The Vlasov continuum limit for the classical microcanonical ensemble

MICHAEL K.-H. KIESLING
Department of Mathematics, Rutgers University
Piscataway NJ 08854, USA

Abstract
For classical Hamiltonian $N$-body systems with mildly regular pair interaction potential (in particular, $\Omega^2_{loc}$ integrability is required) it is shown that when $N \to \infty$ in a fixed bounded domain $\Lambda \subset \mathbb{R}^3$, with energy $E$ scaling as $E \propto N^2$, then Boltzmann’s ergodic ensemble entropy $S_{\Lambda}(N, E)$ has the asymptotic expansion $S_{\Lambda}(N, N^2 \varepsilon) = -N \ln N + s_{\Lambda}(\varepsilon)N + o(N)$; here, the $N \ln N$ term is combinatorial in origin and independent of the rescaled Hamiltonian, while $s_{\Lambda}(\varepsilon)$ is the system-specific Boltzmann entropy per particle, i.e. $-s_{\Lambda}(\varepsilon)$ is the minimum of Boltzmann’s $H$ function for a perfect gas of energy $\varepsilon$ subjected to a combination of externally and self-generated fields. It is also shown that any limit point of the $n$-point marginal ensemble measures is a linear convex superposition of $n$-fold products of the $H$-function-minimizing one-point functions. The proofs are direct, in the sense that (a) the map $E \mapsto S(E)$ is studied rather than its inverse $S \mapsto E(S)$; (b) no regularization of the microcanonical measure $\delta(E - H)$ is invoked, and (c) no detour via the canonical ensemble. The proofs hold irrespective of whether microcanonical and canonical ensembles are equivalent or not.
1 Introduction

The rigorous foundations of equilibrium statistical mechanics have largely been laid long ago [Rue69, Pen70, Len73, ML79], but the most basic problem in classical statistical mechanics, namely the rigorous asymptotic evaluation of Gibbs’ microcanonical ensemble [Gib02] in the limit of a large number \( N \) of particles, has only been treated in an approximate way. The standard way of dealing with the microcanonical ensemble (a.k.a. Boltzmann’s ergodic ensemble [Bol96]) in a rigorous manner [Rue69, Lan73, ML79] has been to replace its singular ensemble measure by a regularized measure (usually also referred to as microcanonical, although quasi-microcanonical would seem a better name). In these approaches one cannot take the limit of vanishing regularization; yet, since one can approximate the singular measure as closely as one pleases, “this is not completely unsatisfactory from a conceptual point of view” ([Lan73], p.4). All the same, Lanford’s wording makes it plain that it is desirable to find a way to remove the regularization or to avoid it altogether.

Recently [Kie09a] the author noticed that after only minor modifications, Ruelle’s method [Rue69] to establish the thermodynamic limit for Boltzmann’s ergodic ensemble entropy, taken per volume (or per particle), works without the need for any regularization of the ensemble measure; a follow-up work on the thermodynamic limit of the correlation functions is planned. Taking “the thermodynamic limit” [Rue69] means that the domain \( \Lambda \) grows “evenly” with \( N \) and such that \( N/\text{Vol}(\Lambda) \to \rho \) with \( \rho \) a fixed number density, and the energy \( \mathcal{E} \) scales such that \( \mathcal{E}/\text{Vol}(\Lambda) \to \varepsilon \) (or \( \mathcal{E}/N \to \varepsilon \), abusing notation), with \( \varepsilon \in \mathbb{R} \) a fixed energy density (or energy per particle) — this limit covers systems of interest in condensed matter physics or chemical physics, such as those with hard core or Lennard-Jones interactions.

In the present paper we will be concerned with another limit \( N \to \infty \), where \( \Lambda \) is fixed and \( \mathcal{E} \) scales such that \( \mathcal{E}/N^2 \to \varepsilon \). This limit covers systems of interest in plasma and astrophysics, such as those with Coulomb or (mollified) Newton interactions. It is variably known\(^1\) as a “thermodynamic mean-field limit,” a “self-averaging limit,” or “Vlasov limit.” We will study the Boltzmann ensemble entropy and the correlation functions.

The remainder of this paper is structured as follows. In section 2 we collect the defining formulas of the ergodic / microcanonical ensemble for finite \( N \) and explain which probabilistic quantities are of physical interest. In section 3 we give a heuristic motivation for the Vlasov limit. In section 4 we state our main theorems, ordered by increasing depth. Their proofs are given in sections 5.1 to 5.3. Section 6 lists some spin-offs of our results, and section 7 closes our paper with an outlook on some open problems.

\(^1\)The first two names refer to a Weiss-type “mean-field approximation” becoming exact in the limit, but we will not invoke any such approximation and speak of the Vlasov limit.
2 A brief review of the ergodic ensemble

For a Newtonian $N$-body system in a domain $\Lambda \subset \mathbb{R}^3$ with Hamiltonian

$$H_\Lambda^{(N)}(p_1, \ldots, q_N) = \sum_{1 \leq i \leq N} \frac{1}{2} |p_i|^2 + \sum_{1 \leq i < j \leq N} W_\Lambda(q_i, q_j) + \sum_{1 \leq j \leq N} V_\Lambda^{(N)}(q_j), \quad (1)$$

the ergodic / microcanonical ensemble is a family $\{X_k^{(N)}|k \in \mathbb{N}\}$ of i.i.d. copies of a random vector $X^{(N)} = (P_1, Q_1; \ldots; P_N, Q_N) \in (\mathbb{R}^3 \times \Lambda)^N$ distributed according to the stationary single-system a-priori probability measure

$$\mu_\epsilon^{(N)}(d^{6N}X) = (N!\Omega'_{H_\Lambda^{(N)}}(\epsilon))^{-1} \delta(\epsilon - H_\Lambda^{(N)}(X^{(N)}))d^{6N}X, \quad (2)$$

where $X^{(N)} := (p_1, q_1; \ldots; p_N, q_N) \in (\mathbb{R}^3 \times \Lambda)^N$ and $d^{6N}X$ is 6N-dimensional Lebesgue measure, and where

$$\Omega'_{H_\Lambda^{(N)}}(\epsilon) = \frac{1}{N!} \int \delta\left(\epsilon - H_\Lambda^{(N)}(X^{(N)})\right) d^{6N}X \quad (3)$$

is known as the structure function here, the $'$ means derivative w.r.t. $\epsilon$ of $\Omega_{H_\Lambda^{(N)}}(\epsilon) = \frac{1}{N!} \int \chi_{\{H_\Lambda^{(N)}(X^{(N)}) < \epsilon\}} d^{6N}X, \quad (4)$

where $\chi_{\{H_\Lambda^{(N)}(X^{(N)}) < \epsilon\}}$ is the characteristic function of the set $\{H_\Lambda^{(N)}(X^{(N)}) < \epsilon\} \in (\mathbb{R}^3 \times \Lambda)^N$, over which the integrals extend. Thus, if $\mathcal{B}$ denotes the Borel sets of $(\mathbb{R}^3 \times \Lambda)^N \subset \mathbb{R}^{6N}, \text{ then } ((\mathbb{R}^3 \times \Lambda)^N, \mathcal{B}, \mu_\epsilon^{(N)})$ is the single-system probability space; so if $B \in \mathcal{B}$ is a Borel set, then the probability of $X^{(N)}$ being in $B$ is

$$\text{Prob}(X^{(N)} \in B) = \mu_\epsilon^{(N)}(B). \quad (5)$$

Clearly, $\text{Prob}(X^{(N)} \in B) = 0$ unless $B \cap \{H_\Lambda^{(N)} = \epsilon\} \neq \emptyset$; put differently, $\text{Prob}(H_\Lambda^{(N)}(X_k^{(N)}) = \epsilon) = 1 \forall k \in \mathbb{N}$. Moreover, $\text{Prob}(X^{(N)} \in d^{6N}X) = \mu_\epsilon^{(N)}(d^{6N}X)$ is the a-priori probability for $X^{(N)}$ to be in $d^{6N}X$ about $X^{(N)}$.

The ergodic ensemble is probabilistically meaningful for all $N \in \mathbb{N}$, yet its thermodynamic significance emerges only in the large $N$ regime (Avogadro’s $N \approx 10^{23}$) when it makes sense to speak of a solid, a liquid, a plasma (etc.) on macroscopic scales of space and time. Since the typical physical characteristics

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2 All particles belong to a single specie. We use units of $mc^2$ for energy, $mc$ for momentum, and $h/mc$ for length, where $m$ is particle mass, $c$ the speed of light, $h$ Planck’s constant.

3 It is understood that $W_\Lambda$ is symmetric, i.e. $W_\Lambda(q, q) = W_\Lambda(q, q)$, and not reducible to a sum of one-body terms; other details of $W$ and $V$ will be specified in the next section.

4 Stationarity is defined w.r.t. the flow generated by the Hamiltonian $H_\Lambda^{(N)}(p_1, \ldots, q_N)$.

5 The $N!$ term was supplied by Gibbs to resolve Gibbs’ paradox. It cancels out in (2).

6 It is tacitly understood that whenever one encounters a physically interesting subset $L$ of a Borel null-set which is not itself Borel measurable, then we use the Lebesgue $\sigma$-algebra.
of solids and liquids (etc.) are not revealed by “picturing” such systems as individual points in \( \mathbb{R}^{6N} \), one associates each microstate \( X^{(N)} \) with a unique family of empirical \( n \)-point “densities” on \( (\mathbb{R}^3 \times \Lambda)^n \), \( n = 1, 2, \ldots, N \). The \textit{normalized one-point “density” with \( N \) atoms} (empirical measure) is given by

\[
\Delta^{(1)}_{X^{(N)}}(p, q) = \frac{1}{N} \sum_{1 \leq i \leq N} \delta(p - p_i)\delta(q - q_i)
\]  

(6)

and the \textit{normalized two-point density with \( N \) atoms} \((U\text{-statistic of order 2})\) by

\[
\Delta^{(2)}_{X^{(N)}}(p, q; p', q') = \frac{1}{N(N-1)} \sum_{1 \leq i \neq j \leq N} \delta(p - p_i)\delta(q - q_i)\delta(p' - p_j)\delta(q' - q_j);
\]

(7)

Similarly the empirical \( n \)-point densities with \( n = 3, \ldots, N \) are defined. The map \( X^{(N)} \to \{\Delta^{(n)}_{X^{(N)}}\}_{n=1}^N \) is bijective if we insist that the particular labeling given to us algebraically with r.h.s.\( \{6\} \) or r.h.s.\( \{7\} \) etc. has an intrinsic meaning; however, considered purely measure theoretically as “density” on \( \mathbb{R}^m \) each \( \Delta^{(n)}_{X^{(N)}} \) is invariant under the permutation group applied to the particular labeling, and since there are \( N! \) distinct \( X^{(N)} \)'s obtained by permuting the particle labels, the map \( X^{(N)} \to \{\Delta^{(n)}_{X^{(N)}}\}_{n=1}^N \) is many-to-one in this sense. Understood in this measure theoretic way the empirical \( n \)-point densities do not depend on the unphysical (though mathematically convenient) labeling of the particles\footnote{So, physically we can identify these \( N! \) distinct \( X^{(N)} \)'s with a single \textit{\( N \)-point configuration in} \( \mathbb{R}^3 \times \Lambda \), which is a point \( \tilde{X}^{(N)} \in \mathbb{R}^{3N} \times \Lambda_{x}^{N}/S_N \). The subscript \( x \) means that coincidence points are removed, and \( S_N \) is the symmetric group of order \( N \). We should also write \( \Delta^{(n)}_{\tilde{X}^{(N)}} \), with the understanding that as measure \( \Delta^{(n)}_{\tilde{X}^{(N)}} \) is given by \( \Delta^{(n)}_{X^{(N)}} \) for \textit{any} of the \( N! \) points \( X^{(N)} \) in the pre-image in \( \mathbb{R}^{6N} \) of \( \tilde{X}^{(N)} \). The map \( \tilde{X}^{(N)} \to \{\Delta^{(n)}_{\tilde{X}^{(N)}}\}_{n=1}^N \) is bijective.}

Hence, the probabilities of interest to physicists will be of the form

\[
\text{Prob}\left(\Delta^{(n)}_{X^{(N)}} \in \tilde{B}\right)
\]

(8)

for physically significant measurable sets \( \tilde{B} \) in \( \mathcal{P}^s((\mathbb{R}^3 \times \Lambda)^n) \), the permutation-symmetric probability measures on \( (\mathbb{R}^3 \times \Lambda)^n \). Among the physically significant sets are balls (w.r.t. a suitable topology, still to be chosen) centered at a representative \( n \)-point density function for a solid, liquid, ... , or complements of such balls. As for the topology, the fine \((TV)\) topology for \( \mathcal{P}^s((\mathbb{R}^3 \times \Lambda)^n) \) is \textit{not} suitable as it is equivalent to discriminating between different \( \Delta^{(n)}_{X^{(N)}} \) w.r.t. the Borel sigma algebra of \( \mathbb{R}^{6N}/S_N \) (see footnote 6). Practically accessible\footnote{Even if the balls in \( TV \) topology \textit{were} practically accessible, for \( N \gg 1 \) the amount of information would be sheer overwhelming and not very illuminating.} are only some considerably less finely resolved events, such as the empirical \( n \)-point densities \( \Delta^{(n)}_{X^{(N)}} \) distinguished w.r.t. the weak topology, quantified by
a convenient Kantorovich-Rubinstein metric $d_{\text{KR}}$ on $\mathfrak{P}^s((\mathbb{R}^3 \times \Lambda)^n)$. Two very different points in $\mathbb{R}^{6N}/S_N$, say $\tilde{X}^{(N)}$ and $\tilde{Y}^{(N)}$, can map into two densities $\Delta_{X^{(N)}}^{(n)}$ and $\Delta_{Y^{(N)}}^{(n)}$ which in weak topology on $\mathfrak{P}^s((\mathbb{R}^3 \times \Lambda)^n)$ are virtually indistinguishable; here $X^{(N)}$ and $Y^{(N)}$ are any two representative points out of the $N!$ points each, which constitute the pre-image in $\mathbb{R}^{6N}$ of $\tilde{X}^{(N)}$, respectively $\tilde{Y}^{(N)}$. So the probabilities of interest to physicists are typically of the form

$$\text{Prob}\left(d_{\text{KR}}\left(\Delta_{X^{(N)}}^{(n)}, f_{\text{eq}}^{(n)}\right) > \delta\right),$$

where $f_{\text{eq}}^{(n)}(p^{(1)}, q^{(1)}; \ldots; p^{(n)}, q^{(n)}) \in (\mathfrak{P} \cap \mathfrak{C}^0)((\mathbb{R}^3 \times \Lambda)^n)$ is an equilibrium density function, defined — in the simplest of all cases — implicitly as the unique function for which (after rescaling of variables and parameters, if necessary)

$$\text{Prob}\left(d_{\text{KR}}\left(\Delta_{X^{(N)}}^{(n)}, f_{\text{eq}}^{(n)}\right) > \delta\right) \xrightarrow{N \to \infty} 0 \quad \forall \delta > 0.$$

In these simplest of all cases, (10) also explains what is meant by a “representative n-point density function;” and whether $f_{\text{eq}}^{(n)}$ represents a solid, liquid, gas, etc., depends on the specific configurational correlations exhibited by $f_{\text{eq}}^{(n)}$. In more complicated (and more interesting) situations, several “competing” equilibrium functions $f_{\text{eq}}^{(n)}$ may exist, and (10) has to be modified accordingly.

The “simplest case” scenario just described was discovered by Boltzmann (p.442 of [Bol96]), based on his explicit evaluation of (2) for the perfect gas. He realized that when $H^{(N)}_\Lambda$ is the perfect gas Hamiltonian and $N \gg 1$, then basically every point of $\{H^{(N)}_\Lambda = \mathcal{E}\}$ (identified with an n-pt. density through the map $X^{(N)} \to \Delta_{X^{(N)}}^{(n)}$) lies in the vicinity (w.r.t. weak topology) of one and the same equilibrium density function $f_{\text{eq}}^{(n)}$ at that energy $\mathcal{E}$, and given $n$. When $H^{(N)}_\Lambda$ sports non-trivial pair interactions, Boltzmann’s description needs to be modified slightly to account for the phenomenon of phase transitions.

While there can hardly be a doubt that Boltzmann’s insight into (2) is correct, the rigorous results which support his assessment have been obtained not for (2) but for some regularized approximation of this singular measure [Rue69, Len73, ML79]. In this paper we will finally vindicate Boltzmann’s ideas in the Vlasov regime of the relevant class of Hamiltonians (1).

### 3 Heuristic considerations on the Vlasov limit

For the ergodic ensemble to exhibit a Vlasov regime the Hamiltonian (1) needs to satisfy additional conditions. In particular, a necessary condition on the symmetric and irreducible pair potential $W_\Lambda$ is local integrability, i.e. $W_\Lambda(q, \cdot) \in L^1(B_r(q) \cap \Lambda) \forall q \in \Lambda$. We remark that for the existence of a dynamical Vlasov regime the local integrability of the forces derived from $W_\Lambda$...
Whenever Boltzmann’s simplest scenario holds, then there is an equilibrium \( W \) as is most easily seen if we assume for a moment that weak compactness estimates, e.g. in some \( L^\infty \) is mandatory, viz. \( \nabla_q W_\Lambda(q, \cdot) \in L^1(B_r(q) \cap \Lambda) \forall q \in \Lambda \). Coulomb’s electrical and Newton’s gravitational interactions belong in either class. Physically meaningful external potentials \( V^{(N)}_\Lambda \) are continuous for \( q \in \Lambda \); it has minor technical advantages to assume that \( V^{(N)}_\Lambda \) is actually continuous also at the boundary, i.e. \( \lim_{q' \to q} V^{(N)}_\Lambda(q') = V^{(N)}_\Lambda(q) \) for all \( q \in \partial \Lambda \) and \( q' \in \Lambda \). For convenience we assume that \( \inf H^{(N)}_\Lambda(p_1, \ldots, q_N) = \min H^{(N)}_\Lambda(p_1, \ldots, q_N) = \mathcal{E}_g(N) > -\infty \), and call \( \mathcal{E}_g(N) \) the \( N \)-body ground state energy.\footnote{Presumably boundedness below is not technically necessary. We expect that pair interactions which diverge logarithmically to \( -\infty \) can be accommodated but require additional weak compactness estimates, e.g. in some \( \mathcal{L}^p \) space; cf. [KiLe97].} Newton’s gravitational interactions need to be regularized to achieve \( \mathcal{E}_g(N) > -\infty \).

In the introduction we have already mentioned that the Vlasov limit scaling for such interactions is \( \mathcal{E} \approx N^2 \varepsilon \) for \( N \gg 1 \). We now explain why. Integrating \( \mathcal{E} \) over \( p \)-space \( \mathbb{R}^3 \) gives a normalized one-point “density” (empirical measure) on \( \Lambda \) with \( N \) atoms, which by abuse of notation we denote as follows,

\[
\Delta^{(1)}_{X^{(N)}}(q) = \int_{\mathbb{R}^3} \Delta^{(1)}_{X^{(N)}}(p, q) d^3p = \frac{1}{N} \sum_{1 \leq i \leq N} \delta(q - q_i). \tag{11}
\]

Whenever Boltzmann’s simplest scenario holds, then there is an equilibrium density \( \rho_{\varepsilon, N} \in (\mathfrak{P} \cap \mathfrak{C}^0_b)(\Lambda) \), depending on \( N(\gg 1) \) and \( \mathcal{E} \), such that \( \Delta^{(1)}_{X^{(N)}}(q) \approx \rho_{\varepsilon, N}(q) \) for overwhelmingly most \( X^{(N)} \) distributed by \([2]\), where “\( \approx \)” means the two “densities” do not differ by much in a conventional Kantorovich-Rubinstein metric \( d_{KR} \). This suggests that when \( \Lambda \subset \mathbb{R}^3 \) is fixed and \( N \to \infty \) together with \( \mathcal{E} \to \infty \) such that \( \mathcal{E}/N^\alpha \to \varepsilon \) for a yet-to-be determined \( \alpha \), then \( \rho_{\varepsilon, N} \to \varepsilon \rho_{\varepsilon} \in (\mathfrak{P} \cap \mathfrak{C}^0_b)(\Lambda) \) and \( \Delta^{(1)}_{X^{(N)}}(q) d^3p \to \varepsilon \rho_{\varepsilon}(q) \), weakly. Implementing this law-of-large-numbers type scenario inevitably leads to \( \alpha = 2 \), as is most easily seen if we assume for a moment that \( W_\Lambda \in \mathfrak{C}^0_b(\Lambda \times \Lambda) \). Then \( q \mapsto W_\Lambda(q, \mathcal{P}) \) is a bounded continuous function in \( \Lambda \) and we can write

\[
H^{(N)}(X^{(N)}) = N \int \left[ \frac{1}{2} |p|^2 \Delta^{(1)}_{X^{(N)}}(p, q) d^3p d^3q 
+ N \int \left( V^{(N)}_\Lambda(q) - \frac{1}{2} W_\Lambda(q, q) \right) \Delta^{(1)}_{X^{(N)}}(p, q) d^3p d^3q \right] \tag{12}
+ N^2 \left[ \int \left( W_\Lambda(q, \mathcal{P}) \Delta^{(1)}_{X^{(N)}}(p, q) d^3p d^3q \Delta^{(1)}_{X^{(N)}}(\mathcal{P}, \mathcal{P}) d^3pd^3\mathcal{P} \right) \Delta^{(1)}_{X^{(N)}}(\mathcal{P}, \mathcal{P}) d^3pd^3\mathcal{P} \right].
\]
and when $\int_{\mathbb{R}^3} \Delta_X^{(1)}(p, q)d^3p \approx \rho_\varepsilon(q)$, we find

$$H^{(N)}(X^{(N)}) \approx N \int \frac{1}{2} |p|^2 \Delta_X^{(1)}(p, q)d^3p + N \left( V^{(N)}_\Lambda(q) - \frac{1}{2} W_\Lambda(q, q) \right) \rho_\varepsilon(q)d^3q + N^2 \int \frac{1}{2} W_\Lambda(q, q) \rho_\varepsilon(q) \rho_\varepsilon(q)d^3qd^3\tilde{q}.$$  \hspace{1cm} (13)

The last term clearly scales $\propto N^2$ because $W_\Lambda$ and $\rho_\varepsilon$ are independent of $N$. In a sense this already establishes the $\mathcal{E} \propto N^2$ scaling. However, we have yet to consider the terms on the first two lines on the r.h.s. of (13). It would seem that these scale $\propto N$ and so, for large $N$, would become insignificant as compared to the one in the last line, but only the $N \int \frac{1}{2} W_\Lambda(q, q) \rho_\varepsilon(q)d^3q$ contribution will surely become insignificant\textsuperscript{10} for large $N$, for the same reasons for why the last one scales $\propto N^2$ ($W_\Lambda$ and $\rho_\varepsilon$ do not depend on $N$). As for the external potential $V^{(N)}_\Lambda(q)$, the superscript ($^{(N)}$) indicates that we may want to adjust it to the number of particles in the system on which it acts in order to retain a noticeable effect when $N$ becomes large. So in particular we can set $V^{(N)}_\Lambda(q) = NV_\Lambda(q)$ [or $= (N - 1)V_\Lambda(q)$], with $V_\Lambda(q)$ independent of $N$, and find $N \int V^{(N)}_\Lambda(q) \rho_\varepsilon(q)d^3q = N^2 \int V_\Lambda(q) \rho_\varepsilon(q)d^3q \ [+O(N)]$, scaling $\propto N^2$ [in leading order], hence remaining significant in (13) as $N$ becomes large. And as to the kinetic energy term, it is important to realize that $\int_{\mathbb{R}^3} \Delta_X^{(1)}(p, q)d^3p \approx \rho_\varepsilon(q) \in (\mathcal{F} \cap \mathcal{C}_0^0)(\mathbb{R}^3)$ does not imply that $\Delta_X^{(1)}(p, q) \approx f_\varepsilon(p, q) \in (\mathcal{F} \cap \mathcal{C}_0^0)(\mathbb{R}^3 \times \Lambda)$. For instance, we can have that $N^{3/2} \Delta_X^{(1)}(N^{1/2}p, q) \approx f_\varepsilon(p, q) \in (\mathcal{F} \cap \mathcal{C}_0^0)(\mathbb{R}^3 \times \Lambda)$ so that a significant fraction of the energy will be distributed over the kinetic degrees of freedom\textsuperscript{11} and then, up to terms of $O(N)$, we find

$$H^{(N)}(X^{(N)}) \approx N^2 \left( \int \left( \frac{1}{2} |p|^2 + V_\Lambda(q) \right) f_\varepsilon(p, q)d^3p \right) + \int \int \int \frac{1}{2} W_\Lambda(q, q) f_\varepsilon(p, q)f_\varepsilon(\tilde{p}, \tilde{q})d^3pd^3qd^3\tilde{q}.$$  \hspace{1cm} (14)

This scaling scenario can be verified explicitly for the perfect gas ($W_\Lambda \equiv 0$) by inspecting Boltzmann’s calculations, and it is reasonable to expect that it will continue to hold for a physically interesting class of $W_\Lambda \neq 0$.

To summarize, the Vlasov limit for the Hamiltonian (11) with $V^{(N)} = NV$ means that $N^{3/2} \Delta_X^{(1)}(N^{1/2}p, q) \to f_\varepsilon(p, q)$ weakly in $\mathcal{P}(\mathbb{R}^3 \times \Lambda)$, with

\textsuperscript{10}Incidentally, this indicates that the Vlasov limit does not require the continuity of $W_\Lambda$, the only purpose of which was to furnish identity (12) which involves $W_\Lambda(q, q)$.

\textsuperscript{11}Unless $\mathcal{E}$ is the ground state energy for which all particle momenta vanish, indeed.
\( f_\varepsilon(\mathbf{p}, \mathbf{q}) \in (\Psi \cap \mathbf{c}_{\varepsilon}^n)(\mathbb{R}^3 \times \Lambda), \) and \( N^{-2}H^{(N)}(X^{(N)}) \xrightarrow{N \to \infty} \varepsilon(f_\varepsilon) = \varepsilon > \varepsilon_g, \) where

\[
\varepsilon(f) = \iint \left( \frac{1}{2} |\mathbf{p}|^2 + V_\Lambda(q) \right) f(\mathbf{p}, \mathbf{q}) \, d^3pd^3q \\
+ \iiint \frac{1}{2}W_\Lambda(q, \tilde{\mathbf{q}})f(\mathbf{p}, \mathbf{q})f(\mathbf{\tilde{p}}, \mathbf{\tilde{q}}) \, d^3pd^3q \, d^3\tilde{p} \, d^3\tilde{q}
\]

(15)
is the “energy of \( f, \)” and where \( \varepsilon_g = \inf_{f \in \Psi(\mathbb{R}^3 \times \Lambda)} \varepsilon(f) \) is given by

\[
\varepsilon_g = \inf_{\rho \in \Psi(\Lambda)} \left( \int V_\Lambda(q) \rho(q) \, d^3q + \int \frac{1}{2}W_\Lambda(q, \tilde{\mathbf{q}}) \rho(q) \rho(\tilde{\mathbf{q}}) \, d^3q \, d^3\tilde{q} \right).
\]

(16)

\section{The Vlasov limit for Boltzmann’s Ergode}

We now state our main results about the Vlasov scaling limit for Boltzmann’s ergodic ensemble of \( N \)-body systems in a format which will be recognized as the familiar folklore by anyone with a joint expertise in Vlasov theory and statistical mechanics. We will also utilize some less familiar notions.

In the following, \( \Lambda \subset \mathbb{R}^3 \) is a bounded, connected domain (open) which does not depend on \( N \). The upshot of the previous section is that if we want the external potential to remain significant when \( N \) gets large, then our \( N \)-body dynamics in \( \Lambda \) will be governed by Hamiltonians (11) of the special type

\[
H_\Lambda^{(N)}(\mathbf{p}_1, \ldots, \mathbf{q}_N) = \sum_{1 \leq i \leq N} \left( \frac{1}{2} |\mathbf{p}_i|^2 + (N - 1)V_\Lambda(q_i) \right) + \sum_{1 \leq i < j \leq N} W_\Lambda(q_i, q_j),
\]

(17)

with the single particle potential \( V_\Lambda \) and the pair interaction \( W_\Lambda \) independent of \( N \). We choose \( N - 1 \) rather than \( N \) as scaling for \( V_\Lambda^{(N)} \) because then we can absorb \( V_\Lambda \) and \( W_\Lambda \) together in a new \( N \)-independent effective pair interaction \( U_\Lambda(q, \tilde{\mathbf{q}}) := W_\Lambda(q, \tilde{\mathbf{q}}) + V_\Lambda(q) + V_\Lambda(\tilde{\mathbf{q}}) \). This doesn’t affect any of our results (as we will prove), but the Hamiltonian (17) can be recast shorter as

\[
H_\Lambda^{(N)}(\mathbf{p}_1, \ldots, \mathbf{q}_N) = \sum_{1 \leq i \leq N} \frac{1}{2} |\mathbf{p}_i|^2 + \sum_{1 \leq i < j \leq N} U_\Lambda(q_i, q_j).
\]

(18)

Since heuristically we expect for a Hamiltonian system with Hamiltonian (18) under Vlasov scaling that \( N^{3/2} \Delta^{(1)}(\mathbb{R}^3) (N^{1/2} \mathbf{p}, \mathbf{q}) \xrightarrow{N \to \infty} f_\varepsilon(\mathbf{p}, \mathbf{q}) \) weakly, with \( f_\varepsilon(\mathbf{p}, \mathbf{q}) \in (\Psi \cap \mathbf{c}_{\varepsilon}^n)(\mathbb{R}^3 \times \Lambda) \), we also expect that the rescaled particle momentum random vectors \( N^{-1/2} \mathbf{P}_i \) converge in distribution, implying that \( \sum \frac{1}{2} |\mathbf{P}_i|^2 \approx N^2 \varepsilon_{\text{kin}} \) for \( \mu^{(N)}_{\varepsilon} \)-most \( X^{(N)} \), where \( \varepsilon_{\text{kin}} \) is the kinetic energy contribution to \( \varepsilon \).

We find it more convenient to work with random variables which themselves converge in distribution and so re-scale the momentum variables as \( \mathbf{p}_k = N^{1/2} \tilde{\mathbf{p}}_k \) in (18); or in more economical notation: we replace \( \mathbf{p}_k \to N^{1/2} \tilde{\mathbf{p}}_k \) in
With this minor additional abuse of notation our Hamiltonian finally reads
\[ H^{(N)}_{\Lambda}(p_1, \ldots, q_N) = N \sum_{1 \leq i \leq N} \frac{1}{2} |p_i|^2 + \sum_{1 \leq i < j \leq N} U_{\Lambda}(q_i, q_j). \] (19)

Our main results will be proved under the following hypotheses on \( U_{\Lambda}(q, \hat{q}) \):

- (H1) Symmetry: \( U_{\Lambda}(q, \hat{q}) = U_{\Lambda}(\hat{q}, q) \)
- (H2) Lower Semi-Continuity: \( U_{\Lambda}(q, \hat{q}) \) is l.s.c. on \( \overline{\Lambda} \times \overline{\Lambda} \)
- (H3) Sublevel Set Regularity: \( \int \int X_{\{U_{\Lambda}(q, \hat{q}) - \min_{\Lambda} U_{\Lambda} < \epsilon\}} d^3q d^3\hat{q} > 0 \)
- (H4) Local Square Integrability: \( U_{\Lambda}(q, \cdot) \in L^2(B_r(q) \cap \Lambda) \forall q \in \Lambda \)
- (H5) Confinement: \( U_{\Lambda}(q, \hat{q}) = +\infty \) whenever \( \hat{q} \notin \overline{\Lambda} \) or \( q \notin \overline{\Lambda} \)

Hypothesis (H1) is a consequence for \( W_{\Lambda} \) of Newton’s “actio equals re-actio,” plus the symmetrized added contribution of \( V_{\Lambda} \), both of which need no further commentary. Hypothesis (H2) is satisfied by many important pair interactions invoked in physics, though not by all. For instance, the Coulomb pair potential \( U_{\Lambda}^{\text{Coul}}(q, \hat{q}) = 1/|q - \hat{q}| \) for \( q \neq \hat{q} \) satisfies (H2) after also setting \( U_{\Lambda}^{\text{Coul}}(q, q) \equiv u \) for any particular \( u \in \mathbb{R} \). On the other hand, the Newton pair potential \( U_{\Lambda}^{\text{Newt}}(q, \hat{q}) = -U_{\Lambda}^{\text{Coul}}(q, \hat{q}) \) does not satisfy (H2) for any choice of \( u \); however, the regularized Newton pair potential \( U_{\Lambda, \text{reg}}^{\text{Newt}}(q, \hat{q}) = -(\chi_{B_r} * U_{\Lambda}^{\text{Coul}} * \chi_{B_r})(q, \hat{q}) \) (where \( * \) denotes the conventional convolution product of \( f \) and \( g \)) does satisfy (H2). By (H2), there exists an \( N \)-dependent ground state energy \( E_g(N) \), i.e. \( H_{\Lambda}^{(N)} \geq E_g(N) > -\infty \), but the ground state configuration can have some unwanted features. Hypothesis (H3) eliminates the possibility of energetically isolated ground states, thus guaranteeing the existence of a fat set of minimizing sequences of configurations. Hypothesis (H4) is a little stronger than necessary, but it allows us to make convenient use of Chebychev’s inequality to prove a law of large numbers for the pair-specific interaction energy; the important Coulomb potential satisfies (H4). Note that (H4) implies local \( L^1 \) integrability of \( U_{\Lambda} \), which is needed in various integrals featuring in the Vlasov limit. Note also that by (H2)&(H4) there exists an \( N \)-independent \( \varepsilon_g \in \mathbb{R} \) defined by [10]. In Appendix A we show that (H1)&(H2) guarantee that the pair-specific ground state energy \( E_g(N)/[N(N - 1)] \equiv \varepsilon_g(N) \) is monotonic increasing with \( N \), and using also (H3) and (H4) we show that \( \varepsilon_g(N) \nearrow \varepsilon_g \) as \( N \to \infty \). In Appendix A we also show that if \( U_{\Lambda} \geq 0 \), then also \( E_g(N)/N^2 \equiv \varepsilon_g(N) \nearrow \varepsilon_g \) as \( N \to \infty \).

\[ \text{For instance, in our example of the amended Coulomb pair potential one can choose} \]
\[ u = 0, \text{but then Thomson’s problem on} \ S^2 \subset \mathbb{R}^3 \text{[Tho04]} \text{yields as ground state configuration always the spurious one (up to SO(3) action) for which all particle positions coincide. To avoid these spurious ground state configurations it is advisable to choose} \ u > 0 \text{huge.} \]
Hypothesis \((H5)\) is really inherited from the dynamical theory of \(N\) particles in \(\Lambda \subset \mathbb{R}^3\), where one sets \(V^{(N)}_\Lambda = +\infty\) for \(q \not\in \Lambda\) to dynamically model confinement in a container; \((H5)\) has a minor notational advantage by allowing us to treat physical space integrals like momentum space integrals as over all \(\mathbb{R}^3\); the spatial cutoff to \(\Lambda\) automatically being provided by the potential \(V_\Lambda\) through \(U_\Lambda\). Usually, \((H5)\) is not listed explicitly as a hypothesis on the interactions even when spatial integrations are explicitly restricted to \(\Lambda\). This concludes our commentary on the list of hypotheses \((H1) - (H5)\).

All our results (except Proposition 7 in Appendix A) will be formulated and proved under the convenient assumption that \(U_\Lambda \geq 0\), so that \(\epsilon_g \geq 0\). Since \(U_\Lambda\) has a minimum in \(\Lambda^2\), by \((H2)\), and since the physics of our dynamical system does not change if we simply add a constant to \(U_\Lambda\), we may assume that \(U_\Lambda \geq 0\) without loss of generality. We emphasize that this choice is merely for convenience, given \((H2)\), and so is not listed as another hypothesis.

The simplest objects of interest are the thermodynamic functions. In the 1960s and hence, techniques based on monotonicity, convexity and superadditivity estimates have been developed to prove their existence and regularity in the limit \(N \to \infty\) which avoids having to control the more sophisticated objects of interest, which are the correlation functions. For the traditional thermodynamic limit scaling, see Ruelle’s book [Rue69] and [Kie09a] for a recent extension of Ruelle’s arguments to Boltzmann’s Ergode proper. For the Vlasov scaling of the canonical ensemble, see [Kie93]. To extend these arguments to Boltzmann’s Ergode proper with Vlasov scaling, our first goal is to show that the logarithm of the structure function \([3]\) for the Hamiltonian \([19]\), which yields Boltzmann’s ergodic ensemble entropy\(^{13}\) (cf. eq.(305) in [Gib02]),

\[
S_{H^{(N)}_\Lambda}(\mathcal{E}) = \ln \Omega'_{H^{(N)}_\Lambda}(\mathcal{E}),
\]

admits the correct type of asymptotic expansion for \(N \to \infty\) with \(\mathcal{E} = N^2 \epsilon\), and has the correct qualitative \(\epsilon\) dependence. The usual strategy can be put to work if we assume just a little more than \((H1) - (H5)\). In this vein we state:

**Theorem 1.** Let \(H^{(N)}_\Lambda\) be given in \([19]\), with \(U_\Lambda\) satisfying conditions \((H1)\) and \((H5)\), but with \((H2), (H3), (H4)\) replaced by the single stronger condition:

\[(H6)\quad \text{Continuity: } U_\Lambda(\mathbf{q}, \mathbf{q}) \text{ is continuous on } \Lambda \times \Lambda.\] (21)

Let \(\epsilon > \epsilon_g\), with \(\epsilon_g \geq 0\) defined as before. Then the ergodic ensemble entropy \([20]\) has the following asymptotic expansion for \(N \gg 1\),

\[
S_{H^{(N)}_\Lambda}(N^2 \epsilon) = -N \ln N + N s_\Lambda(\epsilon) + o(N),
\]

(22)

where \(s_\Lambda(\epsilon)\) is the system-specific Boltzmann entropy per particle. The function \(\epsilon \mapsto s_\Lambda(\epsilon)\) is continuous and strictly increasing for \(\epsilon > \epsilon_g\).

\(^{13}\)Entropy is measured in units of \(k_B\), where \(k_B\) is Boltzmann’s constant.
We remark that the leading term of r.h.s. (22) is purely combinatorial in origin and independent of the Hamiltonian $H^{(N)}_\Lambda$ — it is solely due to the $N!$ in (3). System-specific information begins to show in the next to leading term, which is $O(N)$. The $o(N)$ term in (22) is presumably $O(\ln N)$.

We will also prove two upgrades of Theorem 1 (Theorems 1$^+$ and 1$^{++}$) which involve the decomposition of the system-specific Boltzmann entropy per particle $s_\Lambda(\varepsilon)$ into a “kinetic” and an “interaction” contribution. The discussion of this more technical material is postponed until section 5.1.

While they do yield valuable qualitative information about the thermodynamic functions for the systems under study, in this case $s_\Lambda(\varepsilon)$, existence theorems such as Theorem 1 and their “proofs by sub-additivity” have the disadvantage that they do not characterize the limit objects in a way which would allow their systematic evaluation for physically interesting irreducible pair potentials $W_\Lambda$ and external one-body potentials $V_\Lambda$. It is this type of characterization that we are after, and in section 5.2 we prove that $s_\Lambda(\varepsilon)$ satisfies the familiar maximum entropy variational principle for the entropy per particle of a perfect gas in a combination of self- and externally generated fields. More precisely, we prove the following strengthening of Theorem 1.

**Theorem 2.** Let $H^{(N)}_\Lambda$ be given in (19), with $U_\Lambda \geq 0$ satisfying (H1)–(H5). Let $\varepsilon > \varepsilon_g$. Then the Boltzmann entropy (20) has the asymptotic expansion

$$S_{H^{(N)}_\Lambda}(N^2 \varepsilon) = -N \ln N + Ns_\Lambda(\varepsilon) + o(N)$$

for $N \gg 1$, and the system-specific Boltzmann entropy per particle is given by

$$s_\Lambda(\varepsilon) = -\mathcal{H}_B(f_\varepsilon),$$

where $\mathcal{H}_B(f)$ is “Boltzmann’s H function” of $f$, which reads

$$\mathcal{H}_B(f) = \iint f(p, q) \ln(f(p, q)/e) d^3p d^3q,$$

and where $f_\varepsilon$ is any minimizer of this $H$ functional over the set of trial densities $\mathfrak{A}_\varepsilon = \{f \in (\mathfrak{P} \cap L^1 \cap L^1 \ln L^1)(\mathbb{R}^3 \times \Lambda) : \mathfrak{e}(f) = \varepsilon\}$, where $\mathfrak{e}(f)$ now reads

$$\mathfrak{e}(f) = \iint \frac{1}{2} |p|^2 f(p, q) d^3p d^3q + \iiint U_\Lambda(q, \tilde{q}) f(p, q) f(\tilde{p}, \tilde{q}) d^3p d^3q d^3\tilde{p} d^3\tilde{q}.$$

Any minimizer $f_\varepsilon$ of $\mathcal{H}_B(f)$ over the set $\mathfrak{A}_\varepsilon$ is of the form

$$f_\varepsilon(p, q) = \sigma_\varepsilon(p) \rho_\varepsilon(q),$$

We remark that Euler’s number $e$ in (25) is inherited from the $N!$ term in (20).
where $\rho_\varepsilon(q)$ solves the following fixed point equation on $q$ space,

$$
\rho_\varepsilon(q) = \frac{\exp \left( -\vartheta_\varepsilon(\rho_\varepsilon)^{-1} \int_\Lambda U_\Lambda(q, \tilde{q}) \rho_\varepsilon(\tilde{q}) d^3\tilde{q} \right)}{\int_\Lambda \exp \left( -\vartheta_\varepsilon(\rho_\varepsilon)^{-1} \int_\Lambda U_\Lambda(q, \tilde{q}) \rho_\varepsilon(\tilde{q}) d^3\tilde{q} \right) d\tilde{q}}
$$

(28)

with $\vartheta_\varepsilon(\rho)$ given by

$$
\vartheta_\varepsilon(\rho) = \varepsilon - \int \frac{1}{2} U_\Lambda(q, \tilde{q}) \rho(q) \rho(\tilde{q}) d^3q d^3\tilde{q},
$$

(29)

and where $\sigma_\varepsilon(p) = \sigma(\rho_\varepsilon)(p)$, with $\sigma(\rho)(p)$ defined whenever $\vartheta(\rho) > 0$, by

$$
\sigma(\rho)(p) = \left(2\pi\vartheta(\rho)\right)^{-\frac{3}{2}} \exp \left(-\frac{1}{2} |p|^2 / \vartheta_\varepsilon(\rho)\right).
$$

(30)

Evidently, every minimizer of $H_B(f)$ over $\mathfrak{A}_\varepsilon$ factors into a product of a Maxwellian on $p$ space and a purely space-dependent “self-consistent Boltzmann factor.”\footnote{The expression conventionally known as “Boltzmann factor” results when $W_\Lambda \equiv 0$ so that $U_\Lambda(q, \tilde{q}) = V_\Lambda(q) + V_\Lambda(\tilde{q})$, i.e. for the perfect gas acted on by an external potential $V_\Lambda$.} However, the Maxwellian in (27) is not autonomous from the Boltzmann factor in (27), as is manifest by the functional dependence of the (rescaled) temperature $\vartheta = \vartheta_\varepsilon(\rho_\varepsilon)$ on $\rho_\varepsilon$, see (30). For a subset of $\varepsilon$ values the minimizer of $H_B(f)$ over $\mathfrak{A}_\varepsilon$ may not be unique, but all minimizers produce the same asymptotic formula (23). In such a case of non-uniqueness of minimizers, they always seem to constitute either a finite set (typically a first order phase transition) or a continuous group orbit of a compact group (e.g., when $\Lambda$ is invariant under $SO(2)$ or $SO(3)$ and a minimizer breaks that symmetry), to the best of our knowledge; this seems to cover all physically relevant possibilities.

In addition to the minimizers of $H_B(f)$ there may be non-minimizing critical points of $H_B(f)$ satisfying (27)–(30), but these are irrelevant for (23).

Our Theorem 3, proved in section 5.3 with input from section 5.2, characterizes the Vlasov limit $N \to \infty$ of the marginal measures

$$
\mu^{(N)}_\varepsilon(d^{6n}X) = \mu^{(N)}_\varepsilon(d^{6n}X \times (\mathbb{R}^3 \times \Lambda)^{N-n}), \quad n = 1, 2, \ldots \ (n \text{ fixed})
$$

(31)

in terms of the $f_\varepsilon$. We note that the object of interest in (mathematical) physics is not (2) itself but only the collection of its first few marginal measures (31). To state our theorem, we introduce $\mathcal{P}^s((\mathbb{R}^3 \times \Lambda)^{\mathbb{N}})$, the permutation-symmetric probability measures on the set of infinite sequences in $\mathbb{R}^3 \times \Lambda$. A theorem of de Finetti [deF37], Dynkin [Dyn53], and Hewitt–Savage [HeSa55] (see also [Ell85], App.A.9.) states that $\mathcal{P}^s((\mathbb{R}^3 \times \Lambda)^{\mathbb{N}})$ is uniquely presentable as an average of infinite product measures; i.e., for each $\mu \in \mathcal{P}^s((\mathbb{R}^3 \times \Lambda)^{\mathbb{N}})$ there exists a unique probability measure $\nu(d\tau|\mu)$ on $\mathcal{P}(\mathbb{R}^3 \times \Lambda)$, such that

$$
n_\mu(d^{3n}p d^{3n}q) = \int_{\mathcal{P}(\mathbb{R}^3 \times \Lambda)} \tau^{\otimes n}(d^3p_1 d^3q_1 \cdots d^3p_n d^3q_n) \nu(d\tau|\mu) \quad \forall n \in \mathbb{N},
$$

(32)
where $\mu$ is the $n$-th marginal measure of $\mu$, and $\tau^\otimes n(d^3p_1d^3q_1\cdots d^3p_n d^3q_n)\equiv \tau(d^3p_1d^3q_1)\otimes \cdots \otimes \tau(d^3p_n d^3q_n)$. Equation (32) is also the extremal decomposition for the convex set $\mathcal{P}^s((\mathbb{R}^3 \times \Lambda)^n)$, see [HeSa55].

**Theorem 3.** Under the same assumptions as in Theorem 2, consider (2) with Hamiltonian (19) as extended to a probability on $(\mathbb{R}^3 \times \Lambda)^N$. Then the sequence $\{\mu_{N^2\varepsilon}^{(N)}\} \subset N$ is tight, so one can extract a subsequence $\{\mu_{N^2\varepsilon}^{(N)}\} \subset N$ such that

$$
\lim_{N \to \infty} \mu_{N^2\varepsilon}^{(N)}(d^3p d^3q) = \mu_{\varepsilon}(d^3p d^3q) \in \mathcal{P}^s((\mathbb{R}^3 \times \Lambda)^n) \quad \forall n \in \mathbb{N}.
$$

The decomposition measure $\nu(d\tau | \mu_{\varepsilon})$ of each such limit point $\mu_{\varepsilon}$ is supported by the subset of $\mathcal{P}(\mathbb{R}^3 \times \Lambda)$ which consists of the probability measures $\tau_{\varepsilon}(d^3p d^3q) = f_{\varepsilon}(p, q)d^3p d^3q$ which minimize the $H$ functional $\mathcal{H}_B(f)$ over $\mathcal{A}_\varepsilon$. 

## 5 Proofs

We have stated our Theorems 1,2,3 entirely in terms of the familiar quantities of kinetic theory. These are the one-body density function $f_{\varepsilon}(p, q)$ which minimizes Boltzmann’s $H$-function $\mathcal{H}(f)$ under the familiar energy functional constraint $\varepsilon(f) = \varepsilon$, and the system-specific Boltzmann entropy per particle $s_{\Lambda}(\varepsilon)$ which is given as the negative of Boltzmann’s $H$-function evaluated with $f_{\varepsilon}$. However, in this format our theorems give essentially symmetric weight to the $p$ and $q$ variables, which ignores the fact that the $p$-space integrations involved in (21) and (20) can be carried out explicitly in the same fashion as for the perfect gas. As a consequence the problem reduces to studying the large $N$ asymptotics of the expressions which result from these $p$-space integrations.\(^\text{16}\)

In fact, all the hard analytical work goes into controlling the $q$-space integrations. This is certainly the case as far as the entropy per particle goes, yet also each minimizer $f_{\varepsilon}$ of $\mathcal{H}_B(f)$ over the set $\mathcal{A}_\varepsilon$ is uniquely determined by $\rho_{\varepsilon}$, which signals that all of our Theorems 1 to 3 will be essentially straightforward corollaries of theorems about certain $q$-space expressions. Those theorems take a less familiar form, presumably, which is why their statements have been relegated into this section where we prove Theorems 1 to 3.

### 5.1 Proof of Theorem 1 and its two upgrades

To prove Theorem 1 we first formulate and then prove an upgraded version (Theorem $1^+$), whose proof also proves Theorem 1.

\(^{16}\)All Boltzmann needed for this was that $(1 + x/n)^n \approx e^x$; cf. [Bol96], part II, ch. 3. Of course, things are not quite as straightforward with an irreducible $W_{\Lambda} \neq 0$, or else Boltzmann would not have had to have $W_{\Lambda} \neq 0$ excluded from his analysis.
5.1.1 Theorem 11 and its proof

Carrying out the \( p \) integrations\(^{17} \) in \( \Omega'^{(N)}_{H_{\Lambda}^{(N)}}(\mathcal{E}) \) given by (31), with \( H_{\Lambda}^{(N)} \) given in (19), Boltzmann’s ergodic ensemble entropy (20) becomes

\[
S_{H_{\Lambda}^{(N)}}(\mathcal{E}) = \ln \left( \frac{(2/N)^{3N/2}}{3^N} |S^{3N-1}| \Psi'_{I_{\Lambda}^{(N)}}(\mathcal{E}) \right) 
\]

with \( |S^{3N-1}| \) the standard measure of the unit \( 3N-1 \) sphere \( S^{3N-1} \), and with

\[
\Psi'_{I_{\Lambda}^{(N)}}(\mathcal{E}) = \frac{(3/2)}{(N-1)!} \int \left( \mathcal{E} - I_{\Lambda}^{(N)}(q_1, \ldots, q_N) \right)^{\frac{3N}{2}-1} \chi\{I_{\Lambda}^{(N)} < \mathcal{E}\} d^{3N}q. 
\]

where we introduced the interaction Hamiltonian

\[
I_{\Lambda}^{(N)}(q_1, \ldots, q_N) = \sum_{1 \leq i < j \leq N} U_{\Lambda}(q_i, q_j). 
\]

Implementing the Vlasov limit scaling, i.e. setting \( \mathcal{E} = N^2 \varepsilon \) with \( \varepsilon > \varepsilon_g \geq 0 \), recalling that \( |S^{3N-1}| = \pi^{3N/2}/\Gamma(3N/2) \), and using Stirling’s formula for Euler’s \( \Gamma \) function, we obtain the following asymptotic expansion for (34),

\[
S_{H_{\Lambda}^{(N)}}(N^2 \varepsilon) = -N \ln N + N \ln \left( |\Lambda| \left( \frac{4 \pi \varepsilon}{3} \right)^{3/2} \right) + O(\ln N) 
+ \ln \int \left( 1 - \frac{1}{\varepsilon N^2} I_{\Lambda}^{(N)}(q_1, \ldots, q_N) \right)^{\frac{3N}{2}-1} \lambda(d^{3N}q). 
\]

where \((\cdots)_+\) means the positive part of \((\cdots)\); moreover, \( \lambda(d^{3N}q) \) is the \( N \)-fold product of the normalized Lebesgue measure \( \lambda(d^3q) = |\Lambda|^{-1} d^3q \) on \( \Lambda \). For brevity we wrote \(|\Lambda|\) for the volume \( \text{Vol}(\Lambda) \) of \( \Lambda \).

When \( I_{\Lambda}^{(N)} \equiv 0 \) in \( \Lambda^N \), then \( H_{\Lambda}^{(N)} \) becomes the Hamiltonian of the perfect gas without external fields\(^{18} \) abbreviated as \( K_{\Lambda}^{(N)} \) (for kinetic Hamiltonian). In this case the second line in (37) vanishes, and (37) becomes the asymptotic expansion of the entropy of the spatially uniformly distributed perfect gas, viz.

\[
S_{K_{\Lambda}^{(N)}}(N^2 \varepsilon) = -N \ln N + N \ln \left( |\Lambda| \left( \frac{4 \pi \varepsilon}{3} \right)^{3/2} \right) + O(\ln N). 
\]

The coefficient of the \( O(N) \) term in (38) gives the system-specific Boltzmann entropy per particle of the spatially uniform perfect gas, which we denote by

\[
s_{\Lambda;K}(\varepsilon) = \ln \left( |\Lambda| \left( \frac{4 \pi \varepsilon}{3} \right)^{3/2} \right). 
\]

\(^{17}\)It is understood that \( d^{6N}X \) etc. now involves the \( p \) variables used in (19).

\(^{18}\)It is tacitly understood that the cutoff provided by \( I_{\Lambda}^{(N)} \) remains effective, so that the configurational integrations in (37) are still over \( \Lambda^N \).
Whenever interactions \( I^{(N)}_\Lambda \neq 0 \) of the admitted type are present, Theorem 1 follows if we can show that the second line in (37) is \( O(N) \) and so contributes additively to the system-specific Boltzmann entropy per particle, and provided it has the right monotonicity and regularity. This is expressed in

**Proposition 1.** Under the assumptions stated in Theorem 1, there holds

\[
\lim_{N \to \infty} \frac{1}{N} \ln \left( 1 - \frac{1}{2N} I^{(N)}_\Lambda(q_1, \ldots, q_N) \right) \Rightarrow \lambda(d^3q) = s_{\Lambda,I}(\varepsilon) \tag{40}
\]

The function \( \varepsilon \mapsto s_{\Lambda,I}(\varepsilon) \) is continuous and increasing for \( \varepsilon > \varepsilon_g \geq 0 \).

This concludes the pretext for our first upgrade of Theorem 1, stated next.

**Theorem 1.** Theorem 1 holds, with

\[
s_{\Lambda}(\varepsilon) = s_{\Lambda,K}(\varepsilon) + s_{\Lambda,I}(\varepsilon), \tag{41}
\]

where \( s_{\Lambda,K}(\varepsilon) \) is given in (39), and \( s_{\Lambda,I}(\varepsilon) \) in (40).

**Proof of Theorem 1:**

Clearly, Proposition 1 and formula (37) imply Theorem 1 and the splitting of the system-specific Boltzmann entropy per particle \( s_{\Lambda}(\varepsilon) \) in (22) into a sum of a kinetic and an interaction component, (41). Proposition 1 also adds a piece of information about \( s_{\Lambda,I}(\varepsilon) \) which does not just re-express what is stated in Theorem 1. In fact, by the known strict increase of \( \varepsilon \mapsto \ln \varepsilon \), the increase of \( \varepsilon \mapsto s_{\Lambda,I}(\varepsilon) \) implies the strict increase of \( \varepsilon \mapsto s_{\Lambda}(\varepsilon) \), but the increase of \( \varepsilon \mapsto s_{\Lambda,I}(\varepsilon) \) does not follow from the properties of \( \varepsilon \mapsto \ln \varepsilon \) and the strict increase of \( \varepsilon \mapsto s_{\Lambda}(\varepsilon) \). So Theorem 1 holds and extends Theorem 1.

**Proof of Proposition 1:**

By hypothesis \((H6)\), \( U_\Lambda \) is bounded continuous on \( \Lambda \times \Lambda \), so we can write

\[
N^{-2} I^{(N)}_\Lambda(q_1, \ldots, q_N) = \int \frac{1}{2} U(\tilde{q}, \tilde{q}) \Delta^{(1)}_{X(N)}(\tilde{q}) \Delta^{(1)}_{X(N)}(\tilde{q}) d^3\tilde{q} d^3\tilde{q} - \frac{1}{N} \int \frac{1}{2} U(q, q) \Delta^{(1)}_{X(N)}(q) d^3q,
\]

and we may abbreviate the first term of r.h.s. (42) in bilinear form notation,

\[
\int \frac{1}{2} U(\tilde{q}, \tilde{q}) \Delta^{(1)}_{X(N)}(\tilde{q}) \Delta^{(1)}_{X(N)}(\tilde{q}) d^3\tilde{q} d^3\tilde{q} \equiv \left( \Delta^{(1)}_{X(N)} : \Delta^{(1)}_{X(N)} \right). \tag{43}
\]

The above integrals extend over \( \mathbb{R}^3 \), and we set \( I^{(N)}_\Lambda(q_1, \ldots, q_N) = \infty \) as well as \( \left( \Delta^{(1)}_{X(N)} : \Delta^{(1)}_{X(N)} \right) = \infty \) if any \( q_k \notin \Lambda \). Also by \((H6)\), the term in the second line of r.h.s. (42) is \( O(N^{-1}) \) for all \( X^{(N)} \in \Lambda^N \). Recalling our claim (which we
promised to prove) that the limit \( N \to \infty \) for the ensemble does not change if the Hamiltonian is changed by an additive term of order \( O(N^{-1}) \) relative to the leading terms, we now introduce the configurational integral

\[
\Upsilon^{(N)}_\Lambda(\varepsilon) \equiv \ln \int \left(1 - \frac{1}{\varepsilon} \langle \Delta^{(1)}_{X(N)}, \Delta^{(1)}_{X(N)} \rangle \right)_{+}^{\frac{N-1}{N}} \lambda(d^Nq) \tag{44}
\]

for all \( N > N_U(\varepsilon) \) (to be defined). Note that the integral (44) is generally not well-defined for all \( N \in \mathbb{N} \) because \( \langle \Delta^{(1)}_{X(N)}, \Delta^{(1)}_{X(N)} \rangle \) is bigger than \( N^{-2} I^{(N)}_\Lambda(q_1, ..., q_N) \) by the absolute value of the second line of r.h.s. (42), which reads precisely \( N^{-2} \sum_{k=1}^{N} \frac{1}{2} U_\Lambda(q_k, q_k) \). And while this term = \( O(1/N) \), when \( N \) is not large enough then it is possible that \( \langle \Delta^{(1)}_{X(N)}, \Delta^{(1)}_{X(N)} \rangle > \varepsilon \) everywhere in \( \Lambda^N \), in which case the integral in (44) vanishes, and its logarithm = \( -\infty \), then. Yet, when \( N > N_U(\varepsilon) \) the integral (44) is well-defined, and we conclude that (modulo the proof of precisely the just re-uttered claim that \( O(1/N) \) contributions to the Hamiltonian drop out when \( N \to \infty \)) our proposition I is proved if we can prove the following proposition.

**Proposition 2.** Under the hypotheses on \( U_\Lambda \) in Thm. I when \( N \gg N_U(\varepsilon) \) then

\[
\Upsilon^{(N)}_\Lambda(\varepsilon) = N \gamma_\Lambda(\varepsilon) + o(N). \tag{45}
\]

The function \( \varepsilon \mapsto \gamma_\Lambda(\varepsilon) \) is continuous and increasing for \( \varepsilon > \varepsilon_0 \geq 0 \).

**Proof of Proposition 2:**

We will establish uniform bounds and super-additivity estimates.

For \( 0 < n < N \), we set \( X^{(N)} \equiv (X^{(n)}, Y^{(N-n)}) \), which also defines \( Y^{(N-n)} \). We note the convex linear decomposition

\[
\Delta^{(1)}_{X^{(N)}}(q) = \frac{n}{N} \Delta^{(1)}_{X^{(n)}}(q) + (1 - \frac{n}{N}) \Delta^{(1)}_{Y^{(N-n)}}(q). \tag{46}
\]

Since \( U_\Lambda \geq 0 \) is the kernel of a bilinear form which is positive definite when restricted to the set of probability measures on \( \Lambda \), Jensen’s inequality gives us

\[
\langle \Delta^{(1)}_{X^{(N)}}, \Delta^{(1)}_{X^{(N)}} \rangle \leq \frac{n}{N} \langle \Delta^{(1)}_{X^{(n)}}, \Delta^{(1)}_{X^{(n)}} \rangle + (1 - \frac{n}{N}) \langle \Delta^{(1)}_{Y^{(N-n)}}, \Delta^{(1)}_{Y^{(N-n)}} \rangle. \tag{47}
\]

We of course also have \( 1 = \frac{n}{N} + (1 - \frac{n}{N}) \), and so we conclude that

\[
\left(1 - \frac{1}{\varepsilon} \langle \Delta^{(1)}_{X^{(n)}}, \Delta^{(1)}_{X^{(n)}} \rangle \right)_{+} \geq \left(\frac{n}{N} \left[1 - \frac{1}{\varepsilon} \langle \Delta^{(1)}_{X^{(n)}}, \Delta^{(1)}_{X^{(n)}} \rangle \right] + (1 - \frac{n}{N}) \left[1 - \frac{1}{\varepsilon} \langle \Delta^{(1)}_{Y^{(N-n)}}, \Delta^{(1)}_{Y^{(N-n)}} \rangle \right]\right)_{+}. \tag{48}
\]

Next we recall that, if \( \varphi \) is some function on a domain \( D \), and if \( \Sigma(\varphi_+) \) denotes the support of its positive part, and \( \chi_{\Sigma(\varphi_+)} \) is the characteristic function
of $\Sigma(\varphi_+)$, then the inclusion $\Sigma(\varphi_+) \cap \Sigma(\vartheta_+) \subset \Sigma((\varphi + \vartheta)_+)$ for any two such functions $\varphi$ and $\vartheta$ yields the estimate

$$(\varphi_+ + \vartheta_+)^{X_{\Sigma((\varphi+\vartheta)_+)}} \geq (\varphi_+ + \vartheta_+)^{X_{\Sigma(\varphi_+)}} = (\varphi_+ + \vartheta_+)^{X_{\Sigma(\varphi_+)}},$$

Set $\varphi = \frac{n}{N} \left[ 1 - \frac{1}{\varepsilon} \left\langle \Delta^{(1)}_{X(n)} , \Delta^{(1)}_{X(n)} \right\rangle \right]$ and $\vartheta = (1 - \frac{n}{N}) \left[ 1 - \frac{1}{\varepsilon} \left\langle \Delta^{(1)}_{X(n)} , \Delta^{(1)}_{X(n)} \right\rangle \right]$. Then inequality (49) applies to r.h.s. (48). Applying next the classical inequality between the arithmetic and the geometric means of any two positive numbers $A$ and $B$, viz. $\alpha A + (1 - \alpha) B \geq A^\alpha B^{1-\alpha}$ for any $\alpha \in [0, 1]$, we get

$$\left( 1 - \frac{1}{\varepsilon} \left\langle \Delta^{(1)}_{X(n)} , \Delta^{(1)}_{X(n)} \right\rangle \right)_+ \geq \left[ 1 - \frac{1}{\varepsilon} \left\langle \Delta^{(1)}_{X(n)} , \Delta^{(1)}_{X(n)} \right\rangle \right]^{\frac{n}{N}} + \left[ 1 - \frac{1}{\varepsilon} \left\langle \Delta^{(1)}_{X(n)} , \Delta^{(1)}_{X(n)} \right\rangle \right]^{1 - \frac{n}{N}}.$$  
(50)

We now use (50) to estimate r.h.s. (44). For this, let $N \gg N_U(\varepsilon)$ and let $N_U(\varepsilon) < n < N - N_U(\varepsilon)$. Noting that the resulting integral over $\Lambda^n$ factors into two integrals, one over $\Lambda^n$ and another over $\Lambda^{N-n}$, and working out the powers, we find

$$\ln \left( 1 - \frac{1}{\varepsilon} \left\langle \Delta^{(1)}_{X(n)} , \Delta^{(1)}_{X(n)} \right\rangle \right)^{\frac{3N}{2} - 1} \lambda(d^{3N}q) \geq$$
$$\ln \left( 1 - \frac{1}{\varepsilon} \left\langle \Delta^{(1)}_{X(n)} , \Delta^{(1)}_{X(n)} \right\rangle \right)^{\frac{3N}{2} - 1} \lambda(d^{3n}q) +$$
$$\ln \left( 1 - \frac{1}{\varepsilon} \left\langle \Delta^{(1)}_{X(n)} , \Delta^{(1)}_{X(n)} \right\rangle \right)^{\frac{3(N-n)}{2} - 1} \lambda(d^{3(N-n)}q),$$

where we also relabeled the integration variables under the second integral on r.h.s. (51) from $Y^{(N-n)}$ to $X^{(N-n)}$. Noting next that $0 < \frac{N}{n} < 1$, we resort again to Jensen’s inequality, this time w.r.t. the $\lambda$ measures in the two integrals on r.h.s. (51). Also using $\ln(\cdots)^a = a \ln(\cdots)$, we arrive at

$$\ln \left( 1 - \frac{1}{\varepsilon} \left\langle \Delta^{(1)}_{X(n)} , \Delta^{(1)}_{X(n)} \right\rangle \right)^{\frac{3N}{2} - 1} \lambda(d^{3N}q) \geq$$
$$\left( 1 + \frac{2n/N}{3n-2} \right) \ln \left( 1 - \frac{1}{\varepsilon} \left\langle \Delta^{(1)}_{X(n)} , \Delta^{(1)}_{X(n)} \right\rangle \right)^{\frac{3N}{2} - 1} \lambda(d^{3n}q) +$$
$$\left( 1 + \frac{2n/N}{3(N-n)-2} \right) \ln \left( 1 - \frac{1}{\varepsilon} \left\langle \Delta^{(1)}_{X(n)} , \Delta^{(1)}_{X(n)} \right\rangle \right)^{\frac{3(N-n)}{2} - 1} \lambda(d^{3(N-n)}q).$$
(52)

Formula (52) writes shorter thusly,

$$\Upsilon^{(N)}_{\Lambda}(\varepsilon) \geq \left( 1 + \frac{2n/N}{3n-2} \right) \Upsilon^{(n)}_{\Lambda}(\varepsilon) + \left( 1 + \frac{2n/N}{3(N-n)-2} \right) \Upsilon^{(N-n)}_{\Lambda}(\varepsilon).$$
(53)
So $N \mapsto \mathcal{Y}^{(N)}_\Lambda(\varepsilon)$ is almost super-additive.

To be able to create a properly super-additive function we establish upper and lower bounds of $\ell \mapsto \mathcal{Y}^{(\ell)}_\Lambda(\varepsilon)$ which are linear in $\ell$, whenever $\ell > N_U(\varepsilon)$; we will need those bounds with $\ell \in \{n, N - n\}$, with $\ell > 1$. As a by-product, the upper bound with $\ell = N$ will also guarantee convergence of the constructed super-additive function.

The upper bound is trivial. Recall that by hypothesis $\langle \Delta_X^{(\ell)}(\cdot), \Delta_X^{(\ell)}(\cdot) \rangle \geq 0$ for all $\ell \in \mathbb{N}$. So for $\ell > N_U(\varepsilon)$ and $\varepsilon > \varepsilon_g \geq 0$ we find

$$\frac{2}{\varepsilon^2} \ln \left( 1 - \frac{1}{\varepsilon} \langle \Delta_X^{(\ell)}, \Delta_X^{(\ell)} \rangle \right)^{\frac{2}{\varepsilon}} \lambda(d^3q) \leq 0. \quad (54)$$

As for the lower bound, we distinguish two cases, (a): $\langle |\Lambda|^{-1}, |\Lambda|^{-1} \rangle \leq \varepsilon$, and (b): $\langle |\Lambda|^{-1}, |\Lambda|^{-1} \rangle \geq \varepsilon$. In case (a) we apply Jensen’s inequality w.r.t. $\lambda$ to the convex map $x \mapsto (1 - x)^\theta$ (for $\theta \geq 1$), and also use $\ell - 1 < \ell$, to get

$$\ln \left[ \int \left( 1 - \frac{1}{\varepsilon} \langle \Delta_X^{(\ell)}, \Delta_X^{(\ell)} \rangle \right)^{\frac{2}{\varepsilon}} \lambda(d^3q) \right] \geq \ln \left[ 1 - \frac{1}{\varepsilon} \int \frac{1}{2} U_A(q, q) \lambda(d^3q) - \frac{1}{\varepsilon} \int \frac{1}{2} U_A(\hat{q}, \hat{q}) \lambda(d^3\hat{q}) \lambda(d^3\hat{q}) \right], \quad (55)$$

and r.h.s. $\geq -C > -\infty$ when $\ell > \ell_{\text{crit}}(\varepsilon)$ (given $U_A$), with $C > 0$ independent of $\ell$. Since the interaction entropy exists when $\ell > N_U(\varepsilon)$, clearly $\ell_{\text{crit}} \geq N_U(\varepsilon)$, but after at most an adjustment of $C$, we can conclude that l.h.s. $\geq -C > -\infty$ when $\ell > N_U(\varepsilon)$, with $C > 0$ independent of $\ell$. In case (b), inequality (55) is still true but now trivial, for r.h.s. $= -\infty$ for all $\ell > 1$, then. So instead we now proceed as follows. By hypothesis (H6), the bilinear form $\langle \Delta_X^{(\ell)}, \Delta_X^{(\ell)} \rangle$ takes its minimum $\varepsilon_g^*(\ell) \geq \varepsilon_g$. Clearly, $\varepsilon_g^*(\ell) = \varepsilon_g(\ell) + O(\ell^{-1})$, where $\varepsilon_g(\ell) := \min \ell^{-2} I_\Lambda^{(\ell)}(q_1, \ldots, q_n)$, and since $\varepsilon_g(\ell) \leq \varepsilon_g$ (as proved in Appendix A), we have that $\varepsilon_g^*(\ell) \leq \varepsilon_g + O(\ell^{-1})$; of course, we also assume that $\ell > N_U(\varepsilon)$ so that $\varepsilon_g^*(\ell) < \varepsilon$. By permutation symmetry there are many equivalent minimizers, but possibly also several distinct permutation group orbits of minimizers. We pick any particular minimizer $Q_g^{(\ell)}$ and let $q_{g,k}^{(\ell)} \in \Lambda$ denote the $k$-th coordinate vector in $Q_g^{(\ell)}$. By (H6) again, we can vary all the $q_k$ in the minimizing configuration a little bit, say, each $q_k$ in $B_\delta(q_{g,k}^{(\ell)}) \cap \Lambda$, where $B_\delta(q)$ is a ball centered at $q$, with radius $\delta > 0$ independent of $k$ and $\ell$ but chosen small enough (given $\varepsilon$) so that $\langle \Delta_X^{(\ell)}, \Delta_X^{(\ell)} \rangle$ does not change by more than $(\varepsilon - \varepsilon_g + O(\ell^{-1}))/2$. For brevity we write $B_\delta[k]$ for $B_\delta(q_{g,k}^{(\ell)})$; let $\chi_{B_\delta[k]}$ be the characteristic function of $B_\delta[k]$. We use that $\lambda(d^3q_k) = \chi_{B_\delta[k]}\lambda(d^3q_k) + \chi_{B_\delta[k]}\lambda(d^3q_k)$ where $B_\delta[k] = \Lambda \setminus B_\delta[k]$ is the complement in $\Lambda$ of $B_\delta[k]$, then use that both terms in this decomposition are non-negative so that we get an upper estimate by dropping the contribution...
from $\chi_{B_{\delta}[k]} \lambda(d^3q_k)$ for each $k$. After this step the restriction to the positive part of $(1 - \frac{1}{\varepsilon}(\cdot, \cdot, \cdot))$ is eventually tautological when $\ell$ is sufficiently large so that the $O(\ell^{-1})$ term has gotten sufficiently small. We next apply Jensen’s inequality w.r.t. the probability measure $\prod_{1 \leq k \leq \ell} \lambda(d^3q)^{-1}\chi_{B_{\delta}[k]} \lambda(d^3q_k)$ to the convex map $x_+ \mapsto x_+^\theta$ (for $\theta \geq 1$), finally recall that $0 \leq \varepsilon_g < \varepsilon$, and get

\[
\left[\int \left(1 - \frac{1}{\varepsilon} \langle \Delta_{X(i)}, \Delta_{X(i)} \rangle \right) ^{\frac{3}{2} - 1} \lambda(d^3q) \right] ^{\frac{2}{3} - 2} \geq \left[\int \left(1 - \frac{1}{\varepsilon} \langle \Delta_{X(i)}, \Delta_{X(i)} \rangle \right) ^{\frac{3}{2} - 1} \prod_{1 \leq k \leq \ell} \chi_{B_{\delta}[k]} \lambda(d^3q_k) \right] ^{\frac{2}{3} - 2} \geq (C_\delta \frac{2}{3} - 2) \left(1 - \frac{1}{\varepsilon}(1 + \frac{\varepsilon_g}{\varepsilon}) + O(\ell^{-1})\right) \geq C > 0
\]

for $\ell$ large enough; here

\[
C_\delta = \min_{q'} \int_{B_{\delta}(q') \cap \Lambda} \lambda(d^3q) > 0.
\]

In summary, our list of inequalities (54), (55) and (56), and the finiteness of the number of $\ell$ until “$\ell$ is large enough,” establishes that when $\ell > N_U(\varepsilon)$, then for some $\ell$-independent constant $C_\ast > 0$,

\[
- \left(\frac{3}{2} - 1\right) C_\ast \leq \gamma_A(\varepsilon) \leq 0;
\]

incidentally, our (55) and (56) produce an upper estimate for $N_U(\varepsilon)$.

Recall that in this proof we assume that $N \gg N_U(\varepsilon)$, and that $N_U(\varepsilon) < n < N - N_U(\varepsilon)$. With the help of (58), for $\ell \in \{n, N - n\}$, we conclude from (53) that there exists a $C \in \mathbb{R}$ independent of $n$ and $N$ such that

\[
\gamma_A^{(N)}(\varepsilon) \geq \gamma_A^{(n)}(\varepsilon) + \gamma_A^{(N-n)}(\varepsilon) + C.
\]

Adding that constant $C$ to both sides of the inequality (59) shows that $N \mapsto \gamma_A^{(N)}(\varepsilon) + C$ is a super-additive function for all $\varepsilon > \varepsilon_g \geq 0$. And using (54) with $N$, we also see that $N^{-1}(\gamma_A^{(N)}(\varepsilon) + C)$ is bounded above, and so, by standard facts about super-additive functions, $N^{-1}(\gamma_A^{(N)}(\varepsilon) + C)$ converges as $N \to \infty$,

\[
\lim_{N \to \infty} N^{-1}(\gamma_A^{(N)}(\varepsilon) + C) = \sup_{N \in \mathbb{N}} N^{-1}(\gamma_A^{(N)}(\varepsilon) + C),
\]

and since $N^{-1}C \to 0$, we conclude that $N^{-1}\gamma_A^{(N)}(\varepsilon)$ converges as well, i.e.

\[
\lim_{N \to \infty} \frac{1}{N} \gamma_A^{(N)}(\varepsilon) = \gamma(\varepsilon).
\]
This proves (15).

To prove continuity of $\gamma_{\Lambda}(\varepsilon)$, we establish upper and lower bounds on the derivative of the functions $\varepsilon \mapsto N^{-1} \Upsilon_{\Lambda}^{(N)}(\varepsilon)$ which are uniform in $N > N_U(\varepsilon)$. Differentiating the functions $\varepsilon \mapsto N^{-1} \Upsilon_{\Lambda}^{(N)}(\varepsilon) + \left(\frac{3}{2} - \frac{1}{N}\right) \ln \varepsilon$, we obtain

$$
\frac{1}{N} \Upsilon_{\Lambda}^{(N)'}(\varepsilon) = \left(\frac{3}{2} - \frac{1}{N}\right) \frac{1}{\varepsilon} \left[ \int \left(1 - \frac{1}{\varepsilon} \langle \Delta_{X(N)}^{(1)} \cdot \Delta_{X(N)}^{(1)} \rangle \right) \frac{\Delta_{N}^{N-1}}{3N} \lambda(d^3q) - 1 \right].
$$

(62)

To get a lower bound, we split off a factor $\left(1 - \frac{1}{\varepsilon} \langle \Delta_{X(N)}^{(1)} \cdot \Delta_{X(N)}^{(1)} \rangle \right)_+$ in the integrand of the denominator of r.h.s.(62), and using that $\varepsilon > \varepsilon_g \geq 0$, the positivity of the bilinear form now gives $\left(1 - \frac{1}{\varepsilon} \langle \Delta_{X(N)}^{(1)} \cdot \Delta_{X(N)}^{(1)} \rangle \right)_+ \leq 1$, and so

$$
\frac{1}{N} \Upsilon_{\Lambda}^{(N)'}(\varepsilon) \geq \left(\frac{3}{2} - \frac{1}{N}\right) \frac{1}{\varepsilon} [1 - 1] = 0;
$$

(63)

incidentally, this shows once again monotonicity $\uparrow$ of $\varepsilon \mapsto \gamma_{\Lambda}(\varepsilon)$. To get an $N$-independent upper bound to (62), note that $\frac{3N}{2} - 2 = \left(\frac{3N}{2} - 1\right) \left(1 - \frac{2}{3N-2}\right)$ and that $0 < \left(1 - \frac{2}{3N-2}\right) < 1$ for $N > 1$, then apply Jensen’s inequality w.r.t. $\lambda$ to pull the power $\left(1 - \frac{2}{3N-2}\right)$ out of the integral in the numerator, then note a cancellation versus the denominator. Since $0 < \left(1 - \frac{2}{3N-2}\right) < 1$ for $N > 1$,

$$
\frac{1}{N} \Upsilon_{\Lambda}^{(N)'}(\varepsilon) \leq \left(\frac{3}{2} - \frac{1}{N}\right) \frac{1}{\varepsilon} \left[ \int \left(1 - \frac{1}{\varepsilon} \langle \Delta_{X(N)}^{(1)} \cdot \Delta_{X(N)}^{(1)} \rangle \right) \frac{\Delta_{N}^{N-1}}{3N} \lambda(d^3q) \right] - \frac{2}{3N-2} - 1
$$

(64)

whenever $N > N_U(\varepsilon)$ (so that the integral is non-zero). By the first inequality in (58) with $\ell = N$, the r.h.s. (64) is bounded above independently of $N$. The continuity of $\varepsilon \mapsto \gamma_{\Lambda}(\varepsilon)$ follows.

Proposition 2 is proved. \(\square\)

To complete the proof of Proposition 1 we still need to show that the omission of $\frac{1}{N} \int X_{U_{\Lambda}}(q, q) \Delta_{X(N)}^{(1)}(q) d^3q$ from (42) was justified. This is now straightforward. By hypothesis (H6), $U_{\Lambda}(\geq 0)$ is a bounded continuous function on $X \times \overline{X}$. So there exists an $N$-independent constant $B > 0$ such that

$$
0 \leq \int \frac{1}{2} U_{\Lambda}(q, q) \Delta_{X(N)}^{(1)}(q) d^3q \leq B,
$$

(65)

as long as $X^{(N)} \in \overline{X}$. Thus, and abbreviating the expression in the second line on r.h.s.(37) by $S_{I_{\Lambda}^{(N)}}(N^2 \varepsilon)$, we have the two-sided estimate

$$
\Upsilon_{\Lambda}^{(N)}(\varepsilon) \leq S_{I_{\Lambda}^{(N)}}(N^2 \varepsilon) \leq \Upsilon_{\Lambda}^{(N)}(\varepsilon + BN^{-1}).
$$

(66)

But

$$
\left| \Upsilon_{\Lambda}^{(N)}(\varepsilon + BN^{-1}) - \Upsilon_{\Lambda}^{(N)}(\varepsilon) \right| \leq \int_{\varepsilon}^{\varepsilon + BN^{-1}} \left| \Upsilon_{\Lambda}^{(N)'}(\varsigma) \right| d\varsigma \leq BC,
$$

(67)
the last inequality by (64) and by the first inequality in (58), with \( \ell = N \), and by \( \varepsilon \leq \varsigma \leq 2\varepsilon \). So we conclude that for any \( B > 0 \) we have

\[
\lim_{N \to \infty} \frac{1}{N} S_{\Lambda}^{(N)}(\varepsilon + BN^{-1}) = \gamma_\Lambda(\varepsilon). \tag{68}
\]

Hence, and by (66),

\[
\lim_{N \to \infty} \frac{1}{N} S_I^{(N)}(\varepsilon) = \gamma_\Lambda(\varepsilon), \tag{69}
\]

and Proposition 1 is proved, with \( s_{\Lambda, I}(\varepsilon) = \gamma_\Lambda(\varepsilon) \). This also completes the proof of Theorem 1.

5.1.2 Theorem 1** and its proof

Ruelle’s proof \[Rue69\] of the traditional thermodynamic limit for \( (20) \) per volume proceeded along somewhat different lines, and when adapted to the Vlasov scaling it yields an interesting alternate proof of Theorem 1 which characterizes \( s_\Lambda(\varepsilon) \) in terms of a variational principle (VP) involving \( s_{\Lambda, K}(\varepsilon) \) and yet another (auxiliary) “interaction entropy,” which we denote by \( \varphi_{\Lambda, I}(\varepsilon) \). For technical reasons we now need to assume that \( \varepsilon_g > 0 \) (rather than \( \varepsilon_g \geq 0 \)).

So, following Ruelle \[Rue69\] we introduce the configurational integral

\[
\Xi_{\Lambda}(E) = \int \chi\{\text{some condition}\} \lambda(d^{3N}q). \tag{70}
\]

Up to a purely numerical factor, (70) is quasi the “3N/2-th derivative” w.r.t. \( \varepsilon \) of \( \Psi_{\Lambda}^{(N)}(\varepsilon) \), the first derivative of which is given in (35). For convenience we rewrite (70), with \( E = N^2 \varepsilon \), as

\[
\Xi_{\Lambda}^{(N)}(N^2 \varepsilon) = \int (\varepsilon - N^{-2} I_\Lambda^{(N)}(q_1, ..., q_N))^0_+ \lambda(d^{3N}q). \tag{71}
\]

**Proposition 3.** Assume the hypotheses of Theorem 1, but now let \( \varepsilon_g > 0 \). Then the following limit exists,

\[
\lim_{N \to \infty} \frac{1}{N} \ln \Xi_{\Lambda}^{(N)}(N^2 \varepsilon) = \varphi_{\Lambda, I}(\varepsilon), \tag{72}
\]

and \( \varphi_{\Lambda, I}(\varepsilon) \leq 0 \) is an increasing, right-continuous, function of \( \varepsilon > \varepsilon_g \).

---

19 Actually, Ruelle discussed the entropy of a regularized microcanonical ensemble measure \[Rue69\]. In \[Kie09a\] the author showed that a minor modification of Ruelle’s approach establishes the thermodynamic limit for \( (20) \) per volume without regularization.

20 Instead of the normalized Lebesgue measure \( \lambda(d^{3N}q) \), Ruelle \[Rue69\] uses \( N!^{-1}d^{3N}q \) which gives equivalent results in the thermodynamic limit; not so in the Vlasov limit.
Proof of Proposition 3:

Simplest things first, we note that \( \Xi I^N_{\lambda} (E) \leq 1 \) (obviously), which proves that \( \ln \Xi I^N_{\lambda} (N^2 \varepsilon) \leq 0 \) for all \( N \), and so \( \overline{\sigma}_{\lambda} (\varepsilon) \leq 0 \) whenever this limit exists. The proof that this limit exists and is a monotonically increasing right-continuous function of \( \varepsilon > \varepsilon_0 > 0 \) consists of two main steps.

First, as in our proof of Thm. 1 we temporarily replace \( N^{-2} I^N_{\lambda} (q_1, \ldots, q_N) \) by \( \langle \Delta^{(1)}_{X(N)}, \Delta^{(1)}_{X(N)} \rangle \) in (71) and study its logarithm. For this we need once again to assume that \( N \gg N_U (\varepsilon) \). Inspection of our proof of Proposition 2 reveals that ln \( \Xi \) is either 1 or 0, we conclude that \( \Xi \) is a monotonic increasing function of \( \varepsilon \). Simplest things first, we note that \( \Xi \) is either 1 or 0, we conclude that

\[
\ln \left( \varepsilon - \langle \Delta^{(1)}_{X(N)}, \Delta^{(1)}_{X(N)} \rangle \right)_+ \lambda (d^{3N} q) \geq 0 \quad (73)
\]

which proves super-additivity of \( \Xi \). Without further ado. Furthermore, since \( \langle \cdot \rangle_0^0 \) is either 1 or 0, we conclude that

\[
\ln \left( \varepsilon - \langle \Delta^{(1)}_{X(N)}, \Delta^{(1)}_{X(N)} \rangle \right)_+ \lambda (d^{3N} q) \leq 0. \quad (74)
\]

Moreover, \( \Xi \) is monotonic increasing, since l.h.s. (74) is.

Next we would like to prove continuity of \( \Xi \) as function of \( \varepsilon \) and then conclude the proof as at the end of the proof of Theorem 1 but so far a proof of continuity of \( \Xi \) has eluded us. Fortunately we can bypass this obstacle because \( \Xi \) is a monotonic increasing function of \( \varepsilon \). We define

\[
\Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \Xi \X
where we also introduced the abbreviation
\[ \langle \Delta^{(1)}_{X(N)} \rangle = \int \frac{1}{2} U_\Lambda(q, q) \Delta^{(1)}_{X(N)}(q) d^3q. \] (78)

Since now \( \varepsilon_g > 0 \), there exist constants \( B, \overline{B} \) satisfying \( 0 < B < \overline{B} < \infty \) so that
\[ B \leq \langle \Delta^{(1)}_{X(N)} \rangle \leq \overline{B}. \] (79)

But then, for all \( N > N_U(\varepsilon) \) big enough, we have
\[ \frac{1}{N} \ln \Xi_{I^{(N)}}(N^2 \varepsilon) \geq \tilde{s}_{\Lambda, I}(\varepsilon + N^{-1} B) + o(1) \geq \tilde{s}_{\Lambda, I}(\varepsilon^+) + o(1) \] (80)
where \( o(1) \to 0 \) as \( N \to \infty \). So
\[ \liminf_{N \to \infty} \frac{1}{N} \ln \Xi_{I^{(N)}}(N^2 \varepsilon) \geq \tilde{s}_{\Lambda, I}(\varepsilon^+). \] (81)

On the other hand, for all \( N > N_U(\varepsilon) \) we also have that
\[ \frac{1}{N} \ln \Xi_{I^{(N)}}(N^2 \varepsilon) \leq \tilde{s}_{\Lambda, I}(\varepsilon + N^{-1} \overline{B}) + o(1), \] (82)
and so
\[ \limsup_{N \to \infty} \frac{1}{N} \ln \Xi_{I^{(N)}}(N^2 \varepsilon) \leq \tilde{s}_{\Lambda, I}(\varepsilon^+). \] (83)

The estimates (81) and (83) prove (76).

So \( \tilde{s}_{\Lambda, I}(\varepsilon) = \tilde{s}_{\Lambda, I}(\varepsilon^+) \). Of course, \( \tilde{s}_{\Lambda, I}(\varepsilon) = \tilde{s}_{\Lambda, I}(\varepsilon) \) at all \( \varepsilon \) which are points of continuity of \( \tilde{s}_{\Lambda, I}(\varepsilon) \), and the two functions share their points of discontinuity. At such points \( \tilde{s}_{\Lambda, I}(\varepsilon) \) is right-continuous and may or may not agree with \( \tilde{s}_{\Lambda, I}(\varepsilon) \).

Proposition 3 is proved.

We are now ready to state our second upgrade of our Theorem 1.

**Theorem 1.++** Under the hypotheses of Proposition 3, Theorem 1 holds and the system-specific Boltzmann entropy per particle \( s_\Lambda(\varepsilon) \) given in (22) satisfies the variational principle
\[ s_\Lambda(\varepsilon) = \sup_{0 \leq x \leq 1} \left( s_{\Lambda, K}(x \varepsilon) + \overline{s}_{\Lambda, I}([1 - x] \varepsilon) \right). \] (84)

**Proof of Theorem 1++:**

Integration by parts yields, for any \( \ell > 0 \) and \( \varepsilon > \varepsilon_g \),
\[ \int \left( 1 - \frac{1}{\varepsilon N^2} I_{\Lambda}^{(N)} \right)^\ell \lambda(d^3q) = \int_0^1 \int \left( 1 - \frac{1}{1 - x \varepsilon N^2} I_{\Lambda}^{(N)} \right)^0 \lambda(d^3q) dx^\ell, \] (85)
where we suppressed the arguments \( (q_1, \ldots, q_N) \) from \( I^{(N)}_\Lambda(q_1, \ldots, q_N) \). Setting \( \ell = \frac{3N}{2} - 1 \), recalling (71), and using that \( N^{-1} \ln (\frac{3N}{2} - 1) \to 0 \), we find

\[
s_{\Lambda,I}(\varepsilon) = \lim_{N \to \infty} \frac{1}{N} \ln \int_0^1 \Xi^{(N)}_\Lambda (N^2 [1 - x] \varepsilon) \ x^{\frac{3N}{2} - 2} \ dx.
\] (86)

Proposition 3 and Laplace’s method (cf. sect. II.7 in [Ell85]) now yield

\[
s_{\Lambda,I}(\varepsilon) = \sup_{0 \leq x \leq 1} \left( \frac{3}{2} \ln x + \Xi^{(N)}_\Lambda (\varepsilon) \right); \quad (87)
\]

note that (87) implies that \( \varepsilon \mapsto s_{\Lambda,I}(\varepsilon) \) is continuous even when \( \Xi^{(N)}_\Lambda(\varepsilon) \) is not. Recalling next the definition (39) of \( s_{\Lambda,K}(\varepsilon) \) as well as (41) of Theorem 1++, we see that Theorem 1++ is proved. □

We end this subsection by pointing out that our method of proving Theorem 1++ not only avoids the regularization of Dirac’s \( \delta \) measure, we also tackled the map \( \mathcal{E} \mapsto S(\mathcal{E}) \) directly rather than its inverse \( S \mapsto E(S) \) [Rue69]. The strategy to tackle \( S \mapsto E(S) \) is due to Griffiths [Gri65].

### 5.2 Proof of Theorem 2

Since formula (37) holds also under the assumptions \((H1)–(H5)\) on the interactions, and since it is well-known that the system-specific Boltzmann entropy per particle of the perfect gas (39) minimizes Boltzmann’s \( H \) functional under the constraint of prescribing the value of the kinetic Hamiltonian, it suffices to study the interaction entropy of Boltzmann’s ergodic ensemble,

\[
S^{(N)}_\Lambda(\mathcal{E}) = \ln \int \left( 1 - \frac{1}{\varepsilon} I^{(N)}_\Lambda(q_1, \ldots, q_N) \right)^{\frac{3N}{2} - 1} \lambda(d^3q).
\] (88)

Note that (88) is non-positive, and under hypotheses \((H1)–(H5)\) we also have

\[
\left[ \int \left( 1 - \frac{1}{\varepsilon} I^{(N)}_\Lambda(q_1, \ldots, q_N) \right)^{\frac{3N}{2} - 1} \lambda(d^3q) \right]^{\frac{2}{3N-2}} \geq \left[ \int \left( \frac{1}{\varepsilon} I^{(N)}_\Lambda(q_1, \ldots, q_N) \right)^{\frac{3N}{2} - 1} \prod_{1 \leq k \leq N} \chi_{B_\delta[k]} \lambda(d^3q_k) \right]^{\frac{2}{3N-2}} \geq |C_\delta|^{\frac{2}{3N-2}} \int \left( \frac{1}{\varepsilon} I^{(N)}_\Lambda(q_1, \ldots, q_N) \right) \prod_{1 \leq k \leq N} \frac{\chi_{B_\delta[k]} \lambda(d^3q_k)}{\int_{B_\delta[k]} \lambda(d^3q)}} \lambda(d^3q_k) \geq |C_\delta|^{\frac{2}{3N-2}} \left( 1 - \frac{1}{2} \left( 1 + \frac{\varepsilon_g}{2} \right) \right) > 0,
\] (89)

where again \( C_\delta \) is given in (57), but now with \( \delta(\varepsilon) \) independent of \( k \) and \( N \) chosen so that \( N^{-2} I^{(N)}(q_1, \ldots, q_N) \leq \bar{\varepsilon}_g(N) + (\varepsilon - \varepsilon_g)/2 \) when the \( q_k \)
vary in \( B_\delta(q_{g,k}) \cap \Lambda \), where \((q_{g,1}, \ldots, q_{g,N})\) is a ground state configuration for \( I_{N}^{(N)}(q_1, \ldots, q_N) \) with a fat neighborhood, which exists by \((H2)\&(H3)\). We also used that \( \tilde{\varepsilon}_g(N) = \min N^{-2} I_{N}^{(N)}(q_1, \ldots, q_N) \leq \varepsilon_g \) (see Appendix A). So

\[
\frac{2}{3N-2} S_{I_{\Lambda}^{(N)}}(\mathcal{E}) \geq \ln \left( |C_{\delta}|^\frac{3}{2} \left( 1 - \frac{1}{2} \left( 1 + \frac{2\varepsilon}{\varepsilon_N} \right) \right) \right) > -\infty \tag{90}
\]

for all \( N > 1 \). The estimate \((90)\) guarantees the existence of limit points of the (negative) interaction entropy per particle as \( N \to \infty \). We want to show that the interaction entropy per particle actually has a limit and characterize the limit by the variational principle stated in Theorem \([2]\).

We begin by characterizing \((88)\) by its own maximum entropy principle. We introduce the quasi-interaction energy of \( \varrho^{(N)} \in \mathcal{P}^*(\Lambda^N) \), defined by

\[
Q_{\varepsilon,N}(\varrho^{(N)}) = \frac{3N-2}{2} \int \ln \left( 1 - \frac{1}{\varepsilon N} I_{\Lambda}^{(N)}(q_1, \ldots, q_N) \right) \varrho^{(N)}(d^3q) \tag{91}
\]

whenever \( \text{supp} \varrho^{(N)} \subset \text{supp} (\varepsilon - N^{-2} I_{\Lambda}^{(N)}) \); else we set \( Q_{\varepsilon,N}(\varrho^{(N)}) = -\infty \). The entropy of \( \varrho^{(N)} \) relative to \( \varrho_{ap}^{(N)} \in \mathcal{P}^*(\Lambda^N) \) is defined as usual\(21\) by

\[
\mathcal{R}^{(N)}(\varrho^{(N)}|\varrho_{ap}^{(N)}) = -\int \ln \left( \frac{d\varrho^{(N)}}{d\varrho_{ap}^{(N)}} \right) \varrho^{(N)}(d^3q) \tag{92}
\]

if \( \varrho^{(N)} \) is absolutely continuous w.r.t. the a-priori measure \( \varrho_{ap}^{(N)} \), and provided the integral in \((92)\) exists. In all other cases, \( \mathcal{R}^{(N)}(\varrho^{(N)}|\varrho_{ap}^{(N)}) = -\infty \). Finally, we define what we call the interaction entropy of \( \varrho^{(N)} \) by

\[
S_{\varepsilon,N}(\varrho^{(N)}) \equiv \mathcal{R}^{(N)}(\varrho^{(N)}|\lambda) + Q_{\varepsilon,N}(\varrho^{(N)}) \tag{93}
\]

We are now ready to state our variational principle.

**Proposition 4.** For \( \varepsilon > \varepsilon_g \geq 0 \), the interaction entropy functional \((95)\) achieves its supremum. The maximizer is the unique probability measure

\[
\varrho_{\varepsilon,N}^{(N)}(d^3q) = \frac{\left( 1 - \frac{1}{\varepsilon N} I_{\Lambda}^{(N)}(q_1, \ldots, q_N) \right) \frac{3N}{2} - 1 d^3q}{\int \left( 1 - \frac{1}{\varepsilon N} I_{\Lambda}^{(N)}(q_1, \ldots, q_N) \right) \frac{3N}{2} - 1 d^3q} \in (\mathcal{P}^* \cap \mathcal{L}^\infty)(\Lambda^N); \tag{94}
\]

thus

\[
\max_{\varrho^{(N)} \in \mathcal{P}^*(\Lambda^N)} S_{\varepsilon,N}(\varrho^{(N)}) = S_{\varepsilon,N}(\varrho_{\varepsilon,N}^{(N)}). \tag{95}
\]

Moreover,

\[
S_{\varepsilon,N}(\varrho_{\varepsilon,N}^{(N)}) = S_{\varepsilon,N}(\varrho_{\varepsilon,N}^{(N)}(N^2\varepsilon)). \tag{96}
\]

\(21\)Our physicists’ sign convention of relative entropy is opposite to the probabilists’ one.
Proof of Proposition 4:

Under our hypotheses on \( I^{(N)}_\Lambda \) the measure \( \varphi^{(N)}_{N\varepsilon} \) is absolutely continuous w.r.t. \( \lambda \) and bounded whenever \( \varepsilon > \varepsilon_0 \), so the standard convexity argument due to Boltzmann [Bol96], cf. [Rue69, Ell85], applies and shows that
\[
\mathcal{J}^{(N)}_{I/\varepsilon} (\varphi^{(N)}) - \mathcal{J}^{(N)}_{I/\varepsilon} (\varphi^{(N)}_{N\varepsilon}) \leq 0, \quad \text{with equality holding if and only if } \varphi^{(N)} = \varphi^{(N)}_{N\varepsilon}.
\]
Identity (96) is verified by explicit calculation.

Since ultimately we are interested in the limit \( N \to \infty \) of our finite-\( N \) results, we recall the formalism of probabilities on infinite sequences \( \Lambda \).

Identity (96) is verified by explicit calculation.

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Identity (96) is verified by explicit calculation.

Next we would like to formulate the
\[
\mathcal{J}^{(N)}_{I/\varepsilon} (\varphi^{(N)}) - \mathcal{J}^{(N)}_{I/\varepsilon} (\varphi^{(N)}_{N\varepsilon}) \leq 0, \quad \text{with equality holding if and only if } \varphi^{(N)} = \varphi^{(N)}_{N\varepsilon}.
\]

Identity (96) is verified by explicit calculation.

Since ultimately we are interested in the limit \( N \to \infty \) of our finite-\( N \) results, we recall the formalism of probabilities on infinite sequences \( \Lambda \), as encountered already in section 3 for \((\Lambda \times \mathbb{R}^3)^N\). Thus, by \( \mathcal{P}^s(\Lambda^N) \) we denote the permutation-symmetric probability measures on the set of infinite exchangeable sequences in \( \Lambda \). Let \( \{\varrho_n\}_{n \in \mathbb{N}} \) denote the sequence of marginals of any \( \varrho \in \mathcal{P}^s(\Lambda^N) \). The de Finetti [deF37] – Dynkin [Dyn53] – Hewitt-Savage [HeSa55] decomposition theorem for \( \mathcal{P}^s(\Lambda^N) \) states that every \( \varrho \in \mathcal{P}^s(\Lambda^N) \) is uniquely presentable as a linear convex superposition of infinite product measures, i.e., for each \( \varrho \in \mathcal{P}^s(\Lambda^N) \) there exists a unique probability measure \( \varsigma(d\rho|\varrho) \) on \( \mathcal{P}(\Lambda) \), such that for each \( n \in \mathbb{N} \),
\[
\begin{align*}
\varrho(d^{3n}q) = \int_{\mathcal{P}(\Lambda)} \rho^\otimes_n (d^3q_1 \cdots d^3q_n) \varsigma(d\rho|\varrho),
\end{align*}
\]
where \( \varrho_n \) is the \( n \)-th marginal measure of \( \varrho \), and where \( \rho^\otimes_n (d^3q_1 \cdots d^3q_n) \equiv \rho(d^3q_1) \times \cdots \times \rho(d^3q_n) \). Also, (97) expresses the extreme point decomposition of the convex set \( \mathcal{P}^s(\Lambda^N) \), see [HeSa55].

Next we would like to formulate the \( N = \infty \) analogue of (93), but the naive manipulation of the formulas is not recommended. The functional \( Q^{(N)}_{I/\varepsilon} \) is well-defined by (91) and its accompanying text for all \( N \in \mathbb{N} \); however, since our conditions on \( I^{(N)}_\Lambda(q_1, ..., q_N) \) allow it to be unbounded above when two positions \( q_k \) and \( q_l \) approach each other (for example: Coulomb interactions), we find that \( Q^{(N)}_{I/\varepsilon}(\rho^\otimes_n) = -\infty \) for all product measures \( \rho^\otimes_n \), but these are exactly the \( N \)-point marginals of the extreme points of our set of exchangeable measures on the infinite Cartesian product \( \Lambda^N \). This obstacle can be circumvented by noting that the finite-\( N \) quasi-interaction energy defined in (91) and the line ensuing (91) is the monotone limit of a family of concave functionals in which the integrand function \( \ln(1-x)_+ \) (with \( \ln 0 = -\infty \) understood) is replaced by \( \ln(1-x) \chi_{\{x < 1-\alpha\}} + [\ln \alpha + (1-\alpha-x)/\alpha] \chi_{\{x \geq 1-\alpha\}} \); thus
\[
\begin{align*}
\alpha Q_{I/\varepsilon}^{(N)} (\varphi^{(N)}) & = \frac{3N-2}{2} \int \left( \ln \left( 1 - \frac{1}{\varepsilon N^2} I^{(N)}_\Lambda \right) \chi_{\{I^{(N)}_\Lambda \leq \varepsilon N^2(1-\alpha)\}} \
+ \left[ \ln \alpha + \frac{1}{\alpha} \left( 1 - \frac{1}{\varepsilon N^2} I^{(N)}_\Lambda - \alpha \right) \right] \chi_{\{I^{(N)}_\Lambda \geq \varepsilon N^2(1-\alpha)\}} \right) \varphi^{(N)}(d^3Nq),
\end{align*}
\]
where we omitted the argument \( (q_1, ..., q_N) \) from \( I^{(N)}_\Lambda \), for brevity, and
\[
Q_{I/\varepsilon}^{(N)} (\varphi^{(N)}) = \lim_{\alpha \downarrow 0} \alpha Q_{I/\varepsilon}^{(N)} (\varphi^{(N)}). \quad (99)
\]
We also define \( \bar{\alpha} S(N) (\rho^{(N)}) \) precisely like \( S_{1/\varepsilon}^{(N)} (\rho^{(N)}) \) except that \( \alpha S_{1/\varepsilon}^{(N)} (\rho^{(N)}) \) is replaced by \( \alpha Q_{1/\varepsilon}^{(N)} (\rho^{(N)}) \). We have \( \alpha S_{1/\varepsilon}^{(N)} (\rho^{(N)}) > -\infty \) for all \( \rho \in (\mathcal{P} \cap \mathcal{L}^1 \ln \mathcal{L}^1)(\Lambda) \), and \( \lim_{\varepsilon \downarrow 0} \alpha S_{1/\varepsilon}^{(N)} (\rho^{(N)}) = -\infty \) whenever \( I/\varepsilon \not\in \mathcal{P} \). By \( \alpha Q_{1/\varepsilon}^{(N)} \) we denote the unique maximizer of \( \alpha S_{1/\varepsilon}^{(N)} (\rho^{(N)}) \), easily proven to exist as done for \( S_{1/\varepsilon}^{(N)} (\rho^{(N)}) \). Equally easily we find \( \lim_{\varepsilon \downarrow 0} \alpha S_{1/\varepsilon}^{(N)} (\rho_{N^{2\varepsilon}}^{(N)}) = S_{1/\varepsilon}^{(N)} (\rho_{N^{2\varepsilon}}^{(N)}) \).

We are now ready to formulate the \( N = \infty \) analogue of (93).

To define the mean quasi-interaction energy of \( \varrho \in \mathcal{P}^s(\Lambda^N) \), we introduce the subset \( \mathcal{P}_{U_A}^s(\Lambda^N) \subset \mathcal{P}^s(\Lambda^N) \) for which the expected value of \( U_A^2 \) is finite; i.e. \( \mathcal{P}_{U_A}^2(q, q') = \mathcal{P}(d^3qd^3q') < \infty \), where \( \mathcal{P}(d^3qd^3q') \) is the second marginal measure of \( \varrho \in \mathcal{P}_{U_A}^2(\Lambda^N) \). Also, by \( \mathcal{P}_{U_A}^2(\Lambda) \) we denote the subset of \( \mathcal{P}(\Lambda) \) which consists of Lebesgue-absolutely continuous probability measures \( \varrho \) for which \( \mathcal{P}_{U_A}^2(q, q') \mathcal{P}^s(d^3qd^3q') < \infty \), which implies \( \langle \varrho , \varrho \rangle < \infty \); here we recycled the bilinear form notation (13) for lower semi-continuous (rather than continuous) \( U_A \). If \( \varrho \in \mathcal{P}_{U_A}^s(\Lambda^N) \), then the decomposition measure \( \varsigma(d\varrho|\varrho) \) is concentrated on \( \mathcal{P}_{U_A}^s(\Lambda) \); this can be shown by adapting arguments from [HeSa55]; cf. also [McSp82]. The mean quasi-interaction energy of \( \varrho \in \mathcal{P}_{U_A}^s(\Lambda^N) \) is defined as

\[
\int_{\mathcal{P}_{U_A}^s(\Lambda^N)} (\rho) \equiv \lim_{\varepsilon \downarrow 0} \frac{1}{\varepsilon} \lim_{n \to \infty} \frac{1}{n} \alpha Q_{I/\varepsilon}^{(n)} (\varrho).
\]

We show that \( \bar{Q}_{I/\varepsilon} (\varrho) \) is well-defined. By the linearity of \( \varrho \mapsto \alpha Q_{I/\varepsilon}^{(n)} (\varrho) \), the presentation (97) yields

\[
\alpha Q_{I/\varepsilon}^{(n)} (\varrho) = \int \alpha Q_{I/\varepsilon}^{(n)} (\rho^{(n)}) \varsigma(d\varrho|\varrho),
\]

and on \( \mathcal{P}_{U_A}^s(\Lambda^N) \) the conventional law of large numbers for \( U \) statistics applies (see [Hoe48]) and yields

\[
\lim_{n \to \infty} \frac{1}{n} \alpha Q_{I/\varepsilon}^{(n)} (\rho^{(n)}) = \frac{3}{2} \left[ \ln \left( 1 - \frac{1}{\varepsilon} \langle \rho , \rho \rangle \right) \chi_{\{ \langle \rho , \rho \rangle < (1 - \alpha) \}} + \left( \ln \alpha + \frac{1}{\alpha} \left[ 1 - \alpha - \frac{1}{\varepsilon} \langle \rho , \rho \rangle \right] \right) \chi_{\{ \langle \rho , \rho \rangle \geq (1 - \alpha) \}} \right].
\]

Clearly, when \( \alpha \downarrow 0 \) in (102) the “value” \(-\infty\) is assigned to all \( \rho \) for which \( \langle \rho , \rho \rangle \geq \varepsilon \); the \( \alpha \downarrow 0 \) limit is finite when \( \langle \rho , \rho \rangle < \varepsilon \). We conclude with:

**Lemma 1.** The mean quasi-interaction energy (100) is well-defined and affine linear. For \( \varrho \in \mathcal{P}_{U_A}^s(\Lambda^N) \) having decomposition measure \( \varsigma(d\varrho|\varrho) \) supported entirely by \( \rho \) for which \( \langle \rho , \rho \rangle < \varepsilon \), we have (100) given by

\[
\mathcal{Q}_{I/\varepsilon} (\varrho) = \int \varrho (\rho) \varsigma(d\varrho|\varrho),
\]
where

\[ Q_{I/\varepsilon}(\rho) \equiv \frac{3}{2} \ln \left[ 1 - \frac{1}{\varepsilon} \langle \rho , \rho \rangle \right] ; \quad (104) \]

otherwise, \( Q_{I/\varepsilon}(\rho) = -\infty \).

The \( N = \infty \) analogue of \( (92) \) is the well-known mean (relative) entropy of \( \varrho \in \mathcal{V}^{s}(\Lambda^{\infty}) \), which is well-defined as limit

\[ \mathcal{R}(\varrho) \equiv \lim_{n \to \infty} \frac{1}{n} \mathcal{R}^{(n)}(\varrho|\lambda) . \quad (105) \]

Here, \( \mathcal{R}^{(n)}(\varrho|\lambda) \), \( n \in \{0,1,\ldots\} \), is the relative entropy of \( \varrho \), as defined in \( (92) \); we also set \( \mathcal{R}^{(-k)}(-k\varrho|\lambda) \equiv 0 \) for all \( k \in \mathbb{N} \). The limit \( (105) \) exists or is \(-\infty \). This is a consequence of the next lemma, which holds for \( \varrho \in \mathcal{V}^{s}(\Lambda^{\infty}) \) or \( \varrho \in \mathcal{V}^{s}(\Lambda^{N}) \). If \( \varrho = \varrho^{(N)} \), it is understood that \( k \leq N \) in \( \varrho^{(N)}_{k} \).

**Lemma 2.** Relative entropy \( n \mapsto \mathcal{R}^{(n)}(\varrho|\lambda) \) has the following properties:

(A) Non-positivity: For all \( n \),

\[ \mathcal{R}^{(n)}(\varrho|\lambda) \leq 0; \quad (106) \]

(B) Monotonic decrease: If \( n > m \) then

\[ \mathcal{R}^{(n)}(\varrho|\lambda) \leq \mathcal{R}^{(m)}(\varrho|\lambda); \quad (107) \]

(C) Strong sub-additivity: For \( m, n \leq \ell \), and \( k = \ell - m - n \),

\[ \mathcal{R}^{(\ell)}(\varrho|\lambda) \leq \mathcal{R}^{(m)}(\varrho|\lambda) + \mathcal{R}^{(n)}(\varrho|\lambda) + \mathcal{R}^{(k)}(\varrho|\lambda) - \mathcal{R}^{(-k)}(-\varrho|\lambda). \quad (108) \]

The proof of Lemma 2 is a straightforward adaptation from a proof by Robinson and Ruelle [RoRu67] (section 2, proof of proposition 1) for the standard-thermodynamic-limit problem to the Vlasov limit, studied here, cf. [Kie93].

The next lemma also has an elementary proof which likewise is an adaptation from [RoRu67], proof of their proposition 3, cf. [Kie93].

**Lemma 3.** The mean entropy functional \( (105) \) is affine linear.

Lemma 3 in conjunction with the de Finetti [deF37] – Dynkin [Dyn53] – Hewitt-Savage [HeSa55] decomposition theorem for \( \mathcal{V}^{s}(\Lambda^{N}) \) yields a key formula for the mean entropy which does not hold for the finite-\( N \) entropy. Namely, as a consequence of Lemma 3, the extremal decomposition of \( \varrho \) yields

\[ \mathcal{R}(\varrho) = \int \mathcal{R}(\rho|\lambda) \varsigma(d\rho|\varrho), \quad (109) \]

where we also set \( \mathcal{R}(\rho|\lambda) \equiv \mathcal{R}^{(1)}(\rho|\lambda) \).

Lemma 4, also proved by adaption of a corresponding proof in [RoRu67], proposition 4, ends the listing of properties of mean relative entropy \( (105) \).
Lemma 4. The mean entropy functional is weakly upper semi-continuous.

Finally we define the mean interaction entropy of \( \rho \in \mathfrak{P}^s(\Lambda^N) \),

\[
S_{I/\varepsilon}(\rho) \equiv \mathcal{R}(\rho) + \mathcal{Q}_{I/\varepsilon}(\rho).
\] (110)

By (109) and (103) we have

\[
S_{I/\varepsilon}(\rho) = \int_{\mathfrak{P}(\Lambda)} S_{I/\varepsilon}(\rho) \varsigma(d\rho|\rho),
\] (111)

where we introduced the functional

\[
S_{I/\varepsilon}(\rho) \equiv \mathcal{R}(\rho|\lambda) + \mathcal{Q}_{I/\varepsilon}(\rho),
\] (112)

which is well-defined and finite whenever \( \rho \in (\mathfrak{P} \cap \mathfrak{C}^1(\Lambda^N)) \) and \( \langle \rho , \rho \rangle < \varepsilon \); else we have \( S_{I/\varepsilon}(\rho) = -\infty \). Note that \( S_{I/\varepsilon}(\rho) \leq 0 \), for \( \mathcal{R}(\rho|\lambda) \leq 0 \) and \( \mathcal{Q}_{I/\varepsilon}(\rho) \leq 0 \), the latter because \( U_{\Lambda} \geq 0 \) by hypothesis.

Because of (111) the problem of maximizing \( S_{I/\varepsilon}(\rho) \) reduces to maximizing \( S_{I/\varepsilon}(\rho) \) given in (112).

Proposition 5. \( S_{I/\varepsilon}(\rho) \) is weakly upper semi-continuous for \( \varepsilon > \varepsilon_g \geq 0 \) and takes its finite non-positive maximum at a solution of the fixed point equation

\[
\rho(q) = \frac{\exp \left( -\vartheta^{-1}_\varepsilon(\rho) \int_{\Lambda} U_{\Lambda}(q, \tilde{q}) \rho(\tilde{q}) d^3 \tilde{q} \right)}{\int_{\Lambda} \exp \left( -\vartheta^{-1}_\varepsilon(\rho) \int_{\Lambda} U_{\Lambda}(\tilde{q}, \tilde{q}) \rho(\tilde{q}) d^3 \tilde{q} \right) d\tilde{q}},
\] (113)

where

\[
\vartheta_\varepsilon(\rho) = \frac{2}{3} \left( 1 - \frac{1}{\varepsilon} \langle \rho , \rho \rangle \right) \varepsilon > 0.
\] (114)

Proof of Proposition 5:

Since relative entropy \( \mathcal{R}(\rho|\lambda) \) is weakly upper semi-continuous (ReSi80, Suppl. to IV.5; Ell85, chpt.VIII), and since the functional \( \mathcal{Q}_{I/\varepsilon}(\rho) \) is weakly upper semi-continuous as a consequence of hypothesis \( H2 \) and the positivity of \( U_{\Lambda} \), so is \( S_{I/\varepsilon}(\rho) \). Since \( \Lambda \) is compact, \( S_{I/\varepsilon}(\rho) \) now takes its maximum, which is non-positive because \( S_{I/\varepsilon}(\rho) \leq 0 \), and finite (i.e. \( > -\infty \)) because of the following. Let \( k \mapsto \rho(k) \) in \( (\mathfrak{P} \cap \mathfrak{C}^1(\Lambda^N)) \) be a minimizing sequence for \( \langle \rho , \rho \rangle \). Since \( \Lambda \) is compact, \( S_{I/\varepsilon}(\rho) \) now takes its maximum, which is non-positive because \( S_{I/\varepsilon}(\rho) \leq 0 \), and finite (i.e. \( > -\infty \)) because of the following. Let \( k \mapsto \rho(k) \) in \( (\mathfrak{P} \cap \mathfrak{C}^1(\Lambda^N)) \) be a minimizing sequence for \( \langle \rho , \rho \rangle \). Since \( \varepsilon > \varepsilon_g \geq 0 \), by \( H3 \) there is a \( K \) such that \( \varepsilon_g < \langle \rho(k) , \rho(k) \rangle < \varepsilon \) for all \( k \geq K \). Then \( \max_{\rho} S_{I/\varepsilon}(\rho) \geq S_{I/\varepsilon}(\rho(K)) = 0 + 0 > -\infty \).

Let \( q \mapsto \rho(\epsilon(q)) \) denote any maximizer for \( S_{I/\varepsilon}(\rho) \). Suppose \( \langle \rho_\epsilon , \rho_\epsilon \rangle \geq \varepsilon \). Then \( \mathcal{Q}_{I/\varepsilon}(\rho_\epsilon) = -\infty \), and because \( \mathcal{R}(\rho_\epsilon|\lambda) \leq 0 \) then also \( S_{I/\varepsilon}(\rho_\epsilon) = -\infty \). Therefore \( \langle \rho_\epsilon , \rho_\epsilon \rangle < \varepsilon \) strictly, and since \( \varepsilon > 0 \), this proves (114).

The standard variational argument now shows that the maximizer satisfies the Euler-Lagrange equation for \( S_{I/\varepsilon}(\rho) \), which is (113). \( \square \)
Corollary 1. The functional $\mathcal{S}_{I/\varepsilon}(\rho)$ given in (110) achieves its supremum. If $\rho_\varepsilon$ is a maximizer of $\mathcal{S}_{I/\varepsilon}(\rho)$, then the support of its decomposition measure $\zeta(d\rho|\rho_\varepsilon)$ is the set of maximizers $\{\rho_\varepsilon\}$ of the functional $\mathcal{S}_{I/\varepsilon}(\rho)$ given in (112).

Proof of Corollary 1:

Abstractly, by Lemma 4 and the linearity of the mean quasi-interaction energy functional, the mean interaction entropy functional $\mathcal{S}_{I/\varepsilon}(\rho)$ given in (110) is weakly upper semi-continuous, and so achieves its supremum over the compact set of permutation symmetric probabilities $\mathfrak{P}_U^s(\Lambda^N)$.

Alternatively, by (111) and two obvious estimates, we have right away that

$$\mathcal{S}_{I/\varepsilon}(\rho_\varepsilon) = \mathcal{S}_{I/\varepsilon}(\rho_\varepsilon^N) \leq \sup_{\rho} \mathcal{S}_{I/\varepsilon}(\rho) \leq \max_{\rho} \mathcal{S}_{I/\varepsilon}(\rho) = \mathcal{S}_{I/\varepsilon}(\rho_\varepsilon^N),$$

so $\sup_{\rho} \mathcal{S}_{I/\varepsilon}(\rho) = \max_{\rho} \mathcal{S}_{I/\varepsilon}(\rho) = \mathcal{S}_{I/\varepsilon}(\rho_\varepsilon^N)$. Now let $\rho_\varepsilon$ maximize $\mathcal{S}_{I/\varepsilon}(\rho)$ and suppose that $\text{supp} \zeta(d\rho|\rho_\varepsilon)$ is not a subset of the maximizers $\{\rho_\varepsilon\}$ of $\mathcal{S}_{I/\varepsilon}(\rho)$. Then

$$\mathcal{S}_{I/\varepsilon}(\rho_\varepsilon) = \int_{\mathfrak{P}(\Lambda)} \mathcal{S}_{I/\varepsilon}(\rho) \zeta(d\rho|\rho_\varepsilon) < \max_{\rho} \mathcal{S}_{I/\varepsilon}(\rho) = \mathcal{S}_{I/\varepsilon}(\rho_\varepsilon^N),$$

so $\rho_\varepsilon$ is not a maximizer — a contradiction to the supposition.

We now relate the sequence of maximizers $\{\rho_{N^2\varepsilon}\}_{N \in \mathbb{N}}$ of $\{\mathcal{S}^{(N)}_{I/\varepsilon}\}$ to the set of maximizers $\{\rho_\varepsilon\}$ of $\mathcal{S}_{I/\varepsilon}(\rho)$. We begin with the maxima of $\mathcal{S}^{(N)}_{I/\varepsilon}(\rho^{(N)})$ and $\mathcal{S}_{I/\varepsilon}(\rho)$.

Proposition 6. We have

$$\lim_{N \to \infty} \frac{1}{N} \mathcal{S}^{(N)}_{I/\varepsilon}(\rho_{N^2\varepsilon}^{(N)}) = \mathcal{S}_{I/\varepsilon}(\rho_\varepsilon).$$

Proof of Proposition 6:

For all $\alpha \in (0, 1)$, we have

$$\alpha \mathcal{S}^{(N)}_{I/\varepsilon}(\rho_{N^2\varepsilon}^{\otimes n}) \geq \alpha \mathcal{S}^{(N)}_{I/\varepsilon}(\rho_{\varepsilon}^{\otimes n}).$$

We compute

$$\alpha \mathcal{S}^{(N)}_{I/\varepsilon}(\rho_{\varepsilon}^{\otimes n}) = N \mathcal{R}^{(1)}(\rho_\varepsilon|\lambda) + \alpha \mathcal{Q}_{I/\varepsilon}^{(N)}(\rho_{\varepsilon}^{\otimes n}).$$

Since $\langle \rho_\varepsilon, \rho_\varepsilon \rangle < \varepsilon$, when $\alpha \in (0, 1)$ is sufficiently small we have by (H4) and Proposition 5 that

$$\lim_{N \to \infty} \frac{1}{N} \alpha \mathcal{Q}_{I/\varepsilon}^{(N)}(\rho_{\varepsilon}^{\otimes n}) = \frac{3}{2} \ln \left[1 - \frac{1}{\varepsilon} \langle \rho_\varepsilon, \rho_\varepsilon \rangle \right].$$

Hence, for all sufficiently small $\alpha \in (0, 1),$

$$\lim_{N \to \infty} \frac{1}{N} \alpha \mathcal{S}^{(N)}_{I/\varepsilon}(\rho_{\varepsilon}^{\otimes n}) = \mathcal{S}_{I/\varepsilon}(\rho_\varepsilon).$$
Thus
\[
\liminf_{N \to \infty} \frac{1}{N} \alpha s_{1/\varepsilon}^{(N)}(\mathcal{G}_{N^2 \varepsilon}^{(N)}) \geq s_{1/\varepsilon}(\rho_{\varepsilon})
\]  
(122)
for all sufficiently small $\alpha \in (0, 1)$, and this yields the first desired estimate
\[
\liminf_{N \to \infty} \frac{1}{N} s_{1/\varepsilon}^{(N)}(\mathcal{G}_{N^2 \varepsilon}^{(N)}) \geq s_{1/\varepsilon}(\rho_{\varepsilon}).
\]  
(123)

Now consider (94) as extended to a probability on $\Lambda^N$. Since $\Lambda$ is bounded, $\overline{\Lambda}$ is compact, and then the sequence $\{\varrho(N^2 \varepsilon(N))\} \subseteq \mathbb{N}$ is weakly compact, so
\[
\lim_{N \to \infty} \frac{n}{N} \varrho(N^2 \varepsilon) = \varrho(\varepsilon) \in \mathcal{P}(\overline{\Lambda}^N) \quad \forall n \in \mathbb{N},
\]  
(124)
after extraction of a subsequence $\{\varrho(N^2 \varepsilon(N))\} \subseteq \mathbb{N}$; note that the $\{n \varrho(\varepsilon)\} \subseteq \mathbb{N}$ form a compatible sequence of marginals. Furthermore, we have $\int_{\partial \Lambda} \varrho(\varepsilon) (d\mathcal{L}) = 0$, or else $\mathcal{R}(\varrho(\varepsilon)) = -\infty$, a contradiction; so $n \varrho(\varepsilon) \in \mathcal{P}(\overline{\Lambda}^N)$.

Following [MeSp82, Kie93] we now use sub-additivity of relative entropy (property (C) in Lemma 2) and then negativity of relative entropy (property (A) in Lemma 2) (valid also with $\varrho(N^2 \varepsilon(N))$ in place of $\varrho$), and obtain
\[
\mathcal{R}(N)\varrho(N^2 \varepsilon(N)) \leq \left[ \frac{N}{n} \right] \mathcal{R}(n \varrho(N^2 \varepsilon(N))) + \mathcal{R}(m \varrho(N^2 \varepsilon(N)))
\leq \left[ \frac{N}{n} \right] \mathcal{R}(n \varrho(N^2 \varepsilon(N)))
\]  
(125)
where $[a/b]$ is the integer part of $a/b$, and where $m < n$. Upper semi-continuity for the relative entropy gives
\[
\limsup_{N \to \infty} \mathcal{R}(n \varrho(N^2 \varepsilon(N))) \leq \mathcal{R}(n \varrho(N \varepsilon)),
\]  
(126)
while $\frac{N}{n} \left[ \frac{N}{n} \right] \to \frac{1}{n}$. Hence, dividing (125) by $N[N]$ and letting $N \to \infty$ gives
\[
\limsup_{N \to \infty} \frac{1}{N} \mathcal{R}(N)\varrho(N^2 \varepsilon(N)) \leq \frac{1}{n} \mathcal{R}(n \varrho(N \varepsilon)) \quad \forall n \in \mathbb{N},
\]  
(127)
and now taking the supremum over $n$ (equivalently: the limit $n \to \infty$) we get
\[
\limsup_{N \to \infty} \frac{1}{N} \mathcal{R}(N)\varrho(N^2 \varepsilon(N)) \leq \mathcal{R}(\varrho(\varepsilon)).
\]  
(128)
Lastly, using (109) in (128) yields
\[
\limsup_{N \to \infty} \frac{1}{N} \mathcal{R}(N)\varrho(N^2 \varepsilon(N)) \leq \int \mathcal{R}(\rho | \lambda) (d\rho | \varrho(\varepsilon))
\]  
(129)
where \( \zeta(d\rho|\hat{\rho}_\varepsilon) \) be the Hewitt–Savage decomposition measure for \( \hat{\rho}_\varepsilon \). For each \( \rho \in \text{supp} \zeta(d\rho|\hat{\rho}_\varepsilon) \) we can choose a family of \( \varrho^{(N)}[\rho] \in \Psi^s(\Lambda^N) \) satisfying

\[
\lim_{N \to \infty} \eta^{(N)}[\rho] = \rho^{\otimes n} \tag{130}
\]

for each \( n \in \mathbb{N} \), such that for each \( \hat{N}[N] \), with \( N \in \mathbb{N} \), we have

\[
\varrho^{(N)}_{\hat{N}_\varepsilon}[N] = \int \varrho^{(N)}[\rho] \zeta(d\rho|\hat{\rho}_\varepsilon). \tag{131}
\]

In contrast to the de Finetti-Dynkin-Hewitt-Savage decomposition, this finite \( N \) decomposition is not unique, but this is immaterial. We remark that in the physically (presumably) most important situations, namely when \( \text{supp} \zeta(d\rho|\hat{\rho}_\varepsilon) \) is either a finite set or a continuous group orbit of a compact group, then a decomposition \( \text{(131)} \) satisfying \( \text{(130)} \) can easily be constructed explicitly, as shown in Appendix B.

By \( \text{(131)} \), the linearity of the map \( \varrho^{(N)}(\varrho^{(N)}) \mapsto \alpha Q_{I/\varepsilon}(\varrho^{(N)}) \) gives

\[
\alpha Q_{I/\varepsilon}^{(N)}(\varrho^{(N)}_{\hat{N}_\varepsilon}) = \int \alpha Q_{I/\varepsilon}^{(N)}(\varrho^{(N)}[\rho]) \zeta(d\rho|\hat{\rho}_\varepsilon), \tag{132}
\]

and by the concavity of the map \( I \mapsto \alpha Q_{I/\varepsilon}^{(N)}(\varrho^{(N)}) \), Jensen’s inequality gives

\[
\alpha Q_{I/\varepsilon}^{(N)}(\varrho^{(N)}[\rho]) \leq \frac{3\hat{N} - 2}{2} \left[ \ln \left( 1 - \frac{1}{\varepsilon} \varrho^{(N)}(\varrho^{(N)}) \right) \chi_{\{\varrho^{(N)}(\varrho^{(N)}) < \varepsilon(1 - \alpha)\}} + \left( \ln \alpha + \frac{1}{\alpha} \left[ 1 - \alpha - \frac{1}{\varepsilon} \varrho^{(N)}(\varrho^{(N)}) \right] \right) \chi_{\{\varrho^{(N)}(\varrho^{(N))} \geq \varepsilon(1 - \alpha)\}} \right], \tag{133}
\]

where

\[
\varrho^{(N)}(\varrho^{(N)}) = \left( 1 - \hat{N}^{-1} \right) \int \frac{1}{2} U_\Lambda(q, \dot{q}) \varrho^{(N)}[\rho](d^3q, d^3\dot{q}). \tag{134}
\]

The weak lower semi-continuity of \( U_\Lambda \) now gives

\[
\liminf_{N \to \infty} \int \frac{1}{2} U_\Lambda \varrho^{(N)}[\rho] d^6q \geq \langle \rho, \rho \rangle, \tag{135}
\]

and since \( \hat{N}^{-1} \to 0 \), we find for each convergent subsequence of measures that

\[
\limsup_{N \to \infty} \frac{1}{N} \alpha Q_{I/\varepsilon}^{(N)}(\varrho^{(N)}[\rho]) \leq \frac{3}{2} \ln \left[ 1 - \frac{1}{\varepsilon} \langle \rho, \rho \rangle \right] \chi_{\{\langle \rho, \rho \rangle < \varepsilon(1 - \alpha)\}} \tag{136}
\]

\[
\quad + \left( \ln \alpha + \frac{1}{\alpha} \left[ 1 - \alpha - \frac{1}{\varepsilon} \langle \rho, \rho \rangle \right] \right) \chi_{\{\langle \rho, \rho \rangle \geq \varepsilon(1 - \alpha)\}} \right],
\]

for each \( \alpha \in (0, 1) \). Now suppose that \( \langle \rho, \rho \rangle \geq \varepsilon \); then r.h.s. \( \text{(136)} \) \( \downarrow -\infty \) as \( \alpha \downarrow 0 \), in which case by \( \text{(136)} \) and \( \text{(132)} \) also \( \alpha Q_{I/\varepsilon}^{(N)}(\varrho^{(N)}_{\hat{N}_\varepsilon}) \downarrow -\infty \) as \( \alpha \downarrow 0 \),
and by (99) and (93) and property (A) in Lemma 2, and then Proposition 4, this contradicts the lower bound (90). Therefore, $\langle \rho, \rho \rangle < \varepsilon$ for every $\rho \in \text{supp} \zeta(d\rho|\hat{\varepsilon})$, and so, and recalling (104), we conclude that

$$\limsup_{N \to \infty} \frac{1}{N} S_{\varepsilon}^{(N)}(\hat{\varepsilon}) \leq S_{\varepsilon}/\varepsilon(\rho_\varepsilon).$$

(137)

The estimates (137) and (129) and two obvious estimates now give

$$\limsup_{N \to \infty} \frac{1}{N} S_{\varepsilon}^{(N)}(\hat{\varepsilon}) \leq \limsup_{N \to \infty} \frac{1}{N} R^{(N)}(\rho^{(N)}_{N^2\varepsilon}|\lambda) + \limsup_{N \to \infty} \frac{1}{N} Q_{\varepsilon}^{(N)}(\hat{\varepsilon})$$

$$\leq \int R(\rho|\lambda)(d\rho|\hat{\varepsilon}) + \int Q_{\varepsilon}(\rho)(d\rho|\hat{\varepsilon})$$

$$= \int S_{\varepsilon}(\rho)(d\rho|\hat{\varepsilon})$$

$$\leq \max_\rho S_{\varepsilon}(\rho),$$

(138)

and since this holds for each limit point $\hat{\varepsilon}$ we can drop the dot to get

$$\limsup_{N \to \infty} \frac{1}{N} S_{\varepsilon}^{(N)}(\hat{\varepsilon}) \leq S_{\varepsilon}(\rho_\varepsilon).$$

(139)

By (123) and (139), Proposition 6 is proved.

By Propositions 4, 5, and 6, the interaction entropy per particle for Boltzmann’s ergodic ensemble converges as follows,

$$s_{\Lambda,I}(\varepsilon) \equiv \lim_{N \to \infty} \frac{1}{N} S_{\varepsilon}^{(N)}(\hat{\varepsilon}) = S_{\varepsilon}/\varepsilon(\rho_\varepsilon),$$

(140)

and $s_{\Lambda,I}(\varepsilon)$ is characterized by its own variational principle expressed in Proposition 5. Moreover, by formula (37), which holds under assumptions (H1)–(H5), the expansion (23) now follows, with

$$s_{\Lambda}(\varepsilon) = s_{\Lambda,K}(\varepsilon) + s_{\Lambda,I}(\varepsilon),$$

(141)

where $s_{\Lambda,K}(\varepsilon)$ is given in (39), and $s_{\Lambda,I}(\varepsilon)$ in (140) and Proposition 5. By Proposition 5 any maximizer $\rho_\varepsilon$ of $S_{\varepsilon}/\varepsilon(\rho)$ satisfies (28) and (29).

Lastly, one readily verifies that the just described $s_{\Lambda}(\varepsilon)$ equals the negative minimum of Boltzmann’s $H$ functional over the set of trial densities $A_\varepsilon = \{ f \in (\mathfrak{F} \cap L^1 \cap L^1 \ln L^1)(\mathbb{R}^3 \times \Lambda) : \varepsilon(f) = \varepsilon \}$. This is done by explicitly carrying out the standard variational argument for $H(f)$, taking the constraints into account with the help of Lagrange multipliers which are then eliminated with the help of the very functionals of $\rho_\varepsilon$ displayed in Theorem 2.

This completes the proof of Theorem 2.
5.3 Proof of Theorem 3

We begin with the observation that (94) is clearly the $N$-th configurational marginal measure of (2), i.e. (94) is (2) with the Hamiltonian given by (19), integrated over all the $p$ variables in (19). Put differently, (94) is the joint $N$-point distribution on configuration space $\Lambda^N$ of an $N$-body system with Hamiltonian (19) chosen w.r.t. the a-priori measure (2) on $(\mathbb{R}^3 \times \Lambda)^N$. Hence, our proof of Theorem 2 also proves the following weaker version of Theorem 3.

**Theorem 3.**— Under the same assumptions as in Theorem 2 consider (2) for the Hamiltonian (19) as extended to a probability on $(\mathbb{R}^3 \times \Lambda)^N$. Then the sequence $\{\varrho^{(N)}_{N \varepsilon}\}_{N \in \mathbb{N}}$ of its configuration space marginals, obtained by integrating over all the $p$ variables in (19) and given in (94), is weakly compact in $\mathfrak{P}^*(\Lambda^N)$, so one can extract a subsequence $\{\varrho_{N^2 \varepsilon}^{(N)}\}_{N \in \mathbb{N}}$ such that

$$\lim_{N \to \infty} \varrho_{N \varepsilon}^{(N)} = \hat{\varrho}_\varepsilon \in \mathfrak{P}^*(\Lambda^N),$$

in the sense that

$$\lim_{N \to \infty} \varrho_{N^2 \varepsilon}^{(N)} = \int_{\mathfrak{P}(\Lambda)} \prod_{1 \leq k \leq n} \rho(q_k) d^3 q_k \varsigma(d\rho|\hat{\varrho}_\varepsilon) \quad \forall n \in \mathbb{N}. \quad (143)$$

The decomposition measure $\varsigma(d\rho|\hat{\varrho}_\varepsilon)$ of each such limit point $\hat{\varrho}_\varepsilon$ is supported on the subset of $\mathfrak{P}(\Lambda)$ which consists of the probability measures $\rho_{\varepsilon}(q)d^3 q$ which maximize the functional $s_{I/\varepsilon}(\rho)$.

Since each limit point $\hat{\varrho}_\varepsilon$ of (94) is a convex linear superposition of infinite product measures on $\Lambda^N$ consisting of “Boltzmann factors” $\rho_{\varepsilon}(q)$ on $\Lambda$, satisfying (28) with (29) and maximizing the interaction entropy functional $s_{I/\varepsilon}(\rho)$, and since each such Boltzmann factor is associated with a unique “Maxwellian” $\sigma_\varepsilon(p)$ on $\mathbb{R}^3$ through (30), each such Boltzmann factor thereby defines a unique Maxwell–Boltzmann distribution $\sigma_{\varepsilon}(p)\rho_{\varepsilon}(q)$ on $\mathbb{R}^3 \times \Lambda$ given by the product of this Boltzmann factor with its associated Maxwellian. So the very decomposition measure $\varsigma(d\rho|\hat{\varrho}_\varepsilon)$ of each limit point $\hat{\varrho}_\varepsilon$ on $\Lambda^N$ allows us to define a unique probability measure $\hat{\mu}_\varepsilon$ on $(\mathbb{R}^3 \times \Lambda)^N$, viz.

$$\eta \hat{\mu}_\varepsilon(d^3 p d^3 q) = \int_{\mathfrak{P}(\Lambda)} \prod_{1 \leq k \leq n} \sigma(\rho)(p_k) \rho(q_k) d^3 p_k d^3 q_k \varsigma(d\rho|\hat{\varrho}_\varepsilon) \quad \forall n \in \mathbb{N}, \quad (144)$$

and this measure $\varsigma(d\rho|\hat{\varrho}_\varepsilon)$ on $\mathfrak{P}(\Lambda)$ can be mapped into a unique measure $\nu(d\tau|\hat{\mu}_\varepsilon)$ on $\mathfrak{P}(\mathbb{R}^3 \times \Lambda)$ which is concentrated on those $\tau \in \mathfrak{P}(\mathbb{R}^3 \times \Lambda)$ which are of the form $\tau(d^3 p d^3 q) = \sigma(\rho)(p)\rho(q)d^3 p d^3 q$, with $\sigma(\rho)$ given by (30) and $\rho$ satisfying (28) with (29) and maximizing $s_{I/\varepsilon}(\rho)$, thus

$$\eta \hat{\mu}_\varepsilon(d^3 p d^3 q) = \int_{\mathfrak{P}(\Lambda)} \prod_{1 \leq k \leq n} \tau(d^3 p_k d^3 q_k) \nu(d\tau|\hat{\mu}_\varepsilon) \quad \forall n \in \mathbb{N}. \quad (145)$$
The corresponding infinite product measures $\prod_{1 \leq k \leq \infty} \tau(d^3p_k d^3q_k)$ on $(\mathbb{R}^3 \times \Lambda)^N$ are extreme points of $\mathcal{P}^*((\mathbb{R}^3 \times \Lambda)^N)$, and so (145) is the extremal representation of $\hat{\mu}_\varepsilon$. So, having Theorem 3 and its consequence (145), all we need to do to finish the proof of Theorem 3 is to show that each such defined $\hat{\mu}_\varepsilon$ is indeed a limit point of (2) under the stated hypotheses.

To see this, we use that by Theorem 3 we already know that (143) holds, and we know the support of $\zeta(d\rho|\hat{\phi}_\varepsilon)$. Writing $n_o^{(N\lceil N\rceil)}\hat{\phi}_{N^2\varepsilon}$ explicitly gives

$$n_o^{(N\lceil N\rceil)}\hat{\phi}_{N^2\varepsilon}(d^{3n}q) = \int \left(1 - \frac{1}{\varepsilon N^2} I_A^{(n)}(q_1, \ldots, q_N)\right) \frac{3N-1}{2} d^3(N-n)q$$

where the integral in the numerator runs over the variables $q_{n+1}$ to $q_N$. For any $\hat{N}$ and $1 \leq n < \hat{N}$ we now write

$$I_{\Lambda}^{(\hat{N})}(q_1, \ldots, q_N) = I_A^{(n)}(q_1, \ldots, q_n) + I_A^{(\lceil N\rceil)}(q_1, \ldots, q_N) + I_A^{(\hat{N}-n)}(q_{n+1}, \ldots, q_N)$$

(147)

which defines $I_A^{(\lceil N\rceil)}(q_1, \ldots, q_N)$. Henceforth we omit the arguments from the $I$s to keep the formulas within sight; by (147) the superscripts convey which variables are used. With the help of (147) we rewrite the integrands thusly:

$$\left(1 - \frac{1}{\varepsilon N^2} I_A^{(n)}\right) = \left(1 - \frac{I_A^{(n)} + I_A^{(\lceil N\rceil)}}{N^2(\varepsilon - \hat{N}-2 I_A^{(\hat{N}-n)})}\right) \left(1 - \frac{1}{\varepsilon N^2} I_A^{(\hat{N}-n)}\right)$$

(148)

Now $1 - \left(\varepsilon \hat{N}^2\right)^{-1} I_A^{(\hat{N})}$ vanishes in an open neighborhood of configurations $(q_1, \ldots, q_n)$ for which $I_A^{(\hat{N})} = \infty$, so that $I_A^{(n)} < \infty$ on the support of (148). And for any configuration $(q_1, \ldots, q_n)$ for which $I_A^{(n)} < \infty$, we have $\hat{N}-2 I_A^{(\hat{N})} \rightarrow 0$ as $\hat{N}[N] \rightarrow \infty$. Moreover, by our Theorem 3 and its explication (143), we have that

$$\left(1 - \frac{1}{\varepsilon N^2} I_A^{(\hat{N}-n)}\right) \frac{3(N-n)}{2} d^3(N-n)q$$

interpreted as a measure on the convex set of probability measures $\mathcal{P}(\Lambda)$ with support in the set of empirical one-point “densities” with $\hat{N} - n$ atoms converges (up to normalization) to

22We are using that $(fg)_+ = f_+ g_+ + f_- g_-$ for two arbitrary functions $f$ and $g$, and that in our case $f$ cannot be strictly negative if $g$ is, giving $(fg)_+ = f_+ g_+$ in our case, $f$ and $g$ are the respective expressions between the two pairs of big parentheses at r.h.s. (148).

23If $U_A$ is bounded continuous on $\Lambda^2$, then we already know that we can rewrite $I_A^{(n)}$ as a sum of a bilinear and a linear form on $\mathcal{P}(\Lambda)$ evaluated at a normalized empirical one-point “density” with $N$ atoms; see (12). If $U_A$ is only lower semi-continuous this particular identification ceases to make sense, but happily we can always interpret $I_A^{(n)}$ as a linear form on the convex set of probability measures $\mathcal{P}(\Lambda^2)$ (cf. 123 and 135), evaluated at a normalized empirical two-point “density” with $N$ atoms, and we note that any empirical two-point “density” with $N$ atoms is uniquely determined by its associated empirical one-point “density” with $N$ atoms.
\( \zeta(d\rho|\hat{\nu}_\varepsilon) \), and for any \( \rho \) in the support of \( \zeta(d\rho|\hat{\nu}_\varepsilon) \) we have that \( N^{-1}i^{(N)}_{\Lambda} \to \langle \rho, \rho \rangle \) while \( N^{-1}i^{(n)}_{\Lambda} \to \sum_{1 \leq k \leq n} \int_{\Lambda} U_{\Lambda}(q_k, \bar{q})\rho(\bar{q})d^3q \) when \( N[N] \to \infty \). So for any \( \rho \) in the support of the decomposition measure \( \zeta(d\rho|\hat{\nu}_\varepsilon) \) we have

\[
\left( 1 - \frac{i^{(n)}_{\Lambda} + i^{(n)}_{\Lambda^N}}{N^2(\varepsilon - N^{-2}i^{(N-n)}_{\Lambda})} \right)^{\frac{3(N-n)}{2} - 1} \to \prod_{1 \leq k \leq n} \exp \left( -\frac{1}{\varepsilon}\int_{\Lambda} U_{\Lambda}(q_k, \bar{q})\rho(\bar{q})d^3\bar{q} \right) \tag{149}
\]

with \( \frac{3}{2}\varepsilon = \varepsilon - \langle \rho, \rho \rangle \). After this preparation, we now explicitly compute the marginal \( m^{(N)}_{\Lambda^2\varepsilon} \) and find

\[
m^{(N)}_{\Lambda^2\varepsilon}(d^3p|d^3q) = \frac{\int_{\Lambda} \left( 1 - \frac{i^{(n)}_{\Lambda} + i^{(N)}_{\Lambda^N}}{N^2(\varepsilon - N^{-2}i^{(N-n)}_{\Lambda})} \right)^{\frac{3(N-n)}{2} - 1} d^3q}{\int_{\Lambda} \left( 1 - \frac{i^{(n)}_{\Lambda} + i^{(N)}_{\Lambda^N}}{N^2(\varepsilon - N^{-2}i^{(N-n)}_{\Lambda})} \right)^{\frac{3(N-n)}{2} - 1} d^3q} \tag{150}
\]

where \( K^{(n)}_{\Lambda^N}(p_1, \ldots, p_n) = N\sum_{1 \leq k \leq n} \frac{1}{2}|p_k|^2 \). Using (147) we factor the integrals as in (148), though now we get

\[
\left( 1 - \frac{i^{(n)}_{\Lambda} + i^{(N)}_{\Lambda^N}}{N^2(\varepsilon - N^{-2}i^{(N-n)}_{\Lambda})} \right) = \left( 1 - \frac{i^{(n)}_{\Lambda} + i^{(n)}_{\Lambda^N}}{N^2(\varepsilon - N^{-2}i^{(N-n)}_{\Lambda})} \right) \left( 1 - \frac{1}{N^2}i^{(N-n)}_{\Lambda^N} \right) \tag{151}
\]

and by following essentially verbatim the arguments which lead from (148) to (149), we now find that for any \( \rho \in \text{supp} \zeta(d\rho|\hat{\nu}_\varepsilon) \),

\[
\left( 1 - \frac{i^{(n)}_{\Lambda} + i^{(n)}_{\Lambda^N}}{N^2(\varepsilon - N^{-2}i^{(N-n)}_{\Lambda})} \right)^{\frac{3(N-n)}{2} - 1} \to \prod_{1 \leq k \leq n} \exp \left( -\frac{1}{\varepsilon}|p_k|^2 + \int_{\Lambda} U_{\Lambda}(q_k, \bar{q})\rho(\bar{q})d^3\bar{q} \right) \tag{152}
\]

6 Spin-offs of our results

In this section we list a number of corollaries of our results.

6.1 A weak law of large numbers / ergodic theorem

Whenever \( \mathcal{H}_F(f) \) has a unique minimizer \( f_\varepsilon \) over \( \mathcal{W}_\varepsilon \), then necessarily all limit points in (33) coincide, i.e. any \( \mu_\varepsilon = \mu_\varepsilon \). By the weak compactness of \( \mathcal{P}^*(\Lambda^N) \) (in product topology) we then in fact do have weak convergence,

\[
\lim_{N \to \infty} n^{(N)}_{\Lambda^2\varepsilon}(d^3p|d^3q) = n_{\Lambda^2\varepsilon}(d^3p|d^3q) \in \mathcal{P}^*((\mathbb{R}^3 \times \Lambda)^n) \quad \forall n \in \mathbb{N}. \tag{153}
\]
Since in this case the decomposition measure $\nu(d\tau|\mu)\epsilon$ is a singleton, the limit
$\mu_{\epsilon} = \{\mu_{\epsilon}\}_{n\in\mathbb{N}}$ is of the form

$$n_{\mu_{\epsilon}}(d^{3n}p_{\epsilon}d^{3n}q) = \prod_{1\leq k\leq n} f_{\epsilon}(p_{k}, q_{k})d^{3}p_{k}d^{3}q_{k} \quad (154)$$

with $f_{\epsilon}(p, q) = \sigma_{\epsilon}(p)\rho_{\epsilon}(q)$ as defined in Theorem [2]. As discussed in [Spo91], the factorization property (154) is equivalent to a weak law of large numbers — or to an ergodic theorem, depending on one's point of view. Since the single particle momentum $P$ and position $Q$ of an individual $N$-body system picked from Boltzmann’s Ergode (2), with Hamiltonian (19), are random variables, any bounded continuous single-particle test function $\theta$ on $\mathbb{R}^{3}\times\Lambda$ defines a new random variable $\Theta = \theta(P, Q)$, and so does its sample mean over a single $N$-body system,

$$\langle \Theta \rangle_{N} \equiv \frac{1}{N} \sum_{j=1}^{N} \theta(p_{j}, q_{j}) \quad (155)$$

Theorem [3] in the special case (154) implies that, for all such $\theta$,

$$\lim_{N\to\infty} \langle \Theta \rangle_{N} = \int_{\mathbb{R}^{3}\times\Lambda} \theta(p, q)f_{\epsilon}(p, q)d^{3}p_{\epsilon}d^{3}q \quad (156)$$

in probability. The generalization to $n$-body test functions holds as well.

### 6.2 The Vlasov limit for other thermodynamic potentials

A second corollary, or actually a whole family of corollaries, is the existence of the Vlasov limit for the thermodynamic potentials of the canonical and grandcanonical ensembles under the same hypotheses. We only discuss the Vlasov limit for the thermodynamic potential of the canonical ensemble.

Thus, taking the Laplace transform of (3), i.e. multiplying by $e^{-\beta E}$ and integrating over $E$, yields what is known as the canonical partition function,

$$Z_{H_{\Lambda}^{(N)}(\beta)} = \frac{1}{N!} \int \exp \left( -\beta H_{\Lambda}^{(N)}(X^{(N)}) \right) d^{6N}X. \quad (157)$$

The Hamiltonian $H_{\Lambda}^{(N)}(X^{(N)})$ is given in (19). Clearly (157) factors as follows,

$$Z_{H_{\Lambda}^{(N)}(\beta)} = Z_{K^{(N)}(\beta)}Z_{I_{\Lambda}^{(N)}(\beta)} \quad (158)$$

where

$$Z_{I_{\Lambda}^{(N)}(\beta)} = \int \exp \left( -\beta I_{\Lambda}^{(N)}(q_{1}, ..., q_{N}) \right) \lambda(d^{3N}q) \quad (159)$$
is the canonical configurational integral, with $\lambda(d^3q) = |\Lambda|^{-1}d^3q$ the normalized Lebesgue measure introduced in section 5, and $\lambda(d^3Nq)$ its $N$-fold product, and

$$Z_{K(N)}(\beta) = \frac{|\Lambda|^N}{N^N} \int \exp \left(-\beta K^{(N)}(p_1, \ldots, p_N)\right) d^{3N}p$$

(160)

is the canonical partition function of a spatially uniform perfect gas in $\Lambda$, a Gaussian on the Cartesian product of the $p$ spaces, which evaluates to

$$Z_{K(N)}(\beta) = \frac{|\Lambda|^N}{N^N} \left(2\pi \vartheta\right)^{3N/2};$$

(161)

here, we introduced $N\vartheta = \beta^{-1}$, with $\vartheta$ independent of $N$, not to be confused with $\vartheta_\varepsilon$ which is a functional of $\rho$. Since $\beta^{-1}$ receives the meaning of a temperature of a heat bath (up to the absorbed factor $k_B$), it needs to grow $\propto N$ to compensate for the growth of the system’s energy $E \propto N^2$. Taking the logarithm of (157) gives what we call the canonical thermodynamic potential (canonical $T$-potential, for short) $\Phi_{H^{(N)}}(\beta)$. Using (158) and (161) as well as $\beta = \frac{1}{N\vartheta}$ yields the asymptotic expansion

$$\Phi_{H^{(N)}}(\frac{1}{N\vartheta}) = -N \ln N + N \ln \left(e|\Lambda|(2\pi \vartheta)^{3/2}\right) + O(\ln N)$$

$$+ \ln Z_{I^{(N)}}(\frac{1}{N\vartheta}).$$

(162)

Again, the $N \ln N$ term is due to Gibbs’ $N!$ and purely combinatorial in origin. In the absence of interactions (save the confinement to $\Lambda$) (162) reduces to

$$\Phi_{K^{(N)}}(\frac{1}{N\vartheta}) = -N \ln N + N \ln \left(e|\Lambda|(2\pi \vartheta)^{3/2}\right) + O(\ln N),$$

(163)

the asymptotic expansion of the canonical $T$-potential of the spatially uniform perfect gas. The coefficient of the $O(N)$ term in (163) is the system-specific Helmholtz $T$-potential per particle of the uniform perfect gas in $\Lambda$, denoted by

$$\phi_{\Lambda,K}(\vartheta) = \ln \left(e|\Lambda|(2\pi \vartheta)^{3/2}\right).$$

(164)

The system-specific interaction Helmholtz $T$-potential per particle is defined by

$$\phi_{\Lambda,I}(\vartheta) = \lim_{N \to \infty} \frac{1}{N} \ln Z_{I^{(N)}}(\frac{1}{N\vartheta}).$$

(165)

The limit (165) exists for Hamiltonians satisfying (H1)–(H5), as follows by corollary from Theorem 2, if (H2) is replaced by bounded continuity of the interaction, as explained earlier, then we can also infer the existence of the

$^{24}$Multiplying the canonical $T$-potential by the temperature of the heat bath yields the negative of what is usually called the canonical free energy, which in the thermodynamic limit yields the Helmholtz free energy of the physical systems.
limit (165) from our Theorem 1. The argument is quite standard, cf. [Rue69]. Namely, note that

\[ \frac{1}{N} \ln Z_{H_{\Lambda}^{(N)}}(\beta) = \frac{1}{N} \ln \int e^{-\beta \mathcal{E} + S(\mathcal{E})} d\mathcal{E} \]  

(166)

where \( S(\mathcal{E}) \) is shorthand for \( S_{H_{\Lambda}^{(N)}}(\mathcal{E}) \). Setting \( \mathcal{E} = N^2 \varepsilon \) and \( \beta = \frac{1}{N \vartheta} \) and expanding \( S(\mathcal{E}) \) using (23) (if \( U_{\Lambda} \) is bounded continuous on \( \Lambda^2 \) we can alternately use (22)), we find

\[ \frac{1}{N} \ln Z_{H_{\Lambda}^{(N)}}(\frac{1}{N \vartheta}) = - \ln N + \ln \left[ \int e^{N(-\vartheta^{-1} \varepsilon + s_{\Lambda}(\varepsilon)) + o(N)} d\varepsilon \right] \frac{1}{N} + O\left(\frac{\ln N}{N}\right). \]  

(167)

Clearly, \( \|g\|_N \to \|g\|_\infty \) as \( N \to \infty \), and so the following asymptotic expansion for the canonical \( T \)-potential results,

\[ \Phi_{H_{\Lambda}^{(N)}}(\frac{1}{N \vartheta}) = -N \ln N + N \phi_{\Lambda}(\vartheta) + o(N) \]  

(168)

with

\[ \phi_{\Lambda}(\vartheta) \equiv \sup_{\varepsilon \geq \varepsilon_{\vartheta}} \left( -\vartheta^{-1} \varepsilon + s_{\Lambda}(\varepsilon) \right). \]  

(169)

By (162) and (168), we also have \( N^{-1} \ln Z_{H_{\Lambda}^{(N)}}(\frac{1}{N \vartheta}) \xrightarrow{N \to \infty} \phi_{\Lambda,I}(\vartheta) \), with

\[ \phi_{\Lambda,I}(\vartheta) = \phi_{\Lambda}(\vartheta) - \phi_{\Lambda,K}(\vartheta). \]  

(170)

This concludes our demonstration that the Vlasov limit for the system-specific Helmholtz \( T \)-potential per particle follows from our theorems about the Vlasov limit of the system-specific Boltzmann entropy per particle.

Next we notice that also the familiar “minimum free energy principle” for \( -\phi_{\Lambda}(\vartheta) \) follows from combining the Legendre–Fenchel transform (169) with our “maximum entropy principle” in Theorem 2. Thus, for the system-specific Helmholtz \( T \)-potential per particle we find the variational principle

\[ -\vartheta \phi_{\Lambda}(\vartheta) = \inf_{f \in \mathfrak{A}} \mathcal{F}_\vartheta(f), \]  

(171)

with \( \mathfrak{A} = \{ f \in (\mathfrak{F}_{U_{\Lambda}} \cap L^1 \cap L^1 \ln L^1)(\mathbb{R}^3 \times \Lambda) \} \) the admissible trial densities, and

\[ \mathcal{F}_\vartheta(f) = \mathcal{E}(f) + \vartheta \mathcal{H}_{\vartheta}(f), \]  

(172)

the *Helmholtz free energy functional of \( f \), where \( \mathcal{H}_{\vartheta}(f) \) is Boltzmann’s \( H \) function of \( f \), given in (25), and \( \mathcal{E}(f) \) is the energy functional given in (26).
It also follows directly from our results that $F(\varphi)$ takes its infimum over the set $\mathfrak{A}$, and that any minimizer $f_\varphi$ of $F(\varphi)$ over $\mathfrak{A}$ is of the form

$$f_\varphi(p, q) = \sigma_\varphi(p)\rho_\varphi(q),$$

(173)

where

$$\sigma_\varphi(p) = (2\pi\varphi)^{-\frac{3}{2}}\exp\left(-\varphi^{-\frac{1}{2}}|p|^2\right),$$

(174)

while $\rho_\varphi(q)$ now solves the following fixed point equation on $\varphi$ space,

$$\rho_\varphi(q) = \frac{\exp\left(-\frac{1}{\varphi}\int_{\Lambda} U(\varphi, \tilde{\varphi})\rho_\varphi(\tilde{\varphi})d^3\tilde{\varphi}\right)}{\int_{\Lambda} \exp\left(-\frac{1}{\varphi}\int_{\Lambda} U(\varphi, \tilde{\varphi})\rho_\varphi(\tilde{\varphi})d^3\tilde{\varphi}\right)d\varphi}\tau_{\varphi}$$

(175)

with $\varphi > 0$ prescribed.

We remark that the various possible relationships between the set of maximizers of the maximum entropy variational principle and the set of minimizers of the minimum free energy variational principle have been discussed in great detail in [EHT00, CETT05]. Note that this can be (and was) done without proving that the maximum entropy variational principle characterizes the limit points of Boltzmann’s Ergode (2) proper.

We also remark that the existence of the system-specific Helmholtz $T$-potential per particle in the Vlasov limit for the canonical ensemble was shown previously by various techniques. Sub-additivity arguments, such as those used to prove Theorem 1 are used in [Kie93]. The very strategy which we applied to prove Theorems 2 and 3, which not only yields the variational principle for the system-specific Boltzmann entropy but also identifies the limit points of the sequence of ergodic ensemble measures as convex linear superpositions of infinite products of the optimizers for this maximum entropy principle, was originally applied in [MeSp82] to the canonical ensemble for Lipschitz continuous interactions $\mathcal{I}^{(N)}_\Lambda$; subsequently in [Kie93] and in [CLMP92] this approach to the canonical ensemble was generalized to less regular interactions including the ones studied here; and in [KiSp99] the limit $N \to \infty$ of $N^{-1}\ln Z^{(N)}_{\mathcal{I}_\Lambda}(1/\varphi)$ was obtained by adapting this strategy (note the different $N$ scaling of $\beta$). We emphasize that none of these canonical results implies the existence of the Vlasov limit for the system-specific Boltzmann entropy per particle, nor captures the limit points of the ergodic ensemble measures, unless it is a priori known that the ensembles are (convexly) equivalent, i.e. unless it is known that $\varepsilon \mapsto s_\varepsilon(\varepsilon)$ is concave (more on that in section 7). Our results, by contrast, hold irrespective of whether $\varepsilon \mapsto s_\varepsilon(\varepsilon)$ is concave or not.

### 6.3 The Vlasov limit for subergodic ensembles

Another spin-off, or in this case rather a variation on the theme of our microcanonical results is the straightforward generalization of our Theorems to
subensembles whose invariant measures are concentrated on sub-manifolds of 
\( \{ H = \mathcal{E} \} \) determined by further isolating integrals of the Hamiltonian \((19)\),
such as angular momentum if the domain \( \Lambda \) is rotationally symmetric, or
the Lynden-Bells’ invariant \([\text{LBLB99}, \text{LBLB04}]\) which occurs in a generalization
of the Calogero–Mosser model to particles moving in \( \mathbb{R}^3 \) confined by a
quadratic potential. Hypothesis \((H4)\) does not hold for these interactions, but
can be replaced by a weaker one at the expense of some extra work. In those
cases the entropy maximizer factors into a product of a \textit{locally (at } q \text{) shifted}
Maxwellian on \( p \) space and a purely space-dependent \textit{Boltzmann factor}. The
shifted Maxwellian which generalizes \((27)\) to include angular momentum is
known as a “rotating Maxwellian;” in the case of the Lynden-Bells’ Hamilto-
nian one finds a “rotating-dilating Maxwellian.” An announcement of these
results was made in \([\text{Kie08}]\); details will appear in \([\text{KiLa09}]\).

7 Unfinished business

In this last section of our paper we point out some open problems related to
the ones treated here.

7.1 The maximum interaction entropy principle

To the best of the author’s knowledge, the maximum interaction entropy prin-
ciple formulated in Proposition \([5]\) is new. As made clear in Theorem \([2]\) it offers
a way to directly evaluate the usual variational principle of maximum entropy
with energy constraint. By contrast, the standard approach to evaluate this
constrained maximum entropy principle has been rather indirect. Namely,
a Lagrange parameter (basically \( \vartheta \)) is introduced for the energy constraint,
yielding the corresponding fix point equation \((175)\) for the stationary points
of the free energy functional. After finding all solution families (not just the
minimizers of the free energy functional), a parameter representation of energy
and entropy along the various solution families of \((175)\) results, among which
the one with highest entropy for given energy has then to be selected. Clearly
our new variational approach appears to be more economical than that.

One of the simplest tasks would be to prove the existence of a unique solu-
tion to \((28)\) at sufficiently high energies \( \varepsilon \). For Coulomb interactions a unique
solution is expected for all energies, while for (regularized) Newton interac-
tions multiplicity of solutions is expected for sufficiently low energies. This is
suggested by the detailed numerical evaluations of the standard principle of
maximum entropy with constraints for related equations, cf. \([\text{SKS95}, \text{Cha02}]\).
7.2 Convergence of the ergodic ensemble measures

We already pointed out in subsection 6.1 that the sequence of ergodic ensemble measures converges whenever a unique optimizer exists for the maximum interaction entropy variational principle in Theorem 2 and Proposition 5. We don’t see any reason why the sequence of ergodic ensemble measures should not converge when the entropy maximizer is not unique, and so we expect that the mere existence of limit points concluded in this paper by using weak compactness can actually be upgraded to the existence of a limit.

7.3 Characterization of the de Finetti–Dynkin measure

As also noted in subsection 6.1, the decomposition measure \( \nu(d\tau|\mu_\varepsilon) \) is a singleton whenever a unique optimizer exists for the maximum interaction entropy variational principle in Theorem 2. In more general situations we have little information on the decomposition measure \( \nu(d\tau|\mu_\varepsilon) \), beyond knowing that it reduces to \( \varsigma(d\rho|\varrho_\varepsilon) \) and that \( \varsigma(d\rho|\varrho_\varepsilon) \) is supported on the maximizers of the maximum interaction entropy principle formulated in Proposition 5. Of course, we already mentioned earlier that experience with explicitly studied physical systems suggests that \( \text{supp} \varsigma(d\rho|\varrho_\varepsilon) \) is either a finite set or a continuous group orbit of a compact group, but a general proof or disproof seems not available. More is known for the canonical ensemble [KuTa84], and their approach should apply to the microcanonical ensemble to determine \( \nu(d\tau|\mu_\varepsilon) \).

7.4 Large deviation principles

Whenever \( \mathcal{M}_B(f) \) has a unique minimizer \( \varepsilon \) over \( \mathcal{A}_\varepsilon \), then Theorems 2 and 3 imply that

\[
\text{Prob}\left( d_{KR} \left( \Delta_{X(N)}^{(n)}, f_\varepsilon^\otimes n \right) > \delta \right) \xrightarrow{N \to \infty} 0 \quad \forall \delta > 0,
\]

where “Prob” refers to the ensemble measure (2) with Hamiltonian (19). It is desirable to improve (176) to a large deviation principle, a rigorous variation on the theme of Einstein’s fluctuation formula. Heuristically we expect

\[
\text{Prob}\left( d_{KR} \left( \Delta_{X(N)}^{(n)}, f_\varepsilon^\otimes n \right) > \delta \right) \approx \sup_{f \in \mathcal{A}_\delta} e^{-N(\mathcal{H}(f) - \mathcal{H}(f_\varepsilon))} \quad \forall \delta > 0,
\]

where \( \mathcal{A}_\delta = \{ f \in (\mathcal{B} \cap L^1 \cap L^1 \ln L^1)(\mathbb{R}^3 \times \Lambda) : \varepsilon(f) = \varepsilon \} \backslash \overline{B}_\delta(f_\varepsilon) \). In [EySp93, EHT00, CETT05] such a feat was accomplished for the regularized microcanonical ensembles at the level of the 1-point functions. The recent article [EISc102] establishes some nice large deviation principles for the \( n \)-point...
functions in a strong topology which allows one to handle some singular interactions. We expect that the conjectured large deviation principle can be proved along their lines.

We also refer to Lanford’s article [Lan73] and the books by Varadhan [Var84] and Ellis [Ell85] for mathematical background on large deviation principles and their applications to statistical mechanics, and to [Tou08] for a more recent review.

7.5 Vlasov limit for the canonical ensemble measures

Using the very strategy used in this paper to prove our Theorems 2 and 3, the Vlasov limit for the canonical ensemble measures associated with (157) was established in [MeSp82, CLMP92, Kie93] under various hypotheses on the interactions, covering our (H1)–(H5). This raises the question of whether one can conclude the convergence of the canonical ensemble measures associated with (157) from the convergence of the microcanonical ensemble measures (or, if convergence cannot be shown, the analog for the limit points). Put differently, we ask to extend the conclusions reached at the level of the thermodynamic functions to the level of the measures. In [EHT00, CETT05] such a feat was accomplished for the canonical ensemble measures in terms of regularized microcanonical ensemble measures, using large deviation principle techniques, and issues of equivalence of ensembles were addressed.

7.6 Interactions without lower bound

By hypothesis (H2) we allow the pair interactions to diverge when two particles approach each other infinitely closely. However, $W_{A}(q, \tilde{q})$ is only allowed to diverge to $+\infty$, which happens with the repulsive Coulomb interactions when $q \rightarrow \tilde{q}$. Divergence of $W_{A}(q, \tilde{q})$ to $-\infty$ is excluded from our analysis, because our postulates imply that $I_{A}^{(N)}$ is bounded below by $E_{g}(N) > -\infty$. In particular, the $-\infty$ singularity of the attractive Newton interactions in $\mathbb{R}^{3}$ will have to be regularized.

The canonical ensemble and regularized microcanonical ensembles have been controlled under weaker hypotheses, allowing in particular the interactions to diverge logarithmically to $-\infty$, see [CLMP92, Kie93] for the canonical and [CLMP95, KiLe97, Kie00] for the regularized microcanonical ensembles. It should be possible to adapt the technical arguments in these papers to establish the Vlasov limit for (2) for negative logarithmically singular interactions.
7.7 Unbounded domains

In [KiSp99] and [ChKi00], unbounded $\Lambda$ where allowed for the canonical ensemble, and our microcanonical theorems should similarly be extendible to unbounded domains under a suitable confinement hypothesis which replaces hypothesis (H5), presumably

$$(H5') \quad \text{Confinement: } e^{-U_\Lambda(q,\tilde{q})} \in L^1(\Lambda \times \Lambda). \quad (178)$$

Incidentally, (H5') not only imposes on behavior of $U_\Lambda$ as any of its two arguments is sent to infinity, it also restricts the manner in which $U_\Lambda$ can diverge to $-\infty$, e.g. when its two arguments approach each other infinitely closely, allowing logarithmic divergence.

7.8 Ergodic ensembles of quasi-particles

Our analysis does not cover ergodic ensembles of quasi-particle systems like point vortices moving in two dimensions whose Kirchoff Hamiltonian is of the type (11) without the sum of $|p|^2$ terms. The ergodic point vortex ensemble measures are of the type

$$\mu^{(N)}_\varepsilon(d^{2N}X) = \left(N!\Omega'_{I^{(N)}_\Lambda}(\varepsilon)\right)^{-1} \delta(\varepsilon - I^{(N)}_\Lambda(X^{(N)}))d^{2N}X, \quad (179)$$

where $X^{(N)} := (q_1, ..., q_N) \in \Lambda^N$, where now $\Lambda \subset \mathbb{R}^2$, and $d^{2N}X$ is 2N-dimensional Lebesgue measure, and the pair interactions now feature positive logarithmic singularities (for a single specie of point vortices). Onsager [Ons49] observed that for such systems a critical $\varepsilon$ value exists such that the map $\varepsilon \mapsto S(\varepsilon)$ is decreasing when $\varepsilon > \varepsilon_{\text{crit}}$, giving rise to negative ensemble temperatures. Regularized microcanonical measures for such vortex Hamiltonians have been analyzed in [CLMP95] under an equivalence assumption to the canonical ensemble, and in [KiLe97] [Kie00] without such an equivalence assumption. It is desirable to find a way to handle the proper ergodic ensemble for point vortex and other quasi-particle systems for which the sum of squares of kinematical momenta is absent from their Hamiltonian, but clearly this will require the introduction of new technical ideas. Incidentally, this last sentence applies verbatim also to other scalings than Vlasov scaling, in particular to the conventional thermodynamic limit scaling explained in the introduction.
There is one exception to what we just wrote: precisely at the critical energy $\mathcal{E}_{\text{crit}}$ of a point vortex system it is a priori known that all the $n$-point measures have densities given by $(1/|\Lambda|)^\otimes n$. Taking advantage of this fact, O’Neil and collaborators [ONR91, CON91] found that for a neutral two-species system the vicinity of $\mathcal{E}_{\text{crit}} \propto N \ln N$ can be analyzed directly using $\delta(I - \mathcal{E})$; it turns out to be a small-entropy regime where $S$, not $S/N$, converges to a limit when $N \to \infty$, with $\mathcal{E} - CN \ln N \propto N$. Interestingly enough, this scaling falls in between the conventional thermodynamic limit and the Vlasov scaling.

To the author’s knowledge, so far these are the only results for point vortices obtained for $\delta(I - \mathcal{E})$ proper, i.e. without regularization of the Dirac measure.

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A Monotonicity of the ground state energy

In this appendix we will prove two monotonic convergence results about the ground state energy which are used in the setup of our construction of the Vlasov limit $N \to \infty$. The results and their proofs are rather elementary and presumably known, and quite likely to be found in the vast literature on $U$ statistics; however, my (certainly incomplete) perusal of the pertinent literature has not yet met with success.

Here is our first proposition.

Proposition 7. Let $\Lambda \subset \mathbb{R}^D$ be a bounded and connected domain. Assume the following hypotheses regarding $U_\Lambda(q, \tilde{q})$:

(H1) Symmetry: $U_\Lambda(q, \tilde{q}) = U_\Lambda(q, \hat{q})$

(H2) Lower Semi-Continuity: $U_\Lambda(q, \tilde{q})$ is l.s.c. on $\overline{\Lambda} \times \overline{\Lambda}$

(H3) Sublevel Set Regularity: $\lambda^{\mathbb{R}^2}(\{U_\Lambda(q, \tilde{q}) - \min U_\Lambda < \epsilon\}) > 0$

(H4) Local Square Integrability: $U_\Lambda(q, \cdot) \in \mathcal{L}^2(B_r(q) \cap \Lambda) \ \forall \ q \in \Lambda$

where $\lambda$ is normalized Lebesgue measure for $\Lambda$. For $N \geq 2$ define the pair-specific ground state energy by

$$\varepsilon_g(N) \equiv \min_{\{q_1, \ldots, q_N\}} \frac{1}{N(N-1)} \sum_{1 \leq i < j \leq N} U_\Lambda(q_i, q_j).$$

(180)

Then the sequence $N \mapsto \varepsilon_g(N)$ so defined is monotonic increasing and converges to $\varepsilon_g < \infty$ defined by

$$\varepsilon_g = \min_{\rho \in \mathcal{P}(\Lambda)} \int \int \frac{1}{2} U_\Lambda(q, \tilde{q}) \rho(q) \rho(\tilde{q}) d^D q d^D \tilde{q}.$$ 

(181)

Note that $\varepsilon_g$ as defined in (181) coincides with $\varepsilon_g$ as defined in (16) when $D = 3$ and $U_\Lambda$ is decomposed into the earlier stipulated sum of $V_\Lambda$ and $W_\Lambda$.

Proof of Proposition 7:

We begin with the mandatory observation that under hypotheses (H1) and (H2) the pair-specific ground state energy $\varepsilon_g(N)$ defined in (180) is well-defined; i.e. $\varepsilon_g(N) \in \mathbb{R}$ (note that (H3)&(H4) are immaterial here).

26In fact, I originally did not expect monotonicity results of the type proved here to hold at all. I was prompted to conjecture the results, and then to prove them, by analyzing the numerical results of the computations of the (conjectured) ground state energies $E_g(N)$ for Thomson’s problem [Tho04] reported in [Aetal97, Petal97], which – divided by either $N^2$ or $N(N-1)$ – arranged themselves monotonically increasing when plotted vs. $N$. An interesting spin-off of the monotonicity of the pair-specific Thomson energies is a necessary criterion for minimality which can be used as a test for the empirical numerical experiments. After the present paper was submitted I successfully carried out such a test; see [Kie09b].
We next prove the monotonicity of $N \mapsto \varepsilon_g(N)$, with $N \geq 2$. Elementary (combinatorial) identities and the single inequality that the minimum of a sum is not less than the sum of the minima shows that $\varepsilon_g(N + 1) \geq \varepsilon_g(N)$, viz.

\[
\varepsilon_g(N + 1) = \min_{\{q_1, \ldots, q_{N+1}\}} \frac{1}{(N+1)N} \sum_{1 \leq i < j \leq N+1} U_\Lambda(q_i, q_j)
\]

\[
\geq \frac{1}{(N+1)N} \sum_{1 \leq k \leq N+1} \left[ \min_{\{q_1, \ldots, q_{N+1}\}\setminus\{q_k\}} \frac{1}{N-1} \sum_{1 \leq i < j \leq N+1, i \neq k \neq j} U_\Lambda(q_i, q_j) \right]
\]

\[
= \frac{1}{(N+1)N} (N + 1) \left[ \min_{\{q_1, \ldots, q_N\}} \frac{1}{N-1} \sum_{1 \leq i < j \leq N} U_\Lambda(q_i, q_j) \right]
\]

\[
= \frac{1}{N(N-1)} \sum_{1 \leq i < j \leq N} U_\Lambda(q_i, q_j)
\]

\[
= \varepsilon_g(N),
\]

and the proof of monotonicity of $N \mapsto \varepsilon_g(N)$ is complete.

Next, to prove convergence to $\varepsilon_g$ given by (181) we begin by noting that under hypotheses $(H1)$, $(H2)$ and $(H4)$, the ground state energy $\varepsilon_g$ defined in (181) is well-defined; actually, for this issue we can even relax $(H4)$ to the weaker $L^1_{\text{loc}}(\Lambda)$ condition which is implied by $(H4)$. We now use the density of empirical $N$-point measures in the weakly compact set of all probability measures on $\Lambda^2$, and the existence (by $(H2)$&$(H3)$) of a minimizing sequence $\in C_0^b(\Lambda)$ for $\langle \rho, \rho \rangle$, to prove convergence $\varepsilon_g(N) \rightharpoonup \varepsilon_g$. We let $\Delta^{(2)}_{X_g(N)}$ denote the 2-point measure in $\Lambda^2$ for a ground state $X_g(N) = (0, q_1; \ldots; 0, q_N)_g$ of $N$ points in $\Lambda$ (which need not be unique), and let $\Delta^{(2)}_{X(N)}$ be any other 2-point measure on $\Lambda^2$ with $N$ support points.

We define the linear functional $\gamma_\rho \mapsto U(\gamma_\rho)$ by

\[
U(\gamma_\rho) = \int \int \frac{1}{2} U_\Lambda(\check{q}, \dot{q}) \gamma_\rho(d^D \check{q} d^D \dot{q}).
\]

Note that for product measures $\gamma_\rho = \rho \otimes^2$ we have

\[
U(\rho \otimes^2) = \langle \rho, \rho \rangle.
\]

Note furthermore that the functional $\gamma_\rho \mapsto U(\gamma_\rho)$ is generally not continuous, because we have only (weak) lower semi-continuity of $U_\Lambda$. In particular, while any continuous change in the supporting points of the 2-point measure $\Delta^{(2)}_{X_g(N)}$
on $\Lambda^2$ results in a weakly continuous change of the 2-point measure, the functional $U$ evaluated at these 2-point measures, i.e. $U(\Delta^{(2)}_{X(N)})$, generally changes discontinuously. However, we do have

$$\varepsilon_g(N) = U(\Delta^{(2)}_{X(N)}) \leq U(\Delta^{(2)}_{X(N)}), \quad (185)$$

Now let $\{\rho_n\}_{n \in \mathbb{N}}$ be a minimizing sequence in $(\mathfrak{P} \cap C_0^b)(\Lambda)$ for $\langle \rho, \rho \rangle = U(\rho \otimes 2)$; note that it is not necessary to postulate also that $\rho_n \to \rho$ for any actual minimizer $\rho$, as this will follow automatically from the proof. Then, by (H3), for any $\epsilon > 0$ we can find an $n_\epsilon$ such that $U(\rho_n^{(2)}) \leq \varepsilon_g + \epsilon$ whenever $n \geq n_\epsilon$. So pick any $\epsilon > 0$, let $n = n_\epsilon$, and let $\{q_k\}_{k \in \mathbb{N}}$ be i.i.d. with a-priori measure $\rho_{n_\epsilon} \in (\mathfrak{P} \cap C_0^b)(\Lambda)$ for each $q_k$. Then by (H4) the weak law of large numbers for $U$ statistics (of order 2) holds \cite{Hoe48}, and so, in probability,

$$U(\Delta^{(2)}_{X(N)}) \xrightarrow{N \to \infty} \langle \rho_{n_\epsilon}, \rho_{n_\epsilon} \rangle \leq \varepsilon_g + \epsilon \quad (186)$$

for each $\epsilon > 0$. By (186) and (185) we have

$$\limsup_{N \to \infty} \varepsilon_g(N) = \limsup_{N \to \infty} U(\Delta^{(2)}_{X(N)}) \leq \varepsilon_g. \quad (187)$$

On the other hand, by the compactness of $\Lambda$ and the weak* compactness of $\mathfrak{P}(\Lambda)$ we can extract a *-weakly convergent subsequence $\Delta^{(2)}_{X(N)} \to \ddot{\rho} \in \mathfrak{P}(\Lambda^2)$. Moreover, since any convergent sequence of $n$-point measures $\Delta^{(n)}_{X(N)}$ necessarily converges to an $n$-fold product measure, we have $\ddot{\rho} = \dddot{\rho}^{(2)}$. Now the weak lower semi-continuity of $U$ gives

$$\liminf_{N \to \infty} U(\Delta^{(2)}_{X(N)}) \geq \langle \dddot{\rho}, \dddot{\rho} \rangle \geq \varepsilon_g. \quad (188)$$

Estimates (187) and (188) prove convergence $\varepsilon_g(N) \to \varepsilon_g$.

Convergence and the earlier proved monotonicity of $N \mapsto \varepsilon_g(N)$ completes the proof of Proposition 7. \hfill \square

We notice that our proof of Proposition 7 yields as a “byproduct” that $\langle \dddot{\rho}, \dddot{\rho} \rangle = \varepsilon_g$. Thus we have the following noteworthy corollary:

**Corollary 2.** Any limit point $\dddot{\rho}^{(2)}$ of the sequence of ground state 2-point measures $\{\Delta^{(2)}_{X(N)}\}_{N \in \mathbb{N}}$ minimizes the bilinear form $U(\dddot{\rho}^{(2)}) = \langle \rho, \rho \rangle$.

Here is our second proposition.

**Proposition 8.** Assume the hypotheses on $U_\Lambda(q, \tilde{q})$ stated in the previous proposition, and in addition assume that $U_\Lambda \geq 0$. Then the quasi pair-specific ground state energy, defined by

$$\tilde{\varepsilon}_g(N) \equiv \min_{q_1, \ldots, q_N} \frac{1}{N^2} \sum_{1 \leq i < j \leq N} U_\Lambda(q_i, q_j), \quad (189)$$

is a strictly increasing function of $N$ which converges to $\varepsilon_g$ defined in (187).
Proof of Proposition 8:

First of all, $\tilde{\varepsilon}_g(N)$ is as well-defined as $\varepsilon_g(N)$.

Next, inspection of the monotonicity part of the proof of proposition reveals that the same steps as in (182) now yield

$$\tilde{\varepsilon}_g(N + 1) \geq \frac{N^2}{(N+1)(N-1)} \tilde{\varepsilon}_g(N),$$

(190)

and $\tilde{\varepsilon}_g(N) \geq 0$ because of the here assumed positivity of $U_\Lambda$. The strict monotonicity of $N \mapsto \tilde{\varepsilon}_g(N)$ now follows because

$$(N + 1)(N - 1) < N^2.$$  

(191)

Lastly, since $1 - N^{-1} \to 1$, the limit of $\tilde{\varepsilon}_g(N)$ coincides with that of $\varepsilon_g(N)$.

This concludes the proof of Proposition 8.

B. Decomposition of the finite $N$ measures

Let $\varrho_\varepsilon \in \mathfrak{P}^s(\Lambda^N)$ be the weak limit of $\{\varrho_{N^2\varepsilon}^{(N)} \in \mathfrak{P}^s(\Lambda^N)\}_{N \in \mathbb{N}}$, and let $\varsigma(d\rho|\varrho_\varepsilon)$ be its unique de Finetti-Dynkin-Hewitt-Savage decomposition measure. (If $\{\varrho_{N^2\varepsilon}^{(N)}\}_{N \in \mathbb{N}}$ has several limit points, as accounted for in the main text, the following considerations are valid for the associated converging subsequences of finite $N$ measures.) We now show that if $\text{supp} \varsigma(d\rho|\varrho_\varepsilon)$ is either a finite set or a continuous group orbit of a compact group, then for each $\rho \in \text{supp} \varsigma(d\rho|\varrho_\varepsilon)$ we can explicitly construct a family of $\varrho^{(N)}[\rho] \in \mathfrak{P}^s(\Lambda^N)$ satisfying

$$\lim_{N \to \infty} n \varrho^{(N)}[\rho] = \rho^\otimes n$$

(192)

for each $n \in \mathbb{N}$, such that for each $N \in \mathbb{N}$,

$$\varrho_{N^2\varepsilon}^{(N)} = \int \varrho^{(N)}[\rho] \varsigma(d\rho|\varrho_\varepsilon).$$

(193)

B.1 The support of $\varsigma(d\rho|\varrho_\varepsilon)$ is a finite set

In the simplest case $\varsigma(d\rho|\varrho_\varepsilon)$ is a singleton, so that $\varrho_\varepsilon = \rho_\varepsilon^\otimes N$, i.e.

$$\lim_{N \to \infty} n \varrho_{N^2\varepsilon}^{(N)} = \rho_\varepsilon^\otimes n \quad \forall \quad n \in \mathbb{N}.$$  

(194)

In this case $\int \varrho^{(N)}[\rho] \varsigma(d\rho|\varrho_\varepsilon) = \varrho^{(N)}[\rho_\varepsilon] = \varrho_{N^2\varepsilon}^{(N)}$, and we are done.

Next, assume that $\varsigma(d\rho|\varrho_\varepsilon)$ is an arithmetic mean of two singletons, viz.

$$\varsigma(d\rho|\varrho_\varepsilon) = \nu_1 \delta_{\rho_1}(d\rho) + \nu_2 \delta_{\rho_2}(d\rho)$$

(195)
with \( 0 < \nu_1 = 1 - \nu_2 < 1 \), and let \( d_{\text{KR}}(\rho_1, \rho_2) = D > 0 \) be the usual Kantorovich-Rubinistein distance between \( \rho_1 \) and \( \rho_2 \). Let \( B_{D/2}(\rho_k) \) be the KR-open ball in \( \mathfrak{P}(\Lambda) \) which is centered at \( \rho_k \) and has radius \( D/2 \). Now decompose \( \Lambda^N = \Lambda_1^N \cup \Lambda_2^N \), where \( \Lambda_1 \cap \Lambda_2 = \emptyset \) and \( \mathfrak{g}^{(N)}(\Lambda_k^N) = \nu_k \), such that \( \Lambda_k^N \) contains all points for which \( 1\Delta^{(N)} \in B_{D/2}(\rho_k) \); when \( N \) is too small there may be no such points, but by the weak density in \( \mathfrak{P}(\Lambda) \) of the empirical one-point measures the set of such points \( \in \Lambda^N_k \) has positive \( \nu \) measure when \( N \) is large enough. In fact, since by hypothesis the weak limit of \( \{ \mathfrak{g}^{(N)}_{N^2e} \in \mathfrak{P}(\Lambda^N) \}_{N \in \mathbb{N}} \) is given by \( \mathfrak{g}_e = \nu_1 \rho_1 \otimes \nu_2 \rho_2 \in \mathfrak{P}(\Lambda) \), it follows that when \( N \to \infty \) then the probability w.r.t. \( \mathfrak{g}^{(N)}_{N^2e} \) that \( 1\Delta^{(N)} \in B_{D/2}(\rho_k) \) approaches \( \nu_k \). So if we define

\[
\mathfrak{g}^{(N)}[\rho_k] = \nu_k^{-1} \mathfrak{g}_{N^2e}^{(N)} \chi_{\Lambda_k^N}(196)
\]

and recall that \( \mathfrak{g}^{(N)}_{N^2e}(\Lambda_k^N) = \nu_k\), it follows that

\[
\lim_{N \to \infty} n^{(N)}[\rho_k] = \rho_k \otimes \nu_k(197)
\]

for each \( n \in \mathbb{N} \) and \( k = 1 \) or \( 2 \), and such that for each \( N \in \mathbb{N} \),

\[
\mathfrak{g}^{(N)}_{N^2e} = \nu_1 \mathfrak{g}^{(N)}[\rho_1] + \nu_2 \mathfrak{g}^{(N)}[\rho_2], (198)
\]

which is (193) in the case that \( \varsigma \) is the arithmetic mean of two singletons.

The general case of \( \text{supp} \varsigma \) being a finite set is treated similarly in an obvious manner, with \( D \) now the minimum of the set of distances between any pair \((\rho_k, \rho_l)\) picked from the support of \( \varsigma \).

**B.2 The support of \( \varsigma(d\rho|\rho_e) \) is a continuous group orbit**

For simplicity we assume that we are dealing with a one-parameter continuous group \( G \) acting on the base space, like \( SO(2) \) acting on \( \Lambda \); the generalization to more complicated situations (e.g. \( SO(3) \) acting on \( \Lambda \)) is straightforward. In this case we can pick any particular \( \rho_0 \in \text{supp} \varsigma \) and obtain every other (say) \( \rho_\theta \in \text{supp} \varsigma \) by acting with a group element \( g_\theta \in G \) thusly, \( \rho_\theta = \rho_0 \circ g_\theta \). The de Finetti etc. decomposition of \( \mathfrak{g}_e \) can then be written as an integral w.r.t. Haar measure over the group \( G \) of the infinite product measures \( \rho_\theta \otimes \nu \). The corresponding finite \( N \) presentation is simply obtained by change of variables for \( \mathfrak{g}^{(N)}_{N^2e} \) through factoring out the group \( G \), which gives each \( \mathfrak{g}^{(N)}[\rho_\theta] \) uniquely.
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