

3. The thermodynamic limit for thermodynamic functions: continuous systems

3.1.) Interactions of classical continuous systems

3.2.) Stable interactions

3.3.) Thermodynamic limit for the configurational microcanonical ensemble

3.4.) Thermodynamic limit for the classical ensembles

In the previous section we considered classical and quantum lattice systems in the grand canonical ensemble. We think here of the lattice gas interpretation of the model. In case of the spin interpretation one would rather speak of the canonical ensemble.

In this section we will consider classical continuous systems, for which various new difficulties occur.

For these systems we will consider several ensembles and show that they lead to the same thermodynamic functions in the thermodynamic limit.

The study of continuous quantum systems would require a solid background in functional analysis, and we therefore refrain from following this route here.

The interested reader can find an introduction to this topic in Chapter 3 in [1].

3.1. Interactions of classical continuous systems

In the previous section we were able to prove that the thermodynamic limit exists for the relevant thermodynamic function, and that it is a convex continuous convex function on the Banach space $\mathcal{B}$ of interactions. A similar result can be proved for a class of continuous systems with hard cores (that is, particles have a minimal distance between each other) using the grand canonical ensemble.

If no hard core condition is imposed and/or if we consider other ensembles then we encounter the following new problems:

- (a) The microcanonical ensemble is more difficult to study than the canonical ensemble, which is more difficult than the grand canonical ensemble. Some convexity properties which hold in the grand canonical ensemble in finite volume hold in the other ensembles only in the thermodynamic limit.
- (b) As we will see in Section 3.2. one usually obtains a catastrophic potential (one that does not yield thermodynamic behavior) if one changes the sign of a stable potential yielding thermodynamic behavior. Catastrophic behavior is possible in continuous systems without hard cores because

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an arbitrary large number of particles can occupy a bounded region in space.

The potentials $U(x_1, \dots, x_n)$ of n particles we consider in the following have the following properties:

• $U : \mathbb{R}^{dn} \rightarrow \mathbb{R} \cup \{+\infty\}$ is a measurable function that may take the value $+\infty$ on a set with finite (Lebesgue-) measure. Hard cores with radius $R_0 > 0$ (particles are hard balls) are e.g. implemented by setting $U(x_1, \dots, x_n) = +\infty$ if $\min_{ij} |x_i - x_j| \leq R_0$. Those configurations have probability zero.

$$\bullet \quad U(x_1, \dots, x_i, \dots, x_j, \dots, x_n) = U(x_1, \dots, x_j, \dots, x_i, \dots, x_n) \quad \forall 1 \leq i < j \leq n. \quad (1)$$

$$\text{(Permutation symmetry)} \quad (2)$$

$$\bullet \quad \text{Translation invariance: } U(x_1 + a, \dots, x_n + a) = U(x_1, \dots, x_n) \quad \forall a \in \mathbb{R}^d.$$

$$\bullet \quad \text{We write } U(x_1, \dots, x_n) = \sum_{k=1}^n \sum_{1 \leq i_1 < \dots < i_k \leq n} \Phi^k(x_{i_1}, \dots, x_{i_k}), \quad (3)$$

where $\Phi^1 = \text{const.}$ by translation invariance. We will assume that $\Phi^1 = 0$. In the following we assume $\mathcal{U}$ is given by (3) with $\Phi^k : \mathbb{R}^{dk_k} \rightarrow \mathbb{R} \cup \{+\infty\}$ measurable.

A sequence of potentials $\{\Phi^k\}_{k=2}^{\infty}$ will be called an **interaction**. If $\Phi^k = 0$ for $k > 2$ we call it a **pair interaction**. Because of translation invariance Φ^2 only depends on $x_1 - x_2$ and we write

$$\Phi^2(x_1, x_2) = \Phi^2(x_1 - x_2). \quad (4)$$

Because of permutation symmetry we have

$$\Phi^2(x) = \Phi^2(-x). \quad (5)$$

We say that a pair potential has **finite range** if Φ has compact support. A hard core condition can be implemented by setting $\Phi(x) = +\infty$

if $|x| \leq R_0$.

An interaction is invariant under Euclidean transformations

$$\int \Phi^k(ox_1 \dots ox_k) = \bar{\Phi}^k(x_1 \dots x_k) \quad (6)$$

holds for every rotation o of $\mathbb{R}^d$. In case of a pair potential this implies that $\bar{\Phi}^2$ is only a function of $|x|$. In case of rare gases this is a reasonable assumption.

In order to have thermodynamic behavior we will need that

- (a) the interaction between distant particles is small,
- (b) the interaction must not cause the collapse of infinitely many particles into a bounded region of $\mathbb{R}^d$.

These two conditions will be assured by the temperedness condition that we introduce next, and by the stability condition in section 3.2.

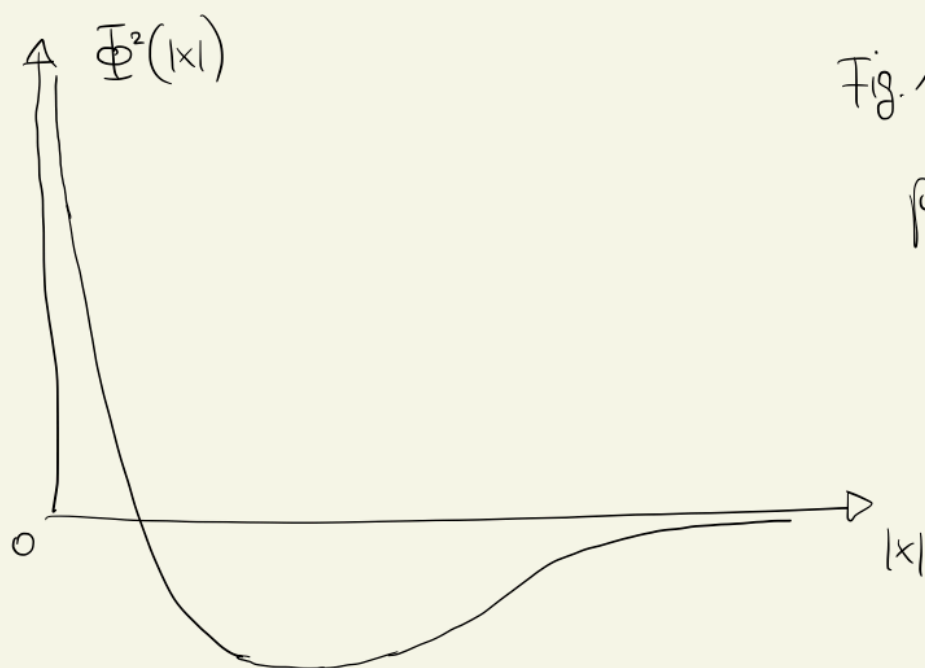


Fig. 1: A typical pair interaction.

We define the mutual interaction energy $W_{u_1 u_2}$ by

$$W_{u_1 u_2}(x_{i_1}^1, \dots, x_{i_{n_1}}^1, x_{j_1}^2, \dots, x_{j_{n_2}}^2) = \sum_{k=1}^{n_1} \sum_{l=1}^{n_2} \sum_{1 \leq i_1 < \dots < i_k \leq u_1} \sum_{1 \leq j_1 < \dots < j_l \leq u_2} \Phi^{k+l}(x_{i_1}^1, \dots, x_{i_k}^1, x_{j_1}^2, \dots, x_{j_l}^2), \quad (7)$$

which allows us to write

$$\begin{aligned} \mathcal{U}(x'_1, \dots, x'_{u_1}, x''_1, \dots, x''_{u_2}) &= \mathcal{U}(x'_1, \dots, x'_{u_1}) + \mathcal{U}(x''_1, \dots, x''_{u_2}) \\ &+ W_{u_1 u_2}(x'_1, \dots, x'_{u_1}; x''_1, \dots, x''_{u_2}). \end{aligned} \quad (8)$$

3.1.1. Definition (tempered interaction): We say

that the interaction $\{\Phi_k\}_{k=2}^{\infty}$ is **tempered** if there exist $\lambda > d$, $R_0 > 0$ and $A \geq 0$ such that

$$W_{u_1 u_2}(x'_1, \dots, x'_{u_1}; x''_1, \dots, x''_{u_2}) \leq A u_1 u_2 r^{-\lambda} \quad (9)$$

whenever $|x''_j - x'_i| \geq r \geq R_0$ for all $i=1, \dots, u_1$, $j=1, \dots, u_2$.

Remark: Temperedness is e.g. assured if

$$W_{u_1 u_2}(x'_1, \dots, x'_{u_1}; x''_1, \dots, x''_{u_2}) \leq 0 \quad (10)$$

whenever $|x''_j - x'_i| \geq r \geq R_0$ for all $i=1, \dots, u_1$, $j=1, \dots, u_2$, that is, the pair interaction in Fig. 1 is tempered.

□ A pair interaction is tempered if and only if

$$\Phi^2(x) \leq A|x|^{-\lambda} \quad \text{for } |x| \geq R_0. \quad (11)$$

To obtain some intuition how temperedness will be used, we consider the situation of a particle at $x=0$ interacting with other particles that are distributed randomly with a density $\rho(x) = \text{const.}$ at a distance $D \geq R_0$ from the particle.

$$\text{Interaction energy: } \int_{|x| \geq D} \Phi^2(x) \underbrace{\rho(x)}_{\text{const.}} dx \quad (12)$$

$$\leq \text{const. } A \int_{|x| \geq D} |x|^{-\lambda} dx = \text{const. } 4\pi A \int_D^\infty \underbrace{r^{d-1-\lambda}}_{< -1} dr$$

$< +\infty$.

Because $d-\lambda < 0$
by assumption.

We note that the r.h.s. tends to zero for $D \rightarrow \infty$.

3.2. Stable interactions

We start with the following definition.

3.2.1. Definition (stable interaction): We say

that the interaction $\{\Phi^k\}_{k=2}^{\infty}$ is stable if there exists $B \geq 0$ such that

$$U(x_1, \dots, x_n) \geq -uB \quad (13)$$

for all $u \geq 0$ and $x_1, \dots, x_n \in \mathbb{R}^d$.

Remark: The condition is satisfied if $\Phi^k \geq 0$ for all $k \geq 2$.

□ The sum of two stable interactions is stable.

Let Λ be a bounded measurable subset of $\mathbb{R}^d$ with volume $|\Lambda|$ and consider the partition function of the grand canonical ensemble

$$Z_\Lambda = 1 + \sum_{n=1}^{\infty} \frac{z^n}{n!} \int_{\Lambda^n} \exp(-\beta U(x_1, \dots, x_n)) d(x_1, \dots, x_n) \quad (14)$$

with $\beta > 0$ and $z > 0$. The stability condition from above implies the convergence of the sum in (14) because

$$\begin{aligned} Z_\Lambda &\leq 1 + \sum_{n=1}^{\infty} \frac{z^n}{n!} |\Lambda|^n \exp(\beta B n) \\ &= \exp(z |\Lambda| \exp(\beta B)). \end{aligned} \quad (15)$$

The divergence of the series in (14) would indicate nonthermodynamic behavior. Next we show that for a large class of potentials the series in (14)

diverges if and only if the stability condition in (13) is violated.

3.2.2. Proposition: Let Φ be a real upper semi-continuous (u.s.c.) function on $\mathbb{R}^d$ such that $\Phi(x) = \Phi(-x)$, and define

$$U(x_1, \dots, x_n) = \sum_{1 \leq i < j \leq n} \Phi(x_i - x_j). \quad (16)$$

Then the following properties are equivalent:

(a) The inequality

$$\sum_{i=1}^n \sum_{j=1}^n \Phi(x_i - x_j) \geq 0 \quad (17)$$

holds for all $n \geq 0$ and $x_1, \dots, x_n \in \mathbb{R}^d$,

(b) there exists $\beta \geq 0$ such that

$$U(x_1, \dots, x_n) \geq -nB$$

(18)

for all $n \geq 0$ and $x_1, \dots, x_n \in \mathbb{R}^d$,

(c) the following series converges for all bounded measurable sets $\Lambda \subset \mathbb{R}^d$

$$Z_\Lambda = 1 + \sum_{n=1}^{\infty} \frac{z^n}{n!} \int_{\Lambda^n} \exp(-\beta U(x_1, \dots, x_n)) d(x_1, \dots, x_n). \quad (19)$$

A function $f: \mathbb{R} \rightarrow \mathbb{R}$ is called u.s.c. if for all $x_0 \in \mathbb{R}$

$$\limsup_{x \rightarrow x_0} f(x) \leq f(x_0)$$

holds.

Example:

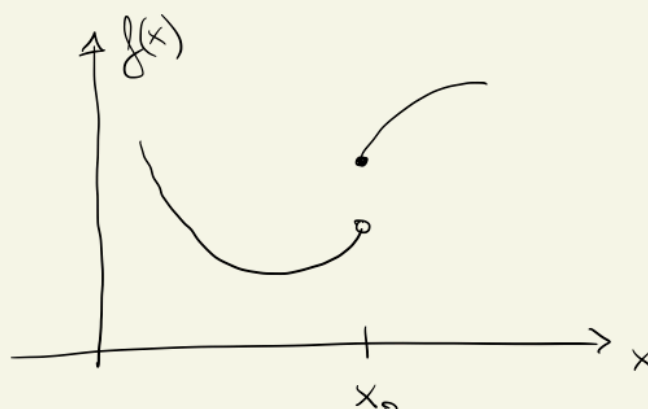


fig. 2

Proof: We first prove (a) $\Rightarrow$ (b) and, to that end, note that

$$\sum_{i=1}^n \sum_{j=1}^n \Phi(x_i - x_j) = n \Phi(0) + 2U(x_1, \dots, x_n). \quad (20)$$

In combination with (17), this implies

$$U(x_1, \dots, x_n) \geq -\frac{n}{2} \Phi(0), \quad (21)$$

hence $\mathcal{B} = \frac{1}{2} \Phi(0)$.

(b) $\Rightarrow$ (c) follows from (15).

Next we consider (c) $\Rightarrow$ (a), which is implied if we can show that (c) does not hold if (a) does not hold. If (a) does not hold then there exist $n \geq 2$ and $\tilde{x}_1, \dots, \tilde{x}_n \in \mathbb{R}^d$ such that

$$\sum_{i=1}^n \sum_{j=1}^n \Phi(\tilde{x}_i - \tilde{x}_j) = -2\varepsilon < 0. \quad (22)$$

Since Φ is u.s.c. we know that the function

$$(y_1, \dots, y_n, z_1, \dots, z_n) \mapsto \sum_{i=1}^n \sum_{j=1}^n \Phi(y_i - z_j) \quad (23)$$

is u.s.c. on $\mathbb{R}^{2dn}$. It takes the value -2ε at

$(\tilde{x}_1, \dots, \tilde{x}_n, \tilde{x}_1, \dots, \tilde{x}_n)$, and hence there exists $\delta > 0$ s.t.

for

$$|y_1 - \tilde{x}_1| < \delta, |z_1 - \tilde{x}_1| < \delta, \dots, |y_n - \tilde{x}_n| < \delta, |z_n - \tilde{x}_n| < \delta$$

we have

$$\sum_{i=1}^n \sum_{j=1}^n \Phi(y_i - z_j) < -\varepsilon. \quad (24)$$

We define the set

$$\mathcal{U}_\delta = \left\{ (x_1, \dots, x_{2n}) \in \mathbb{R}^{2dn} \mid |x_{np+i} - \tilde{x}_i| < \delta \text{ for } p=0, \dots, \delta-1 \text{ and } i=1, \dots, n \right\} \quad (25)$$

and use (24) to see that for $(x_1 \dots x_{su}) \in \mathcal{U}_s$ we have

$$\begin{aligned} \ell(x_1 \dots x_{su}) &= \frac{1}{2} \left[\sum_{p=0}^{s-1} \sum_{q=1}^{s-1} \sum_{i=1}^u \sum_{j=1}^u \Phi(x_{p+u+i} - x_{q+u+j}) \right. \\ &\quad \left. - su\Phi(0) \right] \\ &\leq \frac{1}{2} \left[-s^2\varepsilon - su\Phi(0) \right]. \end{aligned} \quad (26)$$

Let us also define the set

$$\Lambda = \bigcup_{i=1}^u \{x \in \mathbb{R}^d \mid |x - \tilde{x}_i| < s\}. \quad (27)$$

We apply (26) to see that

$$\begin{aligned} Z_\Lambda &= 1 + \sum_{m=1}^{\infty} \frac{z^m}{m!} \int_{\Lambda^m} \exp[-\beta \ell(x_1 \dots x_m)] d(x_1 \dots x_m) \quad (28) \\ &\geq \sum_{s=1}^{\infty} \frac{z^{su}}{(su)!} \int_{\mathcal{U}_s} \exp[-\beta \ell(x_1 \dots x_{su})] d(x_1 \dots x_{su}) \end{aligned}$$

$$\geq \sum_{s=1}^{\infty} \frac{z^{s_n}}{(s_n)!} \underbrace{|\mathcal{B}_s(0)|^{s_n}}_{=\{x \in \mathbb{R}^d \mid |x| < s\}} \exp\left[\frac{\beta}{2}(s^2 \varepsilon + s_n \Phi(0))\right].$$

When we use the bound (see Wikipedia: Stirling's approximation)

$$(s_n)! \leq e (s_n)^{(s_n + \frac{1}{2})} e^{-(s_n)}, \quad (29)$$

we easily check that the r.h.s. of (28) diverges. This proves the claim of the Proposition.



3.2.3. Examples (catastrophic potentials):

• Choose $R_0, a > 0$. By Proposition 3.2.2. the potential

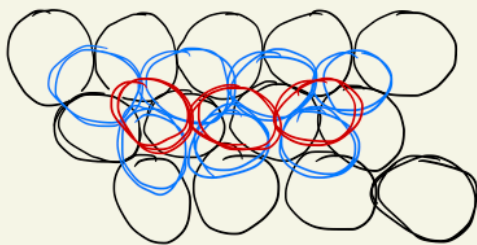
$$\Phi(x) = \begin{cases} -a & \text{for } |x| \leq R_0 \\ 0 & \text{instead} \end{cases} \quad (30)$$

is catastrophic (in the sense that (29) diverges).

Let $0 < a < 2R$ and define the potential

$$\Phi(x) = \begin{cases} 11 & \text{if } 0 \leq |x| < R - \frac{a}{2} \\ -1 & \text{if } R - \frac{a}{2} \leq |x| \leq R + \frac{a}{2} \\ 0 & \text{instead.} \end{cases} \quad (31)$$

If we have hard spheres we can pack them in the following way in $\mathbb{R}^3$:



black = first layer fig. 3
blue = second layer
red = third layer

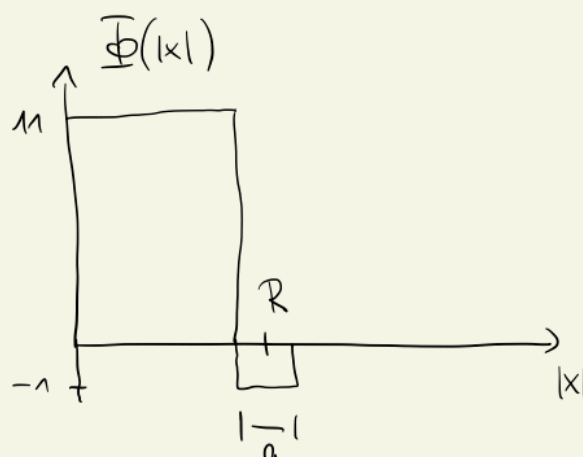
This arrangement is called the face-centered cubic lattice. For more information about this we refer to Wikipedia or almost any book on solid state physics. For us it is only important to note that every sphere in the array has 12 neighbors at the distance R (distance

between the midpoints of the spheres) if R is the radius of the spheres (6 in their own layer, 3 in the layer above and 3 in the layer below).

Let us consider the lattice that we obtain when we take the midpoints of the spheres in fig. 3 and let $x_1, \dots, x_n$ be the lattice points contained in a sphere that is so large that the number of nearest neighbor bonds between $x_1, \dots, x_n$ equals $N > \frac{11n}{2}$ (Please make sure you understand why this is possible.). Then we have

$$\begin{aligned} \sum_{i=1}^n \sum_{j=1}^n \Phi(x_i - x_j) &= n\Phi(0) + 2N\Phi(R) \\ &= 11n - 2N < 11n - 11n = 0. \end{aligned} \quad (32)$$

In combination with Proposition 3.2.2. this proves that Φ is catastrophic.



Other examples of catastrophic potentials are provided by the following result.

3.24. Proposition: Assume that $\Phi \in L^1(\mathbb{R}^d)$ is

such that

$$\int_{\mathbb{R}^d} \Phi(x) dx < 0 \quad (33)$$

holds. Then there exists a bounded measurable set Λ

such that $Z_\Lambda = +\infty$.

Proof: Let $\Lambda \subset \mathbb{R}^d$ be bounded and measurable.

We apply Jensen's inequality to see that

$$\begin{aligned} & \frac{1}{|\Lambda|^n} \int_{\Lambda^n} \exp(-\beta U(x_1, \dots, x_n)) d(x_1, \dots, x_n) \\ & \geq \exp\left(-\frac{\beta}{|\Lambda|^n} \int_{\Lambda^n} U(x_1, \dots, x_n) d(x_1, \dots, x_n)\right) \\ & = \exp\left(-\frac{\beta}{|\Lambda|^2} \frac{n(n-1)}{2} \int_{\Lambda^2} \Phi(x_1 - x_2) d(x_1, x_2)\right) \end{aligned} \quad (34)$$

Eq. (33) implies that

$$-\varepsilon = \frac{1}{|\Lambda|^2} \int_{\Lambda^2} \bar{\Phi}(x_1 - x_2) d(x_1, x_2) < 0 \quad (34)$$

if $\Lambda = [-L/2, L/2]^d$ with L chosen large enough. Accordingly,

$$Z_\Lambda \geq \sum_{n=1}^{\infty} \frac{Z^n}{n!} |\Lambda|^n \exp\left(\beta \frac{n(n-1)}{2} \varepsilon\right) = +\infty. \quad (35)$$

This proves the claim. 

After having discussed catastrophic potentials in some detail we now give examples of potentials, for which the stability condition is satisfied.

3.3.5. Examples (stable potentials):

□ Let Φ be a pair potential with hard core, that is,

$$\Phi(x) = +\infty \quad \text{if } |x| < R \quad (36)$$

and suppose furthermore that there is a constant $B > 0$ s.t.

$$\sum_{i=1}^n \Phi(x_i) \geq -2B \quad (37)$$

holds for all $n \geq 1$ and all sequences $(x_1, \dots, x_n) \in \mathbb{R}^{dn}$ with $|x_i - x_j| \geq R$ for $i \neq j$. In this case the stability condition is satisfied because

$$U(x_1, \dots, x_n) = \frac{1}{2} \sum_{i=1}^n \left[\underbrace{\sum_{j \neq i} \Phi(x_i - x_j)}_{\geq -2B} \right] \geq -nB \quad (38)$$

holds. One easily checks that (37) is satisfied if

there exists a positive, bounded, decreasing function

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$\varphi: [\mathbb{R}, \infty) \rightarrow \mathbb{R}$ with

$$\int_{\mathbb{R}}^{\infty} \varphi(t) t^{d-1} dt < +\infty \quad (39)$$

and

$$\Phi(x) \geq -\varphi(|x|) \quad (40)$$

holds if $|x| \geq R$.

$\square$ A continuous function $f: \mathbb{R}^d \rightarrow \mathbb{C}$ is said to be of **positive type** if for all $x_1, \dots, x_n \in \mathbb{R}^d$ and for all $z_1, \dots, z_n \in \mathbb{C}^n$ one has

$$\sum_{i=1}^n \sum_{j=1}^n \overline{z_i} z_j f(x_i - x_j) \geq 0. \quad (41)$$

Bochner's Theorem tells us that a function is of positive type if and only if it is the Fourier transform of

bounded positive measure on $\mathbb{R}^d$, that is, if f can be written as

$$f(x) = \int_{\mathbb{R}^d} e^{-ipx} \underbrace{d\mu(p)}_{\text{bd. and positive}}. \quad (42)$$

If f is of positive type then $f(-x) = f(x)$ for all $x \in \mathbb{R}^d$ and with the choice $z_1 = z_2 = \dots = z_n = 1$ in (41) we find

$$\sum_{i=1}^n \sum_{j=1}^n f(x_i - x_j) \geq 0, \quad (43)$$

that is, f is a stable pair potential by Proposition 3.2.2.

Let us summarize our findings in a proposition for later reference.

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3.5.6. Proposition: If the pair potential $\bar{\Phi}$ can

be written in the form

$$\bar{\Phi} = \bar{\Phi}_1 + \bar{\Phi}_2 \quad (44)$$

where $\bar{\Phi}_1$ is positive and $\bar{\Phi}_2$ is of positive type, then $\bar{\Phi}$ is stable.

For the sake of completeness we also state the following Proposition without a proof. A proof sketch can be found in [1] in Section 3.2.

3.5.7. Proposition: Let $0 < a_1 < a_2$ and let

φ_1 and φ_2 be positive decreasing functions on $(0, a_1)$, $(a_2, +\infty)$, respectively. Assume furthermore that

$$\int_0^{a_1} \varphi_1(t) t^{d-1} dt = +\infty, \quad \int_{a_2}^{\infty} \varphi_2(t) t^{d-1} dt < +\infty. \quad (45)$$

If the pair potential Φ is bounded from below and satisfies

$$\Phi(x) \geq \varphi_1(|x|) \quad \text{for } |x| \leq a_1 \quad \text{and} \quad (46)$$

$$\Phi(x) \geq -\varphi_2(|x|) \quad \text{for } |x| \geq a_2$$

then Φ is stable.

Remark: It is interesting to consider two species of particles, which we think of as having a positive or a negative electrical charge (depending on the species). The results of this section can easily be generalized to this case. Let us assume the interaction is given by $(x_1, \dots, x_n, y_1, \dots, y_m \in \mathbb{R}^3)$

$$U(\underbrace{x_1, \dots, x_n}_{\text{first species}}, \underbrace{y_1, \dots, y_m}_{\text{second species}}) = \sum_{1 \leq i < j \leq n} \frac{1}{|x_i - x_j|} + \sum_{1 \leq i < j \leq m} \frac{1}{|y_i - y_j|} \quad (47)$$

$$- \sum_{i=1}^n \sum_{j=1}^m \frac{1}{|x_i - y_j|}.$$

Because

$$\int_{\Lambda^2} \exp \left(\beta \frac{1}{|x-y|} \right) d(x,y) = +\infty \quad (48)$$

This system does not show thermodynamic behavior. As is discussed in great detail in Ref. [11] this problem is cured if one considers the quantum mechanical description of the system.

[11] E.H. Lieb, R. Seiringer, The stability of matter in quantum mechanics, Cambridge University Press.

3.3. Thermodynamic limit for the configurational microcanonical ensemble

In this section we assume that an interaction $\{\Phi^k\}_{k=2}^{\infty}$ is given and that

$$U(x_1, \dots, x_n) = \sum_{k \geq 2} \sum_{1 \leq i_1 < \dots < i_k \leq n} \Phi^k(x_{i_1}, \dots, x_{i_k}). \quad (49)$$

Let $\Lambda \subset \mathbb{R}^d$ be a bounded measurable set with volume $|\Lambda|$ and introduce the configurational microcanonical partition function

$$\Omega(\Lambda, n, E) = \frac{1}{n!} \int_{\Lambda^n} \delta^-(U(x_1, \dots, x_n) - E) d(x_1, \dots, x_n) \quad (50)$$

$$= \frac{1}{n!} \left| \left\{ (x_1, \dots, x_n) \in \Lambda^n \mid U(x_1, \dots, x_n) \leq E \right\} \right|.$$

[We define $\Omega(\Lambda, 0, E) = \begin{cases} 1 & \text{if } E \geq 0 \text{ and} \\ 0 & \text{instead} \end{cases}$.]

The configurational entropy is given by

$$S(\lambda, u, E) = \ln(\Omega(\lambda, u, E)), \quad (51)$$

where S may take the value $-\infty$ if $\Omega = 0$.

The entropy $S(\lambda, u, E)$ is an increasing function of E and an increasing function of λ in the sense that $\lambda_1 \subseteq \lambda_2$ implies

$$S(\lambda_1, u, E) \leq S(\lambda_2, u, E). \quad (52)$$

If we allow the values $\pm\infty$ and left possible ambiguities in the definition by choosing it to be left continuous we can define the inverse $E(\lambda, u, S)$ of $S(\lambda, u, E)$ w.r.t. E .

Exercise: Prove that $E(\lambda, u, S)$ is well-defined.

By definition E is an increasing function of S .

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We collect the properties of E in a proposition for later reference.

3.8.1. Proposition: For fixed u , $E(1, u, S)$ is

- (a) an increasing function of S ,
- (b) a decreasing function of 1 (in the sense mentioned above).

Proof: We only need to prove (b). It follows from the fact that E is increasing in S and that S is increasing in 1 .

Let us assume that U is a stable interaction, that is, $U(x_1, \dots, x_n) \geq -uB$ for some $B > 0$. If $E < -uB$ in (56)

then $\Sigma(1, u, E) = 0$ and $S(1, u, E) = -\infty$. In combination

with the definition of $E(\lambda, u, S)$ we conclude that

$$E(\lambda, u, S) \geq -uB. \quad (53)$$

The goal of this section is to prove that

$$\frac{1}{|\lambda|} S(\lambda, u, E) \quad (54)$$

has a limit when $\lambda \uparrow \mathbb{R}^d$ in the sense of Fisher, and when

$$\frac{1}{|\lambda|} u \rightarrow g, \quad \frac{1}{|\lambda|} E \rightarrow e. \quad (55)$$

In order to achieve this goal, we will first establish a similar result for $|\lambda|^{-1} E(\lambda, u, S)$. The first step towards this is the following proposition.

3.3.2. Proposition: Assume that the interaction is

tempered. Then we have the following two statements:

(a) If $\Lambda_1, \Lambda_2 \subset \mathbb{R}^d$ are measurable, bounded, disjoint sets with distance $r \gg R_0$ ($r = \inf_{x \in \Lambda_1, y \in \Lambda_2} |x-y|$), then

$$\begin{aligned} \mathbb{E}(\Lambda_1 \cup \Lambda_2, u_1 + u_2, S_1 + S_2) &\leq \mathbb{E}(\Lambda_1, u_1, S_1) + \mathbb{E}(\Lambda_2, u_2, S_2) \\ &\quad + A u_1 u_2 r^{-\lambda}. \end{aligned} \quad (56)$$

(b) In the case of several such regions $\Lambda_1 \dots \Lambda_m$ with mutual distances $\gg r \gg R_0$ we have

$$\begin{aligned} \mathbb{E}\left(\bigcup_{i=1}^m \Lambda_i, \sum_{i=1}^m u_i, \sum_{i=1}^m S_i\right) &\leq \sum_{i=1}^m \mathbb{E}(\Lambda_i, u_i, S_i) \\ &\quad + \frac{1}{2} A \left(\sum_{i=1}^m u_i\right)^2 r^{-\lambda} \end{aligned} \quad (57)$$

Proof: We start with the proof of (a). Let $x'_1 \dots x'_{n_1} \in \Lambda_1$

and $x''_1 \dots x''_{n_2} \in \Lambda_2$ be such that

$$\mathcal{U}(x'_1 \dots x'_{n_1}) \leq E_1 \quad \text{and} \quad \mathcal{U}(x''_1 \dots x''_{n_2}) \leq E_2. \quad (58)$$

Then we have

$$\begin{aligned} \mathcal{U}(x_1' \dots x_{u_1}', x_1'' \dots x_{u_2}'') &= \mathcal{U}(x_1' \dots x_{u_1}') + \mathcal{U}(x_1'' \dots x_{u_2}'') \\ &\quad + \mathcal{W}(x_1' \dots x_{u_1}', x_1'' \dots x_{u_2}'') \end{aligned} \quad (59)$$

$$\leq E_1 + E_2 + \Delta u_1 u_2 r^{-\lambda},$$

as well as

$$\begin{aligned} \frac{1}{(u_1 + u_2)!} \left| \left\{ (x_1 \dots x_{u_1 + u_2}) \in (\Lambda_1 \cup \Lambda_2)^{u_1 + u_2} \mid \mathcal{U}(x_1 \dots x_{u_1 + u_2}) \right. \right. \\ \left. \left. \leq E_1 + E_2 + \Delta u_1 u_2 r^{-\lambda} \right\} \right| \end{aligned} \quad (60)$$

$$\geq \frac{1}{u_1!} \left| \left\{ (x_1 \dots x_{u_1}) \in \Lambda_1^{u_1} \mid \mathcal{U}(x_1 \dots x_{u_1}) \leq E_1 \right\} \right| \times$$

$$\frac{1}{u_2!} \left| \left\{ (x_1 \dots x_{u_2}) \in \Lambda_2^{u_2} \mid \mathcal{U}(x_1 \dots x_{u_2}) \leq E_2 \right\} \right|.$$

We apply the logarithm on both sides of (60) and

find

$$S(\lambda_1 \cup \lambda_2, u_1 + u_2, E_1 + E_2 + A u_1 u_2 r^{-\lambda}) \quad (61)$$

$$\geq S(\lambda_1, u_1, E_1) + S(\lambda_2, u_2, E_2).$$

Let us call the l.h.s. of (61) S_3 and the r.h.s. $S_1 + S_2$. In combination, the above inequality and Proposition 3.3.1 (a) imply

$$\underbrace{E(\lambda_1 \cup \lambda_2, u_1 + u_2, S_3)}_{\substack{\uparrow \\ E \text{ monotone increasing in third} \\ \text{argument}}} \geq E(\lambda_1 \cup \lambda_2, u_1 + u_2, S_1 + S_2) \quad (62)$$

$\swarrow S_3 \geq S_1 + S_2$

$$= \underbrace{E_1}_{\parallel} + \underbrace{E_2}_{\parallel} + A u_1 u_2 r^{-\lambda}$$

$$= E(\lambda_1, u_1, S_1) + E(\lambda_2, u_2, S_2)$$

This proves (a).

Part (b) can be proved with a repeated application of (a) and the inequality

$$\sum_{i < j} u_i u_j \leq \frac{1}{2} \left(\sum_i u_i \right)^2 \quad (63)$$

(Please check!). This proves the claim.



In the second step we prove the existence of the thermodynamic limit for $N^{-1} E(\Lambda_N, S)$ along a special sequence of cubes that we define now.

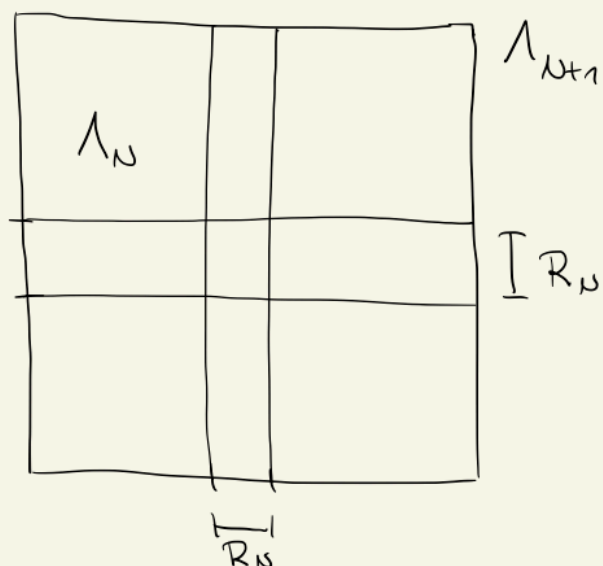


fig. 5
[The cubes Λ_N and Λ_{N+1}]

We choose $\Theta \in \mathbb{R}$ s.t.

$$1 < 2^{d/\lambda} < \Theta < 2, \quad (64)$$

where λ is related to $\{\Phi^k\}_{k=2}^{\infty}$ via the temperedness condition and satisfies $\lambda > d$. Let also R_0 be defined as in the temperedness condition, choose $L, R \in \mathbb{R}$ s.t.

$$L > R = \frac{R_0}{2 - \Theta} \quad (65)$$

holds, and define

$$L_N = 2^N L - \Theta^N R \quad (66)$$

for $N \in \mathbb{N}$. Finally, we define $\Lambda_N \subset \mathbb{R}^d$ to be the cube $[-L_N/2, L_N/2]^d$.

As Fig. 5 indicates it is possible to place 2^d

translates $\Lambda_N^{(i)}$ of Λ_N in Λ_{N+1} at mutual distances at least

$$R_N = L_{N+1} - 2L_N = \Theta^N (2 - \Theta) \underbrace{R_0}_{= \frac{R_0}{2 - \Theta}} = \Theta^N R_0 \geq R_0. \quad (67)$$

From Proposition 3.3.1 (b) we know that

$$\begin{aligned} E\left(\Lambda_{N+1}, \sum_{i=1}^{2^d} u_i, \sum_{i=1}^{2^d} S_i\right) \\ \leq E\left(\bigcup_{i=1}^{2^d} \Lambda_N^{(i)}, \sum_{i=1}^{2^d} u_i, \sum_{i=1}^{2^d} S_i\right), \end{aligned} \quad (68)$$

and Proposition 3.3.2 (b) implies that the r.h.s. of (68) is bounded from above by

$$\sum_{i=1}^{2^d} E(\Lambda_N, u_i, S_i) + \frac{A}{2} \left(\sum_{i=1}^{2^d} u_i \right)^2 R_N^{-\lambda}. \quad (69)$$

In particular,

$$E(\lambda_{N+1}, 2^d u, 2^d s) \leq 2^d E(\lambda_N, u, s) + \frac{A}{2} (2^d u)^2 R_N^{-\lambda}. \quad (70)$$

Now we choose $\delta, \epsilon \in \mathbb{R} \cup \{0\}$ s.t. $2^{Nd} \delta \in \mathbb{N}_0$ and define the sequence

$$\begin{aligned} C_N(\delta, \epsilon) &= 2^{-Nd} E(\lambda_N, 2^{Nd} \delta, 2^{Nd} \epsilon) \\ &\quad - \frac{A}{2} \delta^2 \sum_{u=0}^{N-1} 2^{(u+1)d} R_u^{-\lambda}. \end{aligned} \quad (71)$$

Eq. (70) implies

$$\begin{aligned} C_{N+1}(\delta, \epsilon) &\leq 2^{-Nd} E(\lambda_N, 2^{Nd} \delta, 2^{Nd} \epsilon) \\ &\quad + \frac{A}{2} \delta^2 2^{(N+1)d} R_N^{-\lambda} - \frac{A}{2} \delta^2 \sum_{u=0}^N 2^{(u+1)d} R_u^{-\lambda} \\ &= C_N(\delta, \epsilon). \end{aligned} \quad (72)$$

We also have

$$\lim_{N \rightarrow \infty} \sum_{u=0}^{N-1} \left(2^{(u+1)d} R_u^{-\lambda} \right) = R_0^{-\lambda} 2^d \sum_{u=0}^{\infty} \left(2^d R_0^{-\lambda} \right)^u, \quad (73)$$

which is finite because $2^d \Theta^{-\lambda} < 1$ holds by (64). Moreover, (53) implies

$$2^{-Nd} E(1_N, 2^{Nd} \delta, 2^{Nd} \epsilon) \geq -B\delta. \quad (74)$$

In combination (72), (73) and (74) imply that the sequence $C_N(\delta, \epsilon)$ is bounded from below and monotone decreasing, and therefore has a limit:

$$\lim_{N \rightarrow \infty} C_N(\delta, \epsilon) = C(\delta, \epsilon). \quad (75)$$

Using the result in (73) another time we see that

$$2^{-Nd} E(1_N, 2^{Nd} \delta, 2^{Nd} \epsilon) \quad (76)$$

has a limit. We collect our findings in the following Lemma.

3.3.3. Lemma: Let $\delta, \zeta \in \mathbb{R}$ s.t. $\delta = 2^{-q} p$

with $p, q \in \mathbb{N}_0$ ($\Rightarrow \delta \in \mathbb{Q}$). Then the following limit exists:

$$\lim_{N \rightarrow \infty} 2^{-Nd} \mathbb{E}(\lambda_N, 2^{Nd} \delta, 2^{Nd} \zeta) = \gamma(\delta, \zeta), \quad (77)$$

where

$$\gamma(\delta, \zeta) = c(\delta, \zeta) + \frac{\Lambda}{2} \delta^2 \sum_{u=0}^{\infty} 2^{(u+1)d} R_u^{-\gamma}. \quad (78)$$

We have $\gamma(\delta, \zeta) = +\infty$ if and only if

$$\mathbb{E}(\lambda_N, 2^{Nd} \delta, 2^{Nd} \zeta) = +\infty \text{ for all } N.$$

In the following we investigate the function γ in some more detail. From Proposition 3.3.1 (b) and Proposition 3.3.2. (b) we know that

$$2^{-d(N+1)} \mathbb{E}\left(\lambda_{N+1}, 2^{d(N+1)} \frac{1}{2} (\delta_1 + \delta_2), 2^{d(N+1)} \frac{1}{2} (\zeta_1 + \zeta_2)\right) \leq \dots \quad (79)$$

$$\begin{aligned} \dots &\leq \frac{1}{2} 2^{-dN} E(1_N, 2^{dN} g_1, 2^{dN} G_1) \\ &\quad + \frac{1}{2} 2^{-dN} E(1_N, 2^{dN} g_2, 2^{dN} G_2) \\ &\quad + A 2^{2(N-1)} R_N^{-\lambda}. \end{aligned}$$

We take the limit $N \rightarrow \infty$ on both sides and find

$$\psi\left(\frac{1}{2}g_1 + \frac{1}{2}g_2, \frac{1}{2}G_1 + \frac{1}{2}G_2\right) \leq \frac{1}{2} \psi(g_1, G_1) + \frac{1}{2} \psi(g_2, G_2). \quad (8d)$$

Repeated application of (8d) also shows

$$\psi(\alpha g_1 + (1-\alpha)g_2, \alpha G_1 + (1-\alpha)G_2) \leq \alpha \psi(g_1, G_1) + (1-\alpha) \psi(g_2, G_2) \quad (8e)$$

for $0 \leq \alpha \leq 1$ of the form $\alpha = 2^{-q} p$ with $p, q \in \mathbb{N}_0$.

Next, we check that repeated application of (68) and (69) shows for $n \leq 2^{Nd}$ that

$$\mathbb{E}(\lambda_0, u, uS_n + (2^{Nd} - u)S_0) \leq u \mathbb{E}(\lambda_0, 1, S_n) \quad (82)$$

$$+ (2^{Nd} - u) \mathbb{E}(\lambda_0, 0, S_0) + u \frac{A}{2} \sum_{m=0}^{N-1} 2^{(m+1)d} R_m^{-\lambda}.$$

Using the definitions of R, S and E , we check that

$$\mathbb{E}(\lambda_0, 0, S_0) = 0 \text{ if } S_0 \leq 0 \text{ as well as } \mathbb{E}(\lambda_0, 1, S_n) = 0$$

if $S_n \leq \ln(1.1)$. In combination with (82), this implies

$$\mathbb{E}(\lambda_0, u, S) \leq u \frac{A}{2} \sum_{m=0}^{N-1} 2^{(m+1)d} R_m^{-\lambda} \quad (83)$$

for $u \leq 2^{Nd}$ and $\frac{S}{u} \leq \ln(1.1)$. In particular,

$$\underbrace{\lim_{N \rightarrow \infty} \frac{1}{2^{dN}} \mathbb{E}(\lambda_0, 2^{dN} S, 2^{dN} \phi)}_{= \eta(S, \phi)} \leq \frac{A}{2} \sum_{m=0}^{\infty} 2^{(m+1)d} R_m^{-\lambda} \quad (84)$$

if $0 \leq S \leq 1$ with $S = 2^{-q} p$; $p, q \in \mathbb{N}_0$ and $\phi \leq S \ln(1.1)$.

Our next goal is to prove the following proposition.

Proposition 3.3.4: Let the stability and the temperedness conditions be satisfied. Then there exists a nonempty open convex set $\Delta \subset \mathbb{R}^2$ such that γ extends by continuity to a convex function in Δ , and $\gamma(s, b) = +\infty$ if (s, b) does not belong to the closure $\bar{\Delta}$ of Δ . Furthermore $\gamma(s, b)$ is an increasing function of b .

Proof: The function $\gamma(s, b)$ is defined for $0 \leq s \leq 1$ of the form $s = 2^{-q} p$ with $p, q \in \mathbb{N}_0$ ($\Leftrightarrow$ for $s \in \mathbb{Q} \cap [0, 1]$) and $b \leq s \ln(|\lambda_0|)$. From (84) we know that there is a constant $C > 0$ s.t. $\gamma(s, b) \leq C$ for these points. From stability we obtain the lower bound $\gamma(s, b) \geq -sB \geq -B$.

In the following we will use the convexity of γ in the sense of (81) to show that it can be extended by continuity to the set $0 \leq \delta \leq 1$, $0 \leq \delta \ln(|\lambda|)$.

Let $x = (\delta_1, \delta_1)$ and $y = (\delta_2, \delta_2)$ be rational points and define their norm by $\|z\| = \max\{z_1, z_2\}$. We also assume that $0 < \|x - y\| \leq 1$ and define

$$z = y + \frac{x - y}{\|x - y\|} \quad (85)$$

s.t.

$$x = (1 - \|x - y\|)y + \|x - y\|z. \quad (86)$$

This implies $\gamma(x) \leq (1 - \|x - y\|)\gamma(y) + \|x - y\|\gamma(z)$

$$\Leftrightarrow \gamma(x) - \gamma(y) \leq \|x - y\| (\gamma(z) - \gamma(y)). \quad (87)$$

Similarly, if $w = x + \frac{y-x}{\|x-y\|}$, then

$$\eta(y) - \eta(x) \leq \|x-y\| (\eta(w) - \eta(x)). \quad (88)$$

In combination with the uniform bound $|\eta(s, \ell)| \leq \max\{C, B\}$ which holds for $0 \leq s \leq 1$, $s = 2^{-7}p$, $\ell \leq s \ln(|\mathbf{1}_0|)$, we conclude that

$$|\eta(x) - \eta(y)| \leq 2 \max\{C, B\} \|x-y\| \quad (89)$$

holds for rational points x, y . This allows to show that η can be extended by continuity to the set $0 \leq s \leq 1$, $\ell \leq s \ln(|\mathbf{1}_0|)$ and that the resulting function, which we will still denote by η , is bounded on this set. Moreover, it is continuous and convex.

It remains to study $\eta(s, \ell)$ for points (s, ℓ) that

are not in the above region. To that end, we define

$$\Gamma = \left\{ (s, \zeta) \mid s = 2^{-q} p, \ p, q \in \mathbb{N}_0, \ \zeta \in \mathbb{R}, \right. \quad (90) \\ \left. \nu(s, \zeta) \neq +\infty \right\}$$

and denote by $\bar{\Gamma}$ the closure of Γ in $\mathbb{R}^2$. Using (P1) we show that $\bar{\Gamma}$ is convex. We also define Δ as the interior of $\bar{\Gamma}$ and note that it is a convex open set. From our previous analysis we know that Δ is not empty. If (d, ζ) is any point in Δ , we can find $(s_1, \zeta_1) \in \Gamma$ and $\alpha = 2^{-q} p$, $p, q \in \mathbb{N}_0$, $0 \leq \alpha \leq 1$, s.t.

$$\alpha(s_1, \zeta_1) + (1-\alpha)(s_2, \zeta_2) \quad (91)$$

covers the rational points of a neighborhood of (d, ζ)

If (s_2, ζ_2) varies of the set $0 \leq s_2 \leq 1$, $s_2 = 2^{-q_2} p_2$, $q_2, p_2 \in \mathbb{N}_0$, $\zeta_2 \in S_2 \text{ lin}(\mathbb{N}_0)$. With (P1) we conclude

that η is also bounded from above on the rational points of a neighborhood of (d, ϵ) . Using again the fact that $\eta(s, \epsilon) \geq -sB$, conclude that $|\eta|$ is bounded on the rational points of a neighborhood of every point of Δ . From here on we argue as in the previous case. That $\eta(s, \epsilon)$ is an increasing function of s follows from Proposition 3.3.1.(a). This proves the claim. $\square$

Remark: Let $(s, \epsilon_1), (s, \epsilon_2) \in \Delta$ with $s = 2^{-q}p$; $p, q \in \mathbb{N}$.

The convergence $2^{-Nd} E(1s, 2^{Nd}s, 2^{Nd}\epsilon)$ to $\eta(s, \epsilon)$ is uniform in $\epsilon \in [\epsilon_1, \epsilon_2]$ because pointwise convergence of monotone functions to a continuous function on a compact interval implies uniform convergence.

In the next step we prove the existence of the thermodynamic limit for general sequences $\{\lambda_\alpha\}_{\alpha=1}^\infty$ tending to $\mathbb{R}^d$ in the sense of Fisher.

3.3.5. Proposition: Let $\{\lambda_\alpha\}_{\alpha=1}^\infty$ be a sequence

s.t. $\lambda_\alpha \uparrow \mathbb{R}^d$ in the sense of Fisher and assume

that

$$\frac{n_\alpha}{|\lambda_\alpha|} \rightarrow L^{-d} g, \quad \frac{S_\alpha}{|\lambda_\alpha|} \rightarrow L^{-d} \zeta, \quad (32)$$

where $(g, \zeta) \in \Delta$. Then the limit

$$\lim_{\alpha \rightarrow \infty} \frac{E(\lambda_\alpha, n_\alpha, S_\alpha)}{|\lambda_\alpha|} = L^{-d} \eta(g, \zeta) \quad (33)$$

exists and does not depend on the sequence $\{\lambda_\alpha\}_{\alpha=1}^\infty$.

Proof:- We start by showing that

$$\limsup_{\alpha \rightarrow \infty} \frac{E(\lambda_\alpha, u_\alpha, \delta_\alpha)}{|\lambda_\alpha|} \leq L^{-d} \psi(\delta, \epsilon) \quad (84)$$

holds. Let us choose $\delta_0 = 2^{-Nd} u_0 > \delta$ with $u_0 \in \mathbb{N}_0$ and write

$$\begin{aligned} u_\alpha &= u_\alpha u_0 + r_{0,\alpha} \quad \text{with} \quad 0 \leq r_0 < u_0, \\ r_{0,\alpha} &= p_\alpha 2^{Nd} + r_{1,\alpha} \quad \text{with} \quad 0 \leq r_1 < 2^{Nd}, \\ &\text{and} \quad p \in \mathbb{N}_0. \end{aligned} \quad (85)$$

We keep δ_0 fixed and choose N_α as a function of u_α s.t.

$$\frac{L_{N_\alpha}^d}{u_\alpha} \xrightarrow{\alpha \rightarrow \infty} 0 \quad \text{and} \quad \frac{L_{N_\alpha}^\lambda}{u_\alpha} \xrightarrow{\alpha \rightarrow \infty} \infty. \quad (86)$$

Using the definition of Fisher convergence, we check that λ_α contains $u_{\alpha+p+1}$ disjoint cubes with
for α large enough

file length $\exists L_N$ (Exercise), where

$$1 < \exists < \left(\frac{S_0}{\varepsilon}\right)^{1/d}. \quad (97)$$

Therefore, Λ_α contains $w_\alpha + p + 1$ translates $\Lambda_N^{(i)}$, $i = 1 \dots w_\alpha + p + 1$, of Λ_N with mutual distances at least $(\exists - 1)L_N$.

Using Propositions 3.3.1 (b), 3.3.2. (b) and (83) we check that

$$E(\Lambda_\alpha, u_\alpha, S_\alpha) \leq E\left(\bigcup_{i=1}^{w_\alpha + p + 1} \Lambda_N^{(i)}, \underbrace{u_\alpha}_{u_\alpha u_0 + r_{0,\alpha}}, S_\alpha\right) \quad (98)$$

Via Λ_α this also depends on α .

$$\leq u_\alpha E\left(\Lambda_N, u_0, \frac{1}{u_\alpha} [S_\alpha - r_{0,\alpha} \ln(|\Lambda_0|)]\right)$$

$$+ p_\alpha E(\Lambda_N, 2^{Nd}, 2^{Nd} \ln(|\Lambda_0|))$$

$$+ E(\Lambda_N, r_{1,\alpha}, r_{1,\alpha} \ln(|\Lambda_0|))$$

$$+ \frac{A}{2} u^2 (\exists - 1)^{-\lambda} L_N^{-\lambda}$$

Solution of the exercise with the cubes

1/3

Notation: Let $\lambda_\alpha \uparrow \mathbb{R}^d$ in the sense of Fisher, $\frac{u_\alpha}{|\lambda_\alpha|} \rightarrow \delta$, choose $\delta_0 > \delta$ and define $u_0^\alpha = 2^{N_\alpha} \delta_0$ with $N_\alpha \rightarrow \infty$ in such a way

that

$$\frac{L_{N_\alpha}^d}{u_\alpha} \xrightarrow{\alpha \rightarrow \infty} 0, \quad \frac{\lambda_{N_\alpha}^d}{u_\alpha} \xrightarrow{\alpha \rightarrow \infty} \infty \quad \text{and} \quad \frac{u_0^\alpha}{L_{N_\alpha}^d} \xrightarrow{\alpha \rightarrow \infty} \delta_0 \quad (a)$$

with L_N and λ as on p. 36. Also write

$$u_\alpha = u_\alpha u_0^\alpha + r_{0,\alpha} \quad \text{with} \quad 0 \leq r_{0,\alpha} < u_0, \quad (b)$$

$$r_{0,\alpha} = p_\alpha 2^{N_\alpha d} + r_{1,\alpha} \quad \text{with} \quad 0 \leq r_{1,\alpha} < 2^{N_\alpha d},$$

and $p \in \mathbb{N}_0$.

Problem: Show that λ_α contains $u_\alpha + p + 1$ disjoint cubes with side length $\geq L_{N_\alpha}$, where $1 \leq \beta < \left(\frac{\delta_0}{\delta}\right)^{1/d}$ if $\alpha \geq \alpha_0$ for some $\alpha_0 \in \mathbb{N}$.

Proof: We first note that

$$\begin{aligned} \frac{(u_\alpha + p + 1) L_{N_\alpha}^d}{|\lambda_\alpha|} &= \underbrace{\frac{u_\alpha u_0 L_{N_\alpha}^d}{|\lambda_\alpha| u_0^\alpha}}_{\substack{\leq \frac{u_\alpha}{|\lambda_\alpha|} \frac{L_{N_\alpha}^d}{u_0^\alpha} \xrightarrow{\alpha \rightarrow \infty} \frac{\delta}{\delta_0} \\ \rightarrow \delta \quad \rightarrow 1/\delta_0}} + \underbrace{\frac{p_\alpha 2^{N_\alpha d}}{|\lambda_\alpha|}}_{\rightarrow \frac{1}{\delta_0}} \underbrace{\frac{L_{N_\alpha}^d}{2^{N_\alpha d}}}_{\rightarrow \frac{1}{\delta_0}} + \underbrace{\frac{L_{N_\alpha}^d}{|\lambda_\alpha|}}_{\rightarrow 0} \quad (c) \\ &\leq \frac{r_{0,\alpha}}{|\lambda_\alpha|} = \frac{u_\alpha r_{0,\alpha}}{|\lambda_\alpha|} \frac{1}{u_\alpha} \end{aligned}$$

$$\Rightarrow \boxed{\lim_{\alpha \rightarrow \infty} \frac{(u_\alpha + p + 1) L_{N_\alpha}^d}{|\lambda_\alpha|} = \frac{\delta}{\delta_0} < 1}$$

$$\leq \frac{u_\alpha}{|\lambda_\alpha|} \frac{1}{u_\alpha} \xrightarrow{\alpha \rightarrow \infty} 0$$

$\downarrow$
 δ $u_\alpha \rightarrow \infty$

In other words, the volume of the cubes equals a fraction of the volume of Λ_α that is asymptotically as $\alpha \rightarrow \infty$ strictly smaller than one

Since $\Lambda_\alpha \uparrow \mathbb{R}^d$ in the sense of Fisher, we have

$$\frac{V_{x d(\Lambda_\alpha)}(\Lambda_\alpha)}{|\Lambda_\alpha|} \leq \pi(x) \quad \text{with } \pi(x) \xrightarrow{x \downarrow 0} 0 \quad (d)$$

If $\alpha \geq \alpha_0(x) \in \mathbb{N}$. We chose x s.t. $\pi(x) < 1 - \frac{\delta}{s_0}$ and consider the set $\tilde{\Lambda}_\alpha = \Lambda_\alpha \setminus \{x \in \mathbb{R}^d \mid \text{dist}(x, \partial \Lambda_\alpha) \leq x d(\Lambda_\alpha)\}$. We have $d(\Lambda_\alpha) \geq \text{const. } |\Lambda_\alpha|^{1/d}$, and hence

$$x d(\Lambda_\alpha) \stackrel{(a)}{>} L_{N_\alpha} \quad \text{for } \alpha \text{ large enough.} \quad (e)$$

Let us consider a tiling of $\mathbb{R}^d$ with cubes of side length L_{N_α} and let $\mathcal{C}_\alpha$ be the collection of all cubes in this tiling that have a non-empty intersection with Λ_α . The volume of these cubes is bounded from below by that of $\tilde{\Lambda}_\alpha$. In formulas

$$|\mathcal{C}_\alpha| \geq |\tilde{\Lambda}_\alpha|. \quad (d)$$

Moreover, we have $\mathcal{C}_\alpha \subseteq \Lambda_\alpha$ because of (e). For $|\tilde{\Lambda}_\alpha|$ we have the bound

$$|\tilde{\Lambda}_\alpha| \geq |\Lambda_\alpha| - \underbrace{|V_{x d(\Lambda_\alpha)}(\Lambda_\alpha)|}_{\leq |\Lambda_\alpha| \pi(x)} \geq |\Lambda_\alpha| \underbrace{(1 - \pi(x))}_{< 1 - \frac{\delta}{s_0}} > |\Lambda_\alpha| \frac{\delta}{s_0} \quad (e)$$

for α large enough. In combination, (c), (d) and (e) prove the claim. $\square$

It should be noted that if we replace convergence in the sense of Fisher by convergence in the sense of Van Hove then the statement that we just proved is not true anymore. A counterexample is provided by the sequence of boxes

$$\Lambda_\alpha = [0, \alpha] \times [0, \ln(L_{N_\alpha})] \subset \mathbb{R}^2 \text{ for } \alpha \geq 2.$$

The problem here is that the sidelength of the cubes that we want to place inside Λ_α , and that obeys (a) is growing faster than $\ln(L_{N_\alpha})$. Note that Λ_α converges to $\mathbb{R}^d$ in the sense of Van Hove. The proof is analogous to that given for a similar sequence of sets on p.m in Chapter 2.

$$\leq u_\alpha E(\lambda_\alpha, u_\alpha, \frac{1}{u_\alpha} [S_\alpha - r_{0,\alpha} \ln(|\lambda_\alpha|)]) \\ + r_{0,\alpha} \frac{\Lambda}{2} \sum_{q=0}^{D-1} 2^{(q+1)d} R_q^{-\lambda} + \frac{\Lambda}{2} u^2 \left(\frac{2}{3}-1\right)^{-\lambda} L_N^{-\lambda}$$

$\Rightarrow$

(39)

$$\frac{E(\lambda_\alpha, u_\alpha, S_\alpha)}{|\lambda_\alpha|} \leq \frac{u_\alpha}{|\lambda_\alpha|} \left[\frac{u_\alpha u_0}{u_\alpha} \cdot \frac{1}{S_0} \cdot 2^{-\lambda d} E(\lambda_\alpha, u_\alpha, \frac{1}{u_\alpha} [S_\alpha - r_{0,\alpha} \ln(|\lambda_\alpha|)]) \right. \\ \left. + \frac{r_{0,\alpha} \Lambda}{u_\alpha} \sum_{q=0}^{\infty} 2^{(q+1)d} + \frac{\Lambda}{2} \left(\frac{2}{3}-1\right)^{-\lambda} \frac{u_\alpha}{L_{N_\alpha}^\lambda} \right].$$

When we take $\limsup_{\alpha \rightarrow \infty}$ on both sides, this implies

$$\limsup_{\alpha \rightarrow \infty} \frac{E(\lambda_\alpha, u_\alpha, S_\alpha)}{|\lambda_\alpha|} \leq L^{-d} \frac{S}{S_0} \psi\left(\frac{S_0}{S}, \frac{S_0}{S} \leq\right). \quad (100)$$

To obtain this result, we used $\frac{u_\alpha}{|\lambda_\alpha|} \rightarrow L^{-d} S$, $\frac{r_{0,\alpha}}{|\lambda_\alpha|} \rightarrow 0$

$$2^{-\lambda d} \frac{1}{u_\alpha} S_\alpha = S_0 \underbrace{\frac{u_\alpha}{u_\alpha u_0}}_{\leq 1} \underbrace{\frac{|\lambda_\alpha|}{n_\alpha}}_{\leq \frac{L^d}{S}} \underbrace{\frac{S_\alpha}{|\lambda_\alpha|}}_{\leq L^{-d} S} \rightarrow \frac{S_0}{S} \leq \text{ and } \frac{u_\alpha}{L_{N_\alpha}^\lambda} \rightarrow 0. \quad (96)$$

When we let S_0 approach S from above in (100), this proves (94).

To conclude the proof of the Proposition we will show

that

$$\liminf_{\alpha \rightarrow \infty} \frac{E(\lambda_\alpha, \mu_\alpha, S_\alpha)}{|\lambda_\alpha|} \geq L^{-d} \gamma(S, \epsilon) \quad (101)$$

holds. Since $V_{xd(\lambda_\alpha)}(\lambda_\alpha)$ is larger than the volume of a sphere with radius $xd(\lambda_\alpha)$ (Exercise), we conclude that Fisher convergence implies

$$|\lambda_\alpha| \geq C d(\lambda_\alpha)^d. \quad (102)$$

Accordingly, there exists a constant $C' > 0$ and an integer N'_α s.t. $\lambda_{N'_\alpha}$ contains a translate λ'_α of λ_α

and

$$C' \leq \frac{|\lambda_\alpha|}{|\lambda_{N'_\alpha}|} \leq \frac{1}{2}. \quad (103)$$

We pick $S_n = 2^{-q} p$ with $p, q \in \mathbb{N}_0$, which we think of as being close to S . If $N'_\alpha d \geq q$ we may write $S_n = 2^{-N'_\alpha d} n_{n,\alpha}$. We denote by Λ''_α the set of points in $\Lambda_{N'_\alpha}$ which have a distance to Λ_2 larger than $\Theta^{N'_\alpha} R$. Since $\Lambda_\alpha \uparrow \mathbb{R}^d$ in the sense of Fisher, we have

$$\lim_{\alpha \rightarrow \infty} |\Lambda''_\alpha| = +\infty \quad \text{and} \quad \frac{V_{\times d}(\Lambda''_\alpha)(\Lambda''_\alpha)}{|\Lambda''_\alpha|} \leq \pi(x) \quad (104)$$

for some function π with the same properties than the function in the definition of Fisher convergence (Check this carefully!). Moreover,

$$\lim_{\alpha \rightarrow \infty} \frac{|\Lambda_\alpha| + |\Lambda''_\alpha|}{|\Lambda_{N'_\alpha}|} = 1. \quad (105)$$

Using Propositions 3.3.1 (b) and 3.3.2 (a) we see that

$$\begin{aligned}
& E(\Lambda_{\nu}, 2^{\nu d} S_1, 2^{\nu d} \mathcal{G}) \\
& \leq E(\Lambda_{\alpha} \cup \Lambda_{\alpha}^{\prime\prime}, 2^{\nu d} S_1, 2^{\nu d} \mathcal{G}) \quad (106) \\
& \leq E(\Lambda_{\alpha}, u_{\alpha}, S_2) + E(\Lambda_{\alpha}^{\prime\prime}, u_1 - u_{\alpha}, 2^{\nu' d} \mathcal{G} - S_2) \\
& \quad + \frac{1}{2} A u_1^2 (\Theta^{\nu' d} R)^{-\lambda}
\end{aligned}$$

We divide both sides of (106) by $|\Lambda_{\alpha}|$, take
 $\liminf_{\alpha \rightarrow \infty}$ on both sides and estimate

$$\liminf_{\alpha \rightarrow \infty} \frac{E(\Lambda_{\alpha}, u_{\alpha}, S_2)}{|\Lambda_{\alpha}|} \geq \liminf_{\alpha \rightarrow \infty} \left[\frac{|\Lambda_{\nu_2}|}{|\Lambda_{\alpha}|} L^{-d} 2^{-\nu' d} \times \right. \quad (107)$$

$$\begin{aligned}
& E(\Lambda_{\nu'}, 2^{\nu' d} S_1, 2^{\nu' d} \mathcal{G}) \\
& \left. - \frac{|\Lambda_{\nu_2}| - |\Lambda_{\alpha}|}{|\Lambda_{\alpha}|} \frac{1}{|\Lambda_{\alpha}^{\prime\prime}|} E(\Lambda_{\alpha}^{\prime\prime}, u_1 - u_{\alpha}, 2^{\nu' d} \mathcal{G} - S_2) \right].
\end{aligned}$$

The first term on the r.h.s. behaves asymptotically as

$$\frac{|\lambda_{\alpha_2}|}{|\lambda_{\alpha}|} L^{-d} \left(\eta(\mathcal{S}_{\alpha_1, 6}) + \underbrace{o(1)}_{\text{Vanishes for } \alpha \rightarrow \infty} \right). \quad (108)$$

↳ This holds although $\lambda_{\alpha}^* \notin \mathbb{R}^d$!

For large α , we use (100) to see that the second term is bounded from below by

$$\left(1 - \frac{|\lambda_{\alpha_2}|}{|\lambda_{\alpha}|} \right) L^{-d} \left(\eta(\mathcal{S}_{\alpha_1, 6}) + o(1) \right). \quad (109)$$

In combination with (103) this proves (101).



We also state without proof the following two improvements of Proposition 3.3.5. :

Proposition 3.3.6.: Let the assumptions of Proposition 3.3.5 be satisfied. Then

(a) If $(s, b) \notin \bar{\Delta}$, then

$$\lim_{\alpha \rightarrow \infty} \frac{E(\lambda_\alpha, u_\alpha, S_\alpha)}{|\lambda_\alpha|} = +\infty. \quad (110)$$

(b) If $(s, b) \in \bar{\Delta} \setminus \Delta$, then

$$\liminf_{\alpha \rightarrow \infty} \frac{E(\lambda_\alpha, u_\alpha, S_\alpha)}{|\lambda_\alpha|} \geq \gamma^*(s, b), \quad (111)$$

$$\text{where } \gamma^*(s, b) = \liminf_{\substack{(s^*, b^*) \in \Delta \\ (s^*, b^*) \rightarrow (s, b)}} \gamma(s^*, b^*). \quad (112)$$

Proposition 3.3.7.: The function γ is continuous

on the union of Δ and the half-line $\{(s, b) \mid s=0, b < 0\}$.

If $\lambda_\alpha \uparrow \mathbb{R}^d$ in the sense of Fisher and

$$\frac{n_\alpha}{|\lambda_\alpha|} \rightarrow 0, \quad \frac{S_\alpha}{|\lambda_\alpha|} \rightarrow L^{-d} \zeta < 0 \quad (113) \quad \text{SP}$$

Then

$$\lim_{\alpha \rightarrow \infty} \frac{E(\lambda_\alpha, n_\alpha, S_\alpha)}{|\lambda_\alpha|} = L^{-d} \eta(0, L^{-d} \zeta) = 0. \quad (114)$$

The above results establish the existence of the thermodynamic limit for the function $E(\lambda, n, S)$.

In the following we will use these results to show that the function $S(\lambda, n, E)$ has a limit.

Entropy as a function of energy and density

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Let us formulate the results we just obtained for the energy in a more symmetric way. To that end, we define the set $\Sigma^* \subset \mathbb{R}^3$ as the union of the following sets

(a) The graph $\mathcal{G}$ of η over Δ , that is,

$$\mathcal{G} = \{ (S, \phi, \eta) \mid (S, \phi) \in \Delta, \eta = \eta(S, \phi) \}, \quad (115)$$

(b) the union of the half lines

$$\{ (S, \phi, \eta) \mid S = S^*, \phi = \phi^*, \eta \geq \eta^* \}, \quad (116)$$

where (S^*, ϕ^*) is a point on the boundary of Δ and not of the form (S, ϕ) with $S = 0$ and $\phi < 0$,

and

$$\eta^* = \lim_{\substack{(\delta, \epsilon) \in \Delta \\ (\delta, \epsilon) \rightarrow (\delta^*, \epsilon^*)}} \eta(\delta, \epsilon), \quad (117)$$

(c) the half-line $\{(\delta, \epsilon, \eta) \mid \delta=0, \epsilon < 0, \eta=0\}$.

In the following we use the rescaled variables

$$\varrho = L^{-d} \delta, \quad \varepsilon = L^{-d} \epsilon, \quad \varsigma = L^{-d} \epsilon \quad (118)$$

and denote by Σ the surface corresponding to Σ^* in these new variables. The following Proposition is a direct consequence of Proposition 3.3.5, Proposition 3.3.6 and Proposition 3.3.7.

Proposition 3.3.8: If $\lambda_\alpha \uparrow \mathbb{R}^d$ in the sense of

Fishes and if $|\lambda_\alpha|^{-1} u_\alpha \rightarrow g$, $|\lambda_\alpha|^{-1} E_\alpha \rightarrow e$,

$|\lambda_\alpha|^{-1} S(\lambda_\alpha, u_\alpha, E_\alpha) \rightarrow S$, where g, e, S are finite, then

$(g, e, S) \in \Sigma$.

If $(g, e, S) \in \Sigma$ then we have

$$\varepsilon \geq -g\varepsilon \quad \text{and} \quad \varepsilon \leq g - g \log g. \quad (119)$$

The bound for ε has already been proven on p.43. The bound for the entropy follows from

$$S(\lambda, u, E) \leq \log \left(\frac{|\lambda|^u}{u!} \right), \quad (120)$$

which is a direct consequence of its definition, and Stirling's approximation, that is,

$$\ln(u!) = u \ln(u) - u + O(\ln(u)). \quad (121)$$

More precisely, we have

$$\begin{aligned} \frac{S(\lambda, u, E)}{|\lambda|} &\leq \frac{1}{|\lambda|} \ln\left(\frac{|\lambda|^u}{u!}\right) = \frac{1}{|\lambda|} \left(u \ln(|\lambda|) - \ln(u!) \right) \quad (122) \\ &= \frac{1}{|\lambda|} \left(u \ln(|\lambda|) - u \ln(u) + u + O(\ln(u)) \right) \\ &= g - g \ln(s) + O\left(\frac{\ln(u)}{|\lambda|}\right) \end{aligned}$$

as well as

$$s = \lim_{\alpha \rightarrow \infty} \frac{S(\lambda_\alpha, u_\alpha, E_\alpha)}{|\lambda_\alpha|} \leq g - \ln(s)$$

$$\text{If } \lambda_\alpha \uparrow \mathbb{R}^d \text{ in the sense of Fisher and } \frac{\mu_\alpha}{|\lambda_\alpha|} \rightarrow g, \quad (123)$$

$$\frac{E_\alpha}{|\lambda_\alpha|} \rightarrow \varepsilon.$$

Let us define

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$$g_{\varphi} = \left[\sup_{(g, \varepsilon, s) \in \Sigma} g \right] \in [0, +\infty] \quad (124)$$

as well as for $0 \leq g < g_{\varphi}$ the function

$$\varepsilon_0(g) = \inf \{ \varepsilon \mid (g, \varepsilon, s) \in \Sigma \} \quad (125)$$

We note that $\varepsilon_0(0) = 0$. This follows from (118) and Proposition 3.3.7.

With the above we are prepared to state the following Theorem.

Theorem 3.3.9.: Let $\Sigma(1, u, E)$ be defined by (50) and (51) and let the interaction V be stable and tempered. There exist

(a) $g_{cp} > 0$ or $g_{cp} = +\infty$,

(b) a convex continuous function ε_0 on the interval $[0, g_{cp})$ s.t. $\varepsilon_0(0) = 0$ and $\varepsilon_0(g) \geq -g\beta$,

(c) a concave continuous function δ on the region

$$\Theta = \{(g, \varepsilon) \mid 0 \leq g < g_{cp}, \varepsilon > \varepsilon_0(g)\},$$

increasing in ε for fixed g and s.t. $\delta(0, \varepsilon) = 0$ for $\varepsilon > 0$.

Let $\lambda_\alpha \uparrow \mathbb{R}^d$ in the sense of Fisher and

$$\lim_{\alpha \rightarrow \infty} \frac{u_\alpha}{|\lambda_\alpha|} = g, \quad \lim_{\alpha \rightarrow \infty} \frac{E_\alpha}{|\lambda_\alpha|} = \varepsilon. \quad (126)$$

(a) If $(g, \varepsilon) \in \Theta$ then $\lim_{\alpha \rightarrow \infty} \frac{\mathcal{S}(\lambda_\alpha, u_\alpha, E_\alpha)}{|\lambda_\alpha|} = \mathcal{S}(g, \varepsilon)$.

(b) If (g, ε) belongs to the boundary of Θ then

$$\limsup_{\alpha \rightarrow \infty} \frac{\mathcal{S}(\lambda_\alpha, u_\alpha, E_\alpha)}{|\lambda_\alpha|} \leq \mathcal{S}^*(g, \varepsilon) \quad (127)$$

$$\text{where } S^*(g, \varepsilon) = \limsup_{\substack{(g_i^*, \varepsilon_i^*) \in \Delta \\ (g_i^*, \varepsilon_i^*) \rightarrow (g, \varepsilon)}} S(g_i^*, \varepsilon_i^*). \quad (128)$$

(c) If (g, ε) belongs to the complement of the closure of

$\ominus$ then

$$\lim_{\alpha \rightarrow \infty} \frac{S(\lambda_\alpha, \mu_\alpha, E_\alpha)}{|\lambda_\alpha|} = -\infty. \quad (129)$$

Before we show how the above Theorem follows from our previous results, we discuss a few aspects of convex functions.

Intermezzo (Convex functions):

When working with convex functions on $\mathbb{R}^n$ it is often convenient to allow the values $\pm\infty$. One advantage is that one can always view any convex function as defined on the whole space by defining it to be $+\infty$, wherever it was previously not defined. This is what we will do in the following.

A function $f: \mathbb{R}^n \rightarrow [-\infty, +\infty]$ is called convex if the epigraph

$$\text{epi } f = \{ (x, \mu) \mid x \in \mathbb{R}^n, \mu \in \mathbb{R}, \mu \geq f(x) \} \quad (130)$$

is a convex set.

A convex function is said to be proper if its epigraph is non-empty and contains no vertical lines, i.e., if $f(x) < +\infty$ for at least one x and $f(x) > -\infty$ for every x . Equally, a proper convex function on $\mathbb{R}^n$ is a function obtained

by taking a finite convex function f on a non-empty convex set C and then extending it to all of $\mathbb{R}^n$ by setting $f(x) = +\infty$ for $x \notin C$. A convex function, which is not proper, is called improper.

Example: The function $f: \mathbb{R} \rightarrow [-\infty, +\infty]$ defined by

$$f(x) = \begin{cases} -\infty & \text{if } |x| < 1, \\ 0 & \text{if } |x| = 1, \\ +\infty & \text{if } |x| > 1, \end{cases} \quad (131)$$

is an improper convex function.

We have the following familiar characterizations of convex functions:

(a) The function $f: \mathbb{R} \rightarrow (-\infty, +\infty]$ is convex if and only if

$$f(\lambda x + (1-\lambda)y) \leq \lambda f(x) + (1-\lambda)f(y), \quad 0 < \lambda < 1, \quad (132)$$

for every $x, y \in \mathbb{R}^n$.

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(b) The function $f: \mathbb{R} \rightarrow [-\infty, +\infty]$ is convex $\iff$ and only $\iff$

$$f(\lambda x + (1-\lambda)y) \leq \lambda \alpha + (1-\lambda)\beta, \quad 0 < \lambda < 1 \quad (133)$$

whenever $f(x) < \alpha$ and $f(y) < \beta$.

To prove the convexity of the function ε_0 in (125) we need the following Lemma.

Lemma (Stability under partial minimization):

Assume that $f: \mathbb{R}^n \times \mathbb{R}^m \rightarrow \mathbb{R}$ is convex and let $C \subseteq \mathbb{R}^m$ be a convex set. If the function

$$g(x) = \inf_{y \in C} f(x, y) \quad (134)$$

is proper, i.e. $g(x) > -\infty$ everywhere and $g(x_0) < +\infty$ for at least one x_0 , then g is convex.

Proof:- We want to show that $x, x' \in \mathbb{R}^n$ and $\lambda \in [0, 1]$

$$g(\lambda x + (1-\lambda)x') \leq \lambda g(x) + (1-\lambda)g(x') \quad (135)$$

holds. Given $\varepsilon > 0$ we can find points y and y' s.t.

$$g(x) + \varepsilon \geq f(x, y) \quad \text{and} \quad g(x') + \varepsilon \geq f(x', y'). \quad (136)$$

Taking the weighted sum of these two inequalities shows

$$\lambda g(x) + (1-\lambda)g(x') + \varepsilon \geq \lambda f(x, y) + (1-\lambda)f(x', y') \quad (137)$$

$$\begin{array}{l} \text{Convexity} \\ \text{of } f \end{array} \quad \rightarrow \geq f(\lambda x + (1-\lambda)x', \lambda y + (1-\lambda)y')$$

$$\begin{array}{l} \text{Definition of } g \end{array} \quad \rightarrow \geq g(\lambda x + (1-\lambda)x').$$

The inequality holds for any $\varepsilon > 0$, and therefore proves the claim. $\square$

Lemma: Let $\Delta \subseteq \mathbb{R}^n$ be a convex open set and let

$f: \Delta \rightarrow (-\infty, +\infty)$ be a convex function. Then

the function $\tilde{f}: \bar{\Delta} \rightarrow (-\infty, +\infty]$ defined by

$$\tilde{f}(x) = \begin{cases} f(x) & \text{if } x \in \Delta, \\ \liminf_{\substack{x_n \rightarrow x \\ x_n \in \Delta}} f(x) & \text{if } x \in \partial\Delta, \end{cases} \quad (135)$$

is convex.

Proof: We need to show that

$$\tilde{f}(\lambda x + (1-\lambda)y) \leq \lambda\alpha + (1-\lambda)\beta \quad \text{for all } 0 \leq \lambda \leq 1$$

if $f(x) \leq \alpha$ and $f(y) \leq \beta$. If $x, y \in \Delta$ this follows

from the convexity of f . It also follows easily from

the convexity of f and the fact that $f(x) > -\infty$ for

all $x \in \Delta$ that $\tilde{f}(x) > -\infty$ for all $x \in \partial\Delta$. One can

actually show that $\tilde{f}(x) = -\infty$ for one $x \in \partial\Delta$ already

implies $f(x) = -\infty$ for all $x \in \Delta$. Let us consider the case $x \in \Delta$, $y \in \partial\Delta$ (the case $x, y \in \partial\Delta$ can be proved similarly). By the definition of $\tilde{f}$ we know that for every $\varepsilon > 0$ exists a point $\tilde{y} \in \Delta$ s.t.

$$|\tilde{y} - y| + |\tilde{f}(y) - \tilde{f}(\tilde{y})| < \varepsilon. \quad (136)$$

Pick a sequence $\varepsilon_n \downarrow 0$ and denote by $\tilde{y}_n$ the related sequence of points converging to $y \in \partial\Delta$. We have

$$\begin{aligned} \tilde{f}(\lambda x + (1-\lambda)\tilde{y}_n) &\leq \lambda \tilde{f}(x) + (1-\lambda)\tilde{f}(\tilde{y}_n) \\ &\leq \lambda \tilde{f}(x) + (1-\lambda)\tilde{f}(y) + \varepsilon_n. \end{aligned} \quad (137)$$

When we take the $\liminf_{n \rightarrow \infty}$ on both sides, this proves the claim (the right side converges by continuity).

We are now prepared to prove Theorem 3.3.9

Proof of Theorem 3.3.3.: We start by

showing that the function $\varepsilon_0(g)$ in (125) is convex.

Let us write $\Sigma = \Sigma_a \cup \Sigma_b \cup \Sigma_c$ where $\Sigma_{a,b,c}$ are the components of Σ on p. 59 and 60. For $g \in [0, g_{cp})$ we have

$$\varepsilon_0(g) = \min \left\{ \inf \{ e \mid (e, g, s) \in \Sigma_a \}, \right. \quad (138)$$

$$\inf \{ e \mid (e, g, s) \in \Sigma_b \},$$

$$\left. \inf \{ e \mid (e, g, s) \in \Sigma_c \} \right\}.$$

This is equivalent to saying that

$$\varepsilon_0(g) = \inf \{ \tilde{\varepsilon}(g, s) \mid (g, s) \in \overline{\Delta} \}, \quad (139)$$

where

$$\tilde{\varepsilon}(g, s) = \begin{cases} \varepsilon(g, s) & \text{if } (g, s) \in \Delta \\ \liminf_{\substack{(g^*, s^*) \in \Delta \\ (g^*, s^*) \rightarrow (g, s)}} \varepsilon(g^*, s^*) & \text{if } (g, s) \in \partial \Delta \end{cases} \quad (140)$$

From the second Lemma of the intermezzo we know that $\tilde{E}(g, s)$ is a convex function, and we can apply the first Lemma of the intermezzo to see that $E_0(g)$ is convex.

The function $S(g, \varepsilon)$ is the inverse function of $E(g, s)$ for fixed g (as one should expect because $E(1, u, S)$ is defined as the inverse of $S(1, u, E)$ for fixed 1 and u). We know that $s \mapsto E(g, s)$ is monotone increasing and convex. Accordingly, it has no jumps and can be constant only on an interval of the form $(-\infty, a]$ with some $a \in \mathbb{R}$.

Apart from that it is a strictly monotone and continuous function. See fig. 6 for how typical curves look like.

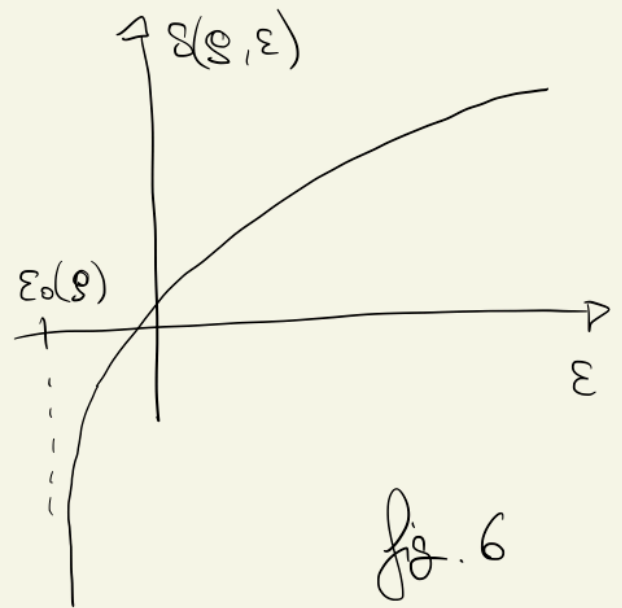
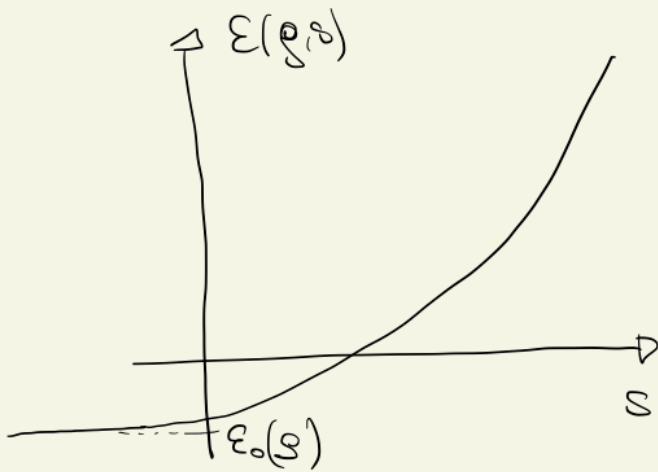


fig. 6

Because $s(s, \varepsilon)$ is the inverse of $E(s, s)$ we know that it is a jointly concave function of its arguments:

$$\begin{array}{c} \nearrow \\ \varepsilon_3 \end{array} E(\lambda s_1 + (1-\lambda)s_2, \lambda s_1 + (1-\lambda)s_2) \leq \lambda \underset{\uparrow \varepsilon_1}{E(s_1, s_1)} + (1-\lambda) \underset{\uparrow \varepsilon_2}{E(s_2, s_2)} \quad (141)$$

monotonicity of
 $\varepsilon \mapsto s(s, \varepsilon)$

$$\begin{aligned} \Rightarrow s(\lambda s_1 + (1-\lambda)s_2, \varepsilon_3) &\leq s(\lambda s_1 + (1-\lambda)s_2, \lambda \varepsilon_1 + (1-\lambda)\varepsilon_2) \quad (142) \\ &= \lambda s_1 + (1-\lambda)s_2 = \lambda s(s_1, s_1) + (1-\lambda)s(s_2, s_2). \end{aligned}$$

Moreover, $S(0, \varepsilon) = 0$ for $\varepsilon > 0$ follows from $S(1, 0, \varepsilon) = 0$ for $\varepsilon > 0$, which follows from $\Omega(1, 0, \varepsilon) = 1$ for $\varepsilon > 0$ (this was our definition of Ω for $u=0$).

Assume that $\lambda_\alpha \uparrow \mathbb{R}^d$ in the sense of Fisher and that

$$\frac{u_\alpha}{|\lambda_\alpha|} \rightarrow g \text{ as well as}$$

$$E_\alpha \rightarrow \frac{E(\lambda_\alpha, u_\alpha, S_\alpha)}{|\lambda_\alpha|} \rightarrow \varepsilon > \varepsilon_0(g) \quad (143)$$

Let us first assume that the sequence $\frac{S_\alpha}{|\lambda_\alpha|}$

is bounded. In this case we can use the strict monotonicity of $S(g, \varepsilon)$ to prove that $\frac{S_\alpha}{|\lambda_\alpha|}$

converges. In case of a general sequence S_α

we write $\frac{S_\alpha}{|\lambda_\alpha|}$ as a sum of a two sub-

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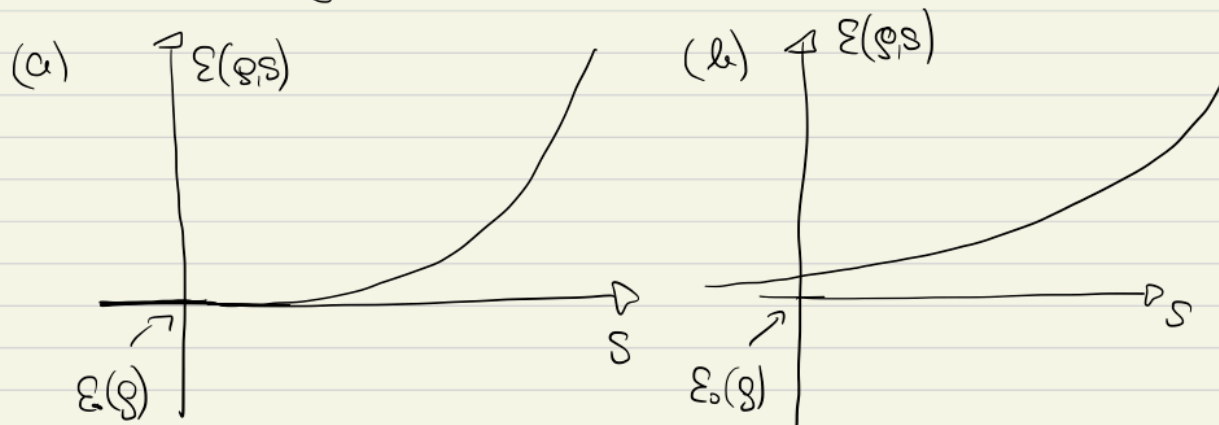
sequences, S_α^d and S_α^b , where $\frac{S_\alpha^b}{|\lambda_\alpha|}$ is bounded and $\frac{S_\alpha^d}{|\lambda_\alpha|}$ is diverging to $-\infty$ (recall that $\frac{S_\alpha}{|\lambda_\alpha|}$ is bounded from above). We apply the previous argument to the subsequence $\frac{S_\alpha^b}{|\lambda_\alpha|}$ and show that it converges. Using the strict monotonicity the map $\varepsilon \mapsto \delta(\varepsilon)$ and $\varepsilon > \varepsilon_0(\delta)$, we afterwards show that the full sequence $\frac{S_\alpha}{|\lambda_\alpha|}$ converges^(*). This proves (a). The points (b) and (c) follow from similar arguments and we omit the details. Please check them as an exercise. $\square$

Remark 3.3.10: Let $K \subset \Theta$ be a compact set and assume that $\lambda_\alpha \uparrow \mathbb{R}^d$ in the sense of Fisher.

Remark on (*) (More details)

1/1

The function $\varepsilon(g, s)$ with fixed g can qualitatively look like that (follows from monotonicity and convexity):



If $\frac{S_n}{|I_n|} \rightarrow -\infty$ we define a new sequence $\tilde{S}_n^c$ s.t.

$$\tilde{S}_n^c = \begin{cases} S_n & \text{if } \frac{S_n}{|I_n|} > -c, \\ -c & \text{instead.} \end{cases}$$

Choosing c large enough we obtain in both cases a contradiction because we assumed that $\varepsilon > \varepsilon_0(g)$. If $\frac{S_n}{|I_n|}$ is unbounded from below we choose a subsequence with $\frac{S_n}{|I_n|} \rightarrow -\infty$ and obtain with the above construction a contradiction. Accordingly, the sequence $\frac{S_n}{|I_n|}$ is bounded. By the argument in the proof for this case it needs to converge.

It is not difficult to see that

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$$\left| \frac{1}{|A_\alpha|} S(\lambda_\alpha, u_\alpha, E_\alpha) - s\left(\frac{u_\alpha}{|A_\alpha|}, \frac{E_\alpha}{|A_\alpha|}\right) \right| \quad (144)$$

converges to zero uniformly for $\left(\frac{1}{|A_\alpha|} u_\alpha, \frac{1}{|A_\alpha|} E_\alpha\right) \in K$.

Remark 3.3.11: In his book Fuelle claims that

with the above results one can also prove that

$$\frac{1}{|A_\alpha|} \text{lee } S^\Delta(\lambda_\alpha, u_\alpha, E_\alpha) \rightarrow s(s, e) \quad (145)$$

holds for fixed Δ , where

$$S^\Delta(\lambda, u, E) = \frac{1}{u!} \int \mathbb{1}(E - \Delta \leq \text{ll}(x_1 \dots x_u) < E) d(x_1 \dots x_u), \quad (146)$$

see Section 3.3.14 in [1] on p.51. Unfortunately, I

do not understand this. If you have an idea how this may work please let me know.

3.4. Thermodynamic limit for the classical ensembles

Throughout this section we assume that all interactions are tempered and stable.

3.4.1. Microcanonical ensemble

In this section we consider the (modified) microcanonical ensemble with partition function

$$\Omega_{\text{tot}}(1, n, E) = \frac{1}{n!} \int \mathbb{1} \left(\sum_{i=1}^n p_i^2 + U(x_1, \dots, x_n) < E \right) d(p_1, \dots, p_n) d(x_1, \dots, x_n). \quad (147)$$

We call this ensemble modified because we consider $\mathbb{1}(H < E)$ instead of $\delta(H - E)$.

Let us define the kinetic partition function

$$\begin{aligned}\Omega_{\text{kin}}(u, E) &= \int_{\mathbb{R}^{du}} \delta\left(\sum_{i=1}^u p_i^2 - E\right) d(p_1, \dots, p_u) \\ &= \frac{(\pi E)^{du/2}}{E \Gamma(du/2)},\end{aligned}\quad (148)$$

$\swarrow$ volume of surface of sphere

where Γ denotes the Gamma function. The full partition function can be written as

$$\begin{aligned}\Omega_{\text{tot}}(\lambda, u, E) &= \int_0^\infty \int_{\mathbb{R}^{du}} \delta\left(\sum_{i=1}^u p_i^2 - t\right) d(p_1, \dots, p_u) \\ &\quad \times \frac{1}{u!} \int_{\Lambda^u} \mathbb{1}\left(\ell(x_1, \dots, x_u) + t - E < 0\right) d(x_1, \dots, x_u) dt \\ &= \int_0^\infty \Omega_{\text{kin}}(u, t) \Omega(\lambda, u, E - t) dt.\end{aligned}\quad (149)$$

Let $\lambda_\alpha \uparrow \mathbb{R}^d$ in the sense of Fisher, $\frac{u_\alpha}{|\lambda_\alpha|} \rightarrow \rho$, $\frac{E_\alpha}{|\lambda_\alpha|} \rightarrow \varepsilon$.

Using (121), we show that

$$\begin{aligned} \lim_{\alpha \rightarrow \infty} \frac{1}{|\lambda_\alpha|} \ln \Omega_{\text{kin}}(u_\alpha, E_\alpha) \\ = \frac{d\mathcal{G}}{2} \left(\ln \left(\frac{2\pi E}{d\mathcal{G}} \right) + 1 \right) =: \mathcal{S}_{\text{kin}}(\mathcal{G}, E) \end{aligned} \quad (150)$$

holds.

For $0 \leq \mathcal{G} < \mathcal{G}_{\text{cp}}$ and $E > E_0(\mathcal{G})$ we define

$$\mathcal{S}_{\text{tot}}(\mathcal{G}, E) = \sup_{E' \in (0, E - E_0(\mathcal{G}))} \left[\mathcal{S}_{\text{kin}}(\mathcal{G}, E') + \mathcal{S}(\mathcal{G}, E - E') \right]. \quad (151)$$

We use Theorem 3.3.9 and (150) to see that there exists a nonempty interval (t_1, t_2) s.t. for given $\mathcal{S} > 0$ and $t \in (t_1, t_2)$ we have

$$\Omega_{\text{kin}}(u_\alpha, t) \Omega(\lambda_\alpha u_\alpha, E_\alpha - t) > \exp(|\lambda_\alpha| (\mathcal{S}_{\text{tot}}(\mathcal{G}, E) - \mathcal{S})) \quad (152)$$

If α is large enough. In combination with (152),

this implies

$$\liminf_{\alpha \rightarrow \infty} \frac{1}{|\lambda_\alpha|} \lim \underbrace{\Omega_{\text{tot}}(\lambda_\alpha, u_\alpha, E_\alpha)}_{(153)}$$

$$\lim \underbrace{\int_0^\infty \Omega_{\text{lin}}(u_\alpha, t) \Omega(\lambda_\alpha, u_\alpha, E_\alpha - t) dt}_{(153)}$$

$$\geq (t_2 - t_1) \exp(|\lambda_\alpha| (S_{\text{tot}}(g, \varepsilon) - \delta))$$

$$\geq S_{\text{tot}}(g, \varepsilon) - \delta,$$

and hence,

$$\liminf_{\alpha \rightarrow \infty} \frac{1}{|\lambda_\alpha|} \lim \Omega_{\text{tot}}(\lambda_\alpha, u_\alpha, E_\alpha) \geq S_{\text{tot}}(g, \varepsilon). \quad (154)$$

We also claim that for given $\delta > 0$, we have

$$\Omega_{\text{lin}}(u_\alpha, t) \Omega(\lambda_\alpha, u_\alpha, E_\alpha - t) < \exp(|\lambda_\alpha| (S_{\text{tot}}(g, \varepsilon) + \delta)) \quad (155)$$

for all t as long as α is chosen large enough.

To prove this, we note that the stability condition implies that the left side vanishes for large t (of the order $|\lambda|$), that is, we can assume that t is in a compact interval of the form $[0, |\lambda|t']$.

Using Remark 3.3.10 we can easily deduce a contradiction if (165) was not satisfied for t in that interval. We conclude that

$$\limsup_{\alpha \rightarrow \infty} \frac{1}{|\lambda_\alpha|} \text{Le } \Omega_{\text{tot}}(\lambda_\alpha, u_\alpha, E_\alpha) \leq S_{\text{tot}}(g, \varepsilon). \quad (166)$$

We collect our findings in the following Proposition for later reference.

Proposition 34.1.1. Let $\lambda_\alpha \uparrow \mathbb{R}^d$ in the sense

of Fisher and $\frac{u_\alpha}{|\lambda_\alpha|} \rightarrow g$, $\frac{E_\alpha}{|\lambda_\alpha|} \rightarrow \varepsilon$, where

$0 \leq g < g_{cp}$ and $\varepsilon_0(g) < \varepsilon$. Then we have

$$\lim_{\alpha \rightarrow \infty} \frac{1}{|\Lambda_\alpha|} \log \Omega_{\text{tot}}(\lambda_\alpha, u_\alpha, E_\alpha) = S_{\text{tot}}(g, \varepsilon). \quad (157)$$

Remark 3.4.1.2: One can treat the cases where

$(g, \varepsilon) \notin \mathcal{G}$ similarly.

Next, we consider the canonical ensemble. Before that we quickly introduce and discuss Legendre transformations.

Notes on Legendre transformation

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Definition: Let $f: \mathbb{R} \rightarrow (-\infty, +\infty]$ be a proper convex function. The Legendre transform of f is defined by

$$f^*(y) := \sup_{x \in \mathbb{R}} \{yx - f(x)\}, \quad y \in \mathbb{R}. \quad (158)$$

Since f is proper, we have $f^*(y) > -\infty$.

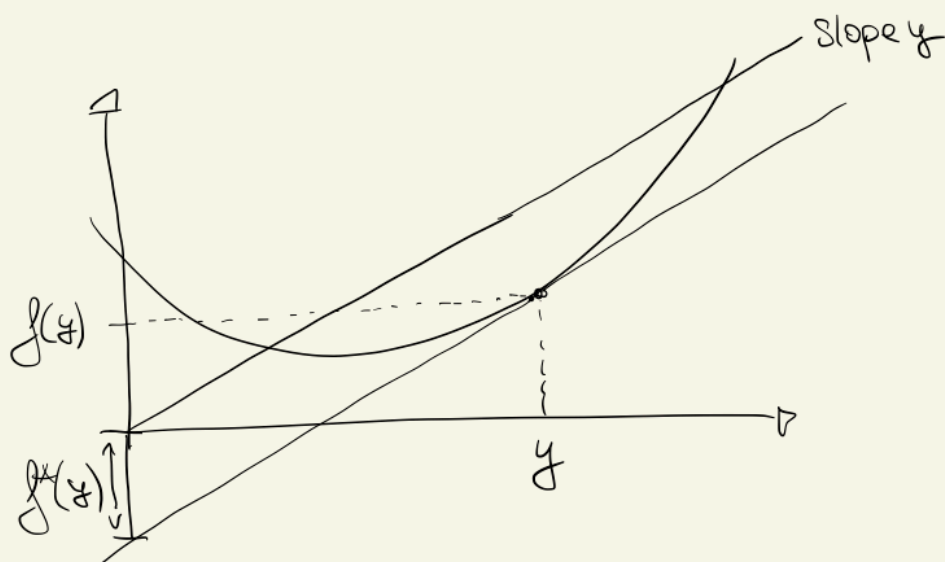


fig. 7

For a given $y \in \mathbb{R}$, $f^*(y)$ is the largest difference between the straight line $x \mapsto yx$ and the graph of f .

I recommend the following exercises:

Exercise 1: Show that any Legendre transform is convex.

Exercise 2: Compute the Legendre transform of

the following functions: (159)

$$f_1(x) = \frac{1}{2}x^2, \quad f_2(x) = x^4, \quad f_3(x) = \begin{cases} 0 & \text{if } x \in (-1, 1) \\ +\infty & \text{instead.} \end{cases}$$

Compute also $f_i^{**} = (f_i^*)^*$ for $i=1,2,3$.

From the second exercise we learn that f^{**} does not necessarily equal f .

Exercise 3: Show that $f^{**} \leq f$ holds p.w. for all proper convex functions f .

The following two examples make the geometrical effect of applying two successive Legendre transformations transparent:

Exercise 4: Let $f(x) = ||x|-1|$ and show

that

$$f^{**}(x) = \begin{cases} -x-1 & \text{if } x < -1, \\ 0 & \text{if } |x| \leq 1, \\ x+1 & \text{if } x > 1. \end{cases} \quad (160)$$

Exercise 5: Let $f(x) = x^4 - x^2$. Using the

geometric picture in fig. 7, study qualitatively f^* and f^{**} .

We recall that a function f is called lower semi-continuous at x if

$$\liminf_{u \rightarrow x} f(x_u) \geq f(x) \quad (161)$$

holds for any sequence $x_u \rightarrow x$.

Exercise 6: Show that any Legendre transform is lower semi-continuous.

Definition: The convex envelope (or convex hull)

of f , denoted $CE f$, is defined as the unique convex function g whose epigraph is

$$C := \bigcap \{ F \subset \mathbb{R}^2 \mid F \text{ closed, convex, } F \supset \text{epi}(f) \}.$$

That is,

$$CE f(x) := \inf \{ y \mid (x, y) \in C \}. \quad (162)$$

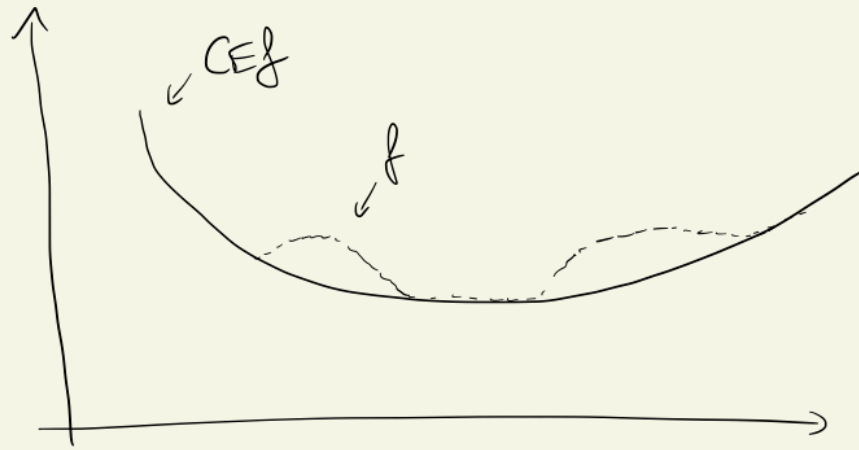


fig. 8

We state the following two Theorems without proof.

Theorem 1: If $f: \mathbb{R} \rightarrow \mathbb{R}$ is lower semi-continuous, then

$$f^{**} = CE f. \quad (163)$$

Theorem 2: If $f: \mathbb{R} \rightarrow (-\infty, +\infty]$ is a proper convex

and lower semi-continuous function then

$$f^{**} = f. \quad (164)$$

3.4.3. Canonical ensemble

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The canonical partition function is given by

$$\begin{aligned} \frac{1}{u!} \int_{\mathbb{R}^{du}} \int_{\Lambda^u} \exp(-\beta (\sum_{i=1}^u p_i^2 + \mathcal{U}(x_1, \dots, x_u))) d(p_1, \dots, p_u) d(x_1, \dots, x_u) \\ = \left(\frac{\pi}{\beta}\right)^{\frac{ud}{2}} Q(\Lambda, u, \beta) \end{aligned}$$

with the configurational partition function

$$Q(\Lambda, u, \beta) = \frac{1}{u!} \int_{\Lambda^u} \exp(-\beta \mathcal{U}(x_1, \dots, x_u)) d(x_1, \dots, x_u). \quad (165)$$

For $0 \leq g < g_{cp}$ and $\beta > 0$ we define the free energy

$$f(g, \beta) = \inf_{\varepsilon > \varepsilon_0(g)} \left\{ \varepsilon - \beta^{-1} s(g, \varepsilon) \right\}. \quad (166)$$

The free energy is convex in g by the Lemma on

p. 68 and, as an infimum over affine functions*, it is concave in β . We also note that $\beta g(\beta, g)$ is concave in β because the Legendre transform of a convex function is convex. 30

* Let f_α be a family of concave functions (e.g. affine functions). Then

$$g(x) = \inf_{\alpha} f_{\alpha}(x) \quad (167)$$

is concave because

$$\begin{aligned} f_{\alpha}(\lambda x + (1-\lambda)y) &\geq \lambda f_{\alpha}(x) + (1-\lambda)f_{\alpha}(y) \\ &\geq \lambda g(x) + (1-\lambda)g(y). \end{aligned} \quad (168)$$

When we take the infimum over α on both sides,

↳ This proves the claim. ↘

For given $\delta > 0$ we can find $\tilde{\varepsilon}$ s.t.

$$\beta \tilde{\varepsilon} - S(\mathcal{G}, \tilde{\varepsilon}) < \beta f(\mathcal{G}, \beta) + \delta. \quad (169)$$

Assume that $\lambda_\alpha \uparrow \mathbb{R}^d$ in the sense of Fisher and $|\lambda_\alpha|^{-1} u_\alpha \rightarrow \mathcal{G}$, and define $\tilde{E}_\alpha = \tilde{\varepsilon} |\lambda_\alpha|$.

We have

$$Q(\lambda_\alpha, u_\alpha, \beta) \geq \frac{1}{u_\alpha!} \int_{\Lambda_\alpha^{u_\alpha}} \mathbb{1}(\mathcal{U}(x_1 \dots x_{u_\alpha}) < \tilde{E}_\alpha) \exp(-\beta \mathcal{U}(x_1 \dots x_{u_\alpha})) d(x_1 \dots x_{u_\alpha})$$

$$> \frac{\exp(-\beta \tilde{E}_\alpha)}{u_\alpha!} \underbrace{\int_{\Lambda_\alpha^{u_\alpha}} \mathbb{1}(\mathcal{U}(x_1 \dots x_{u_\alpha}) < \tilde{E}_\alpha) d(x_1 \dots x_{u_\alpha})}_{\Omega(\lambda_\alpha, u_\alpha, \tilde{E}_\alpha)}$$

α large enough

$$\downarrow \geq \exp\left(|\lambda_\alpha|(-\beta \tilde{\varepsilon} + S(\mathcal{G}, \tilde{\varepsilon}) - \delta)\right) \quad (170)$$

$$> \exp\left(|\lambda_\alpha|(-\beta f(\mathcal{G}, \beta) - 2\delta)\right).$$

Eq. (170) implies

$$\liminf_{\alpha \rightarrow \infty} \frac{1}{|\Lambda_\alpha|} \ln Q(\Lambda_\alpha, u_\alpha, \beta) \geq -\beta f(g, \beta). \quad (171)$$

To obtain a reverse inequality, we write

$$Q(\Lambda_\alpha, u_\alpha, \beta) = \sum_{i=1}^m Q_{i,\alpha} + \tilde{Q}_\alpha \quad \text{with} \quad (172)$$

$$Q_{i,\alpha} = \frac{1}{u_\alpha!} \int_{\Lambda_\alpha^{u_\alpha}} \mathbb{1}(\Xi_i^\alpha < u(x_1 \dots x_{u_\alpha}) \leq \Xi_{i+1}^\alpha) \exp(-\beta \ell(x_1 \dots x_{u_\alpha})) d(x_1 \dots x_{u_\alpha}).$$

Here $\Xi_i^\alpha = |\Lambda_\alpha| \Xi_i$, where $\{\Xi_i\}_{i=1}^{u+1}$ is chosen st.

$$\Xi_1 < \Xi_2 < \dots < \Xi_{u+1}, \quad (173)$$

$\Xi_1 < -g\beta$ and $\beta \Xi_i - S(g, \Xi_{i+1}) > \beta f(g, \beta) - \delta$. Moreover,

$$\tilde{Q}_\alpha \leq \frac{|\Lambda_\alpha|^{u_\alpha}}{u_\alpha!} \exp(-\beta \Xi_{u+1}^\alpha). \quad (174)$$

To proceed with our analysis we need the following Lemma.

Lemma 3.4.3.1. : Assume that $\lambda_\alpha \uparrow \mathbb{R}^d$ in the

sense of Fisher, $\frac{u_\alpha}{|\lambda_\alpha|} \rightarrow g$, $\frac{E_\alpha}{|\lambda_\alpha|} \rightarrow \varepsilon$ and that (g, ε) , $(g, \varepsilon - \delta) \in \Theta$ for $\delta > 0$. Then we have

$$\lim_{\alpha \rightarrow \infty} \frac{1}{|\lambda_\alpha|} \Omega^{S|\lambda_\alpha|}(\lambda_\alpha, u_\alpha, E_\alpha) = S(g, \varepsilon).$$

More precisely,

$$\begin{aligned} \frac{1}{|\lambda_\alpha|} \ln \Omega^{S|\lambda_\alpha|}(\lambda_\alpha, u_\alpha, E_\alpha) &= \frac{1}{|\lambda_\alpha|} \ln \Omega(\lambda_\alpha, u_\alpha, E_\alpha) \quad (175) \\ &\quad + \frac{1}{|\lambda_\alpha|} \ln(1 - \exp(-|\lambda_\alpha| R_\alpha(g, \varepsilon, \delta))) \end{aligned}$$

where the function R_α obeys the bounds

$$\begin{aligned} 2 \left[S(g, \varepsilon - \delta) - S(g, \varepsilon) \right] &\leq R_\alpha(g, \varepsilon, \delta) \quad (176) \\ &\leq \frac{1}{2} \left[S(g, \varepsilon - \delta) - S(g, \varepsilon) \right]. \end{aligned}$$

Remarks. $\square$ Eq. (175) is a direct consequence of (176).

□ This answers the question on p. 77 for $\Delta_\alpha = |\lambda_\alpha| \delta$.

Our proof does not work for fixed Δ s.t. $\frac{\Delta}{|\lambda_\alpha|} \rightarrow 0$ for $\alpha \rightarrow \infty$.

Proof: We have

$$\Omega(\lambda, u, E) = \Omega(\lambda, u, E - \Delta) + \Omega^\Delta(\lambda, u, E) \quad (177)$$

$\Leftrightarrow$

$$\Omega^\Delta(\lambda, u, E) = \Omega(\lambda, u, E) \left(1 - \frac{\Omega(\lambda, u, E - \Delta)}{\Omega(\lambda, u, E)} \right)$$

$\Rightarrow$

$$\begin{aligned} \frac{1}{|\lambda|} \ln \Omega^\Delta(\lambda, u, E) &= \frac{1}{|\lambda|} \ln \Omega(\lambda, u, E) \\ &\quad + \frac{1}{|\lambda|} \ln \left(1 - \frac{\Omega(\lambda, u, E - \Delta)}{\Omega(\lambda, u, E)} \right). \end{aligned}$$

Assume that $\lambda_\alpha \uparrow \mathbb{R}^d$ in the sense of Fisher, $\frac{u_\alpha}{|\lambda_\alpha|} \rightarrow g$,

$\frac{E_\alpha}{|\lambda_\alpha|} \rightarrow \varepsilon$ and that $(g, \varepsilon), (g, \varepsilon - \delta) \in \Theta$, $\delta > 0$. Then we have

$$\begin{aligned} \frac{1}{|\lambda_\alpha|} \ln \Omega^{S|\lambda_\alpha|}(\lambda_\alpha, u_\alpha, E_\alpha) &= \frac{1}{|\lambda_\alpha|} \ln \Omega(\lambda_\alpha, u_\alpha, E_\alpha) \\ &+ \frac{1}{|\lambda_\alpha|} \ln \left(1 - \exp \left(S(\lambda_\alpha, u_\alpha, E_\alpha - |\lambda_\alpha| S) - S(\lambda_\alpha, u_\alpha, E_\alpha) \right) \right), \end{aligned} \quad (178)$$

where the first term on the r.h.s. converges to $S(g, \varepsilon)$ for $\alpha \rightarrow \infty$. The exponent in the second term can be written as

$$\begin{aligned} &S(\lambda_\alpha, u_\alpha, E_\alpha - |\lambda_\alpha| S) - S(\lambda_\alpha, u_\alpha, E_\alpha) \\ &= |\lambda_\alpha| \left(S(g, \varepsilon - s) - S(g, \varepsilon) \right. \\ &\quad + \frac{S(\lambda_\alpha, u_\alpha, E_\alpha - s|\lambda_\alpha|)}{|\lambda_\alpha|} - S(g, \varepsilon - s) \\ &\quad \left. - \frac{S(\lambda_\alpha, u_\alpha, E_\alpha)}{|\lambda_\alpha|} + S(g, \varepsilon) \right). \end{aligned} \quad (179)$$

Accordingly, there exists $\alpha_0 \in \mathbb{N}$ s.t.

$$\begin{aligned} 2|\lambda_\alpha| \left[S(g, \varepsilon - s) - S(g, \varepsilon) \right] &\leq S(\lambda_\alpha, u_\alpha, E_\alpha - |\lambda_\alpha| S) - S(\lambda_\alpha, u_\alpha, E_\alpha) \quad (180) \\ &\leq \frac{1}{2} |\lambda_\alpha| \left[S(g, \varepsilon - s) - S(g, \varepsilon) \right] \end{aligned}$$

holds for $\alpha \geq \alpha_0$. When we define

$$R_\alpha(\mathcal{Q}, \varepsilon, \delta) = \frac{1}{|\Lambda_\alpha|} \left(S(\lambda_\alpha, \mu_\alpha, E_\alpha - |\Lambda_\alpha| \delta) - S(\lambda_\alpha, \mu_\alpha, E_\alpha) \right) \quad (181)$$

this proves the claim. $\square$

Let's continue with the upper bound for the free energy.

We write

$$\frac{1}{|\Lambda_\alpha|} \ln \left(\sum_{i=1}^m \underbrace{Q_{i,\alpha}} + \tilde{Q}_\alpha \right) \quad (182)$$

$$= \frac{1}{|\Lambda_\alpha|} \int_{\Lambda_\alpha^{\mu_\alpha}} \underbrace{\mathbb{1}(E_i^\alpha < \mathcal{H}(x_1, \dots, x_\alpha) \leq E_{i+1}^\alpha)}_{\downarrow} \underbrace{\exp(-\beta \mathcal{H}(x_1, \dots, x_\alpha))}_{d(x_1, \dots, x_\alpha)}$$

$$\leq \exp(-\beta E_i^\alpha)$$

$$\leq \exp(-\beta E_i^\alpha) \underbrace{\Omega^{\vec{E}_{i+1}^\alpha - E_i^\alpha}(\lambda_\alpha, \mu_\alpha, E_{i+1}^\alpha)}$$

$$\stackrel{\text{Lemma 3.4.3.1}}{\rightarrow} = \underbrace{\Omega(\lambda_\alpha, \mu_\alpha, E_{i+1}^\alpha)}_{\exp(S(\lambda_\alpha, \mu_\alpha, E_{i+1}^\alpha))} \left(1 - \exp(|\Lambda_\alpha| R_\alpha(\mathcal{Q}, \varepsilon_{i+1}, \varepsilon_{i+1} - \varepsilon_i)) \right)$$

$$= \exp\left(-|\lambda_\alpha| \left(\underbrace{\beta \varepsilon_i - S(\mathcal{S}, \varepsilon_{i+1})}_{(1)} + \underbrace{S(\mathcal{S}, \varepsilon_{i+1}) - \frac{S(\lambda_\alpha, \mu_\alpha, E_{i+1}^\kappa)}{|\lambda_\alpha|}}_{(2)} \right)\right) \quad 97$$

$$\times \left(1 - \exp(|\lambda_\alpha| R_\alpha(\mathcal{S}_\alpha, \varepsilon_{i+1}, \varepsilon_{i+1} - \varepsilon_i))\right).$$

By our choice of $\{\varepsilon_i\}_{i=1}^m$ we have

$$(1) > \beta f(\mathcal{S}, \beta) - \delta, \quad (183)$$

$$(2) > -\delta \text{ for } \alpha \geq \alpha_0 \text{ and } \alpha_0 \in \mathbb{N} \text{ (uniformly in } i=1, \dots, m).$$

Accordingly,

$$\frac{1}{|\lambda_\alpha|} \ln \left(\sum_{i=1}^m Q_{i,\alpha} + \tilde{Q}_\alpha \right) \leq \frac{1}{|\lambda_\alpha|} \ln \left[m \exp\left(-|\lambda_\alpha| \left(\beta f(\mathcal{S}, \beta) - 2\delta \right)\right) \times \right. \quad (184)$$

$$\left. \left(1 - \exp\left(2|\lambda_\alpha| \max_{i=1, \dots, m} \left\{ S(\mathcal{S}, \varepsilon_i) - S(\mathcal{S}, \varepsilon_{i+1}) \right\} \right) \right) \right. \\ \left. + \tilde{Q}_\alpha \right) \geq -C/2$$

$$\leq -\beta f(\mathcal{S}, \beta) + 2\mathcal{S} + \frac{1}{|\Lambda_2|} \ln \left(1 - \exp(-c|\Lambda_2|) \right) + \frac{1}{|\Lambda_2|} \ln(u) \\ + \frac{1}{|\Lambda_2|} \ln \left(1 - \frac{\tilde{Q}_\alpha}{\underbrace{\left(1 - \exp(-c|\Lambda_2|) \right)}_{(*)} u} \exp(|\Lambda_2|(\beta f(\mathcal{S}, \beta) - 2\mathcal{S})) \right)$$

Using (174), we easily check that $(*)$ behaves as $\exp(-\tilde{c}|\Lambda_2|)$ for some $\tilde{c} > 0$ as long as $\tilde{\mathcal{E}}_{m+1}$ is chosen large enough.

This proves

$$\limsup_{\alpha \rightarrow \infty} \frac{1}{|\Lambda_2|} \ln Q(\Lambda_2, \Lambda_2, \beta) \leq -\beta f(\mathcal{S}, \beta) + 2\mathcal{S} \quad (185)$$

for all $\mathcal{S} > 0$ (and therefore for $\mathcal{S} = 0$). In combination with (171), it shows

$$\lim_{\alpha \rightarrow \infty} \frac{1}{|\Lambda_2|} \ln Q(\Lambda_2, \Lambda_2, \beta) = -\beta f(\mathcal{S}, \beta). \quad (186)$$

Analogue results can be obtained when $\frac{1}{|\Lambda_2|} u_2 \geq \beta_{cp}$ but we do not discuss the details. We collect our findings

in the following Theorem.

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Theorem 8.4.4.2 : The function $f(s, \beta)$ defined

for $0 \leq s < s_{cp}$ and $\beta > 0$ by

$$f(s, \beta) = \inf_{\varepsilon \in \varepsilon_0(s)} \{ \varepsilon - \beta^{-1} s(s, \varepsilon) \} \quad (187)$$

is a concave function of β^{-1} and a convex function of s , $s^{-1} f(s, \beta)$ is a convex and decreasing function of s^{-1} .

Let $\lambda_n \in \mathbb{R}^d$ in the sense of Fisher and $\frac{1}{|\lambda_n|} u_n \rightarrow s$.

(a) If $0 \leq s < s_{cp}$ then $\lim_{n \rightarrow \infty} \frac{1}{|\lambda_n|} \ln Q(\lambda_n, u_n, \beta) = -\beta f(s, \beta)$

(b) If $s = s_{cp}$ then $\limsup_{n \rightarrow \infty} \frac{1}{|\lambda_n|} \ln Q(\lambda_n, u_n, \beta) \leq -\beta f^*(\beta)$,

where $f^*(\beta) = \lim_{\substack{s \rightarrow s_{cp} \\ s < s_{cp}}} f(s, \beta).$

(c) If $s > s_{cp}$ then $\lim_{n \rightarrow \infty} \frac{1}{|\lambda_n|} \ln Q(\lambda_n, u_n, \beta) = -\infty.$

Remarks: $\square$ The function f is known as specific free energy (free energy per unit volume). The free energy per particle $\rho^{-1}f(s, \beta)$ is a decreasing function of ρ^{-1} because $Q(1, u, \beta)$ is, for fixed u, β , an increasing function of $|A|$.

$\square$ Eq. (187) establishes a relation between the parameters of the canonical and the microcanonical ensemble.

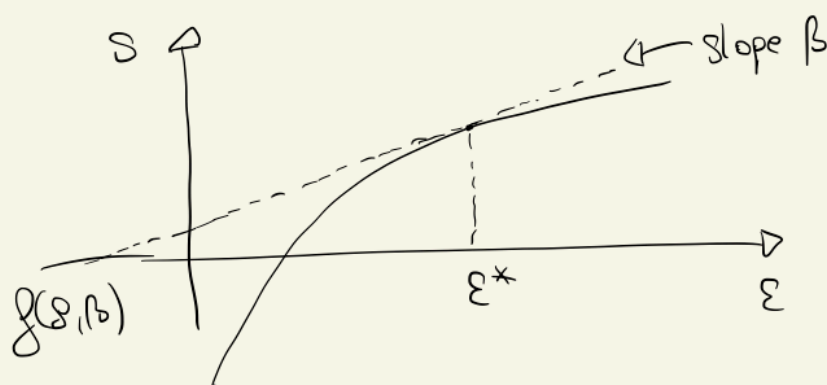


fig. 3

Assuming differentiability (because of convexity derivatives exist almost everywhere) we obtain the following standard thermodynamic relations

$$f(\beta, g) = \varepsilon^* - \beta^{-1} S(g, \varepsilon^*), \quad (188)$$

$$\beta = \frac{\partial S(g, \varepsilon^*)}{\partial \varepsilon^*},$$

$$S(g, \varepsilon^*) = \beta^2 \frac{\partial f(g, \beta)}{\partial \beta}.$$

This concludes our discussion of the canonical ensemble.
Next, we consider the grand canonical ensemble.

3.4.4. Grand canonical ensemble

The grand canonical partition function is given by

$$\Theta(\lambda, z, \beta) = 1 + \sum_{u \geq 1} \frac{e^{\beta \mu u}}{u!} \int_{\mathbb{R}^{du} \times \Lambda^u} \exp(-\beta (\sum_{i=1}^u p_i^2 + \ell(x_1, \dots, x_u))) d(p_1, \dots, p_u) d(x_1, \dots, x_u)$$

$$= \sum_{u=0}^{\infty} z^u Q(\lambda, u, \beta), \quad (189)$$

with the activity

$$z = \left(\frac{\pi}{\beta}\right)^{d/2} e^{\beta\mu}. \quad (190)$$

Here we used $Q(1,0,\beta) = 1$. The pressure of the system is defined by

$$p(z,\beta) = \sup_{0 \leq \beta \leq \beta_{cp}} \left\{ \beta^{-1} \ln(z) - f(\beta, \beta) \right\}. \quad (191)$$

It is a convex function of $\ln(z)$ and β . The supremum in (191) is reached if the slope of a tangent to the curve $\beta \mapsto f(\beta, \beta)$ has the value $\beta^{-1} \ln(z)$ for $\beta = \beta^*$; $-\beta p(z, \beta)$ is the ordinate of the intersection of this tangent with the β axis, see fig. 10 below.

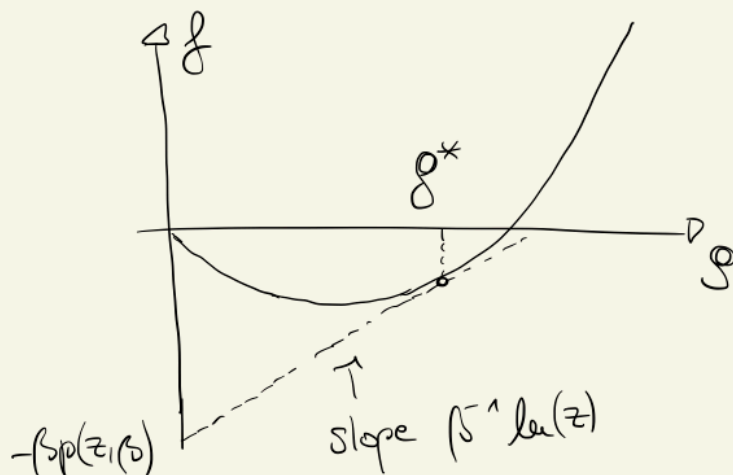


fig. 10

Assume that $\lambda_\alpha \uparrow \mathbb{R}^d$ in the sense of Fisher. For given $S > 0$ we can find $\tilde{g} \in [0, g_{\text{cr}})$ s.t.

$$\beta^{-1} \tilde{g} \ln(z) - f(\tilde{g}, \beta) \geq p(z, \beta) - \beta^{-1} S. \quad (192)$$

We choose $\tilde{u}_\alpha = \tilde{g} / |\lambda_\alpha|$ and note that

$$\Theta(\lambda_\alpha, z, \beta) \geq z^{\tilde{u}_\alpha} Q(\lambda_\alpha, \tilde{u}_\alpha, \beta) \quad (193)$$

as well as for given $S > 0$

$$Q(\lambda_\alpha, \tilde{u}_\alpha, \beta) = \exp(\ln Q(\lambda_\alpha, \tilde{u}_\alpha, \beta)) \quad (194)$$

$$= \exp(-|\lambda_\alpha| \beta f(\tilde{g}, \beta) + \ln Q(\lambda_\alpha, \tilde{u}_\alpha, \beta) + |\lambda_\alpha| \beta f(\tilde{g}, \beta))$$

$$\alpha \gg \alpha_0(S)$$

$\downarrow$

$$\geq \exp(-|\lambda_\alpha| (\beta f(\tilde{g}, \beta) + S))$$

$$\stackrel{(192)}{\rightarrow} \geq \exp(|\lambda_\alpha| (\beta p(z, \beta) - 2S)) \exp(-|\lambda_\alpha| \beta \tilde{g} \ln(z)).$$

$$\text{Since } \exp(-|\lambda_\alpha| \tilde{g} \ln(z)) \underbrace{z^{\tilde{u}_\alpha}}_{\exp(\tilde{u}_\alpha \ln(z))} = \exp(-|\lambda_\alpha| \tilde{g} \ln(z) + |\lambda_\alpha| \tilde{g} \ln(z)) = 1$$

we thus have

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$$\Theta(\lambda, z, \beta) \geq \exp(|\lambda|(\rho(z, \beta) - 2\beta)), \quad (195)$$

which implies

$$\liminf_{\alpha \rightarrow \infty} \frac{1}{|\lambda|} \log \Theta(\lambda, z, \beta) \geq \beta \rho(z, \beta). \quad (196)$$

Let's look for a reverse inequality. The stability condition implies

$$z^n Q(\lambda, n, \beta) \leq \frac{1}{n!} \left(z |\lambda| e^{\beta\beta} \right)^n \leq \left(z \frac{|\lambda|}{n} e^{\beta\beta+1} \right)^n \quad (197)$$

$$n! \geq \sqrt{2\pi n} n^{n+\frac{1}{2}} e^{-n} \geq n^n e^{-n}$$

$$\Rightarrow \frac{1}{n!} \leq \frac{1}{n^n} e^n$$

We define $v_0 = \frac{1}{2} z^{-1} e^{-\beta\beta-1}$ and note that (197) implies

$$\sum_{n > v_0^{-1} |\lambda|} z^n Q(\lambda, n, \beta) \leq \sum_{n > v_0^{-1} |\lambda|} \left(\frac{1}{2} \right)^n \quad (198)$$

Let $\lambda_\alpha \uparrow \mathbb{R}^d$ in the sense of Fisher, let $\frac{u_\alpha}{|\lambda_\alpha|} \rightarrow g$,
 let $S > 0$ be given and assume that $\frac{u_\alpha}{|\lambda_\alpha|} \in [0, v_0^{-1}]$.

There exists $\alpha_0(S) \in \mathbb{N}$ s.t. for all $\alpha \geq \alpha_0$ we have

$$\begin{aligned} z^{u_\alpha} Q(\lambda_\alpha, u_\alpha, \beta) &= \exp\left(|\lambda_\alpha| \left(\frac{u_\alpha}{|\lambda_\alpha|} \log(z) - \beta f\left(\frac{u_\alpha}{|\lambda_\alpha|}, \beta\right) \right. \right. \\ &\quad \left. \left. + \log Q(\lambda_\alpha, u_\alpha, \beta) + |\lambda_\alpha| \beta f\left(\frac{u_\alpha}{|\lambda_\alpha|}, \beta\right) \right) \right) \\ &\leq \exp\left(|\lambda_\alpha| \left(\beta \rho(z, \beta) + S \right)\right). \end{aligned} \quad (199)$$

In combination, (198) and (199) imply

$$\begin{aligned} \Theta(\lambda_\alpha, z, \beta) &\leq v_0^{-1} |\lambda_\alpha| \exp\left(|\lambda_\alpha| \left(\beta \rho(g, \beta) + S \right)\right), \\ &\quad + \sum_{u > v_0^{-1} |\lambda_\alpha|} \left(\frac{1}{2}\right)^u \end{aligned} \quad (200)$$

and hence

$$\limsup_{\alpha \rightarrow \infty} \frac{1}{|\lambda_\alpha|} \log \Theta(\lambda_\alpha, z, \beta) \leq \beta \rho(z, \beta). \quad (201)$$

We collect our findings in the following Theorem.

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Theorem 3.4.4.1: For $z > 0$ and $\beta > 0$ let

$$\rho(z, \beta) = \sup_{0 \leq g < g_\infty} \{ \beta^{-1} g \log z - f(g, \beta) \}. \quad (202)$$

$\beta \rho(z, \beta)$ is a convex function of $\log(z)$ and β , $\rho(z, \beta) \geq 0$ and $z \mapsto \rho(z, \beta)$ is increasing.

Let $\lambda_\alpha \uparrow \mathbb{R}^d$ in the sense of Fisher, then

$$\lim_{\alpha \rightarrow \infty} \frac{1}{|\lambda_\alpha|} \log \Theta(\lambda_\alpha, z, \beta) = \beta \rho(z, \beta). \quad (203)$$

Remark: Assuming differentiability we have the following thermodynamic relations

$$\begin{aligned} \beta \rho(z, \beta) &= g^* \log(z) - \beta f(g^*, \beta), \\ \beta^{-1} \log z &= \frac{\partial f(g^*, \beta)}{\partial g^*}, \quad \text{and} \\ g^* &= \frac{\partial(\beta \rho(z, \beta))}{\partial(\log z)}. \end{aligned} \quad (204)$$

This ends our discussion of the existence of the
thermodynamic limit for thermodynamic functions
and the equivalence of the ensembles.