1)), we arrive at

$$\mu_{P,0}(u) \geq \prod_{j=1}^K \left[\frac{T}{\lambda_j} (1 - e^{-\lambda_j/T}) \right] \mu_{0,K}(u). \quad (8.21)$$

Using

$$\frac{1 - e^{-t}}{t} \geq 1 - \frac{t}{2}, \quad \forall t > 0$$

and Bernoulli's inequality, recalling (8.3) we can estimate

$$\prod_{j=1}^K \left[\frac{T}{\lambda_j} (1 - e^{-\lambda_j/T}) \right] \geq \prod_{j=1}^K \left(1 - \frac{\lambda_j}{2T} \right) \geq 1 - \frac{\Lambda_e K}{2T} \geq 1 - \frac{\text{Tr}[h^{-p}] \Lambda_e^{p+1}}{T}. \quad (8.22)$$

Thus

$$\mu_{P,0}(u) \geq \left(1 - \text{Tr}[h^{-p}] T^{-1} \Lambda_e^{p+1} \right) \mu_{0,K}(u), \quad (8.23)$$

which implies

$$(\mu_{P,0} - \mu_{0,K})_-(u) \leq \text{Tr}[h^{-p}] T^{-1} \Lambda_e^{p+1} \mu_{0,K}(u)$$

where $f_- = \max(-f, 0)$ is the negative part. Integrating over $u \in P\mathfrak{H}$ we find

$$\int_{P\mathfrak{H}} (\mu_{P,0} - \mu_{0,K})_- \leq \text{Tr}[h^{-p}] T^{-1} \Lambda_e^{p+1}.$$

Notice then that

$$0 = \int_{P\mathfrak{H}} (\mu_{P,0} - \mu_{0,K}) = \int_{P\mathfrak{H}} (\mu_{P,0} - \mu_{0,K})_+ - \int_{P\mathfrak{H}} (\mu_{P,0} - \mu_{0,K})_-$$

so we get as announced that

$$\int_{P\mathfrak{H}} |\mu_{P,0} - \mu_{0,K}| \leq 2 \text{Tr}[h^{-p}] T^{-1} \Lambda_e^{p+1}.$$

□

With the above lemma we now conclude the

Proof of Proposition 8.1. Using Lemma 8.4 and the fact that $\mathcal{D}_K[u] \geq 0$, we can estimate

$$\int_{P\mathfrak{H}} e^{-\mathcal{D}_K[u]} d\mu_{P,0}(u) \leq 2 \operatorname{Tr}(h^{-p}) T^{-1} \Lambda_e^{p+1} + \int_{P\mathfrak{H}} e^{-\mathcal{D}_K[u]} d\mu_{0,K}(u). \quad (8.24)$$

Inserting this bound in the right side of (8.19), we arrive at the lower bound

$$-\log \frac{\mathcal{Z}_\lambda}{\mathcal{Z}_0} \geq -\log \left(\int_{P\mathfrak{H}} e^{-\mathcal{D}_K[u]} d\mu_{0,K}(u) + CT^{-1} \Lambda_e^{p+1} \right) - \operatorname{Err} \quad (8.25)$$

where Err is the error term in (8.17). Moreover, note that when $T \rightarrow \infty$, we have $K \rightarrow \infty$ since $\Lambda_e \rightarrow \infty$, and hence $\mathcal{D}_K[u] \rightarrow \mathcal{D}[u]$ in $L^1(\mu_0)$ by Lemma 5.3. Consequently,

$$\lim_{T \rightarrow \infty} \int_{P\mathfrak{H}} e^{-\mathcal{D}_K[u]} d\mu_{0,K}(u) = \int e^{-\mathcal{D}[u]} d\mu_0(u) \quad (8.26)$$

by the dominated convergence Theorem. Using the fact that $\log(1+t) = O(t)$ for $|t|$ small, we obtain

$$-\log \left(\int_{P\mathfrak{H}} e^{-\mathcal{D}_K[u]} d\mu_{0,K}(u) + CT^{-1} \Lambda_e^{p+1} \right) \geq -\log \left(\int_{P\mathfrak{H}} e^{-\mathcal{D}_K[u]} d\mu_{0,K}(u) \right) - CT^{-1} \Lambda_e^{p+1}.$$

Thus our final lower bound is

$$\begin{aligned} & -\log \frac{\mathcal{Z}_\lambda}{\mathcal{Z}_0} \geq -\log \left(\int_{P\mathfrak{H}} e^{-\mathcal{D}_K[u]} d\mu_{0,K}(u) \right) \\ & - C \left(T^{-1} \Lambda_e^{p+1} + T^{-1} \Lambda_e^{2p-1} + T^{\frac{61p-65}{32}} \Lambda_e^{\frac{2-p}{128}} + T^{\frac{3(p-1)}{4}} \Lambda_e^{-\frac{2-p}{16}} + T^{-\frac{3(p-1)}{4}} \Lambda_e^{-\frac{7(2-p)}{16}} \right). \end{aligned} \quad (8.27)$$

After inspection one sees that the smallest and largest terms to optimize are

$$T^{-1} \Lambda_e^{p+1} + T^{\frac{3(p-1)}{4}} \Lambda_e^{-\frac{2-p}{16}},$$

which provides the value

$$\boxed{\Lambda_e = T^{\frac{4(3p+1)}{15p+18}}} \quad (8.28)$$

and an error term going to zero under the condition that

$$\frac{4(3p+1)}{15p+18}(p+1) < 1$$

which is equivalent to $12p^2 + p - 14 < 0$, or

$$\boxed{p < p_c = \frac{\sqrt{673} - 1}{24} \simeq 1.039.}$$

This is the condition (3.49). For this choice of Λ_e and this constraint on p , all the other terms are negligible, which yields the final inequality

$$-\log \frac{\mathcal{Z}_\lambda}{\mathcal{Z}_0} \geq -\log \left(\int_{P\mathfrak{H}} e^{-\mathcal{D}_K[u]} d\mu_{0,K}(u) \right) - CT^{-\eta} \quad (8.29)$$

with

$$\boxed{\eta := \frac{14 - 12p^2 - p}{15p + 18} > 0.} \quad (8.30)$$

The desired lower bound (8.1) follows. \square

9. FREE ENERGY UPPER BOUND

Now we complete the proof of (3.4) by providing a free-energy upper bound which complements Proposition 8.1:

Proposition 9.1 (Free-energy upper bound).

Let h satisfy (3.45)-(3.46) with p as in (3.49). Let z_r be the classical relative partition function defined in Lemma 5.3. In the limit $T \rightarrow \infty, \lambda T \rightarrow 1$ we have

$$-\log \frac{Z_\lambda}{Z_0} = \frac{F_\lambda - F_0}{T} \leq -\log z_r + CT^{-\frac{14-12p^2-p}{15p+18}} \quad (9.1)$$

This part is easier than the free-energy lower bound. We rely on the variational principle and simply evaluate the free-energy of a suitable trial state. We split the proof into two main steps:

- *Reduction to a finite-dimensional estimate, Section 9.1.* Our trial state coincides with the free Gibbs states on high kinetic energy modes, and with a projected finite-dimensional interacting Gibbs state on low modes. We prove that the calculation of its free-energy reduces to that of the projected state, up to affordable errors. This is fairly similar to the analysis in Sections 7 and 8.1, but somewhat simpler. Some details will thus be skipped.
- *Finite-dimensional semi-classics, Section 9.2.* Once we are reduced to treating a problem posed in a finite dimensional one-particle space, we are on more familiar terrain [89, 121, 73, 54], see e.g. [109, 110, Appendix B]. We provide a proof of the needed free-energy upper bound for self-containedness and because we need to keep track of the dependence on the finite, but large, dimension.

9.1. Reduction to a finite-dimensional estimate. We use similar low- and high-kinetic energy projectors as previously:

$$P = \mathbb{1}_{h \leq \Lambda_e}, \quad Q = 1 - P, \quad \Lambda_e \text{ given by (8.28).}$$

Let us define the interacting Gibbs state in $\mathcal{F}(P\mathfrak{H})$:

$$\Gamma_{\lambda, P} = \frac{e^{-(d\Gamma(P)h + \lambda \mathbb{W}_P^{\text{ren}})/T}}{\text{Tr}_{\mathcal{F}(P\mathfrak{H})} e^{-(d\Gamma(P)h + \lambda \mathbb{W}_P^{\text{ren}})/T}} \quad (9.2)$$

where $\mathbb{W}_P^{\text{ren}}$ is the localized interaction⁹

$$\begin{aligned}\mathbb{W}_P^{\text{ren}} &= \frac{1}{2} \int_{\mathbb{R}^2} \widehat{w}(k) \left| \text{d}\Gamma(Pe^{ik \cdot x} P) - \left\langle \text{d}\Gamma(Pe^{ik \cdot x} P) \right\rangle_0 \right|^2 dk \\ &= \frac{1}{2} \int_{\mathbb{R}^2} \widehat{w}(k) \left| \text{d}\Gamma(P \cos(k \cdot x) P) - \left\langle \text{d}\Gamma(P \cos(k \cdot x) P) \right\rangle_0 \right|^2 dk \\ &\quad + \frac{1}{2} \int_{\mathbb{R}^2} \widehat{w}(k) \left| \text{d}\Gamma(P \sin(k \cdot x) P) - \left\langle \text{d}\Gamma(P \sin(k \cdot x) P) \right\rangle_0 \right|^2 dk.\end{aligned}\tag{9.3}$$

Note that $\Gamma_{\lambda,P}$ does not coincide with the state $(\Gamma_\lambda)_P$ obtained by P -localizing the full interacting Gibbs state, except in the non-interacting case

$$\Gamma_{\lambda=0,P} = (\Gamma_0)_P.$$

Let

$$F_\lambda^P := -T \log \left(\text{Tr} \left(e^{-(\text{d}\Gamma(P_h) + \lambda \mathbb{W}_P^{\text{ren}})/T} \right) \right)$$

be the free-energy of the P -localized problem.

In this subsection we prove the following, which reduces the proof of Proposition 9.1 to an estimate on the corresponding problem of finite dimensional sets in $P\mathfrak{H}$.

Lemma 9.2 (Reduction to low kinetic energy modes).

Let $h > 0$ satisfy $\text{Tr}(h^{-p}) < \infty$ with p as in (3.49) and Λ_ϵ given by (8.28). Then

$$\begin{aligned}-\log \frac{\mathcal{Z}_\lambda}{\mathcal{Z}_0} &= \frac{F_\lambda - F_0}{T} \leq \mathcal{H}(\Gamma_{\lambda,P}, (\Gamma_0)_P) + T^{-2} \text{Tr}[\mathbb{W}_P^{\text{ren}} \Gamma_{\lambda,P}] + CT^{3(p-1)/4} \Lambda_\epsilon^{(p-2)/16}. \\ &= \frac{F_\lambda^P - F_0^P}{T} + CT^{3(p-1)/4} \Lambda_\epsilon^{(p-2)/16}.\end{aligned}\tag{9.4}$$

Before proving this we interject the

Lemma 9.3 (Entropy relative to a product state).

Let \mathfrak{H}_1 and \mathfrak{H}_2 be two complex separable Hilbert spaces. Let A be a state on $\mathfrak{H}_1 \otimes \mathfrak{H}_2$ with the partial traces $A_1 = \text{Tr}_{\mathfrak{H}_2} A$, $A_2 = \text{Tr}_{\mathfrak{H}_1} A$ and let B_1, B_2 be states on $\mathfrak{H}_1, \mathfrak{H}_2$. Then

$$\mathcal{H}(A, B_1 \otimes B_2) = \mathcal{H}(A, A_1 \otimes A_2) + \mathcal{H}(A_1, B_1) + \mathcal{H}(A_2, B_2).$$

Proof. Writing the spectral decompositions of B_1, B_2 one can easily see that

$$\log(B_1 \otimes B_2) = \log(B_1) \otimes \mathbf{1} + \mathbf{1} \otimes \log(B_2)$$

and thus we can write

$$\begin{aligned}\mathcal{H}(A, B_1 \otimes B_2) &= \text{Tr} (A(\log A - \log(B_1 \otimes B_2))) \\ &= \text{Tr} (A(\log A - \log(A_1 \otimes A_2))) + \text{Tr} (A(\log(A_1) \otimes \mathbf{1} - \log(B_1) \otimes \mathbf{1})) \\ &\quad + \text{Tr} (A(\mathbf{1} \otimes \log(A_2) - \mathbf{1} \otimes \log(B_2))) \\ &= \mathcal{H}(A, A_1 \otimes A_2) + \mathcal{H}(A_1, B_1) + \mathcal{H}(A_2, B_2).\end{aligned}$$

□

⁹Note that the expectation $\langle \text{d}\Gamma(Pe^{ik \cdot x} P) \rangle_0$ in Γ_0 is the same as that in $(\Gamma_0)_P$.

Proof of Lemma 9.2. In the last identity of (9.4) we use fact that $(\Gamma_0)_P$ and $\Gamma_{\lambda,P}$ are the free and interacting Gibbs states in $\mathcal{F}(P\mathfrak{H})$, similarly as in (4.2). The inequality is proved by a trial state argument.

Step 1: Trial state. Using the unitary (5.18), we define

$$\tilde{\Gamma} = \mathcal{U}^* \Gamma_{\lambda,P} \otimes (\Gamma_0)_Q \mathcal{U} \quad (9.5)$$

where $\Gamma_{\lambda,P}$ is as in (9.2) and $(\Gamma_0)_Q$ is the Q -localization of the free Gibbs state, cf Definition 5.5. Importantly, from (5.19) and (2.8) one shows that

$$\tilde{\Gamma}^{(1)} = P\Gamma_{\lambda,P}^{(1)}P + Q\Gamma_0^{(1)}Q \quad (9.6)$$

and

$$\tilde{\Gamma}^{(2)} = P^{\otimes 2}\Gamma_{\lambda,P}^{(2)}P^{\otimes 2} + Q^{\otimes 2}\Gamma_0^{(2)}Q^{\otimes 2} + \left(\Gamma_{\lambda,P}^{(1)} \otimes Q\Gamma_0^{(1)}Q + Q\Gamma_0^{(1)}Q \otimes \Gamma_{\lambda,P}^{(1)} \right). \quad (9.7)$$

Also, since the relative entropy is unaffected by the partial isometry and the free Gibbs state is factorized,

$$\Gamma_0 = \mathcal{U}^*(\Gamma_0)_P \otimes (\Gamma_0)_Q \mathcal{U},$$

we obtain from Lemma 9.3 that

$$\begin{aligned} \mathcal{H}(\tilde{\Gamma}, \Gamma_0) &= \text{Tr} [\Gamma_{\lambda,P} \otimes (\Gamma_0)_Q (\log (\Gamma_{\lambda,P} \otimes (\Gamma_0)_Q) - \log ((\Gamma_0)_P \otimes (\Gamma_0)_Q))] \\ &= \mathcal{H}(\Gamma_{\lambda,P}, (\Gamma_0)_P). \end{aligned}$$

Hence, by the variational principle (4.2)

$$-\log \frac{\mathcal{Z}_\lambda}{\mathcal{Z}_0} \leq \mathcal{H}(\tilde{\Gamma}, \Gamma_0) + T^{-2} \text{Tr}[\mathbb{W}^{\text{ren}}\tilde{\Gamma}] = \mathcal{H}(\Gamma_{\lambda,P}, (\Gamma_0)_P) + T^{-2} \text{Tr}[\mathbb{W}^{\text{ren}}\tilde{\Gamma}]$$

and there remains to evaluate the energy of the trial state.

Step 2: Bound on the renormalized energy. We finish the proof of (9.4) with the following claim:

$$T^{-2} \text{Tr}[\mathbb{W}^{\text{ren}}\tilde{\Gamma}] \leq T^{-2} \text{Tr}[\mathbb{W}_P^{\text{ren}}\Gamma_{\lambda,P}] + CT^{3(p-1)/4}\Lambda_e^{(p-2)/16}. \quad (9.8)$$

This is very similar in spirit to Lemma 8.2 and we shall skip some details for brevity. In particular, since $(\Gamma_0)_P$ and $\Gamma_{\lambda,P}$ are the free and the interacting Gibbs states in the Fock space $\mathcal{F}(P\mathfrak{H})$, we can adapt to them (with the same proofs) most of the bounds on Γ_0 and Γ_λ we used previously.

First, using (9.6) and arguing as for the proof of (6.28), we have

$$\text{Tr} \left| h^\alpha (\tilde{\Gamma}^{(1)} - \Gamma_0^{(1)}) h^\alpha \right| = \text{Tr} \left| h^\alpha (\Gamma_{\lambda,P}^{(1)} - (\Gamma_0)_P^{(1)}) h^\alpha \right| \leq CT \quad (9.9)$$

with $\alpha = (2-p)/4$ as in Lemma 6.8. Consequently, if we use again the notation

$$e_k^- = Pe_kP, \quad e_k^+ = e_k - e_k^-$$

with e_k being either $\cos(k \cdot x)$ or $\sin(k \cdot x)$, then similarly to (7.23) we have

$$T^{-1} \text{Tr} \left[d\Gamma(e_k^+) (\tilde{\Gamma} - \Gamma_0) \right] = T^{-1} \text{Tr} [e_k^+ (\tilde{\Gamma}^{(1)} - \Gamma_0^{(1)})] \leq C\Lambda_e^{-\alpha}. \quad (9.10)$$

Also, following the proof of Theorem 7.1, we obtain the variance estimate

$$T^{-2} \text{Tr} \left[\left| d\Gamma(e_k^+) - \text{Tr}[d\Gamma(e_k^+)\tilde{\Gamma}] \right|^2 \tilde{\Gamma} \right] \leq C(1 + |k|^2)^2 T^{2p-3} + CT^{3(p-1)/2}\Lambda_e^{(p-2)/8},$$

and hence, by combining with (9.10),

$$T^{-2} \operatorname{Tr} \left[\left| d\Gamma(e_k^+) - \langle d\Gamma(e_k^+) \rangle_0 \right|^2 \tilde{\Gamma} \right] \leq C(1 + |k|^2)^2 T^{2p-3} + CT^{3(p-1)/2} \Lambda_e^{(p-2)/8}. \quad (9.11)$$

By using the Cauchy-Schwarz inequality

$$\left| d\Gamma(e_k) - \langle d\Gamma(e_k) \rangle_0 \right|^2 \leq (1 + \delta) \left| d\Gamma(e_k^-) - \langle d\Gamma(e_k^-) \rangle_0 \right|^2 + (1 + \delta^{-1}) \left| d\Gamma(e_k^+) - \langle d\Gamma(e_k^+) \rangle_0 \right|^2$$

we find that

$$\begin{aligned} T^{-2} \operatorname{Tr} \left[\left| d\Gamma(e_k) - \langle d\Gamma(e_k) \rangle_0 \right|^2 \tilde{\Gamma} \right] &\leq (1 + \delta) T^{-2} \operatorname{Tr} \left[\left| d\Gamma(e_k^-) - \langle d\Gamma(e_k^-) \rangle_0 \right|^2 \tilde{\Gamma} \right] \\ &\quad + C(1 + \delta^{-1}) \left((1 + |k|^2)^2 T^{2p-3} + T^{3(p-1)/2} \Lambda_e^{(p-2)/8} \right). \end{aligned} \quad (9.12)$$

Next, we integrate (9.12) against $\hat{w}(k)$ for $|k| \leq L$, then use (3.42) for the left side and use

$$\int \hat{w}(k) \operatorname{Tr} \left[\left| d\Gamma(e_k^-) - \langle d\Gamma(e_k^-) \rangle_0 \right|^2 \tilde{\Gamma} \right] dk = \operatorname{Tr} [\mathbb{W}_P^{\text{ren}} \Gamma_{\lambda, P}]$$

for the right side, and finally optimize over L similarly as in (8.10). We conclude that

$$T^{-2} \operatorname{Tr} \left[\mathbb{W}^{\text{ren}} \tilde{\Gamma} \right] \leq (1 + \delta) T^{-2} \operatorname{Tr} [\mathbb{W}_P^{\text{ren}} \Gamma_{\lambda, P}] + CT^{3(p-1)/2} \Lambda_e^{(p-2)/8} \quad (9.13)$$

There only remains to note that $T^{-2} \operatorname{Tr} [\mathbb{W}_P^{\text{ren}} \Gamma_{\lambda, P}]$ is bounded uniformly in T . This follows by inserting the trial state $(\Gamma_0)_P$ in a variational formula similar to (4.2), and the fact that $\mathbb{W}_P^{\text{ren}} \geq 0$. The desired result (9.8) thus follows from (9.13) by optimizing over $\delta > 0$. \square

9.2. Finite-dimensional semi-classics. The missing ingredient for the proof of Proposition (9.1) is the analysis of the partition functions in $\mathcal{F}(P\mathfrak{H})$ appearing in the right-hand side of (9.4). We have

Lemma 9.4 (Finite-dimensional semi-classics).

Let $h > 0$ satisfy $\operatorname{Tr}(h^{-p}) < \infty$ with p as in (3.49) and Λ_e given by (8.28). Then

$$\frac{F_\lambda^P - F_0^P}{T} \leq -\log \left(\int_{P\mathfrak{H}} e^{-\mathcal{D}_K[u]} d\mu_{0, K}(u) \right) + CT^{-1} \Lambda_e^{p+1}, \quad (9.14)$$

where \mathcal{D}_K is the truncated renormalized interaction from Lemma 5.3.

Proof. Recall that (6.1) yields

$$\operatorname{Tr} e^{-d\Gamma(P_h)/T} = \prod_{j=1}^K \frac{1}{1 - e^{-\lambda_j/T}} \quad (9.15)$$

where $\{\lambda_j\}_{j=1}^K$ are the eigenvalues of $P_h P$ and that

$$\frac{F_\lambda^P - F_0^P}{T} = -\log \frac{\operatorname{Tr} e^{-(d\Gamma(P_h) + \lambda \mathbb{W}_P^{\text{ren}})/T}}{\operatorname{Tr} e^{-d\Gamma(P_h)/T}}.$$

To estimate the interacting partition function in the right-hand side, we use (a rescaled version of) the coherent-state resolution of the identity (5.25):

$$(T/\pi)^K \int_{P\mathfrak{H}} \left| \xi(\sqrt{T}u) \right\rangle \left\langle \xi(\sqrt{T}u) \right| du = \mathbf{1}_{\mathcal{F}(P\mathfrak{H})}$$

and the Peierls-Bogoliubov inequality $\langle x, e^A x \rangle \geq e^{\langle x, Ax \rangle}$ to obtain

$$\begin{aligned} \mathrm{Tr} e^{-(d\Gamma(P_h) + \lambda \mathbb{W}_P^{\mathrm{ren}})/T} &= (T/\pi)^K \int_{P\mathfrak{H}} \mathrm{Tr} \left[e^{-(d\Gamma(P_h) + \lambda \mathbb{W}_P^{\mathrm{ren}})/T} \left| \xi(\sqrt{T}u) \right\rangle \left\langle \xi(\sqrt{T}u) \right| \right] du \\ &= (T/\pi)^K \int_{P\mathfrak{H}} \left\langle \xi(\sqrt{T}u), e^{-(d\Gamma(P_h) + \lambda \mathbb{W}_P^{\mathrm{ren}})/T} \xi(\sqrt{T}u) \right\rangle du \\ &\geq (T/\pi)^K \int_{P\mathfrak{H}} \exp \left[- \left\langle \xi(\sqrt{T}u), \frac{d\Gamma(P_h) + \lambda \mathbb{W}_P^{\mathrm{ren}}}{T} \xi(\sqrt{T}u) \right\rangle \right] du. \end{aligned} \quad (9.16)$$

Then, for $u \in P\mathfrak{H}$, similarly as in the proof of Lemma 8.4

$$\left\langle \xi(\sqrt{T}u), \frac{d\Gamma(P_h)}{T} \xi(\sqrt{T}u) \right\rangle = \langle u, hu \rangle.$$

Moreover, calculating as in (8.12) and recalling (5.23), (8.13) we have

$$\begin{aligned} &\left\langle \xi(\sqrt{T}u), \frac{|d\Gamma(e_k^-) - \langle d\Gamma(e_k^-) \rangle_0|^2}{T^2} \xi(\sqrt{T}u) \right\rangle \\ &= \langle u, e_k^- u \rangle^2 - 2T^{-1} \langle u, e_k^- u \rangle \mathrm{Tr} \left[e_k^- \Gamma_0^{(1)} \right] + T^{-2} \left(\mathrm{Tr} \left[e_k^- \Gamma_0^{(1)} \right] \right)^2 + T^{-1} \langle u, (e_k^-)^2 u \rangle \\ &\leq (\langle u, e_k^- u \rangle - \langle u, e_k^- u \rangle_{\mu_0})^2 + C \|u\|^2 T^{-1} \Lambda_e. \end{aligned} \quad (9.17)$$

Since $\hat{w} \in L^1$, we find that

$$\left\langle \xi(\sqrt{T}u), \frac{\lambda \mathbb{W}_P^{\mathrm{ren}}}{T}, \xi(\sqrt{T}u) \right\rangle \leq \mathcal{D}_K[u] + C \|u\|^2 T^{-1} \Lambda_e. \quad (9.18)$$

Inserting the latter bound in (9.16) we arrive at

$$\mathrm{Tr} e^{-(d\Gamma(P_h) + \lambda \mathbb{W}_P^{\mathrm{ren}})/T} \geq (T/\pi)^K \int_{P\mathfrak{H}} \exp \left[- \langle u, hu \rangle - \mathcal{D}_K[u] - C \|u\|^2 T^{-1} \Lambda_e \right] du. \quad (9.19)$$

Combining with (9.15), we find

$$\frac{\mathrm{Tr} e^{-(d\Gamma(P_h) + \lambda \mathbb{W}_P^{\mathrm{ren}})/T}}{\mathrm{Tr} e^{-d\Gamma(P_h)/T}} \geq \left[\prod_{j=1}^K \frac{T}{\lambda_j} (1 - e^{-\lambda_j/T}) \right] \int_{P\mathfrak{H}} \exp \left[- \mathcal{D}_K[u] - C \|u\|^2 T^{-1} \Lambda_e \right] d\mu_{0,K}(u) \quad (9.20)$$

where $d\mu_{0,K}$ is the cylindrical projection of $d\mu_0$ on $P\mathfrak{H}$, defined in (5.1). Then, recall from (8.22) that

$$\prod_{j=1}^K \left[\frac{T}{\lambda_j} (1 - e^{-\lambda_j/T}) \right] \geq 1 - CT^{-1} \Lambda_e^{p+1}.$$

Using that $\mathcal{D}_K[u] \geq 0$ by Lemma 5.3, we have

$$\begin{aligned} \exp \left[- \mathcal{D}_K[u] - C \|u\|^2 T^{-1} \Lambda_e \right] &= \exp \left[- \mathcal{D}_K[u] \right] \exp \left[- C \|u\|^2 T^{-1} \Lambda_e \right] \\ &\geq \exp \left[- \mathcal{D}_K[u] \right] (1 - C \|u\|^2 T^{-1} \Lambda_e) \\ &\geq \exp \left[- \mathcal{D}_K[u] - C \|u\|^2 T^{-1} \Lambda_e \right]. \end{aligned}$$

Moreover, by (5.2) and (2.16) we can bound

$$\int_{P\mathfrak{H}} \|u\|^2 d\mu_{0,K}(u) = \text{Tr}[Ph^{-1}] \leq \text{Tr}[(\Lambda_e/h)^{p-1}h^{-1}] \leq C\Lambda_e^{p-1}.$$

Thus we infer

$$\begin{aligned} & \int_{P\mathfrak{H}} \exp[-\mathcal{D}_K[u] - C\|u\|^2 T^{-1}\Lambda_e] d\mu_{0,K}(u) \\ & \geq \int_{P\mathfrak{H}} (\exp[-\mathcal{D}_K[u]] - C\|u\|^2 T^{-1}\Lambda_e) d\mu_{0,K}(u) \\ & \geq \int_{P\mathfrak{H}} \exp[-\mathcal{D}_K[u]] d\mu_{0,K}(u) - CT^{-1}\Lambda_e^p. \end{aligned}$$

Therefore, it follows from (9.20) that

$$\begin{aligned} \frac{\text{Tr} e^{-(d\Gamma(Ph) + \lambda W_P^{\text{ren}})/T}}{\text{Tr} e^{-d\Gamma(Ph)/T}} & \geq (1 - CT^{-1}\Lambda_e^{p+1}) \left[\int_{P\mathfrak{H}} e^{-\mathcal{D}_K[u]} d\mu_{0,K}(u) - CT^{-1}\Lambda_e^p \right] \\ & \geq \int_{P\mathfrak{H}} e^{-\mathcal{D}_K[u]} d\mu_{0,K}(u) - CT^{-1}\Lambda_e^{p+1}. \end{aligned}$$

Taking the log and using the fact that $\log(1+t) = O(t)$ for $|t|$ small concludes the proof. \square

Now we can conclude the

Proof of Proposition 9.1. Inserting (9.14) in (9.4) we get

$$-\log \frac{\mathcal{Z}_\lambda}{\mathcal{Z}_0} \leq -\log \left(\int_{P\mathfrak{H}} e^{-\mathcal{D}_K[u]} d\mu_{0,K}(u) \right) + C \left[T^{-1}\Lambda_e^{p+1} + T^{3(p-1)/4}\Lambda_e^{(p-2)/16} \right].$$

and conclude that

$$-\log \frac{\mathcal{Z}_\lambda}{\mathcal{Z}_0} \leq -\log \left(\int_{P\mathfrak{H}} e^{-\mathcal{D}_K[u]} d\mu_{0,K}(u) \right) + CT^{-\eta} \quad (9.21)$$

with η given in (8.30). When p is as in (3.49), then $\eta > 0$, and the desired upper bound (9.1) follows from (9.21) and (8.26).

The proof of Proposition 9.1, hence that of (3.4) is complete. \square

10. CONVERGENCE OF DENSITY MATRICES

In this section we prove the convergence of reduced density matrices stated in our main results. We will always take Λ_e as in (8.28) and denote

$$P = \mathbb{1}_{h \leq \Lambda_e}, \quad Q = \mathbb{1} - P.$$

10.1. Collecting useful bounds. First, we collect several positive terms previously dropped in our analysis, and use them to derive some new information.

Lemma 10.1 (Trace-class estimates for projected states).

Let h satisfy (3.45)-(3.46) with p as in (3.49) and let η be as in (8.30). For the P and Q

localized states, we have

$$\mathrm{Tr} \left| (\Gamma_\lambda)_Q - (\Gamma_0)_Q \right| \leq CT^{-\eta/2} \quad (10.1)$$

$$\mathrm{Tr} \left| \Gamma_\lambda - (\Gamma_\lambda)_P \otimes (\Gamma_\lambda)_Q \right| \leq CT^{-\eta/2}. \quad (10.2)$$

Moreover, we have

$$\|\mu_{P,\lambda} - \tilde{\mu}\|_{L^1(P\mathfrak{H})} \leq CT^{-\eta/2}, \quad (10.3)$$

where

$$d\tilde{\mu}(u) := \frac{e^{-\mathcal{D}_K[u]} d\mu_{0,K}(u)}{\int_{P\mathfrak{H}} e^{-\mathcal{D}_K(v)} d\mu_{0,K}(v)}. \quad (10.4)$$

Here $\mu_{P,\lambda}$ is the lower symbol of the Gibbs state Γ_λ associated with P and the scale $\varepsilon = T^{-1}$ as in (5.24), $\mu_{0,K}$ is the cylindrical free Gibbs measure and $\mathcal{D}_K[u]$ is the truncated renormalized interaction (all defined in Section 5).

Note that (10.1)-(10.2) precisely confirm the expectation that the interacting and free Gibbs states almost coincide on high kinetic energy modes, whereas (10.3) quantifies the precision of the mean-field/semi-classical approximation on low kinetic energy modes.

Proof of Lemma 10.1. After conjugating by the unitary (5.18), the free Gibbs state is factorized:

$$\Gamma_0 = \mathcal{U}^* (\Gamma_0)_P \otimes (\Gamma_0)_Q \mathcal{U}. \quad (10.5)$$

Hence we may apply the previous lemma to deduce

$$\mathcal{H}(\Gamma_\lambda, \Gamma_0) = \mathcal{H}(\Gamma_\lambda, (\Gamma_\lambda)_P \otimes (\Gamma_\lambda)_Q) + \mathcal{H}((\Gamma_\lambda)_P, (\Gamma_0)_P) + \mathcal{H}((\Gamma_\lambda)_Q, (\Gamma_0)_Q). \quad (10.6)$$

Here $(\Gamma_\lambda)_P$ and $(\Gamma_\lambda)_Q$ are the localized states in $\mathcal{F}(P\mathfrak{H})$ and $\mathcal{F}(Q\mathfrak{H})$, respectively, obtained by the localization method in Section 5.2. Combining (10.6) with (8.4) we obtain

$$\begin{aligned} -\log \frac{\mathcal{Z}_\lambda}{\mathcal{Z}_0} &= \mathcal{H}(\Gamma_\lambda, \Gamma_0) + T^{-2} \mathrm{Tr}[\mathbb{W}^{\mathrm{ren}} \Gamma_\lambda] \\ &\geq \mathcal{H}(\Gamma_\lambda, (\Gamma_\lambda)_P \otimes (\Gamma_\lambda)_Q) + \mathcal{H}((\Gamma_\lambda)_P, (\Gamma_0)_P) + \mathcal{H}((\Gamma_\lambda)_Q, (\Gamma_0)_Q) \\ &\quad + \int_{P\mathfrak{H}} \mathcal{D}_K[u] d\mu_{P,\lambda}(u) + O(T^{-\eta}). \end{aligned} \quad (10.7)$$

Here recall that $\mu_{P,\lambda}$ is the lower symbol of $(\Gamma_\lambda)_P$. By the Berezin-Lieb inequality (8.18) and the classical variational principle (4.3), we refine (8.19) to

$$\begin{aligned} &\mathcal{H}((\Gamma_\lambda)_P, (\Gamma_0)_P) + \int_{P\mathfrak{H}} \mathcal{D}_K[u] d\mu_{P,\lambda}(u) \\ &\geq \mathcal{H}_{\mathrm{cl}}(\mu_{P,\lambda}, \mu_{P,0}) + \int_{P\mathfrak{H}} \mathcal{D}_K[u] d\mu_{P,\lambda}(u) \\ &= \mathcal{H}_{\mathrm{cl}}(\mu_{P,\lambda}, \mu') - \log \left(\int_{P\mathfrak{H}} e^{-\mathcal{D}_K[u]} d\mu_{P,0}(u) \right). \end{aligned} \quad (10.8)$$

where $\mu_{P,0}$ is the corresponding lower symbol of $(\Gamma_0)_P$ and

$$d\mu'(u) := \frac{e^{-\mathcal{D}_K[u]} d\mu_{P,0}(u)}{\int_{P\mathfrak{H}} e^{-\mathcal{D}_K(v)} d\mu_{P,0}(v)}. \quad (10.9)$$

We have already proved in (8.24) that

$$-\log \left(\int_{P\mathfrak{H}} e^{-\mathcal{D}_K[u]} d\mu_{P,0}(u) \right) \geq -\log \left(\int_{P\mathfrak{H}} e^{-\mathcal{D}_K[u]} d\mu_{0,K}(u) \right) - CT^{-\eta}. \quad (10.10)$$

Putting (10.7), (10.8) and (10.10) together, we find that

$$\begin{aligned} -\log \frac{\mathcal{Z}_\lambda}{\mathcal{Z}_0} &\geq \mathcal{H}(\Gamma_\lambda, (\Gamma_\lambda)_P \otimes (\Gamma_\lambda)_Q) + \mathcal{H}((\Gamma_\lambda)_Q, (\Gamma_0)_Q) + \mathcal{H}_{\text{cl}}(\mu_{P,\lambda}, \tilde{\mu}) \\ &\quad - \log \left(\int_{P\mathfrak{H}} e^{-\mathcal{D}_K[u]} d\mu_{0,K}(u) \right) - CT^{-\eta}. \end{aligned} \quad (10.11)$$

On the other hand, we have the upper bound (9.21):

$$-\log \frac{\mathcal{Z}_\lambda}{\mathcal{Z}_0} \leq -\log \left(\int_{P\mathfrak{H}} e^{-\mathcal{D}_K[u]} d\mu_{0,K}(u) \right) + CT^{-\eta},$$

so that

$$\mathcal{H}_{\text{cl}}(\mu_{P,\lambda}, \mu') + \mathcal{H}((\Gamma_\lambda)_Q, (\Gamma_0)_Q) + \mathcal{H}(\Gamma_\lambda, (\Gamma_\lambda)_P \otimes (\Gamma_\lambda)_Q) \leq CT^{-\eta}. \quad (10.12)$$

Thanks to the (quantum and classical) Pinsker inequalities,

$$\mathcal{H}(A, B) \geq \frac{1}{2}(\text{Tr} |A - B|)^2, \quad \mathcal{H}_{\text{cl}}(\mu, \nu) \geq \frac{1}{2}(|\mu - \nu|(\mathfrak{H}))^2,$$

the bound (10.12) implies the desired estimates (10.1), (10.2) and

$$\|\mu_{P,\lambda} - \mu'\|_{L^1(P\mathfrak{H})} \leq CT^{-\eta/2}.$$

Finally, from (8.20) it follows that

$$\|\tilde{\mu} - \mu'\|_{L^1(P\mathfrak{H})} \leq CT^{-\eta/2}.$$

Thus (10.3) follows by the triangle inequality. \square

10.2. Lower density matrices in optimal norms. In this subsection we prove the convergence in the optimal p -Schatten space of the lower density matrices $1 \leq k < \frac{\eta}{2(p-1)}$. For convenience we restate the result (this corresponds to Theorem 3.5, Items 3 and part of 2):

Lemma 10.2 (Optimal convergence for low density matrices).

Let h satisfy (3.45)-(3.46). Assume that the first case in (3.52) holds, namely

$$1 \leq k < \frac{\eta}{2(p-1)} \quad (10.13)$$

with $\eta > 0$ in (8.30). Then in the limit $T \rightarrow \infty, \lambda T \rightarrow 1$, we have (3.51),

$$\frac{k!}{T^k} \Gamma_\lambda^{(k)} \rightarrow \int |u^{\otimes k}\rangle \langle u^{\otimes k}| d\mu(u)$$

strongly in the Schatten space \mathfrak{S}^p . Moreover, if (10.13) holds for $k = 1$, then

$$\text{Tr} \left| \frac{1}{T} \left(\Gamma_\lambda^{(1)} - \Gamma_0^{(1)} \right) - \int |u\rangle \langle u| (d\mu(u) - d\mu_0(u)) \right| \rightarrow 0.$$

In particular, this concludes the proof of Theorem 3.1 because in the homogeneous case h satisfies (3.45)-(3.46) for all $p > 1$. Note that so far we have not used the condition (3.47).

Lemma 10.1 gives some information on the states themselves. To exploit the above consequences on reduced density matrices, the following observation is helpful.

Lemma 10.3 (From states to density matrices, trace-class estimate).

Let Γ, Γ' be two states on Fock space that commute with the number operator \mathcal{N} . Then for all $q, q' > 1$ with $1/q + 1/q' = 1$ we have

$$\mathrm{Tr} |\Gamma^{(k)} - \Gamma'^{(k)}| \leq (\mathrm{Tr} |\Gamma - \Gamma'|)^{1/q'} \left(\mathrm{Tr} [\mathcal{N}^{qk} (\Gamma + \Gamma')] \right)^{1/q}. \quad (10.14)$$

Proof. We write

$$\Gamma = \bigoplus_{n=0}^{\infty} G_n, \quad \Gamma' = \bigoplus_{n=0}^{\infty} G'_n$$

where G_n, G'_n are operators on the n -particle sectors, and denote

$$G_n^{(k)} = \mathrm{Tr}_{k+1 \rightarrow n} [G_n].$$

By Hölder's inequality we may estimate

$$\begin{aligned} \mathrm{Tr} |\Gamma^{(k)} - \Gamma'^{(k)}| &\leq \sum_{n=k}^{\infty} n^k \mathrm{Tr} |G_n^{(k)} - G'_n{}^{(k)}| \\ &\leq \left(\sum_{n=0}^{\infty} \mathrm{Tr} |G_n^{(k)} - G'_n{}^{(k)}| \right)^{1/q'} \left(\sum_{n=0}^{\infty} n^{qk} \mathrm{Tr} |G_n^{(k)} - G'_n{}^{(k)}| \right)^{1/q} \\ &\leq \left(\sum_{n=0}^{\infty} \mathrm{Tr} |G_n - G'_n| \right)^{1/q'} \left(\sum_{n=0}^{\infty} n^{qk} (\mathrm{Tr} G_n + \mathrm{Tr} G'_n) \right)^{1/q} \\ &\leq (\mathrm{Tr} |\Gamma - \Gamma'|)^{1/q'} \left(\mathrm{Tr} [\mathcal{N}^{qk} (\Gamma + \Gamma')] \right)^{1/q}. \end{aligned}$$

□

We may now provide the

Proof of Lemma 10.2. For convenience, denote

$$\tilde{\Gamma}_\lambda = \mathcal{U}^* (\Gamma_{\lambda, P} \otimes \Gamma_{\lambda, Q}) \mathcal{U}. \quad (10.15)$$

Under the condition (10.13) we can choose $q' > 1$ such that $-\eta/(2q') + k(p-1) < 0$. Then from (10.14), (10.2) and (6.30) it follows that

$$T^{-k} \mathrm{Tr} \left| \Gamma_\lambda^{(k)} - \tilde{\Gamma}_\lambda^{(k)} \right| \leq C_k T^{-\eta/(2q') + k(p-1)} \rightarrow 0. \quad (10.16)$$

Next, from the action (5.19) of the partial isometry \mathcal{U} on creation/annihilation operators one can compute that

$$\tilde{\Gamma}_\lambda^{(k)} = P^{\otimes k} \Gamma_\lambda^{(k)} P^{\otimes k} + Q^{\otimes k} \Gamma_\lambda^{(k)} Q^{\otimes k} + \mathrm{Cross} \quad (10.17)$$

where Cross is a sum of finite coefficients (depending only on k) times terms of the form

$$\mathrm{Cross}_l = A_1^{\otimes j_1} \Gamma_\lambda^{(j_1)} A_1^{\otimes j_1} \otimes \dots \otimes A_l^{\otimes j_l} \Gamma_\lambda^{(j_l)} A_l^{\otimes j_l} \quad (10.18)$$

where $\sum_{i=1}^l j_i = k$ and $A_i = P$ or Q , but not all A_i are simultaneously equal to P or Q . The precise expression does not matter for us, but we have already used the expressions for $k = 1, 2$, so let us write them explicitly once more:

$$\begin{aligned}\tilde{\Gamma}_\lambda^{(1)} &= P\Gamma_\lambda^{(1)}P + Q\Gamma_\lambda^{(1)}Q, \\ \tilde{\Gamma}_\lambda^{(2)} &= P^{\otimes 2}\Gamma_\lambda^{(2)}P^{\otimes 2} + Q^{\otimes 2}\Gamma_\lambda^{(2)}Q^{\otimes 2} + P\Gamma_\lambda^{(1)}P \otimes Q\Gamma_\lambda^{(1)}Q + Q\Gamma_\lambda^{(1)}Q \otimes P\Gamma_\lambda^{(1)}P.\end{aligned}\quad (10.19)$$

The rest of the proof is as follows. After dividing everything by T^k , the main claim is that the P -localized term (first term in (10.17)) converges to the desired limit strongly in \mathfrak{S}^1 . Next, the Q -localized term (second term in (10.17)) is close in trace-class to the corresponding free term, which converges to 0 strongly in \mathfrak{S}^p as per (6.12). Combining these two facts, the cross-terms must also converge to 0 strongly in \mathfrak{S}^p , which will conclude the proof of (3.5). We obtain (3.6) because for the first density matrix there are no cross-terms.

Analysis of P -localized terms. We use the quantitative quantum de Finetti theorem 5.8. Recalling the lower symbol $\mu_{P,\lambda}$ of $(\Gamma_\lambda)_P$, we have from (5.26)

$$\int_{P\mathfrak{H}} |u^{\otimes k}\rangle\langle u^{\otimes k}| d\mu_{P,\lambda}(u) = \frac{k!}{T^k} P^{\otimes k} \Gamma^{(k)} P^{\otimes k} + \frac{k!}{T^k} \sum_{\ell=0}^{k-1} \binom{k}{\ell} P^{\otimes \ell} \Gamma^{(\ell)} P^{\otimes \ell} \otimes_s \mathbb{1}_{\otimes_s^{k-\ell} P\mathfrak{H}}. \quad (10.20)$$

Using Lemma 6.9, (8.3), (10.13) and the choice of Λ_e in (8.28), we can estimate

$$\mathrm{Tr} \left| k! T^{-k} P^{\otimes k} \Gamma_\lambda^{(k)} P^{\otimes k} - \int_{P\mathfrak{H}} |u^{\otimes k}\rangle\langle u^{\otimes k}| d\mu_{P,\lambda}(u) \right| \leq C_k T^{k(p-1)-p} \Lambda_e^p \rightarrow 0. \quad (10.21)$$

Consequently

$$\int_{P\mathfrak{H}} \|u\|^{2k} d\mu_{P,\lambda}(u) \leq C_k T^{k(p-1)}. \quad (10.22)$$

An estimate similar to (10.22) holds with $d\mu_{P,\lambda}(u)$ replaced by $d\tilde{\mu}(u)$ in (10.4) because

$$\int_{P\mathfrak{H}} |u^{\otimes k}\rangle\langle u^{\otimes k}| d\tilde{\mu} \leq C \int_{P\mathfrak{H}} |u^{\otimes k}\rangle\langle u^{\otimes k}| d\mu_{0,K} = C k! (Ph^{-1})^{\otimes k}. \quad (10.23)$$

Then using Hölder's inequality and (10.3), with $1/q + 1/q' = 1$ we have

$$\begin{aligned}\mathrm{Tr} \left| \int_{P\mathfrak{H}} |u^{\otimes k}\rangle\langle u^{\otimes k}| (d\mu_{P,\lambda}(u) - d\tilde{\mu}(u)) \right| &\leq \int_{P\mathfrak{H}} \|u\|^{2k} |d\mu_{P,\lambda} - d\tilde{\mu}|(u) \\ &\leq \left(\int_{P\mathfrak{H}} |d\mu_{P,\lambda} - d\tilde{\mu}|(u) \right)^{1/q'} \left(\int_{P\mathfrak{H}} \|u\|^{2qk} |d\mu_{P,\lambda} - d\tilde{\mu}|(u) \right)^{1/q} \\ &\leq C_k T^{-\eta/(2q') + k(p-1)} \rightarrow 0.\end{aligned}\quad (10.24)$$

Here again, thanks to (10.13) we can choose $q' > 1$ such that $-\eta/(2q') + k(p-1) < 0$.

In summary, putting (10.21) and (10.24) together we get by the triangle inequality,

$$\mathrm{Tr} \left| k! T^{-k} P^{\otimes k} \Gamma_\lambda^{(k)} P^{\otimes k} - \int_{P\mathfrak{H}} |u^{\otimes k}\rangle\langle u^{\otimes k}| d\tilde{\mu}(u) \right| \rightarrow 0. \quad (10.25)$$

Thus by the definitions of the Gibbs measure μ and the truncated measure $\tilde{\mu}$ in (10.4), we have, under condition (10.13),

$$\mathrm{Tr} \left| k! T^{-k} P^{\otimes k} \Gamma_\lambda^{(k)} P^{\otimes k} - \int |u^{\otimes k}\rangle \langle u^{\otimes k}| d\mu(u) \right| \rightarrow 0. \quad (10.26)$$

Analysis of Q -localized terms. Now we use (10.14) with $(\Gamma_\lambda)_Q$ and $(\Gamma_0)_Q$, then combine with (10.1), (6.14) and (6.30). This gives

$$T^{-k} \mathrm{Tr} \left| Q^{\otimes k} \left(\Gamma_\lambda^{(k)} - \Gamma_0^{(k)} \right) Q^{\otimes k} \right| = T^{-k} \mathrm{Tr} \left| (\Gamma_\lambda)_Q^{(k)} - (\Gamma_0)_Q^{(k)} \right| \leq CT^{-\eta/(2q') + k(p-1)} \rightarrow 0. \quad (10.27)$$

On the other hand, it follows from (6.12) and (2.18) that

$$Q^{\otimes k} \frac{\Gamma_0^{(k)}}{T^k} Q^{\otimes k} \rightarrow 0$$

strongly in $\mathfrak{S}^p(\mathfrak{H}_k)$. Combining with (10.27), we also have

$$Q^{\otimes k} \frac{\Gamma_\lambda^{(k)}}{T^k} Q^{\otimes k} \rightarrow 0 \quad (10.28)$$

strongly in $\mathfrak{S}^p(\mathfrak{H}_k)$.

Conclusion. We first prove (3.5). Use (10.16), then multiply (10.17) by $k!T^{-k}$. The first term has the desired limit, for (10.26) holds in the trace-class, a fortiori in \mathfrak{S}^p . The second term goes to 0 as per (10.28). All cross terms must also vanish in the limit because they are products of P -localized terms, which are bounded even in trace-class, and of at least one Q -localized term, whose \mathfrak{S}^p norm vanishes. Thus (3.5) is proved.

To obtain (3.6), note that there are no cross-terms in this case. Since we already have proven that both terms converge separately, we certainly have

$$P \frac{\Gamma_\lambda^{(1)} - \Gamma_0^{(1)}}{T} P \xrightarrow{T \rightarrow \infty} \int |u\rangle \langle u| d\mu(u) - h^{-1}$$

strongly in trace-class norm. Now it follows from either (6.28) or (10.27) that

$$Q \frac{\Gamma_\lambda^{(1)} - \Gamma_0^{(1)}}{T} Q \xrightarrow{T \rightarrow \infty} 0$$

strongly in the trace-class. Combining with (10.16), (10.19) and (10.5) concludes the proof of (3.6). This ends the proof of Lemma 10.2. \square

Remark 10.4 (Relative higher density matrices).

It can be seen from the above proof that for every $k \geq 2$, the difference $T^{-k}(\Gamma_\lambda^{(k)} - \Gamma_0^{(k)})$ is *not* bounded in trace class. For example, when $k = 2$, using (10.19) we can write

$$\begin{aligned} T^{-2}(\tilde{\Gamma}_\lambda^{(2)} - \Gamma_0^{(2)}) &= T^{-2} P^{\otimes 2} (\Gamma_\lambda^{(2)} - \Gamma_0^{(2)}) P^{\otimes 2} + T^{-2} Q^{\otimes 2} (\Gamma_\lambda^{(2)} - \Gamma_0^{(2)}) Q^{\otimes 2} \\ &\quad + T^{-2} P \Gamma_\lambda^{(1)} P \otimes Q (\Gamma_\lambda^{(1)} - \Gamma_0^{(1)}) Q + T^{-2} Q (\Gamma_\lambda^{(1)} - \Gamma_0^{(1)}) Q \otimes P \Gamma_\lambda^{(1)} P \\ &\quad + T^{-2} P (\Gamma_\lambda^{(1)} - \Gamma_0^{(1)}) P \otimes Q \Gamma_0^{(1)} Q + T^{-2} Q \Gamma_0^{(1)} Q \otimes P (\Gamma_\lambda^{(1)} - \Gamma_0^{(1)}) P. \end{aligned}$$

From (10.26) and (10.27) it follows that the first four terms on the right side converge in trace class, but the last two terms are unbounded in trace norm (because $T^{-1}P(\Gamma_\lambda^{(1)} - \Gamma_0^{(1)})P$

converges strongly to a non-zero limit but $T^{-1}Q\Gamma_0^{(1)}Q$ is unbounded in trace norm). Thus $T^{-2}(\tilde{\Gamma}_\lambda^{(2)} - \Gamma_0^{(2)})$ is unbounded in trace norm, and hence (10.16) implies that $T^{-2}(\Gamma_\lambda^{(2)} - \Gamma_0^{(2)})$ is also unbounded in trace norm. \diamond

10.3. All density matrices in Hilbert-Schmidt norm. In this subsection we are not assuming that $k < \eta/(p-1)$ as in (3.52), but instead we derive the Hilbert-Schmidt convergence for all density matrices using condition (3.47). This is the only missing item in the statement of Theorem 3.5, which we restate for convenience:

Lemma 10.5 (Hilbert-Schmidt convergence of all density matrices). *Let h satisfy (3.45)-(3.46)-(3.47) with p in (3.49) and let w satisfy (3.30). Then in the limit $T \rightarrow \infty, \lambda T \rightarrow 1$, for all $k \geq 1$ we have*

$$\frac{k!}{T^k} \Gamma_\lambda^{(k)} \rightarrow \int |u^{\otimes k}\rangle \langle u^{\otimes k}| d\mu(u)$$

strongly in the Hilbert-Schmidt space \mathfrak{S}^2 .

We will follow a similar strategy as in the proof of Lemma 10.2, plus two additional inputs. The first one is a uniform bound on all density matrices in the Hilbert-Schmidt norm. This is the only place where we need the condition (3.47).

Lemma 10.6 (Hilbert-Schmidt estimates).

Let h satisfy (3.45),(3.47) with some $p \leq 2$ and let w satisfy (3.30). Then for every $k \geq 1$, we have

$$\left\| T^{-k} \Gamma_\lambda^{(k)} \right\|_{\mathfrak{S}^2} \leq C_k.$$

Proof. From the positivity $e^{-th}(x, y) \geq 0$ and $\lambda \mathbb{W}^{\text{ren}} \geq 0$, a standard argument using the Trotter product formula (see e.g. [107, Theorem VIII.30] or [122, Theorem 1.1]) and the relative bound on partition functions in Lemma 6.7, we obtain the kernel estimate

$$0 \leq \Gamma_\lambda^{(k)}(X_k; Y_k) \leq C_k \Gamma_0^{(k)}(X_k; Y_k).$$

See e.g. [85, Lemma 4.3] for a detailed explanation. Consequently, for every $k \geq 1$ we have the Hilbert-Schmidt estimate

$$\left\| T^{-k} \Gamma_\lambda^{(k)} \right\|_{\mathfrak{S}^2} \leq C_k \left\| T^{-k} \Gamma_0^{(k)} \right\|_{\mathfrak{S}^2} = C_k \left\| \frac{1}{T^k (e^{h/T} - 1)} \right\|_{\mathfrak{S}^2} \leq C_k \|h^{-1}\|_{\mathfrak{S}^2}^k.$$

Note that the bound is uniform in T and depends on h only via $\|h^{-1}\|_{\mathfrak{S}^2}$. \square

Next, we have an adaption of Lemma 10.3 to the Hilbert-Schmidt norm.

Lemma 10.7 (From states to density matrices, Hilbert-Schmidt estimate).

Let Γ, Γ' be two states on Fock space that commute with the number operator \mathcal{N} . Then for all $k \geq 1$, we have the Hilbert-Schmidt norm estimate on the associated density matrices

$$\|\Gamma^{(k)} - \Gamma'^{(k)}\|_{\mathfrak{S}^2}^2 \leq C_k \left(\text{Tr} |\Gamma - \Gamma'| \right) \left(\sum_{\ell=k}^{2k} \left(\|\Gamma^{(\ell)}\|_{\mathfrak{S}^2} + \|\Gamma'^{(\ell)}\|_{\mathfrak{S}^2} \right) \right). \quad (10.29)$$

Proof. Let A_k be a non-negative Hilbert-Schmidt operator on $\mathfrak{H}^{\otimes_s k}$ and \mathbb{A}_k the associated second-quantized operator on the Fock space from Definition 2.1. Using (2.6) we have

$$\begin{aligned} \left| \text{Tr} \left[A_k(\Gamma^{(k)} - \Gamma'^{(k)}) \right] \right|^2 &= \left| \text{Tr} \left[\mathbb{A}_k(\Gamma - \Gamma') \right] \right|^2 \\ &\leq \left(\text{Tr} |\Gamma - \Gamma'| \right) \left(\text{Tr} \left[(\mathbb{A}_k)^2 |\Gamma - \Gamma'| \right] \right) \\ &\leq \left(\text{Tr} |\Gamma - \Gamma'| \right) \left(\text{Tr} \left[(\mathbb{A}_k)^2 (\Gamma + \Gamma') \right] \right). \end{aligned} \quad (10.30)$$

On the n -particle sector, we can compute explicitly

$$\begin{aligned} \left(\sum_{1 \leq i_1 < \dots < i_k \leq n} (A_k)_{i_1, \dots, i_k} \right)^2 &= \sum_{\substack{1 \leq i_1 < \dots < i_k \leq n \\ 1 \leq j_1 < \dots < j_k \leq n}} (A_k)_{i_1, \dots, i_k} (A_k)_{j_1, \dots, j_k} \\ &= \sum_{\ell=k}^{\min\{2k, n\}} \sum_{1 \leq i_1 < \dots < i_\ell \leq n} (B_\ell)_{i_1, i_2, \dots, i_\ell} \end{aligned}$$

where B_ℓ is an operator on $\mathfrak{H}^{\otimes_s \ell}$ defined by

$$(B_\ell)_{1, 2, \dots, \ell} := \sum_{\substack{1 \leq i_1 < \dots < i_k \leq \ell \\ 1 \leq j_1 < \dots < j_k \leq \ell \\ \{i_1, \dots, i_k\} \cup \{j_1, \dots, j_k\} = \{1, \dots, \ell\}}} (A_k)_{i_1, \dots, i_k} (A_k)_{j_1, \dots, j_k}. \quad (10.31)$$

Therefore we have

$$\mathbb{A}_k^2 = \sum_{\ell=k}^{2k} \mathbb{B}_\ell$$

where \mathbb{B}_ℓ is the second quantization of B_ℓ , as in Definition 2.1 again.

On the other hand, since A_k is a Hilbert-Schmidt operator on $\mathfrak{H}^{\otimes_s k}$, we can prove that B_ℓ is a Hilbert-Schmidt operator on $\mathfrak{H}^{\otimes_s \ell}$ and

$$\|B_\ell\|_{\mathfrak{S}^2} \leq C_k \|A_k\|_{\mathfrak{S}^2}^2. \quad (10.32)$$

To prove (10.32), let us come back to the definition (10.31). Consider a general ℓ -particle operator of the form

$$\mathbb{A} = (A_k)_{X, Y} (A_k)_{X, Z}$$

with $(X, Y), (X, Z)$ are k -particle variables. If the kernel of (A_k) is $(A_k)(X, Y; X', Y')$, then the kernel of \mathbb{A} is

$$\mathbb{A}(X, Y, Z; X', Y', Z') = \int dX'' (A_k)(X, Y; X'', Y') (A_k)(X'', Z; X', Z').$$

By the Cauchy-Schwarz inequality we have

$$|\mathbb{A}(X, Y, Z; X', Y', Z')|^2 \leq \left(\int dX'' |(A_k)(X, Y; X'', Y')|^2 \right) \left(\int dX'' |(A_k)(X'', Z; X', Z')|^2 \right).$$

Therefore,

$$\begin{aligned}
\|\mathbb{A}\|_{\mathfrak{S}^2}^2 &= \int dXdYdZdX'dY'dZ' |\mathbb{A}(X, Y, Z; X', Y', Z')|^2 \\
&\leq \int dXdYdZdX'dY'dZ' \left(\int dX'' |(A_k)(X, Y; X'', Y')|^2 \right) \times \\
&\quad \left(\int dX'' |(A_k)(X'', Z; X', Z')|^2 \right) \\
&= \left(\int dXdYdX'dY' |(A_k)(X, Y; X', Y')|^2 \right)^2 = \|A_k\|_{\mathfrak{S}^2}^4.
\end{aligned}$$

We thus obtain (10.32) immediately from the definition (10.31).

Using (10.32), we can estimate

$$\begin{aligned}
\mathrm{Tr} \left[\mathbb{A}_k^2 \Gamma \right] &= \sum_{\ell=k}^{2k} \left[\mathbb{B}_\ell \Gamma \right] = \sum_{\ell=k}^{2k} \mathrm{Tr} \left[B_\ell \Gamma^{(\ell)} \right] \\
&\leq \sum_{\ell=k}^{2k} \|B_\ell\|_{\mathfrak{S}^2} \|\Gamma^{(\ell)}\|_{\mathfrak{S}^2} \leq C_k \|A_k\|_{\mathfrak{S}^2}^2 \sum_{\ell=k}^{2k} \|\Gamma^{(\ell)}\|_{\mathfrak{S}^2}. \tag{10.33}
\end{aligned}$$

Inserting (10.33) and a similar estimate for Γ' in (10.30) we arrive at

$$\left| \mathrm{Tr} \left[A_k(\Gamma^{(k)} - \Gamma'^{(k)}) \right] \right|^2 \leq C_k \|A_k\|_{\mathfrak{S}^2}^2 \left(\mathrm{Tr} |\Gamma - \Gamma'| \right) \left(\sum_{\ell=k}^{2k} \left(\|\Gamma^{(\ell)}\|_{\mathfrak{S}^2} + \|\Gamma'^{(\ell)}\|_{\mathfrak{S}^2} \right) \right). \tag{10.34}$$

This being true for all k -body Hilbert-Schmidt operator A_k leads to the desired bound (10.29) by duality. \square

Now we are ready to conclude

Proof of Lemma 10.5. As in the proof of Lemma 10.2, we can reduce the consideration to the diagonal terms $P^{\otimes k} \Gamma_\lambda P^{\otimes k}$ and $Q^{\otimes k} \Gamma_\lambda Q^{\otimes k}$.

Analysis of P -localized terms. From the lower symbol expression (10.20), taking the Hilbert-Schmidt norm both sides, using the uniform bound in Lemma 10.6 and the fact that $\dim(P\mathfrak{H}) \leq C\Lambda_e^p \ll T$, we find that for every $k \geq 1$,

$$\left\| \frac{k!}{T^k} P^{\otimes k} \Gamma^{(k)} P^{\otimes k} - \int_{P\mathfrak{H}} |u^{\otimes k}\rangle \langle u^{\otimes k}| d\mu_{P,\lambda}(u) \right\|_{\mathfrak{S}^2} \rightarrow 0. \tag{10.35}$$

Consequently,

$$\left\| \int_{P\mathfrak{H}} |u^{\otimes k}\rangle \langle u^{\otimes k}| d\mu_{P,\lambda}(u) \right\|_{\mathfrak{S}^2} \leq C_k. \tag{10.36}$$

A similar estimate with $\mu_{P,\lambda}$ replaced by $\tilde{\mu}$ in (10.4) holds thanks to (10.23).

Next, for every Hilbert-Schmidt operator $X \geq 0$ on $\mathfrak{H}^{\otimes s^k}$, we can estimate

$$\begin{aligned}
 & \left| \text{Tr} \left[X \left(\int_{P\mathfrak{H}} |u^{\otimes k}\rangle\langle u^{\otimes k}| (d\mu_{P,\lambda} - d\tilde{\mu})(u) \right) \right] \right|^2 \\
 &= \left| \int_{P\mathfrak{H}} \langle u^{\otimes k}, X u^{\otimes k} \rangle (d\mu_{P,\lambda} - d\tilde{\mu})(u) \right|^2 \\
 &\leq \left(\int_{P\mathfrak{H}} |\langle u^{\otimes k}, X u^{\otimes k} \rangle|^2 d\mu_{P,\lambda} - d\tilde{\mu}(u) \right) \left(\int_{P\mathfrak{H}} |d\mu_{P,\lambda} - d\tilde{\mu}|(u) \right) \\
 &\leq \left(\int_{P\mathfrak{H}} \langle u^{\otimes 2k}, X \otimes X u^{\otimes 2k} \rangle (d\mu_{P,\lambda} + d\tilde{\mu})(u) \right) |\mu_{P,\lambda} - \tilde{\mu}|(P\mathfrak{H}) \\
 &= \text{Tr} \left[X \otimes X \left(\int_{P\mathfrak{H}} |u^{\otimes 2k}\rangle\langle u^{\otimes 2k}| (d\mu_{P,\lambda} + d\tilde{\mu})(u) \right) \right] |\mu_{P,\lambda} - \tilde{\mu}|(P\mathfrak{H}) \\
 &\leq \|X \otimes X\|_{\mathfrak{H}^2} \left\| \int_{P\mathfrak{H}} |u^{\otimes 2k}\rangle\langle u^{\otimes 2k}| (d\mu_{P,\lambda} + d\tilde{\mu})(u) \right\|_{\mathfrak{S}^2} |\mu_{P,\lambda} - \tilde{\mu}|(P\mathfrak{H}) \\
 &\leq C_k \|X\|_{\mathfrak{S}^2}^2 T^{-\eta/2}.
 \end{aligned}$$

Here in the last inequality we have used (10.3) and (10.36). By duality we deduce

$$\left\| \int_{P\mathfrak{H}} |u^{\otimes k}\rangle\langle u^{\otimes k}| (d\mu_{P,\lambda} - d\tilde{\mu})(u) \right\|_{\mathfrak{S}^2} \leq C_k T^{-\eta/4} \rightarrow 0. \quad (10.37)$$

Thus, by the triangle inequality,

$$\left\| k! T^{-k} P^{\otimes k} \Gamma_\lambda^{(k)} P^{\otimes k} - \int_{P\mathfrak{H}} |u^{\otimes k}\rangle\langle u^{\otimes k}| d\tilde{\mu}(u) \right\|_{\mathfrak{S}^2} \leq C T^{-\eta/4} \rightarrow 0. \quad (10.38)$$

Therefore, for all $k \geq 1$,

$$\left\| k! T^{-k} P^{\otimes k} \Gamma_\lambda^{(k)} P^{\otimes k} - \int |u^{\otimes k}\rangle\langle u^{\otimes k}| d\mu(u) \right\|_{\mathfrak{S}^2} \rightarrow 0. \quad (10.39)$$

Analysis of Q -localized terms. Using Lemma 10.7, Lemma 10.6 and (10.1) we can estimate

$$\begin{aligned}
 \left\| Q^{\otimes k} \frac{\Gamma_\lambda^{(k)} - \Gamma_0^{(k)}}{T^k} Q^{\otimes k} \right\|_{\mathfrak{S}^2}^2 &= \left\| \frac{(\Gamma_\lambda)_Q^{(k)} - (\Gamma_0)_Q^{(k)}}{T^k} \right\|_{\mathfrak{S}^2}^2 \\
 &\leq C_k T^{-2k} \left(\text{Tr} |(\Gamma_\lambda)_Q - (\Gamma_0)_Q| \right) \sum_{\ell=k}^{2k} \left(\|(\Gamma_\lambda)_Q^{(\ell)}\|_{\mathfrak{S}^2} + \|(\Gamma_0)_Q^{(\ell)}\|_{\mathfrak{S}^2} \right) \\
 &\leq C_k T^{-\eta/2} \rightarrow 0
 \end{aligned} \quad (10.40)$$

for all $k \geq 1$. From (10.39) and (10.40) we can go back to (10.17), control all the cross terms, and conclude that

$$\left\| k! T^{-k} \Gamma_\lambda^{(k)} - \int |u^{\otimes k}\rangle\langle u^{\otimes k}| d\mu(u) \right\|_{\mathfrak{S}^2} \rightarrow 0$$

for all $k \geq 1$. This ends the proof of Lemma 10.5, as well as that of Theorem 3.5. \square

APPENDIX A. THE COUNTER-TERM PROBLEM

Here we prove Lemma 3.2 and make some comments on Theorem 3.3.

A.1. Proof of Lemma 3.2. Our proof works in any dimension $d \geq 1$. Let V be a locally integrable non-negative function, tending to $+\infty$ at infinity, such that

$$\int_{\mathbb{R}^d} e^{-V(x)/T} dx < \infty.$$

Then the first eigenvalue of the Friedrichs realization of $h = -\Delta + V$ is positive. In addition, we have

$$\mathrm{Tr}[e^{-h/T}] \leq (2\pi)^{-d} \int_{\mathbb{R}^d} e^{-p^2/T} dp \int_{\mathbb{R}^d} e^{-V(x)/T} dx < \infty,$$

by the Golden-Thompson inequality, see [120, Section 8.1]. The same properties holds if we shift V by $\nu \in \mathbb{R}$ and only keep the positive part. Then we obtain

$$\begin{aligned} & \mathrm{Tr}(-\Delta + (V - \nu)_+) \gamma - T \mathrm{Tr}[(1 + \gamma) \log(1 + \gamma) - \gamma \log \gamma] \\ & \geq \frac{1}{2} \mathrm{Tr}(-\Delta) \gamma + T \mathrm{Tr} \left(\log \left(1 - e^{-\frac{-\Delta/2 + (V - \nu)_+}{T}} \right) \right) \end{aligned} \quad (\text{A.1})$$

for all $\gamma \geq 0$. In order to prove that the reduced-Hartree functional $\mathcal{F}^{\mathrm{rH}}$ is bounded from below, it therefore remains to show that

$$-\int_{\mathbb{R}^d} \rho(x)(V - \nu)_-(x) dx + \frac{\lambda}{2} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} w(x - y) \rho(x) \rho(y) dx dy$$

is bounded from below, uniformly in $\rho \geq 0$, under the assumption that $\widehat{w} \geq 0$ and $w \neq 0$. Since $w \in L^1(\mathbb{R}^d)$, we can find a $k_0 \in \mathbb{R}^d$ and a small radius $r > 0$ such that the continuous non-negative function \widehat{w} is at least equal to $\widehat{w}(k_0)/2$ on $B(k_0, r)$. We then choose φ in the Schwartz class such that $\varphi > 0$ and $\widehat{\varphi} \geq 0$ with $\mathrm{supp}(\widehat{\varphi}) \subset B(k_0, r)$. Since $V \geq 0$ and $V \rightarrow +\infty$ at infinity, the function $(V - \nu)_-$ has compact support and is bounded by ν_+ . Therefore, we have

$$(V - \nu)_- \leq C\varphi$$

for $C = \|\varphi^{-1}(V - \nu)_-\|_{L^\infty(\mathbb{R}^d)} < \infty$. After completing the square and using $\widehat{w} \geq 0$, we then

$$\begin{aligned} & -\int_{\mathbb{R}^d} (V - \nu)_- \rho + \frac{\lambda}{2} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} w(x - y) \rho(x) \rho(y) dx dy \\ & \geq -C \int_{\mathbb{R}^d} \varphi \rho + \frac{\lambda}{2} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} w(x - y) \rho(x) \rho(y) dx dy \geq -\frac{C^2}{2\lambda} \int_{\mathbb{R}^d} \frac{|\widehat{\varphi}(k)|^2}{\widehat{w}(k)} dk \geq -\frac{C^2 \|\widehat{\varphi}\|_{L^2}^2}{\lambda \widehat{w}(k_0)}. \end{aligned}$$

Combining with (A.1) we find as stated that

$$\inf_{\gamma = \gamma^* \geq 0} \mathcal{F}^{\mathrm{rH}}[\gamma] > -\infty,$$

for all $\nu \in \mathbb{R}$.

Let us now prove the existence of a minimizer. Writing

$$\mathcal{F}_\nu^{\mathrm{rH}}[\gamma] = \mathcal{F}_{\nu+1}^{\mathrm{rH}}[\gamma] + \mathrm{Tr} \gamma \geq \inf_{\gamma'} \mathcal{F}_{\nu+1}^{\mathrm{rH}}[\gamma'] + \mathrm{Tr}(\gamma),$$

where we have displayed the parameter ν for convenience, we obtain that minimizing sequences $\{\gamma_n\}$ for $\mathcal{F}_\nu^{\mathrm{rH}}$ are necessarily bounded in the trace-class. In particular, $\|\gamma_n\|$ is also

bounded. In addition, the inequality (A.1) implies that $\text{Tr}(-\Delta)\gamma_n$ is bounded. From the Hoffmann-Ostenhof inequality [66]

$$\text{Tr}(-\Delta)\gamma \geq \int_{\mathbb{R}^d} \left| \nabla \sqrt{\rho_\gamma(x)} \right|^2 dx$$

and the Sobolev inequality, we deduce that ρ_{γ_n} is bounded in $L^{p^*/2}(\mathbb{R}^d)$ where $p^* = +\infty$ in dimension $d = 1$, $p^* < \infty$ arbitrarily in dimension $d = 2$ and $p^* = 2d/(d - 2)$ in dimensions $d \geq 3$. Hence, up to extraction of a subsequence, we have $\gamma_n \rightharpoonup \gamma$ weakly- $*$ in \mathfrak{S}^1 and $\rho_{\gamma_n} \rightharpoonup \rho_\gamma$ weakly in $L^1(\mathbb{R}^d) \cap L^{p^*/2}(\mathbb{R}^d)$. Using Fatou's lemma and the concavity (hence weak upper semi-continuity) of the entropy, we obtain that γ is a minimizer for $\mathcal{F}_\nu^{\text{rH}}$. The nonlinear equation follows from classical arguments. \square

A.2. Comments on Theorem 3.3. Let us briefly discuss Theorem 3.3. In [47, Section 5], the existence of the solution V_T to (3.16) was established by means of a fixed-point argument (which requires that $d \leq 3$ and that κ is sufficiently large). The fixed point is performed in the (complete) metric space

$$B(V) = \left\{ f \in L^\infty_{\text{loc}}(\mathbb{R}^d) : \|f\|_{B(V)} = \left\| \frac{f}{V} - 1 \right\|_{L^\infty} < 1/2 \right\}$$

for the unknown $u = V_T - \kappa$ and provides the Hilbert-Schmidt convergence

$$\text{Tr} \left| (-\Delta + V_T)^{-1} - (-\Delta + V_\infty)^{-1} \right|^2 \rightarrow 0.$$

Our notation here is slightly different from [47] as we shift potentials by a constant. Moreover, since $V_T - \kappa \in B(V)$ we have

$$\frac{V}{2} \leq V_T - \kappa \leq 3\frac{V}{2}.$$

Then by the Lieb-Thirring inequality in [42, Theorem 1] and the last assumption in (3.22), we get

$$\text{Tr}(-\Delta + V_T)^{-p} \leq C_p$$

uniformly in T . The convergence (3.26) thus follows in \mathfrak{S}^q for all $p < q \leq 2$, by interpolation. From the inequality $V_T \geq V/2 + \kappa$ we have pointwise bound on the operator kernels

$$(-\Delta + V_T)^{-p}(x; x) \leq (-\Delta + V/2 + \kappa)^{-p}(x; x)$$

by the Feynman-Kac formula as in Lemma 10.5, since

$$h^{-p} = \Gamma(p)^{-1} \int_0^\infty e^{-th} t^{p-1} dt.$$

In addition, $\text{Tr}(-\Delta + V/2 + \kappa)^{-p} < \infty$ since $V/2$ satisfies the last condition in (3.22) as well. Hence we can conclude from the dominated convergence theorem that

$$\begin{aligned} \lim_{T \rightarrow \infty} \text{Tr}(-\Delta + V_T)^{-p} &= \lim_{T \rightarrow \infty} \int_{\mathbb{R}^d} (-\Delta + V_T)^{-p}(x; x) dx \\ &= \int_{\mathbb{R}^d} (-\Delta + V_\infty)^{-p}(x; x) dx = \text{Tr}(-\Delta + V_\infty)^{-p}. \end{aligned}$$

The convergence in \mathfrak{S}^p follows from Gr\"umm's theorem [120, Chap. 2].

There remains to discuss the nonlinear equation (3.27) for V_∞ , which we can rewrite in the form

$$V_\infty = w * \left(V + \kappa + \rho \left[(-\Delta + V_\infty)^{-1} - (-\Delta + \kappa)^{-1} \right] \right). \quad (\text{A.2})$$

Here we just need to pass to the limit in the similar equation at $T > 0$

$$V_T = w * \left(V + \kappa + \rho \left[\frac{1}{T \left(e^{-\frac{-\Delta + V_T}{T}} - 1 \right)} - \frac{1}{T \left(e^{-\frac{-\Delta + \kappa}{T}} - 1 \right)} \right] \right).$$

Since we know that $V_T/V \rightarrow V_\infty/V$ in L^∞ , we have $V_T \rightarrow V_\infty$ in L^∞_{loc} and it suffices to prove the convergence of the density on the right side, which we denote for simplicity

$$\rho_T^{V_T}(x) := \left[\frac{1}{T \left(e^{-\frac{-\Delta + V_T}{T}} - 1 \right)} - \frac{1}{T \left(e^{-\frac{-\Delta + \kappa}{T}} - 1 \right)} \right] (x; x).$$

In [47, Eq. (5.21)] it is shown that

$$|\rho_T^{V_T}(x)| \leq C \kappa^{d/2-2} \left\| \frac{V_T - \kappa}{V} \right\|_{L^\infty} V(x). \quad (\text{A.3})$$

Hence from the dominated convergence theorem and the assumptions on w , it suffices to prove that

$$\rho_T^{V_T}(x) \rightarrow \left((-\Delta + V_\infty)^{-1} - (-\Delta + \kappa)^{-1} \right) (x; x)$$

almost everywhere. Applying again [47, Eq. (5.21)] we find that

$$\left| \left(\frac{1}{T \left(e^{-\frac{-\Delta + V_T}{T}} - 1 \right)} - \frac{1}{T \left(e^{-\frac{-\Delta + V_\infty}{T}} - 1 \right)} \right) (x; x) \right| \leq C \kappa^{d/2-2} \left\| \frac{V_T - V_\infty}{V} \right\|_{L^\infty} V(x)$$

which tends to 0 in L^∞_{loc} since $(V_T - V_\infty)/V \rightarrow 0$. Hence we can replace V_T by V_∞ throughout. Next we write, following [47, Eq. (5.16)],

$$\rho_T^{V_\infty}(x) = - \int_0^1 ds \int_{\mathbb{R}^d} dz \frac{e^{s(-\Delta + V_\infty)/T}}{T \left(e^{(-\Delta + V_\infty)/T} - 1 \right)} (x; z) V_\infty(z) \frac{e^{(1-s)(-\Delta + \kappa)/T}}{T \left(e^{(-\Delta + \kappa)/T} - 1 \right)} (z; x).$$

Using that $V_\infty \geq \kappa$, we have the pointwise bound on the operator kernels

$$0 \leq \frac{e^{s(-\Delta + V_\infty)/T}}{T \left(e^{(-\Delta + V_\infty)/T} - 1 \right)} (x; z) \leq \frac{e^{s(-\Delta + \kappa)/T}}{T \left(e^{(-\Delta + \kappa)/T} - 1 \right)} (x; z)$$

by the same argument as in Lemma 10.5 and in [47, Eq. (5.17)]. Using [47, Lemma 5.4] we see that we get a convergent domination. So by the dominated convergence theorem, the strong local convergence of $\rho_T^{V_\infty}$ follows from that of the kernels

$$\begin{aligned} \frac{e^{s(-\Delta + V_\infty)/T}}{T \left(e^{(-\Delta + V_\infty)/T} - 1 \right)} (x; z) &\rightarrow \frac{1}{-\Delta + V_\infty} (x; z), \\ \frac{e^{s(-\Delta + \kappa)/T}}{T \left(e^{(-\Delta + \kappa)/T} - 1 \right)} (x; z) &\rightarrow \frac{1}{-\Delta + \kappa} (x; z). \end{aligned}$$

In fact this convergence is strong in $L^2(\mathbb{R}^d \times \mathbb{R}^d)$ since the corresponding operators converge in the Hilbert-Schmidt norm, by [47, Lemma C.1]. Passing to the limit, this proves the strong local convergence

$$\begin{aligned} \rho_T^{V_\infty}(x) &\xrightarrow{T \rightarrow \infty} - \int_0^1 ds \int_{\mathbb{R}^d} dz \frac{1}{-\Delta + V_\infty}(x; z) V_\infty(z) \frac{1}{-\Delta + \kappa}(z; x) \\ &= \left((-\Delta + V_\infty)^{-1} - (-\Delta + \kappa)^{-1} \right) (x; x), \end{aligned}$$

where in the last equality we have used the resolvent formula. The uniform bound (A.3) then allows to pass to the limit in the equation for V_T and obtain (A.2). \square

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