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ENSEMBLE DEPENDENCE OF FLUCTUATIONS AND THE CANONICAL/MICRO-CANONICAL EQUIVALENCE OF ENSEMBLES.

NICOLETTA CANCRINI AND STEFANO OLLA

ABSTRACT. We study the equivalence of microcanonical and canonical ensembles in continuous systems, in the sense of the convergence of the corresponding Gibbs measures. This is obtained by proving a local central limit theorem and a local large deviations principle. As an application we prove a formula due to Lebowitz-Percus-Verlet. It gives mean square fluctuations of an extensive observable, like the kinetic energy, in a classical micro canonical ensemble at fixed energy.

1. INTRODUCTION

The relation between averages of observables of a physical system with respect to different phase-space ensembles permits to prove what is called the *equivalence of ensembles*. That is, in the thermodynamic limit (size of the system goes to ∞), the expected value of a phase function, corresponding to intensive or per particle properties of the system, is independent of the ensemble used. There are many different aspects and approaches to the equivalence of ensembles, and it will be too long to review all the literature on the subject. For some general mathematical work we mention [14] and [15]. We are interested here, for a system of finite N particles, in the difference between the micro canonical average of an observable A on a given energy shell (micro canonical manifold), and the canonical average of A at the corresponding temperature:

$$\Delta_N(A, u) = \langle A|u \rangle_N - \langle A \rangle_{N, \beta_N(u)} \quad (1.1)$$

where Nu is the value of the energy fixed in the micro canonical average, while $\beta_N(u)$ is the corresponding inverse temperature determined such that the canonical average of the energy per particle is u . We will restrict our considerations to situations far from phase transitions (far from thermodynamic singularities), and we expect that the difference (1.1) goes to 0 in the thermodynamic limit ($N \rightarrow \infty$). As the micro canonical average is just a conditional expectation of the canonical average for a given value of the total energy, this is a consequence of the concentration of the distribution of the energy per particle in the canonical distribution around the expected value, due to the law of large numbers. If A is uniformly bounded in N , or local, and the micro canonical expectation $\langle A|u \rangle_N$ is enough regular in u , $\Delta_N(A, u) \rightarrow 0$ is an easy consequence of a large deviation principle for the distribution of the energy under the canonical distribution (see [section 4](#)). But here we are principally interested in

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extensive observables, like the total kinetic energy K_N , and their fluctuations in the micro canonical ensemble. In particular the micro canonical fluctuations of the total kinetic energy is greatly affected, and reduced, by the global constraint on the total energy and the asymptotic micro canonical variance, properly normalized, differs from the canonical one. In order to study such difference we need to compute explicitly the first order of $\Delta_N(A, u)$.

More precisely, let $\langle K_N; K_N | u \rangle_N = \langle K_N^2 | u \rangle_N - \langle K_N | u \rangle_N^2$, the micro canonical variance of the kinetic energy, that typically has order N . The canonical variance of K_N depends only on the maxwellian distribution on the velocities and is equal to $\frac{Nn}{2\beta^2}$, where n is the spacial dimension. It follows from the results contained in [section 5](#) that

$$\lim_{N \rightarrow \infty} \frac{1}{N} \langle K_N; K_N | u \rangle_N = \frac{n}{2\beta^2} \left(1 - \frac{n}{2C(\beta)} \right) \quad (1.2)$$

where the energy u and inverse temperature β are connected by the thermodynamic relation, and $C(\beta)$ is the heat capacity per particle, defined as $C(\beta) = \frac{d}{d\beta^{-1}} u(\beta)$. Formula (1.2) was formally derived in [11], and its rigorous derivation is the main motivation for the present article. We actually prove (1.2) under some regularity conditions on the micro canonical expectations, and in its finite N version, where we also compute explicitly the next order term (see formula (5.17)). We then provide one explicit example where these regularity conditions are satisfied, but we expect that they are verified for a large class of systems. Formula (1.2) is actually a consequence of a more general formula (5.2), also formally deduced in [11], that gives the explicit first order correction for $\Delta_N(A, u)$.

In the proof of (5.2) we use a strong form of the large deviations for the energy distribution under the canonical measure, i.e. the asymptotic expression (3.11) for the density of the canonical probability distribution of the energy. This strong *local* large deviation expression is proven in [section 3](#), as consequence of an Edgeworth expansion in the corresponding local central limit theorem. This expansion is obtained in [section 2](#) under some condition of uniform bounds in N for the first 4 derivatives of the free energy $f_N(\beta)$ of the canonical measure of the N -system.

Even though many of the arguments and results in sections 2,3 and 4 are well known in particular in the probabilistic literature, we decided to present this article as self contained as possible. For example the Edgeworth expansion argument we use in [section 2](#) is essentially the same as used in Feller book [7] for independent variables, but we could not find a precise reference for this statement for dependent continuous variables under canonical Gibbs distributions (in discrete setting see [4], and general setting for dependent variables is treated in [9]).

2. THE LOCAL CENTRAL LIMIT THEOREM AND ITS EDGEWORTH EXPANSION

Consider N particles, the momentum and coordinates given by $\mathbf{p} := (p_1, \dots, p_N)$, $p_i \in \mathbb{R}^n$ and $\mathbf{q} := (q_1, \dots, q_N)$, $q_i \in M$, where M is a manifold of dimension n . The phase space is $\Omega^N = (\mathbb{R}^n \times M)^N$. Let $\bar{\mathbf{q}}_i = (q_1, \dots, q_{i-1}, q_{i+1}, \dots, q_N)$ be the coordinates of all the particles except that of the i particle. To simplify the notation we take $n = 1$.

We want to consider systems whose Hamiltonian can be written as

$$H_N = \sum_{i=1}^N X_i$$

where

$$X_i := \frac{p_i^2}{2} + V(q_i, \bar{\mathbf{q}}_i) \quad i = 1, \dots, N$$

where V is a regular functions. Define for $\beta > 0$:

$$f_N(\beta) := \frac{1}{N} \log \int_{\Omega^N} e^{-\beta H_N} d\mathbf{p} d\mathbf{q}.$$

Notice that the integration in the \mathbf{p} can always be done explicitly and

$$f_N(\beta) = \frac{1}{2} \log(2\pi\beta^{-1}) + \frac{1}{N} \log \int_{M^N} e^{-\beta \sum_i^N V(q_i, \bar{\mathbf{q}}_i)} d\mathbf{q}.$$

Assumption: We assume that there is an interval of values of β such that $f_N(\beta)$ exists, together with its first four derivatives, and that are uniformly bounded in N :

$$\sup_N |f_N^{(j)}(\beta)| \leq C_\beta, \quad j = 0, 1, 2, 3, 4 \quad (2.1)$$

with C_β locally bounded in closed bounded intervals not including $\beta = 0$.

The canonical Gibbs measure associated to H_N and temperature β^{-1} is defined by

$$\nu_{\beta, N}(d\mathbf{p} d\mathbf{q}) = \exp\{-\beta H_N(\mathbf{p}, \mathbf{q}) - N f_N(\beta)\} d\mathbf{p} d\mathbf{q} \quad (2.2)$$

Defining $h_N := H_N/N$, direct calculations give:

$$\begin{aligned} f_N'(\beta) &= -\langle h_N \rangle_{\beta, N} = -u_N(\beta), \\ f_N''(\beta) &= N \langle (h_N - u_N(\beta))^2 \rangle_{\beta, N} \\ f_N'''(\beta) &= -N^2 \langle (h_N - u_N(\beta))^3 \rangle_{\beta, N} \\ f_N''''(\beta) &= N^3 \langle (h_N - u_N(\beta))^4 \rangle_{\beta, N} - 3N f_N''(\beta)^2. \end{aligned} \quad (2.3)$$

where we indicated $\langle \cdot \rangle_{\beta, N}$ the average w.r.t. the canonical measure defined in (2.2).

Notice that, thanks to the presence of the kinetic energy,

$$\inf_N f_N''(\beta) := \sigma_-(\beta) > \frac{1}{2\beta}.$$

Define the centered energy

$$S_N := \sum_{j=1}^N (X_j - u_N(\beta))$$

and its characteristic function

$$\varphi_{\beta, N}(t) := \langle e^{it S_N} \rangle_{\beta, N}, \quad t \in \mathbb{R}. \quad (2.4)$$

By performing explicitly the integration over \mathbf{p} , we have

$$\varphi_{\beta, N}(t) = \left(\frac{1}{1 - it\beta^{-1}} \right)^{N/2} \langle e^{it \sum_j (V(q_j, \bar{\mathbf{q}}_j) - u_N)} \rangle_{N, \beta}$$

where $Nv_N = \langle \sum_j (V(q_i, \bar{q}_i)) \rangle_{N,\beta}$. Consequently we have the bound:

$$|\varphi_{\beta,N}(t)| \leq \left(\frac{\beta^2}{t^2 + \beta^2} \right)^{\frac{N}{4}}, \quad (2.5)$$

thus $|\varphi_{\beta,N}(t)| < 1$ for $t \neq 0$ (i.e. is a characteristic function of a non-lattice distribution). Furthermore $|\varphi_{\beta,N}(t)|$ is integrable for $N \geq 3$, and by the Fourier inversion theorem (see chapter XV.3 of [7]) the probability density function of the variable S_N exists for $N \geq 3$. Observe also that

$$\begin{aligned} \varphi'_N(0) &= 0, \quad \varphi''_N(0) = -N f''_N(\beta), \quad \varphi'''_N(0) = -iN f'''_N(\beta) \\ \varphi''''_N(0) &= N f''''_N(\beta) + 3N^2 f''_N(\beta)^2. \end{aligned} \quad (2.6)$$

In the following we denote the normal gaussian density by

$$\phi(x) = \frac{1}{\sqrt{2\pi}} e^{-x^2/2}.$$

Let $\{H_j(x)\}_{j \geq 0}$ the Hermite polynomials defined by

$$\frac{d^j}{dx^j} \phi(x) = (-1)^j H_j(x) \phi(x) \quad (2.7)$$

The characteristic property of Hermite polynomials is that the Fourier transform of $H_j(x)\phi(x)$ is given by

$$\int_{-\infty}^{+\infty} H_j(x) \phi(x) e^{itx} dx = (it)^j \hat{\phi}(t)$$

where $\hat{\phi}(t) = e^{-t^2/2}$. Recall that $H_0 = 1$, $H_1(x) = x$, $H_3(x) = x^3 - 3x$, $H_4(x) = x^4 - 6x^2 + 3$ and $H_6(x) = x^6 - 15x^4 + 45x^2 - 15$.

We can now state the Local Central Limit Theorem we need in the rest of the article.

Theorem 2.1. *Assume that β is such that the conditions (2.1) are satisfied. Define*

$$Y_N := \frac{\sum_{i=1}^N (X_i - u_N(\beta))}{\sqrt{N f''_N(\beta)}},$$

then the density distribution $g_{\beta,N}(x)$ of Y_N for $N \geq 3$ exists and as $N \rightarrow \infty$

$$g_{\beta,N}(x) - \phi(x) - \phi(x) \left(\frac{Q_{\beta,N}^{(3)}(x)}{\sqrt{N}} + \frac{Q_{\beta,N}^{(4)}(x)}{N} \right) = o\left(\frac{1}{N}\right) K_N(\beta) \quad (2.8)$$

where

$$Q_{\beta,N}^{(3)}(x) = \frac{f'''_N(\beta)}{3! f''_N(\beta)^{\frac{3}{2}}} H_3(x) \quad (2.9)$$

$$Q_{\beta,N}^{(4)}(x) = \frac{f''''_N(\beta)}{4! f''_N(\beta)^2} H_4(x) + \frac{1}{2} \left(\frac{f'''_N(\beta)}{3! f''_N(\beta)^{\frac{3}{2}}} \right)^2 H_6(x) \quad (2.10)$$

and $K_N(\beta)$ is bounded in N , uniformly on bounded closed intervals of $\beta > 0$.

Proof. We follow the proof of theorem 2 in chapter XVI.2 of [7] for independent random variables. By (2.5) and the Fourier inversion theorem the left hand side of (2.8) exists for $N \geq 3$. To simplify the notation we do not write the dependence on β of $f_{\beta,N}$, $\varphi_{\beta,N}$ and their derivatives. Consider the function

$$\widehat{\Phi}_N(t) = \varphi_N\left(\frac{t}{\sqrt{Nf_N''}}\right) - e^{-\frac{t^2}{2}} \left(1 + P_N\left(\frac{it}{\sqrt{Nf_N''}}\right)\right) \quad (2.11)$$

where $\varphi_N(t/\sqrt{Nf_N''})$ is the Fourier transform of $g_{\beta,N}$ (see (2.4)) and $P_N(it)$ is an appropriate polynomial in the variable it . We want to show that

$$\Delta_N = \int_{-\infty}^{\infty} |\widehat{\Phi}_N(t)| dt = o\left(\frac{1}{N}\right). \quad (2.12)$$

Choose $\delta > 0$ arbitrary but fixed. There exists a number $q_\delta < 1$ such that $\left(\frac{\beta^2}{t^2 + \beta^2}\right)^{\frac{1}{4}} < q_\delta$ for $|t| \geq \delta$. The contribution of the intervals $|t| > \delta\sqrt{f_N''N}$ to the integral (2.12), using (2.5), is bounded by

$$q_\delta^{N-3} \int_{-\infty}^{\infty} \left(\frac{\beta^2}{(t/\sqrt{f_N''N})^2 + \beta^2}\right)^3 dt + \int_{|t| > \delta\sqrt{Nf_N''}} e^{-\frac{t^2}{2}} |P_N\left(\frac{it}{\sqrt{Nf_N''}}\right)| dt \quad (2.13)$$

and this tends to zero more rapidly than any power of $1/N$.

We now estimate the contribution to Δ_N from the region $|t| \leq \delta\sqrt{Nf_N''(\beta)}$. Let us rewrite

$$\Delta_N = \int_{-\infty}^{\infty} e^{-\frac{t^2}{2}} \left| e^{\psi_N\left(t/\sqrt{f_N''}\right)} - 1 - P_N\left(\frac{it}{\sqrt{Nf_N''}}\right) \right| dt \quad (2.14)$$

where¹

$$\psi_N(t) = \log \varphi_N(t) + \frac{1}{2} N f_N'' t^2.$$

The function $\psi_N(t)$ is four times differentiable and in $t = 0$ its derivatives are given by

$$\psi_N'(t) = \frac{\varphi_N'(t)}{\varphi_N(t)} + N f_N'' t, \quad \psi_N'(0) = 0.$$

$$\psi_N''(t) = \frac{\varphi_N''(t)}{\varphi_N(t)} - \frac{\varphi_N'(t)^2}{\varphi_N(t)^2} + N f_N'', \quad \psi_N''(0) = 0.$$

$$\psi_N'''(t) = \frac{\varphi_N'''(t)}{\varphi_N(t)} - \frac{\varphi_N'(t)\varphi_N''(t)}{\varphi_N(t)^2} - \frac{2\varphi_N'(t)\varphi_N''(t)}{\varphi_N(t)^2} + \frac{2\varphi_N'(t)^3}{\varphi_N(t)^3}, \quad \psi_N'''(0) = -iN f_N'''.$$

$$\psi_N''''(t) = \frac{\varphi_N''''(t)}{\varphi_N(t)} - \frac{3\varphi_N'(t)\varphi_N'''(t)}{\varphi_N(t)^2} - \frac{3\varphi_N''(t)^2}{\varphi_N(t)^2} + \frac{4\varphi_N'(t)^2\varphi_N''(t)}{\varphi_N(t)^3} + \frac{6\varphi_N'(t)^2\varphi_N''(t)}{\varphi_N(t)^3} - \frac{6\varphi_N'(t)^4}{\varphi_N(t)^4}$$

$$\psi_N''''(0) = \varphi_N''''(0) - 3\varphi_N''(0)^2 = N f_N''''.$$

¹For a complex number z such that $|z| < 1$, we define $\log(1+z) = \sum_n \frac{(-z)^n}{n}$.

where we used relations (2.6). Let $(it)^2\gamma_N(it)$ be the Taylor approximation for $\psi_N(t)/N$. Where $\gamma_N(it)$ is a polynomial of degree 2 with $\gamma_N(0) = 0$; it is uniquely determined by the property

$$\psi_N(t) - N(it)^2\gamma_N(it) = No(|t|^4) \quad (2.15)$$

and it is given by

$$\gamma_N(it) := \frac{f_N'''}{3!} it + \frac{f_N''''}{4!} (it)^2$$

We choose

$$P_N(it) := \sum_{k=1}^2 \frac{1}{k!} [N(it)^2\gamma_N(it)]^k$$

then $P_N(it)$ is a polynomial in the variable it with real coefficients depending on N and β . We use the inequality

$$\left| e^\alpha - 1 - \sum_{k=1}^2 \frac{\beta^k}{k!} \right| \leq |e^\alpha - e^\beta| + \left| e^\beta - 1 - \sum_{k=1}^2 \frac{\beta^k}{k!} \right| \leq e^\gamma \left(|\alpha - \beta| + \frac{|\beta|^3}{3!} \right)$$

with $\gamma = \max\{|\alpha|, |\beta|\}$. Furthermore we choose δ so small that for $|t| < \delta$

$$|\psi_N(t) - N(it)^2\gamma_N(it)| \leq \epsilon (f_N'')^2 N|t|^4$$

and

$$|\psi_N(t)| < N \frac{1}{4} f_N'' t^2 \quad |\gamma_N(it)| \leq a_N |t| \leq \frac{1}{4} f_N''$$

provided that $a_N > 1 + |f_N''|$. For $|t| < \delta \sqrt{N f_N''}$ the integrand in (2.14) can be bounded by

$$e^{-\frac{1}{4}t^2} \left(\epsilon \frac{t^4}{N} + \frac{a_N^3}{3!} \left(\frac{|t|^3}{\sqrt{N f_N''}} \right)^3 \right) \quad (2.16)$$

As ϵ is arbitrary we have that (2.12) is proved. The function $\Phi_N(t)$ defined in (2.11) is the Fourier transform of

$$g_{\beta,N}(x) - \phi(x) - \phi(x) \sum_{k=1}^8 b_{Nk} H_k(x) \quad (2.17)$$

where b_{Nk} are appropriate coefficients depending on N and $H_k(x)$ are the Hermite polynomials defined in (2.7). If we rearrange the terms of the sum in ascending powers of $1/\sqrt{N}$ we get an expression of the form postulated in the theorem plus terms involving powers $1/N^k$ with $k > 1$ that can be dropped and obtain the result. \square

The same argument leads to higher order expansions, but the terms cannot be expressed by simple explicit formulas. We have the following

Theorem 2.2. *Assume that $f_N''(\beta), \dots, f_N^{(k)}(\beta)$ exist and are uniformly bounded in N . Define*

$$Y_N := \frac{\sum_{i=1}^N (X_i - u_N(\beta))}{\sqrt{N f_N''(\beta)}}$$

then the density distribution $g_{\beta,N}(x)$ of Y_N for $N \geq 3$ exists and as $N \rightarrow \infty$

$$g_{\beta,N}(x) - \phi(x) - \phi(x) \sum_{j=3}^k \frac{1}{N^{\frac{1}{2}j-1}} Q_{\beta,N}^{(j)}(x) = o\left(\frac{1}{N^{\frac{1}{2}k-1}}\right) \quad (2.18)$$

uniformly in x . Here $\phi(x)$ is the standard normal density, $Q_{\beta,N}^{(j)}$ is a real polynomial depending only on $f_N''(\beta), \dots, f_N^{(k)}(\beta)$, and whose coefficients are uniformly bounded in N .

Note that Theorem 2.1 is Theorem 2.2 for $k = 4$ and taking $k > 4$ does not improve our estimates and results.

Remark 2.3. Theorem 2.1 is stated for continuous random variables X_i . It can be stated also for discrete random variables, in the same form once $|\varphi_{\beta,N}(t)|$, the characteristic function of S_N , is integrable. In spin systems with finite range interacting potentials, like the Ising model, this is the case, see [5] and [2] where a Gaussian upper bound on the characteristic function is proved.

3. LOCAL LARGE DEVIATIONS AND BOLTZMANN FORMULA

In this section we study the energy distribution under the canonical measure. With reasonable conditions on the interaction potential V , $f_N(\beta)$ is finite for every $\beta > 0$. We can extend its definition to all $\beta \in \mathbb{R}$ denoting $f_N(\beta) = +\infty$ for $\beta \leq 0$.

We define the Fenchel-Legendre transform of $f_N(\beta)$:

$$f_{N*}(u) := \sup_{\beta} \{-\beta u - f_N(\beta)\} = \sup_{\beta > 0} \{-\beta u - f_N(\beta)\} \quad (3.1)$$

Let $\mathcal{D}_{f_N}, \mathcal{D}_{f_{N*}}$ the corresponding domain of definition. For any $u \in \mathcal{D}_{f_{N*}}$ there exists a unique $\beta \in \mathcal{D}_{f_N}$ such that

$$u = -f_N'(\beta) \quad \text{and} \quad \beta = -f_{N*}'(u). \quad (3.2)$$

Under the canonical measure (2.2) h_N can be seen as a normalized sum of random variables. We denote by $\mathcal{F}_{N,\beta}(u)$ the density of its probability distribution. For any integrable function $F: \mathbb{R} \rightarrow \mathbb{R}$

$$\int_{\Omega^N} F(h_N) d\nu_{\beta,N} = \int_{\mathbb{R}} F(u) \mathcal{F}_{N,\beta}(u) du = \int_{\mathbb{R}} F(u) e^{-N[\beta u + f_N(\beta)]} W_N(u) du \quad (3.3)$$

where

$$W_N(u) := \frac{d}{du} \int_{h_N \leq u} dp dq \quad (3.4)$$

Theorem 3.1. Let $u \in \mathcal{D}_{f_{N*}}$ and $\gamma = \gamma_N(u)$ defined by (3.2) be such that $f_N(\gamma)$ satisfies (2.1). Then, for large N ,

$$W_N(u) = e^{-N f_{N*}(u)} \sqrt{\frac{N f_{N*}''(u)}{2\pi}} \left(1 + \frac{Q_{\gamma(u),N}^{(4)}(0)}{N} + o\left(\frac{1}{N}\right) K_N(\gamma(u)) \right) \quad (3.5)$$

where $K_N(\gamma)$ and $Q_{\gamma(u),N}^{(4)}(0)$ are defined in (2.8) and (2.10) respectively.

Proof. Let $\omega = (\mathbf{p}, \mathbf{q}) \in \Omega^N$, $\mathbf{X}(\omega) = (X_1(\omega), \dots, X_N(\omega))$, and $\mathbf{x} = (x_1, \dots, x_N) \in \mathbb{R}^N$. Consider the positive measure $\alpha_N(d\mathbf{x})$ on \mathbb{R}^N defined, for any integrable function F on \mathbb{R}^N , by

$$\int_{\Omega^N} F(\mathbf{X}(\omega)) d\omega = \int_{\mathbb{R}^N} F(\mathbf{x}) \alpha_N(d\mathbf{x}) \quad (3.6)$$

so that for any γ we have

$$\int_{\Omega^N} F(\mathbf{X}(\omega)) \nu_{\gamma, N}(d\omega) = \int_{\mathbb{R}^N} F(\mathbf{x}) e^{-\gamma \sum_{i=1}^N x_i - N f_N(\gamma)} \alpha_N(d\mathbf{x}) \quad (3.7)$$

For any integrable function $G : \mathbb{R} \rightarrow \mathbb{R}$ we can write

$$\int_{\mathbb{R}^N} G\left(\frac{1}{N} \sum_{j=1}^N x_j\right) \alpha_N(d\mathbf{x}) = \int_{-\infty}^{+\infty} G(s) W_N(s) ds \quad (3.8)$$

Take $u \in \mathcal{D}_{f_{N^*}}$, let $\gamma = \gamma_N(u) \in \mathcal{D}_{f_N}$ as in the hypotheses of the theorem. For any integrable function $G : \mathbb{R} \rightarrow \mathbb{R}$ we have

$$\begin{aligned} \int_{\mathbb{R}^N} G\left(\frac{1}{N \sqrt{f_N''(\gamma)}} \sum_{j=1}^N (x_j - u)\right) e^{-\gamma \sum_{j=1}^N x_j - N f_N(\gamma)} \alpha_N(d\mathbf{x}) \\ = \int_{\mathbb{R}} G\left(\frac{s - u}{\sqrt{f_N''(\gamma)}}\right) e^{-\gamma N s - N f_N(\gamma)} W_N(s) ds \\ = e^{N f_{N^*}(u)} \sqrt{f_N''(\gamma)} \int_{\mathbb{R}} G(y) e^{-\beta N \sqrt{f_N''(\gamma)} y} W_N(\sqrt{f_N''(\gamma)} y + u) dy \end{aligned}$$

In order to apply theorem 2.1 we identify

$$e^{N f_{N^*}(u)} \sqrt{f_N''(\gamma)} e^{-\gamma N \sqrt{f_N''(\gamma)} y} W_N(\sqrt{f_N''(\gamma)} y + u) = \sqrt{N} g_{\gamma, N}(\sqrt{N} y)$$

so that for $y = 0$

$$e^{N f_{N^*}(u)} \sqrt{f_N''(\gamma)} W_N(u) = \sqrt{N} g_{\gamma, N}(0) = \sqrt{\frac{N}{2\pi}} \left(1 + \frac{Q_{\gamma(u), N}^{(4)}(0)}{N} + o\left(\frac{1}{N}\right) K_N(\gamma(u)) \right). \quad (3.9)$$

and using $f_N''(\gamma) = 1/f_{N^*}''(u)$

$$W_N(u) = e^{-N f_{N^*}(u)} \sqrt{\frac{N f_{N^*}''(u)}{2\pi}} \left(1 + \frac{Q_{\gamma(u), N}^{(4)}(0)}{N} + o\left(\frac{1}{N}\right) K_N(\gamma(u)) \right)$$

□

We can resume the above result more explicitly, by using the bounds and the explicit form of the polynomial $Q_{\gamma, N}^{(4)}(0) = \frac{\gamma}{4} f_N'''(\gamma)$,

$$\left| W_N(u) e^{N f_{N^*}(u)} \sqrt{\frac{2\pi}{N f_{N^*}''(u)}} - 1 \right| \leq \frac{\beta_N(u) C_{\gamma_N(u)}}{4N} + o\left(\frac{1}{N}\right) K(\gamma_N(u)). \quad (3.10)$$

where $\gamma(u) = -f_{N^*}'(u)$.

Theorem 3.1 allows to write the probability density function in (3.3) as

$$\mathcal{F}_{N,\beta}(u) = e^{-NI_{N,\beta}(u)} \sqrt{\frac{N}{2\pi} f''_{N^*}(u)} \left(1 + \frac{Q_{\gamma(u),N}^{(4)}(0)}{N} + o\left(\frac{1}{N}\right) K_N(\gamma(u)) \right) \quad (3.11)$$

where $\gamma(u) = -f'_{N^*}(u)$ and

$$I_{N,\beta}(u) := \beta u + f_N(\beta) + f_{N^*}(u) = \beta(u - u_N(\beta)) - f_{N^*}(u_N(\beta)) + f_{N^*}(u).$$

As $\beta = -f'_{N^*}(u_N(\beta))$, we can thus rewrite

$$I_{N,\beta}(u) := f_{N^*}(u) - f_{N^*}(u_N(\beta)) - f'_{N^*}(u_N(\beta))(u - u_N(\beta)) \quad (3.12)$$

The functional $I_{N,\beta}(u)$ is convex, derivable and has a minimum in $u_{\beta,N}$ where $u_{\beta,N} := \langle h_N \rangle_{\beta,N}$,

$$I'_{N,\beta}(u_{\beta,N}) = 0,$$

and

$$I''_{N,\beta}(u_{\beta,N}) = f''_{N^*}(u_{\beta,N}) = 1/f''_N(\beta).$$

Equation (3.11) says that the sequence h_N satisfies a local large deviation principle, also called *Large Deviation Principle in the Strong Form*, see [4] where the principle is defined for discrete random variables with assumptions that are generally stronger than (2.1).

4. MICRO-CANONICAL DISTRIBUTION AND EQUIVALENCE OF ENSEMBLES.

We here define the equivalence of ensembles. Given an observable A on Ω_N , we define the micro canonical average $\langle A|u \rangle_N$ as a conditional expectation by the classic formula:

$$\langle AF(h_N) \rangle_{N,\beta} = \langle \langle A|h_N \rangle F(h_N) \rangle_{N,\beta} = \int F(u) \langle A|u \rangle_N \mathcal{F}_{N,\beta}(u) du, \quad (4.1)$$

for any measurable function $F(u)$ on \mathbb{R} . It is an easy exercise to see that these conditional expectations do not depend on β . Of course (4.1) defines the conditional expectation only a.s. with respect to the Lebesgue measure. But under the regularity assumptions on the interaction potential V , the microcanonical surface

$$\Sigma_N(u) = \{(\mathbf{p}, \mathbf{q}) \in \Omega_N : h_N = u\} \quad (4.2)$$

is regular enough such that co-area formulas (cf. [10]) can be applied and give the existence of a regular conditional distribution on $\Sigma_N(u)$, defined for every value of u . We will assume in the following various conditions on the function $u \mapsto \langle A|u \rangle_N$, that have to be verified in the various applications.

By equivalence of ensembles we mean here the convergence of

$$\langle A \rangle_{\beta,N} - \langle A|u_N(\beta) \rangle_N \xrightarrow{N \rightarrow \infty} 0, \quad (4.3)$$

for a certain class of functions. We are in particular interested in the rate of convergence in (4.3).

For the simple case when A is a bounded function such that $\langle A|u \rangle_N$ is continuous around $u = u_N(\beta)$ uniformly in N , all we need is:

$$\begin{aligned} f_N(\beta) &< +\infty, & \forall \beta > 0 \\ f_N(\beta) &\text{ twice differentiable in } \beta \\ \inf_N f_N''(\beta) &\geq \sigma_-^2 > 0. \end{aligned} \tag{4.4}$$

By the uniform continuity of $\langle A|u \rangle_N$, for any $\epsilon > 0$, there exists $\delta_\epsilon > 0$ such that $|\langle A|u \rangle_N - \langle A|u_N(\beta) \rangle_N| < \epsilon$ if $|u - u_N(\beta)| < \delta_\epsilon$. Then

$$|\langle A \rangle_{\beta, N} - \langle A|u_N(\beta) \rangle_N| \leq 2\|A\|_\infty \int_{|u - u_N(\beta)| \geq \delta_\epsilon} \mathcal{F}_{N, \beta}(u) du + \epsilon$$

Let us split the large deviation term:

$$\int_{|u - u_N(\beta)| \geq \delta_\epsilon} \mathcal{F}_{N, \beta}(u) du = \int_{u > u_N(\beta) + \delta_\epsilon} \mathcal{F}_{N, \beta}(u) du + \int_{u < u_N(\beta) - \delta_\epsilon} \mathcal{F}_{N, \beta}(u) du.$$

Let us estimate the first term of the RHS (the second term is analogous). To shorten notation, denote $\bar{u} = u_N(\beta) + \delta_\epsilon$. By exponential Chebichef inequality, for any $\lambda > 0$:

$$\int_{u > \bar{u}} \mathcal{F}_{N, \beta}(u) du \leq e^{-N[\lambda \bar{u} - f_N(\beta - \lambda) + f_N(\beta)]}.$$

Notice that

$$\begin{aligned} I_{N, \beta}(\bar{u}) &= \sup_{\lambda > 0} (\lambda \bar{u} - f_N(\beta - \lambda)) + f_N(\beta) & u > u_N(\beta) \\ I_{N, \beta}(\bar{u}) &= \sup_{\lambda < 0} (\lambda \bar{u} - f_N(\beta - \lambda)) + f_N(\beta) & u < u_N(\beta). \end{aligned} \tag{4.5}$$

Consequently optimizing the estimate over $\lambda > 0$ we have

$$\int_{u > \bar{u}} \mathcal{F}_{N, \beta}(u) du \leq e^{-NI_{N, \beta}(\bar{u})}$$

and similar estimate for the term of the deviation on the other side.

Our conditions on $f_N''(\beta)$ implies the strong convexity of $I_{N, \beta}(\bar{u})$ in an interval around $u_N(\beta)$, uniform in N . This means exists $a > 0$ such that

$$I_{N, \beta}(u_N(\beta) \pm \delta) \geq a\delta^2$$

It follows that

$$\int_{|u - u_N(\beta)| \geq \delta_\epsilon} \mathcal{F}_{N, \beta}(u) du \leq 2e^{-Na\delta_\epsilon^2} \tag{4.6}$$

that converge exponentially to 0 for any $\epsilon > 0$. Taking $\epsilon \rightarrow 0$ concludes the argument.

In the next section we will analyse closer this convergence, allowing observables A that are extensive.

5. LEBOWITZ-PERCUS-VERLET FORMULAS FOR FLUCTUATIONS

In this section A is a function on Ω_N , eventually extensive, such that satisfies the following:

- (i) $\|A\|_{2,\beta,N}$ is finite, where $\|A\|_{2,\beta,N}$ is the L^2 norm of A with respect to the canonical measure $\nu_{\beta,N}$ defined in (2.2)
- (ii) For $j = 0, 1, 2$ there exists $C_\beta > 0$ such that

$$\left| \frac{d^j}{du^j} \langle A|u \rangle_N \Big|_{u_N(\beta)} \right| \leq C_\beta N^{j/2} \|A\|_{2,\beta,N},$$

- (iii) Let $\delta_N := b \sqrt{\log N/N}$ for some $b > 0$, then there exists $C_\beta > 0$ such that

$$B_{N,\beta} := \sup_{|u-u_N(\beta)| \leq \delta_N} \left| \frac{d^3}{du^3} \langle A|u \rangle_N \right| \leq C_\beta \frac{N^{1/2}}{\log N} \|A\|_{2,\beta,N}. \quad (5.1)$$

Theorem 5.1. *Under conditions (i)-(iii) above the following formula holds*

$$\langle A|u_N(\beta) \rangle_N = \langle A \rangle_{\beta,N} - \frac{1}{2N} \frac{d}{d\beta} \left[\frac{1}{f_N''(\beta)} \frac{d}{d\beta} \langle A \rangle_{\beta,N} \right] + o\left(\frac{1}{N}\right) \|A\|_{2,\beta,N}. \quad (5.2)$$

Proof. Since expression (5.2) is homogeneous in A , we can divide by $\|A\|_{2,\beta,N}$ and consider functions A such that $\|A\|_{2,\beta,N} = 1$. We write the difference between the canonical and micro canonical expectations as

$$\langle A \rangle_{\beta,N} - \langle A|u_N(\beta) \rangle_N = \int \mathcal{F}_{N,\beta}(u) [\langle A|u \rangle_N - \langle A|u_{\beta,N} \rangle_N] du \quad (5.3)$$

Denote

$$G_N(u) = \langle A|u \rangle_N - \langle A|u_N(\beta) \rangle_N - \frac{d}{du} \langle A|u \rangle_N \Big|_{u_N(\beta)} (u - u_N(\beta)) - \frac{1}{2} \frac{d^2}{du^2} \langle A|u \rangle_N \Big|_{u_N(\beta)} (u - u_N(\beta))^2$$

Obviously $G_N(u_N(\beta)) = G'_N(u_N(\beta)) = G''_N(u_N(\beta)) = 0$. We want to prove that

$$\int \mathcal{F}_{N,\beta}(u) G_N(u) \sim o\left(\frac{1}{N}\right). \quad (5.4)$$

Under conditions, (i) – (iii) above, using (2.1), the properties of the norm and Schwarz inequality, we have that $\|G_{N,\beta}\|_{\beta,N}^2 \leq C'_\beta$. For a given $\delta_N > 0$, consider the bounded function

$$G_{N,\delta_N}(u) = G_N(u) 1_{[|u-u_N(\beta)| < \delta_N]}$$

Then we can split the integral and, using Schwarz inequality, obtain

$$\left| \int \mathcal{F}_{N,\beta}(u) G_N(u) du \right| \leq \sqrt{C'_\beta} \int \mathcal{F}_{N,\beta}(u) 1_{[|u-u_N(\beta)| \geq \delta_N]} du + \left| \int \mathcal{F}_{N,\beta}(u) G_{N,\delta_N}(u) du \right|$$

By (4.6), and choosing $\delta_N = b \sqrt{\log N/N}$, the first term on the RHS of the above is bounded by

$$\int \mathcal{F}_{N,\beta}(u) 1_{[|u-u_N(\beta)| \geq \delta_N]} du \leq 2N^{-ab^2} \quad (5.5)$$

and we take b such that $ab^2 > 1$.

For the second term, by Jensen's inequality and (3.11), for any $\alpha > 0$ we have

$$\begin{aligned} \left| \int \mathcal{F}_{N,\beta}(u) G_{N,\delta_N}(u) du \right| &\leq \frac{1}{\alpha N} \log \int e^{\alpha N G_{N,\delta_N}(u)} \mathcal{F}_{N,\beta}(u) du \\ &= \frac{1}{\alpha N} \log \left[\int_{|u-u_N(\beta)| < \delta_N} e^{-N(I_{N,\beta}(u) - \alpha G_{N,\delta}(u))} \sqrt{\frac{N}{2\pi} f''_{N^*}(u)} (1 + O(N^{-1})) du + 2N^{-ab^2} \right]. \end{aligned}$$

Since, by Taylor formula and condition (iii) above, $|G_{N,\delta_N}(u)| \leq B_{N,\beta} |u - u_N(\beta)|^3$, and $I_{N,\beta}(u) \geq a(u - u_N(\beta))^2$, with a independent of N , we have that

$$\begin{aligned} I_{N,\beta}(u) - \alpha G_{N,\delta}(u) &\geq (u - u_N(\beta))^2 (a - \alpha B_{N,\beta} |u - u_N(\beta)|) \\ &\geq (u - u_N(\beta))^2 (a - \alpha B_{N,\beta} \delta_N) \end{aligned} \quad (5.6)$$

Choose α as a sequence $\alpha_N \rightarrow \infty$, for $n \rightarrow \infty$, and such that $\alpha_N B_N \delta_N < a$, we have

$$I_{N,\beta}(u) - \alpha_N G_{N,\delta}(u) \geq 0, \quad \text{if } |u - u_N(\beta)| < \delta_N.$$

Then we have:

$$\begin{aligned} N \left| \int \mathcal{F}_{N,\beta}(u) G_{N,\delta_N}(u) du \right| &\leq \frac{1}{\alpha_N} \log \left[2\delta_N \sqrt{\frac{N}{2\pi}} \sup_{|u-u_N(\beta)| < \delta_N} \sqrt{f''_{N^*}(u)} (1 + O(N^{-1})) + 2N^{-ab^2} \right] \\ &= \frac{1}{\alpha_N} \log \left[b\sqrt{\log N} \sqrt{\frac{2}{\pi}} \sup_{|u-u_N(\beta)| < \delta_N} \sqrt{f''_{N^*}(u)} (1 + O(N^{-1})) + 2N^{-ab^2} \right]. \end{aligned}$$

If α_N grows faster than $\log \log N$ the last term above tends to 0 as $N \rightarrow \infty$. If we choose $\alpha_N = \sqrt{\log N}$, we also satisfy that $\alpha_N B_N \delta_N < a$.

We can thus rewrite equation (5.3) as

$$\langle A \rangle_{\beta,N} = \langle A | u_N(\beta) \rangle_N + \frac{f''_N(\beta)}{2N} \frac{d^2}{du^2} \langle A | u \rangle_N \Big|_{u=u_N(\beta)} + o\left(\frac{1}{N}\right) \|A\|_{2,\beta,N} \quad (5.7)$$

Note that for any differentiable function $g(u)$

$$\frac{d}{du} g(u) \Big|_{u=u_N(\beta)} = -\frac{1}{f''_N(\beta)} \frac{d}{d\beta} g(u_N(\beta)) \quad (5.8)$$

$$f''_N(\beta) \frac{d^2}{du^2} g(u) \Big|_{u=u_N(\beta)} = \frac{d}{d\beta} \left[\frac{1}{f''_N(\beta)} \frac{d}{d\beta} g(u_N(\beta)) \right] \quad (5.9)$$

By (5.9) we can write (5.7) as

$$\langle A | u_N(\beta) \rangle_N = \langle A \rangle_{\beta,N} - \frac{1}{2N} \frac{d}{d\beta} \left[\frac{1}{f''_N(\beta)} \frac{d}{d\beta} \langle A | u_N(\beta) \rangle_N \right] + o\left(\frac{1}{N}\right) \|A\|_{2,\beta,N}. \quad (5.10)$$

By lemma 5.2 below:

$$\frac{d}{d\beta} \left[\frac{1}{f''_N(\beta)} \frac{d}{d\beta} \left(\langle A \rangle_{\beta,N} - \langle A | u_N(\beta) \rangle_N \right) \right] \sim o\left(\frac{1}{N}\right) \|A\|_{2,\beta,N}$$

and (5.2) follows. \square

Lemma 5.2. *Under the conditions of Theorem 5.1 the following relations hold*

$$\begin{aligned} \frac{d}{d\beta} \left(\langle A \rangle_{\beta, N} - \langle A | u_N(\beta) \rangle_N \right) &= \frac{f_N'''(\beta)}{2N} \frac{d^2}{du^2} \langle A | u \rangle_N \Big|_{u=u_N(\beta)} + o\left(\frac{1}{N}\right) \|A\|_{2, \beta, N} \\ \frac{d^2}{d\beta^2} \left(\langle A \rangle_{\beta, N} - \langle A | u_N(\beta) \rangle_N \right) &= \frac{f_N''''(\beta)}{2N} \frac{d^2}{du^2} \langle A | u \rangle_N \Big|_{u=u_N(\beta)} + o\left(\frac{1}{N}\right) \|A\|_{2, \beta, N} \end{aligned} \quad (5.11)$$

Proof. Note that by (5.3)

$$\begin{aligned} &\frac{d}{d\beta} \left(\langle A \rangle_{\beta, N} - \langle A | u_N(\beta) \rangle_N \right) \\ &= -N \int (\langle A | u \rangle_N - \langle A | u_N(\beta) \rangle_N) (u - u_N(\beta)) \mathcal{F}_{\beta, N}(u) du - \frac{d}{d\beta} \langle A | u_N(\beta) \rangle_N \end{aligned} \quad (5.12)$$

and, using the definition of $G_N(u)$ above and (5.4), that this is equal to

$$\begin{aligned} &= -f_N''(\beta) \frac{d}{du} \langle A | u \rangle_N \Big|_{u=u_N(\beta)} - \frac{d}{d\beta} \langle A | u_N(\beta) \rangle_N \\ &+ \frac{f_N'''(\beta)}{2N} \frac{d^2}{du^2} \langle A | u \rangle_N \Big|_{u=u_N(\beta)} + o\left(\frac{1}{N}\right) \|A\|_{2, \beta, N} \\ &= \frac{f_N''''(\beta)}{2N} \frac{d^2}{du^2} \langle A | u \rangle_N \Big|_{u=u_N(\beta)} + o\left(\frac{1}{N}\right) \|A\|_{2, \beta, N}. \end{aligned}$$

This proves the first of (5.11). For the second one:

$$\begin{aligned} &\frac{d^2}{d\beta^2} \left(\langle A \rangle_{\beta, N} - \langle A | u_N(\beta) \rangle_N \right) \\ &= N^2 \int (\langle A | u \rangle_N - \langle A | u_N(\beta) \rangle_N) (u - u_N(\beta))^2 \mathcal{F}_{\beta, N}(u) du \\ &\quad - N f_N''(\beta) \left(\langle A \rangle_{\beta, N} - \langle A | u_N(\beta) \rangle_N \right) - \frac{d^2}{d\beta^2} \langle A | u_N(\beta) \rangle_N \end{aligned} \quad (5.13)$$

and again using the definition of $G_N(u)$ above and (5.4), we have that this is equal to

$$\begin{aligned}
& N^2 \frac{d}{du} \langle A|u \rangle_N \Big|_{u=u_N(\beta)} \int (u - u_N(\beta))^3 \mathcal{F}_{\beta,N}(u) du \\
& + \frac{N^2}{2} \frac{d^2}{du^2} \langle A|u \rangle_N \Big|_{u=u_N(\beta)} \int (u - u_N(\beta))^4 \mathcal{F}_{\beta,N}(u) du + \\
& - \frac{1}{2} \frac{d^2}{du^2} \langle A|u \rangle_N \Big|_{u=u_N(\beta)} (f_N''(\beta))^2 - \frac{d^2}{d\beta^2} \langle A|u_N(\beta) \rangle_N + o\left(\frac{1}{N}\right) \|A\|_{2,\beta,N} \\
& = -f_N'''(\beta) \frac{d}{du} \langle A|u \rangle_N \Big|_{u=u_N(\beta)} + \left(\frac{1}{2N} f_N''''(\beta) + \frac{3}{2} (f_N''(\beta))^2 \right) \frac{d^2}{du^2} \langle A|u \rangle_N \Big|_{u=u_N(\beta)} \\
& - \frac{1}{2} (f_N''(\beta))^2 \frac{d^2}{du^2} \langle A|u \rangle_N \Big|_{u=u_N(\beta)} - \frac{d^2}{d\beta^2} \langle A|u_N(\beta) \rangle_N + o\left(\frac{1}{N}\right) \|A\|_{2,\beta,N} \\
& = -f_N'''(\beta) \frac{d}{du} \langle A|u \rangle_N \Big|_{u=u_N(\beta)} + \frac{1}{2N} f_N''''(\beta) \frac{d^2}{du^2} \langle A|u \rangle_N \Big|_{u=u_N(\beta)} \\
& + (f_N''(\beta))^2 \frac{d^2}{du^2} \langle A|u \rangle_N \Big|_{u=u_N(\beta)} - \frac{d^2}{d\beta^2} \langle A|u_N(\beta) \rangle_N + o\left(\frac{1}{N}\right) \|A\|_{2,\beta,N} \\
& = \frac{f_N'''(\beta)}{f_N''(\beta)} \frac{d}{d\beta} \langle A|u_N(\beta) \rangle_N + \frac{1}{2N} f_N''''(\beta) \frac{d^2}{du^2} \langle A|u \rangle_N \Big|_{u=u_N(\beta)} \\
& + f_N''(\beta) \frac{d}{d\beta} \frac{1}{f_N''(\beta)} \frac{d}{d\beta} \langle A|u_N(\beta) \rangle_N - \frac{d^2}{d\beta^2} \langle A|u_N(\beta) \rangle_N + o\left(\frac{1}{N}\right) \|A\|_{2,\beta,N} \\
& = \frac{1}{2N} f_N''''(\beta) \frac{d^2}{du^2} \langle A|u \rangle_N \Big|_{u=u_N(\beta)} + o\left(\frac{1}{N}\right) \|A\|_{2,\beta,N}.
\end{aligned}$$

This proves the second of (5.11). □

Let A and B two functions such that they and their product satisfies the assumptions of Theorem (5.1). Applying formula (5.2) to AB we obtain

$$\langle AB|u_N(\beta) \rangle_N = \langle AB \rangle_{N,\beta} - \frac{1}{2N} \frac{d}{d\beta} \left[\frac{1}{f_N''(\beta)} \frac{d \langle AB \rangle_{N,\beta}}{d\beta} \right] + o\left(\frac{1}{N}\right) \|AB\|_{2,\beta,N}.$$

while

$$\begin{aligned}
\langle A|u_N(\beta) \rangle_N \langle B|u_N(\beta) \rangle_N &= \langle A \rangle_{N,\beta} \langle B \rangle_{N,\beta} - \frac{1}{2N} \left(\langle A \rangle_{N,\beta} \frac{d}{d\beta} \left[\frac{1}{f_N''(\beta)} \frac{d \langle B \rangle_{N,\beta}}{d\beta} \right] + \right. \\
&\quad \left. + \langle B \rangle_{N,\beta} \frac{d}{d\beta} \left[\frac{1}{f_N''(\beta)} \frac{d \langle A \rangle_{N,\beta}}{d\beta} \right] \right) + C_N \\
&= \frac{1}{N} \frac{1}{f_N''(\beta)} \frac{d \langle A \rangle_{N,\beta}}{d\beta} \frac{d \langle B \rangle_{N,\beta}}{d\beta} - \frac{1}{2N} \frac{d}{d\beta} \left[\frac{1}{f_N''(\beta)} \frac{d (\langle A \rangle_{N,\beta} \langle B \rangle_{N,\beta})}{d\beta} \right] + C_N
\end{aligned}$$

where C_N contains all term of smaller order and is bounded by

$$|C_N| \leq o\left(\frac{1}{N}\right) \|A\|_{2,\beta,N} \|B\|_{2,\beta,N}.$$

Then defining the correlations

$$\begin{aligned}\langle A; B|u_N(\beta)\rangle_N &:= \langle AB|u_N(\beta)\rangle_N - \langle A|u_N(\beta)\rangle_N \langle B|u_N(\beta)\rangle_N, \\ \langle A; B\rangle_{\beta,N} &:= \langle AB\rangle_{\beta,N} - \langle A\rangle_{\beta,N} \langle B\rangle_{\beta,N},\end{aligned}\tag{5.14}$$

we get the formula for the equivalence of the correlations:

$$\begin{aligned}\langle A; B|u_N(\beta)\rangle_N &= \langle A; B\rangle_{N,\beta} - \frac{1}{N} \frac{1}{f_N''(\beta)} \frac{d\langle A\rangle_{N,\beta}}{d\beta} \frac{d\langle B\rangle_{N,\beta}}{d\beta} - \frac{1}{2N} \frac{d}{d\beta} \left[\frac{1}{f_N''(\beta)} \frac{d\langle A; B\rangle_{N,\beta}}{d\beta} \right] \\ &+ o\left(\frac{1}{N}\right) (\|AB\|_{2,\beta,N} + \|A\|_{2,\beta,N} \|B\|_{2,\beta,N}).\end{aligned}\tag{5.15}$$

Remark 5.3. *This formula is different than the one of reference [11]. The term with the derivative of the canonical correlation is in general smaller than the others. It can be even smaller than the error term as we will see evaluating the fluctuations of the kinetic energy below.*

Remark 5.4. *For extensive variables, like $A = \sum_{i=1}^N p_i^2$, typically we have $\|A\|_{2,\beta,N} \sim N$, that implies that the error in (5.15) is of order $o(N)$. But in these cases the other terms are of order N .*

5.1. Fluctuations of kinetic energy. Consider the kinetic energy

$$K(\mathbf{p}) = \sum_{j=1}^N \frac{p_j^2}{2}.$$

Then, if n is the space dimension,

$$\langle K\rangle_{N,\beta} = \frac{Nn}{2\beta}, \quad \langle K^2\rangle_{N,\beta} = \frac{N(N+2)n^2}{4\beta^2} \quad \langle K; K\rangle_{N,\beta} = \frac{Nn^2}{2\beta^2}$$

and

$$\frac{d\langle K\rangle_{N,\beta}}{d\beta} = -\frac{Nn}{2\beta^2}, \quad \frac{d\langle K; K\rangle_{N,\beta}}{d\beta} = -\frac{Nn^2}{\beta^3}$$

applying equation (5.15) we obtain

$$\begin{aligned}\langle K; K|u_N(\beta)\rangle_N - \langle K; K\rangle_{N,\beta} &= -\frac{n^2 N}{4\beta^4 f_N''(\beta)} + \frac{1}{2} \frac{d}{d\beta} \left(\frac{n^2}{f_N'' \beta^3} \right) \\ &+ o\left(\frac{1}{N}\right) (\|K^2\|_{2,\beta,N} + \|K\|_{2,\beta,N}^2).\end{aligned}\tag{5.16}$$

Observe that as $\|K\|_{2,\beta,N} \sim N/\beta$ and $\|K^2\|_{2,\beta,N} \sim N^2/\beta^2$ the second term in the r.h.s of (5.16) is smaller than the error term. Dividing by N , we obtain for the variances of K/\sqrt{N} :

$$\frac{1}{N} \langle K; K|u_N(\beta)\rangle_N = \frac{n}{2\beta^2} - \frac{n^2}{4\beta^4 f_N''(\beta)} + o(1) = \frac{n}{2\beta^2} \left(1 - \frac{n}{2C_N(\beta)} \right) + o(1)\tag{5.17}$$

The quantity $C_N(\beta) = \beta^2 f_N''(\beta)$ is called heat capacity (per particle). This is in fact equal to $\frac{d}{d\beta^{-1}} u_N(\beta)$. Notice that (5.17) coincide, up to terms of lower order in N , to formula (3.7) in [11].

Notice in particular that the asymptotic canonical and microcanonical variances of $\frac{1}{\sqrt{N}}K_N$ are different. Denoting by V the total potential energy, since $K + V$ is constant under the microcanonical measure, we have that $\langle K; K|u_N(\beta) \rangle_N = \langle V; V|u_N(\beta) \rangle_N$, so the same formula is valid for $\langle V; V|u_N(\beta) \rangle_N$.

It remains to prove the conditions of theorem 5.1 are satisfied by $\langle K_N; K_N|u \rangle_N$, but this in general depends on the model considered, i.e. on the interaction between the particles.

In section 3 we have defined

$$W_N(u) = \frac{d}{du} \Omega_N(u)$$

where

$$\Omega_N(u) = \int_{\mathbb{R}^N} d\mathbf{p} \int_{\mathbb{R}^N} d\mathbf{q} \theta(N(u - h_N(\mathbf{p}, \mathbf{q})))$$

where the Heaviside unit step function $\theta(x)$ is defined by $\theta(x) = 0$ for $x < 0$ and $\theta(x) = 1$ for $x \geq 0$. Using the N-spherical coordinates on the momentum variables, this can be written as

$$\begin{aligned} \Omega_N(u) &= S_{N-1} \int_{\mathbb{R}^N} d\mathbf{q} \int_0^\infty \rho^{N-1} \theta\left(Nu - \frac{\rho^2}{2} - V(\mathbf{q})\right) d\rho \\ &= S_{N-1} \int_{\mathbb{R}^N} d\mathbf{q} \theta(Nu - V(\mathbf{q})) \int_0^{\sqrt{2(Nu - V(\mathbf{q}))}} \rho^{N-1} d\rho \\ &= S_{N-1} \frac{2^{N/2}}{N} \int_{\mathbb{R}^N} d\mathbf{q} (Nu - V(\mathbf{q}))^{\frac{N}{2}} \theta(Nu - V(\mathbf{q})) \end{aligned}$$

where $S_{N-1} = 2\pi^{N/2}/\Gamma(N/2)$ is the surface of the $N - 1$ dimensional unit sphere. Consequently

$$W_N(u) = \frac{(2\pi)^{N/2} N}{\Gamma(N/2)} \int_{\mathbb{R}^N} d\mathbf{q} (Nu - V(\mathbf{q}))^{\frac{N}{2}-1} \theta(Nu - V(\mathbf{q})) \quad (5.18)$$

This formula goes back to Gibbs ([8], chapter 8, (308)), one can prove that $W_N(u)$ is at least $[\frac{N}{2} - 1]$ times differentiable see [6].

For any observable A , the micro canonical mean can be written as

$$\langle A|u \rangle_N = \frac{\frac{\partial}{\partial u} \int d\mathbf{p} d\mathbf{q} \theta(Nu - H(\mathbf{p}, \mathbf{q})) A(\mathbf{p}, \mathbf{q})}{W_N(u)} \quad (5.19)$$

Using the N dimensional spherical momentum coordinates as above, one can write for the micro canonical mean of the kinetic energy as

$$\begin{aligned} \langle K|u \rangle_N &= W_N(u)^{-1} \left(\frac{2(2\pi)^{N/2} N}{\Gamma(N/2)} \int_{\mathbb{R}^N} d\mathbf{q} (Nu - V(\mathbf{q}))^{\frac{N}{2}} \theta(Nu - V(\mathbf{q})) \right) \\ &= \frac{N^2 \Omega_N(u)}{W_N(u)} = \frac{2 \int_{\mathbb{R}^N} d\mathbf{q} (Nu - V(\mathbf{q}))^{\frac{N}{2}} \theta(Nu - V(\mathbf{q}))}{\int_{\mathbb{R}^N} d\mathbf{q} (Nu - V(\mathbf{q}))^{\frac{N}{2}-1} \theta(Nu - V(\mathbf{q}))} \end{aligned}$$

Of course we have the trivial bound $\langle K | u \rangle_N \leq Nu$. Furthermore, since the micro canonical distribution is symmetric in the $\{p_j, j = 1, \dots, N\}$, we have

$$\frac{1}{2} \langle p_j^2 | u \rangle_N = \frac{2 \int_{\mathbb{R}^N} d\mathbf{q} (Nu - V(\mathbf{q}))^{\frac{N}{2}} \theta(Nu - V(\mathbf{q}))}{N \int_{\mathbb{R}^N} d\mathbf{q} (Nu - V(\mathbf{q}))^{\frac{N}{2}-1} \theta(Nu - V(\mathbf{q}))} \quad (5.20)$$

An analogous calculation brings to

$$\langle K^2 | u \rangle_N = \frac{2^2 \int_{\mathbb{R}^N} d\mathbf{q} (Nu - V(\mathbf{q}))^{\frac{N}{2}+1} \theta(Nu - V(\mathbf{q}))}{\int_{\mathbb{R}^N} d\mathbf{q} (Nu - V(\mathbf{q}))^{\frac{N}{2}-1} \theta(Nu - V(\mathbf{q}))} \quad (5.21)$$

We can rewrite these expression by using the micro canonical potential energy weight:

$$\widetilde{W}_N(v) := \frac{d}{dv} \int_{\mathbb{R}^N} \theta(Nv - V(\mathbf{q})) d\mathbf{q}. \quad (5.22)$$

then

$$\langle K | u \rangle_N = N \frac{2 \int_0^u (u-v)^{\frac{N}{2}} \widetilde{W}_N(v) dv}{\int_0^u (u-v)^{\frac{N}{2}-1} \widetilde{W}_N(v) dv}$$

and

$$\langle K^2 | u \rangle_N = 4N^2 \frac{2 \int_0^u (u-v)^{\frac{N}{2}+1} \widetilde{W}_N(v) dv}{\int_0^u (u-v)^{\frac{N}{2}-1} \widetilde{W}_N(v) dv} \quad (5.23)$$

These formulas imply that these microcanonical averages are at least $[N/2]$ times differentiable in u and the derivatives can be explicitly computed.

Starting from expression (5.21) we give a qualitative argument to understand why conditions (i)-(iii) in section 5 should be satisfied for extensive observables. We then present an example where most calculations can be made exactly. From (5.21) one can see that dimensionally the micro canonical mean of K^2 behaves as $N^2 u^2$ and that the derivatives with respect to u are well defined till the order $N/2 - 1$. The third derivative of $\langle K^2 | u \rangle_N$ behaves dimensionally as N^2/u . Thus, as the canonical norm $\|K\|_{2,\beta,N}^2 = N(N+2)/(4\beta)$ and $u_N(\beta)$ does not grow in N , the required conditions are, at least dimensionally, satisfied. The same reasoning can be extended to any extensive or intensive quantity looking directly expression (5.19).

5.2. Exactly solvable one dimensional model. We here introduce the one dimensional model system studied in [6] where conditions (5.1) can be explicitly satisfied.

Consider N identical point particles confined by a one dimensional box of size L . The Hamiltonian is

$$H(\mathbf{p}, \mathbf{q}) = \sum_{i=1}^N \frac{p_i^2}{2m} + V(\mathbf{q}) = E \quad (5.24)$$

The potential energy $V = V_{\text{int}} + V_{\text{box}}$ is determined by the interaction potential

$$V_{\text{int}}(\mathbf{q}) = \frac{1}{2} \sum_{\substack{i,j=1 \\ i \neq j}} V_{\text{pair}}(|q_i - q_j|)$$

and the box potential

$$V_{\text{box}}(\mathbf{q}) = \begin{cases} 0 & \mathbf{q} \in [0, L]^N \\ +\infty & \text{otherwise.} \end{cases}$$

The pair potential is given by

$$V_{\text{pair}}(r) = \begin{cases} \infty & r \leq d_{hc} \\ -U_0 & d_{hc} < r < d_{hc} + r_0 \\ 0 & r \geq d_{hc} + r_0 \end{cases}$$

where $d_{hc} > 0$ is the hard core diameter of a particle with respect to pair interactions. The pair potential above can be viewed as a simplified Lennard-Jones potential. The depth of the potential well is determined by the binding energy parameter $U_0 > 0$ and the interaction range by the parameter r_0 . It is assumed

$$0 < r_0 \leq d_{hc}$$

the latter condition ensures that particles may interact with their nearest neighbors only. In order to have the volume sufficiently large for realizing the completely dissociated state, corresponding to $V = 0$ it is $L > L_{\min} \equiv (N - 1)(d_{hc} + r_0)$. The energy E of the system can take values between the ground state energy $E_0 = -(N - 1)U_0$ and infinity. Following the calculations of [6] expression (5.21) for this model becomes

$$\langle K^2 | u \rangle_N = \frac{\sum_{k=0}^{N-1} \omega_k (Nu + kU_0)^{\frac{N}{2}+1} \theta(Nu + kU_0)}{\sum_{k=0}^{N-1} \omega_k (Nu + kU_0)^{\frac{N}{2}-1} \theta(Nu + kU_0)} \quad (5.25)$$

where ω_k are positive coefficient depending on N and L see [6] for more details. Furthermore the canonical mean energy per particle

$$u_N(\beta) = \frac{1}{2\beta} - \frac{U_0}{N} \frac{\sum_{k=0}^{N-1} k \omega_k e^{-\beta k U_0}}{\sum_{k=0}^{N-1} \omega_k e^{-\beta k U_0}}.$$

so that

$$\frac{1}{2\beta} - U_0 \leq u_N(\beta) \leq \frac{1}{2\beta} \quad (5.26)$$

Expression (5.25) shows that $\langle K^2 | u \rangle_N$ does not vanish iff $u + \frac{N-1}{N}U_0 \geq 0$ this implies $u + U_0 > 0$. Expression (5.25) is explicit but complicate. To verify that $\langle K^2 | u \rangle_N$ satisfies conditions (i)-(iii) we consider the particular case of $-1 + 2/N \leq u < -1 + 3/N$ so that

$$\langle K^2 | u \rangle_N = \frac{\omega_{N-1} + \omega_{N-2} \left(1 - \frac{1}{N} \frac{U_0}{u+U_0}\right)^{N/2+1}}{\omega_{N-1} + \omega_{N-2} \left(1 - \frac{1}{N} \frac{U_0}{u+U_0}\right)^{N/2-1}} N^2 (u + U_0)^2$$

where we use to simplify the formulas $u + \frac{N-1}{N}U_0 \sim u + U_0$ for N large. Calculating the derivatives of (5.25) (we omit the calculation) one can show that there exists a positive

constant A such that

$$\begin{aligned} \langle K^2 | u \rangle_N &\leq N^2(u + U_0)^2 \\ \left| \frac{d}{du} \langle K^2 | u \rangle_N \right| &\leq A N^2(u + U_0) \\ \left| \frac{d^2}{du^2} \langle K^2 | u \rangle_N \right| &\leq A N^2 \left(\frac{U_0}{u + U_0} + \frac{U_0^2}{(u + U_0)^2} \right) \\ \left| \frac{d^3 \langle K^2 | u \rangle_N}{du^3} \right| &\leq A N^2 \left[\frac{U_0}{(u + U_0)^2} + \frac{U_0^2}{(u + U_0)^3} + \frac{U_0^3}{(u + U_0)^4} \right] \end{aligned} \quad (5.27)$$

Remembering that

$$\langle K^2 \rangle_{N,\beta} = \frac{N(N+2)}{4\beta^2}$$

by (5.26) and (5.27) conditions (i)-(iii) of theorem 5.1 are satisfied.

6. THERMODYNAMIC LIMIT

All the statements in the previous sections are for finite N , under the assumption that $f_N(\beta)$ is bounded in N along with the first four derivatives. By definition $f_N(\beta)$ is analytical in β . Assume now that $f_N(\beta)$ converges to $z(\beta)$ which is analytical in β . Then all the derivatives of $f_N(\beta)$ converge to the derivatives of $z(\beta)$ and conditions (2.1) are satisfied. We thus have

$$f'_N(\beta) \rightarrow z'(\beta) = -u(\beta), \quad f''_N(\beta) \rightarrow z''(\beta) = \chi(\beta)$$

Usual thermodynamic notations denote $F(\beta^{-1}) = -\beta^{-1}z(\beta)$ the *free energy*, $\chi(\beta)$ *heat capacity*, and $s(u) = -z^*(u) = -\lim_{N \rightarrow \infty} f_{N^*}(u)$ the *thermodynamic entropy*. It follows the Boltzmann formula:

$$s(u) = \lim_{N \rightarrow \infty} \frac{1}{N} \log W_N(u) \quad (6.1)$$

Also we denote

$$I_\beta(u) = \lim_{N \rightarrow \infty} I_{\beta,N}(u) = \beta u - s(u) + z(\beta) \quad (6.2)$$

that is the rate function for the large deviations of h_N is the infinite Gibbs state defined by DLR equations.

In absence of phase transition, i.e. $I_\beta(u) = 0$ only for $u = z'(\beta)$, then the equivalence on ensembles follows from (5.3). Differentiability of the limit of $f_N(\beta)$ depends on the system we are considering. In next section we give examples where analyticity of $z(\beta)$ is assured at least for β small enough.

7. EXAMPLES

7.1. Independent case. Consider a system of N noninteracting particles in a potential. This is the case $V(q_i, \bar{\mathbf{q}}_i) = V(q_i)$. The Hamiltonian can be written as the sum of N identical terms

$$H_N(\mathbf{p}, \mathbf{q}) = \sum_{i=1}^N h(p_i, q_i) \quad (7.1)$$

Consequently $f_N(\beta)$ does not depend on N and is a smooth function of β if V is a nice reasonable potential.

7.1.1. *Independent harmonic oscillators.* Consider a system of N harmonic oscillators in dimension d . The Hamiltonian is given by

$$H = \sum_{i=1}^N \left[\frac{p_i^2}{2} + \frac{q_i^2}{2} \right] \quad (7.2)$$

To simplify notations take $n = 1$. Explicitely we have

$$f(\beta) = \log(2\pi\beta^{-1})$$

and $z'(\beta) = -\beta^{-1}$, $z''(\beta) = \beta^{-2}$, so that the heat capacity here is $z''(\beta)\beta^2 = 1$.

If we calculate the expected value of the kinetic energy K with respect to the canonical measure at inverse temperature β we obtain

$$\langle K \rangle_\beta = \frac{N}{2\beta} \quad (7.3)$$

The fluctuations (the *variance*) of K are given by

$$\langle K; K \rangle_\beta = \frac{N}{2\beta^2} \quad (7.4)$$

The expected value of K in the with respect to the microcanonical measure is given by

$$\langle K|u \rangle_N = \frac{Nu}{2} \quad (7.5)$$

and

$$\langle K^2|u \rangle_N = \frac{N+2}{4(N+1)} (Nu)^2 \quad (7.6)$$

This imply that the microcanonical variance is given by

$$\langle K; K|u \rangle_N = \langle K^2|u \rangle_N - \langle K|u \rangle_N^2 = \frac{(Nu)^2}{4(N+1)} \quad (7.7)$$

Since $\langle h_N \rangle_\beta = u_N(\beta) = \frac{1}{\beta}$, we have

$$\langle K; K|u_N(\beta) \rangle_N - \langle K; K \rangle_{N,\beta} = \frac{N^2}{4(N+1)\beta^2} - \frac{N}{2\beta^2} = -\frac{N}{4\beta^2} \left(1 + \frac{1}{N+1} \right), \quad (7.8)$$

that coincide with the general formula (5.16).

7.2. Mean Field.

$$h_N = \frac{1}{N} \sum_1^N \frac{p_i^2}{2} + \frac{1}{N^2} \sum_{i,j=1}^N V(q_i, q_j) \quad (7.9)$$

Where V is a symmetric reasonable potential such that $\int e^{-\beta V} dq_1 dq_2 < +\infty$ for any $\beta > 0$. One can check by direct computation, using the symmetry of the potential that $f_N^{(j)}(\beta)$ are uniformly bounded in N .

7.3. Massless surface. On the lattice \mathbb{Z}^{ν} :

$$h_N = \frac{1}{N^{\nu}} \sum_1^{N^{\nu}} \frac{p_i^2}{2} + \frac{1}{N^{\nu}} \sum_{\langle i,j \rangle}^{N^{\nu}} V(q_i - q_j) \quad (7.10)$$

For $\nu = 1$ defining $r_i = q_i - q_{i-1}$, we are back to the independent case.

For $\nu \geq 2$, under certain conditions on V , there is a polynomial decay of correlations. *Check Spencer review*

7.4. Real Gas. Consider a system of N particles interacting with a stable and tempered pair potential $V: \mathbb{R}^d \rightarrow \mathbb{R} \cup \{\infty\}$, i.e., there exists $B \geq 0$ such that:

$$\sum_{1 \leq i < j \leq N} V(q_i - q_j) \geq -BN$$

for all N and all q_1, \dots, q_N and the integral

$$C(\beta) = \int_{\mathbb{R}^d} |e^{-\beta V(q)} - 1| dq$$

is convergent for some $\beta > 0$ (and hence for all $\beta > 0$). In [13] it has been proved the validity of cluster expansion for the canonical partition function in the high temperature - low density regime. This implies that the thermodynamic free energy is analytic in β if β and the density are small enough. Conditions (2.1) are thus satisfied.

7.5. Unbounded spin systems with finite range potential. We consider here the unbounded spin systems studied in [1]. For any domain Λ of \mathbb{Z}^d , with $|\Lambda| = N$, we consider the following ferromagnetic Hamiltonian on the phase space \mathbb{R}^{Λ} defined as follows

$$H_N(\mathbf{q}) = \sum_{j=1}^N \left[\phi(q_j) + \sum_{i \sim j} V(q_i, q_j) \right] = \sum_{j=1}^N X_j$$

where $i \sim j$ means that the sum is over the sites that are at distance $R > 0$ from j . Here ϕ is a one particle phase on \mathbb{R} with at least quadratic increase at infinity, V is a convex function on \mathbb{R} with bounded second derivative, i.e. $|V''(t)| \leq C$. As the kinetic energy term is not present to use Theorem 2.2 we need to prove that the characteristic function $\varphi_N(t)$ of the centered energy has modulus $|\varphi_N(t)| < 1$ and $|\varphi_N(t)|$ is integrable. We have to prove an analogous of (2.5) which assures that the probability density function of the variable S_N exists. The finite range of the potential is sufficient to prove both properties. Define a $\Lambda_R \subset \Lambda$

$$\Lambda_R = \{i \in \Lambda : d(i, j) > 2R\}$$

and

$$Y_k = \phi(q_k) + 2 \sum_{i \sim k} V(q_i, q_k)$$

we can write the Hamiltonian as

$$H_N(\mathbf{q}) = \sum_{k \in \Lambda_R} Y_k + H_{\Lambda \setminus \Lambda_R}$$

where $H_{\Lambda \setminus \Lambda_R}$ depends only on the variables in $\Lambda \setminus \Lambda_R$. For any $\Lambda \subset \mathbb{Z}^d$, let $\nu_{\beta, \Lambda}$ be the canonical measure defined by the Hamiltonian defined above and indicate by $E_{\beta, \Lambda}$ the expectation value w.r.t. $\nu_{\beta, \Lambda}$. Then

$$\begin{aligned} \varphi_N(t) &= E_{\beta, \Lambda}(e^{it \sum_{k \in \Lambda_R} Y_k + it H_{\Lambda \setminus \Lambda_R}}) = E_{\beta, \Lambda}(e^{it H_{\Lambda \setminus \Lambda_R}} E_{\beta, \Lambda_R}(e^{it \sum_{k \in \Lambda_R} Y_k})) \\ &= E_{\beta, \Lambda}(e^{it H_{\Lambda \setminus \Lambda_R}} \prod_{k=1}^{|\Lambda_R|} E_{\beta, k}(e^{it Y_k})) \end{aligned}$$

where in the last equality we used independence of the $\{Y_k\}$ variables due to the finite range potential. We thus have

$$|\varphi_N(t)| \leq E_{\beta, \Lambda}(\prod_{k=1}^{|\Lambda_R|} |E_{\beta, k}(e^{it Y_k})|) = E_{\beta, \Lambda}(\prod_{k=1}^{|\Lambda_R|} |\varphi_k(t)|)$$

The variables $\{Y_k\}$ have finite probability density. This implies that their characteristic functions $\{\varphi_k(t)\}$ have modulus strictly less than one for $t \neq 0$ (see [7]). Furthermore such density is in L^2 so that, by Plancherel equality, $|\varphi_k(t)|^2$ is integrable (see [7]). These two properties of $\varphi_k(t)$ assure that the modulus of $\varphi_N(t)$ is strictly less than one for $t \neq 0$ and integrable for $|\Lambda_R|$ large enough so that, by the Fourier inversion theorem, the probability density function of the centered energy exists.

In [1] exponential decay of correlations is proven for β small enough which implies analyticity of the free energy in the thermodynamic limit.

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