

# Statistical Mechanics of the Isothermal Lane–Emden Equation

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For classical point particles in a box  $\Lambda$  with potential energy  $H^{(N)} = N^{-1}(1/2) \sum_{i \neq j=1}^N V(x_i, x_j)$  we investigate the canonical ensemble for large  $N$ . We prove that as  $N \rightarrow \infty$  the correlation functions are determined by the global minima of a certain free energy functional. Locally the distribution of particles is given by a superposition of Poisson fields. We study the particular case  $\Lambda = [-\pi L, \pi L]$  and  $V(x, y) = -\beta \cos(x - y)$ ,  $L > 0$ ,  $\beta > 0$ .

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**KEY WORDS:** Classical point particles; Lane–Emden equation; canonical ensemble; instable interactions; mean field limit; equilibrium states.

## 1. INTRODUCTION

Let us consider a finite box  $\Lambda$  into which more and more classical point particles are thrown. To keep the energy of all particles proportional to their number we assume a potential energy of the form

$$H^{(N)} = N^{-1} \frac{1}{2} \sum_{i \neq j=1}^N V(x_i, x_j) \quad (1.1)$$

This corresponds to a weak, as  $1/N$ , interaction. The particles are distributed inside the box according to the canonical ensemble  $Z(N)^{-1} \exp[-\beta H^{(N)}]$ . We want to know then the structure of typical particle configurations for large  $N$ .

The motivation for this work is fourfold.

(i) The particular case of gravitating particles,  $V(x, y) = -\kappa|x - y|^{-1}$ , has been studied extensively.<sup>(1-4)</sup> The canonical ensemble is expected

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to model either the distributions of stars in a star cluster or in a galaxy or the distribution of the galaxies themselves. Formally in the limit as  $N \rightarrow \infty$  the potential  $\psi$  generated by the mass distribution is determined by the isothermal Lane–Emden equation

$$\Delta\psi = 4\pi\kappa e^{-\beta\psi} \quad (1.2)$$

cf. Ref. 5 for a discussion of this and related equations and for an historical account. For a statistical mechanics derivation of that equation one has to confine the system to a box and has to smoothen out the local singularity of the gravitational potential.

(ii) In the temperature-dependent Thomas–Fermi theory one considers fermions in  $\Lambda$  with the scaled quantum mechanical Hamiltonian<sup>(6–8)</sup>

$$H^{(N)} = N^{-2/3} \sum_{j=1}^N (2m)^{-1} p_j^2 + N^{-1} \frac{1}{2} \sum_{i \neq j=1}^N V(x_i, x_j) \quad (1.3)$$

(The spatial scale is here chosen already as the one on which the Thomas–Fermi density varies.) The cases of physical interest are when  $V$  is either the gravitational potential or the electronic repulsive Coulomb potential together with the external potential provided by the nuclei. In the latter case usually the ground state, corresponding to  $\beta = \infty$ , is considered. Our problem is then the classical counterpart to the usual Thomas–Fermi theory.

(iii) If the potential  $V$  is not stable, as is the case for the gravitational potential, then the usual thermodynamic limit does not exist. The scaling (1.1) offers a possibility of still to investigate the canonical distribution for large  $N$ .

(iv) The dynamics of classical particles interacting through the potential (1.1) for large  $N$  has been investigated in Refs. 9–11. In this limit the particle density in the one particle phase space is governed by the Vlasov equation. We study here the static problem.

In statistical mechanics the problem we posed is well known as a mean field limit, because a given particle should roughly see the mean potential field produced by all the other particles. This kind of limit has been extensively studied; cf. Refs. 12 and 13 as review articles. Therefore, first of all, we have to explain why we think that our problem has not yet been covered.

In the van der Waals limit for a continuous particle system one takes first the thermodynamic limit and subsequently the limit of a weak force. The idea behind is that the weak part of the potential has still a range which is small compared to the size of the system. In our case the size of the system and the range of the potential are of the same order. Consequently no comparable results can be expected.

Although rather unnatural from a physical point of view, we may

think of (1.1) as the Hamiltonian of a one-dimensional spin system. The single-site space is then  $(\Lambda, dx)$ . In this context our problem has been studied for the particular case  $V(x_i, x_j) = x_i x_j$ .<sup>(1, 13–15, 19)</sup> These models are referred to as Curie–Weiss models. The limit  $N \rightarrow \infty$  is proved using the sine–Gordon transformation.<sup>(15)</sup> Our argument is based on the subadditivity of entropy and works for a general class of potentials. In other work<sup>(13, 14)</sup> one assumes certain conditions (as KMS) that the infinite volume equilibrium state has to satisfy and investigates then the class of solutions. This procedure has two drawbacks. Firstly, it leaves open the connection to the original finite  $N$  problem. Secondly, by this method it seems hard to rule out solutions which are stationary points of the free energy but not global minima.

One can also consider the lattice gas approximation to (1.1), i.e.,  $\Lambda$  is replaced by a lattice with lattice spacing  $1/N$  and there is at most one particle per lattice site. For  $\Lambda = [0, 1]$  our model is then a special case of the circle model with single-site measure  $\delta_0 + \delta_1$ . If  $V(x, y)$  is positive definite the circle model has been investigated in Refs. 20 and 21 and for general  $V$  in the recent preprint Ref. 22. Of course, the mean field equation for the circle model with single-site measure  $\delta_0 + \delta_1$  turns out to be identical to ours. The proof in Ref. 22 uses however Laplace’s method in function space.

We will show that the mass distribution is, in the limit  $N \rightarrow \infty$ , a superposition of the *global minima* of the free energy functional

$$\begin{aligned}
 F(\rho) &= \frac{1}{2} \int_{\Lambda} \int_{\Lambda} dx dy \rho(x) \rho(y) V(x, y) + \beta^{-1} \int_{\Lambda} dx \rho(x) \log \rho(x) \\
 \rho &\geq 0, \quad \int_{\Lambda} dx \rho(x) = 1
 \end{aligned}
 \tag{1.4}$$

Stationary points of  $F$  satisfy the appropriate generalization of the Lane–Emden equation. Locally the distribution of particles is a superposition of Poisson fields. On the superposition itself, in general, we have no information. Typical cases where it can be determined are when either the minimum of  $F$  is unique or certain symmetries are present.

This result leaves open to determine the global minima of  $F$ . We will prove that for potentials of positive type  $F$  has a unique minimum and that, in general, for sufficiently small  $V$ , i.e., at high temperatures,  $F$  has a unique minimum. At low temperatures one expects the occurrence of several global minima corresponding to the existence of a phase transition.

To have an example for this phenomenon we investigate a one-dimensional system in the box  $\Lambda = [-\pi L, \pi L]$  with the interaction potential  $V(x, y) = -\beta \cos(x - y)$ ,  $\beta > 0$ ,  $L > 0$ . (Note that this potential is unstable.) If  $L$  is not an integer, then  $F$  has a unique minimum. If  $L$  is an integer, then for  $\beta \leq 2$   $F$  has a unique minimum and the mass is uniformly

distributed over the box. For  $\beta > 2$  the system clusters. Since the location of the cluster is not fixed, the mass distribution is a uniform superposition over all possible locations.

## 2. WEAK CONVERGENCE OF THE CANONICAL DISTRIBUTIONS AS $N \rightarrow \infty$

Let  $\Lambda \subset \mathbb{R}^d$  be compact. We consider  $N$  classical point particles in  $\Lambda$  distributed according to the canonical equilibrium measure

$$\mu^{(N)}(dx_1, \dots, dx_N) = Z(N)^{-1} \exp[-H^{(N)}(x_1, \dots, x_N)] dx_1 \dots dx_N \quad (2.1)$$

The energy of a particle configuration  $(x_1, \dots, x_N) \in \Lambda^N$  is given by

$$H^{(N)}(x_1, \dots, x_N) = N^{-1} \frac{1}{2} \sum_{i \neq j=1}^N V(x_i, x_j) \quad (2.2)$$

We are interested in the limit  $N \rightarrow \infty$ . Then the number of particles in every region however small increases proportional to  $N$ . However, because of the mean field scaling (2.2) of the potential, the energy of any given particle remains finite.

For any Borel set  $\Delta \subset \Lambda$  let  $n^{(N)}(\Delta)$  be the number of particles in  $\Delta$ . The superscript  $(N)$  indicates that the random variables  $n^{(N)}(\Delta)$  depend on  $N$  through the probability distribution  $\mu^{(N)}$ . Our goal is to investigate the random field

$$\left\{ \frac{1}{N} n^{(N)}(\Delta) / \Delta \subset \Lambda \right\} \quad (2.3)$$

as  $N \rightarrow \infty$ . We will show that the limit field is supported by those absolutely continuous mass distributions which minimize the free energy functional (1.4). Locally the limit field is a generally nondegenerate superposition of Poisson fields.

Let  $\Omega = \Lambda^{\mathbb{N}}$ . We consider  $\mu^{(N)}$  as a probability measure on  $\Omega$  and investigate the weak limit of  $\mu^{(N)}$  as  $N \rightarrow \infty$ . From this the claimed properties of the random field  $\{(1/N)n^{(N)}(\Delta)\}$  will be deduced. The proof is based on two observations:

(i) Any weak limit point of  $\{\mu^{(N)}/N = 1, 2, \dots\}$  is a permutation invariant measure on  $\Lambda^{\mathbb{N}}$ . The Hewitt–Savage decomposition theorem ensures then that any limit measure is an integral over product measures.

(ii) By subadditivity of the entropy the free energy per particle exists as  $N \rightarrow \infty$  and equals the free energy of any limit point of  $\{\mu^{(N)}/N = 1, 2, \dots\}$ .

(i) combined with (ii) implies the desired support properties. In specific examples one often has additional information, such as symmetry, which

ensures the weak convergence of  $\mu^{(N)}$  and as a consequence the weak convergence of the random field  $\{(1/N)n^{(N)}(\Delta)\}$ .

The potential is assumed to have the following two properties (a)  $V$  is symmetric, i.e.,  $V(x, y) = V(y, x)$ , and (b)  $V$  is Lipschitz continuous, i.e.,

$$|V(x, y) - V(x', y')| \leq L(|x - x'| + |y - y'|) \tag{2.4}$$

Since  $\Lambda$  is compact, by (2.4),  $\sup|V(x, y)| = M_+$  is finite. Lipschitz continuity is a somewhat restrictive assumption. For our technique we need it in order to be able to conclude from the weak convergence of the  $n$ th marginal distribution the convergence of its entropy.

Let

$$f_n^{(N)}(x_1, \dots, x_n) = Z(N)^{-1} \int dx_{n+1} \dots dx_N \exp[-H^{(N)}(x_1, \dots, x_N)] \tag{2.5}$$

be the density of the  $n$ th marginal measure,  $f_n^{(N)}(x_1, \dots, x_n) dx_1 \dots dx_n = \mu_n^{(N)}(dx_1 \dots dx_n)$ .

**Lemma 1.** For each  $n, N$  with  $1 \leq n < N$  and for each  $n$ -tuple  $(x_1, \dots, x_n) \in \Lambda^n$

$$0 \leq f_n^{(N)}(x_1, \dots, x_n) \leq |\Lambda|^{-n} \exp(2nM_+) \tag{2.6}$$

where  $|\Lambda|$  denotes the volume of  $\Lambda$ .

*Proof.* Let  $\tilde{H}^{(n)}(x_1, \dots, x_n) = (1/N)(1/2)\sum_{i \neq j=1}^n V(x_i, x_j)$ ,  $\tilde{H}^{(N-n)}(x_{n+1}, \dots, x_N) = (1/N)(1/2)\sum_{i \neq j=n+1}^N V(x_i, x_j)$ , and  $W^{(n, N-n)}(x_1, \dots, x_N) = (1/N)\sum_{i=1}^n \sum_{j=n+1}^N V(x_i, x_j)$ . Then

$$\begin{aligned} f_n^{(N)}(x_1, \dots, x_n) &\leq Z(N)^{-1} \int dx_{n+1} \dots dx_N \exp(-\tilde{H}^{(n)} - W^{(n, N-n)} - \tilde{H}^{(N-n)}) \\ &\leq e^{nM_+} Z(N)^{-1} \int dx_{n+1} \dots dx_N \exp(-\tilde{H}^{(N-n)}) \end{aligned} \tag{2.7}$$

By Jensen’s inequality

$$\begin{aligned} &[|\Lambda|^{-n} \int dx_1 \dots dx_N \exp(-\tilde{H}^{(N-n)})]^{-1} \\ &\quad \times \int dx_1 \dots dx_N \exp(-\tilde{H}^{(n)} - W^{(n, N-n)} - \tilde{H}^{(N-n)}) \\ &\geq |\Lambda|^n \exp\left\{-\int dx_1 \dots dx_N (\tilde{H}^{(n)} + W^{(n, N-n)}) \exp(-\tilde{H}^{(N-n)})\right. \\ &\quad \left. \times \left[\int dx_1 \dots dx_N \exp(-\tilde{H}^{(N-n)})\right]^{-1}\right\} \\ &\geq |\Lambda|^n \exp(-nM_+) \quad \blacksquare \end{aligned} \tag{2.8}$$

**Lemma 2.** There exist positive numbers  $M$  and  $a$ , such that for all  $n < N$  and  $(x_1, \dots, x_n), (y_1, \dots, y_n) \in \Lambda^n$

$$|f_n^{(N)}(x_1, \dots, x_n) - f_n^{(N)}(y_1, \dots, y_n)| \leq Ma^n \sum_{j=1}^n |x_j - y_j| \quad (2.9)$$

with  $M, a$  independent of  $n$  and  $N$ .

*Proof.* We reformulate

$$\begin{aligned} & |f_n^{(N)}(x_1, \dots, x_n) - f_n^{(N)}(y_1, \dots, y_n)| \\ &= \left| \int_0^1 dt Z(N)^{-1} \int dx_{n+1} \dots dx_N \right. \\ &\quad \times \exp \left[ -tH^{(N)}(y_1, \dots, y_n, x_{n+1}, \dots, x_N) \right. \\ &\quad \left. \left. - (1-t)H^{(N)}(x_1, \dots, x_N) \right] \right. \\ &\quad \left. \times \left\{ H^{(N)}(x_1, \dots, x_N) - H^{(N)}(y_1, \dots, y_n, x_{n+1}, \dots, x_N) \right\} \right| \end{aligned} \quad (2.10)$$

By (2.4)

$$|H^{(N)}(x_1, \dots, x_N) - H^{(N)}(y_1, \dots, y_n, x_{n+1}, \dots, x_N)| \leq L \sum_{j=1}^n |x_j - y_j| \quad (2.11)$$

The remaining estimate is identical to the one of Lemma 1. ■

Let  $\mathfrak{S}$  be the set of all probability measures on  $\Lambda^N = \Omega$  which are invariant under permutations, i.e.,  $\mu \in \mathfrak{S}$  if and only if  $\mu(A_1 \times \dots \times A_m) = \mu(A_{p(1)} \times \dots \times A_{p(m)})$  for arbitrary Borel sets  $A_1, \dots, A_m \subset \Lambda$ , all permutations  $p$  and all  $m$ . Let  $\mathfrak{S}_a \subset \mathfrak{S}$  be the set of all permutation invariant measures  $\mu$  on  $\Omega$  such that

$$(i) \quad \mu \uparrow \Lambda^n \equiv \mu_n(dx_1 \dots dx_n) = f_n(x_1, \dots, x_n) dx_1 \dots dx_n$$

(ii) the densities  $f_n$  are Lipschitz continuous with Lipschitz constant  $Ma^n$  in the sense of (2.9) for some  $M$ .

**Lemma 3.** The set of weak limit points of  $\{\mu^{(N)} / N = 1, 2, \dots\}$  is contained in  $\mathfrak{S}_a$ .

*Proof.* Since  $\Lambda$  is compact,  $\Omega$  is compact in the product topology. Therefore any weak limit point is a probability measure and, since  $\mu^{(N)}$  is symmetric, necessarily in  $\mathfrak{S}$ . Let  $\mu_n^{(N)} \rightharpoonup \mu_n$  weakly. Then  $\lim_N f_n^{(N)} = f_n$  pointwise. Therefore  $f_n$  satisfies (2.9). ■

We want to write measures in  $\mathfrak{S}_a$  as integrals over product measures.

Let  $\mathfrak{M}^1$  be the set of all probability measures on  $\Lambda$ . For  $\rho \in \mathfrak{M}^1$  we define the product measure  $\mu_\rho = \rho \times \rho \times \dots$  on  $\Omega$ . According to the theorem of Hewitt and Savage<sup>(16)</sup> to each  $\mu \in \mathfrak{S}$  there exists a unique probability measure  $\nu(d\rho | \mu)$  on  $\mathfrak{M}^1$  such that

$$\mu = \int_{\mathfrak{M}^1} \nu(d\rho | \mu) \mu_\rho \tag{2.12}$$

For the definition of the integral we refer to Ref. 16.

Let  $\mathfrak{M}_a \subset \mathfrak{M}^1$  be the set of all probability measures  $\rho$  on  $\Lambda$  with  $\mu_\rho \in \mathfrak{S}_a$ .

**Lemma 4.** Let  $\mu \in \mathfrak{S}_a$ . Then  $\nu(d\rho | \mu)$  is concentrated on  $\mathfrak{M}_a$ .

*Proof.*  $\mathfrak{S}_a$  is a convex set. We have to show that the extreme points of  $\mathfrak{S}_a$  are the product measures in  $\mathfrak{S}_a$ . Then the claim follows from the proof given in Ref. 16.

Reference 16, Theorem 5.2 implies that  $\mu_\rho$  with  $\rho \in \mathfrak{M}_a$  is an extreme point of  $\mathfrak{S}_a$ . Conversely let  $\mu \in \mathfrak{S}_a$  be an extreme point with  $\mu_n(dx_1 \dots dx_n) = f_n(x_1, \dots, x_n) dx_1 \dots dx_n$ . For some  $\Delta \subset \Lambda$  let us define the probability measures  $\mu^1, \mu^2 \in \mathfrak{S}$  by

$$\begin{aligned} \mu_n^1(dx_1 \dots dx_n) &= \left[ \int_\Delta f_1(x) dx \right]^{-1} \int_\Delta dx f_{n+1}(x, x_1, \dots, x_n) dx_1 \dots dx_n \\ \mu_n^2(dx_1 \dots dx_n) &= \left[ \int_{\Lambda \setminus \Delta} f_1(x) dx \right]^{-1} \int_{\Lambda \setminus \Delta} dx f_{n+1}(x, x_1, \dots, x_n) dx_1 \dots dx_n \end{aligned} \tag{2.13}$$

Clearly,  $\mu^1, \mu^2 \in \mathfrak{S}_a$  and

$$\mu = \left[ \int_\Delta f_1(x) dx \right] \mu^1 + \left[ \int_{\Lambda \setminus \Delta} f_1(x) dx \right] \mu^2 \tag{2.14}$$

Since  $\mu$  is supposed to be extremal, necessarily  $\mu_n^1 = \mu_n^2$  for all  $\Delta$  and  $n$ . This implies  $f_n(x_1, \dots, x_n) = \prod_{j=1}^n f_1(x_j)$  and therefore  $\mu$  is a product measure. ■

We come now to the thermodynamic part of our argument. For  $\mu \in \mathfrak{S}_a$  let

$$S(\mu_n) = - \int dx_1 \dots dx_n f_n(x_1, \dots, x_n) \log f_n(x_1, \dots, x_n) \tag{2.15}$$

be the entropy of the  $n$ th marginal measure. Then the mean entropy of  $\mu$  is defined by

$$s(\mu) = \lim_{n \rightarrow \infty} \frac{1}{n} S(\mu_n) \tag{2.16}$$

Note that for  $\mu \in \mathfrak{S}_a$   $(1/n)S(\mu_n)$  is bounded independently of  $\mu_n$ , since the  $\mu_n$ 's are uniformly bounded and since  $\Lambda$  is compact. Let

$$E(\mu_n) = \mu_n(H^{(n)}) \tag{2.17}$$

be the average energy of  $\mu_n$ . Then the mean energy of  $\mu$  is defined by

$$e(\mu) = \lim_{n \rightarrow \infty} \frac{1}{n} E(\mu_n) \tag{2.18}$$

Finally we define the free energy and the mean free energy by

$$F(\mu_n) = E(\mu_n) - S(\mu_n), \quad f(\mu) = e(\mu) - s(\mu) \tag{2.19}$$

**Lemma 5.** For  $\mu \in \mathcal{S}_a$

$$s(\mu) = \int \nu(d\rho | \mu) s(\mu_\rho) = \int \nu(d\rho | \mu) S(\rho) \tag{2.20}$$

and

$$e(\mu) = \int \nu(d\rho | \mu) e(\mu_\rho) = \frac{1}{2} \int \mu_2(dx_1 dx_2) V(x_1, x_2) \tag{2.21}$$

*Proof.* (2.21) follows from the definition and (2.12). (2.20) is proved in Ref. 17.

**Theorem 1.** Let  $N(k)$  be any subsequence such that  $\lim_{k \rightarrow \infty} \mu^{(N(k))} = \mu$  weakly. Then

$$\lim_{N \rightarrow \infty} \frac{1}{N} F(\mu^{(N)}) = f(\mu) = \inf_{\mu' \in \mathcal{S}_a} f(\mu') \tag{2.22}$$

*Proof.* Since  $\mu^{(N(k))} \rightarrow \mu$  weakly,

$$\lim_{k \rightarrow \infty} \frac{1}{N(k)} E(\mu^{(N(k))}) = e(\mu) \tag{2.23}$$

By subadditivity of entropy for any  $N$  and  $n$

$$\frac{1}{N} S(\mu^{(N)}) \leq \frac{1}{N} \left[ \frac{N}{n} \right] S(\mu_n^{(N)}) + \frac{1}{N} S(\mu_{N-n\lfloor N/n \rfloor}^{(N)}) \tag{2.24}$$

where  $[b]$  stands for the integer part of  $b$ . By Lemma 1  $S(\mu_{N-n\lfloor N/n \rfloor}^{(N)})$  is bounded independently of  $N$ . By Lemma 2 the densities  $f_n^{(N(k))}$  converge pointwise to the limit density  $f_n$ . Therefore

$$\lim_{k \rightarrow \infty} S(\mu_n^{(N(k))}) = S(\mu_n) \tag{2.25}$$

We conclude that

$$\begin{aligned} \limsup_{k \rightarrow \infty} \frac{1}{N(k)} S(\mu^{(N(k))}) &\leq \limsup_{k \rightarrow \infty} \frac{1}{N(k)} \left[ \frac{N(k)}{n} \right] S(\mu_n^{(N(k))}) \\ &= \frac{1}{n} S(\mu_n) \end{aligned} \tag{2.26}$$



Since  $n$  is arbitrary, by definition (2.16)

$$\limsup_{k \rightarrow \infty} \frac{1}{N(k)} S(\mu^{(N(k))}) \leq s(\mu) \tag{2.27}$$

and therefore, by (2.23),

$$\liminf_{k \rightarrow \infty} \frac{1}{N(k)} F(\mu^{(N(k))}) \geq f(\mu) \tag{2.28}$$

On the other hand, by the finite volume variational principle,

$$\frac{1}{N} F(\mu^{(N)}) \leq \inf_{\mu' \in \mathfrak{S}_a} \frac{1}{N} F(\mu'_N) \tag{2.29}$$

Therefore

$$\limsup_{k \rightarrow \infty} \frac{1}{N(k)} F(\mu^{(N(k))}) \leq \inf_{\mu' \in \mathfrak{S}_a} f(\mu') \leq f(\mu) \tag{2.30}$$

(2.28) and (2.30) prove the claim. ■

Let us consider the free energy functional on  $\mathfrak{N}_a$  defined by

$$F(\rho) = f(\mu_\rho) = \frac{1}{2} \int dx dy \rho(x)\rho(y) V(x, y) + \int dx \rho(x) \log \rho(x) \tag{2.31}$$

On  $\mathfrak{N}_a$   $F$  is bounded and continuous in the sup-norm. Let  $\mathfrak{N}_f \subset \mathfrak{N}_a$  be the set of such  $\rho$ 's for which  $F$  takes its global minimum.

**Theorem 2.** Let  $\mu$  be any weak limit point of  $\{ \mu^{(N)} / N = 1, 2, \dots \}$ . Then its decomposition measure  $\nu(d\rho | \mu)$  is concentrated on  $\mathfrak{N}_f$ .

*Proof.* By definition, for all  $\rho \in \mathfrak{N}_f$   $F(\rho) = f = \inf_{\mu' \in \mathfrak{S}_a} f(\mu')$ . Suppose that  $\nu(d\rho | \mu)$  is not concentrated on  $\mathfrak{N}_f$ . Then  $f(\mu) = \int \nu(d\rho | \mu) f(\mu_\rho) > f$  which contradicts Theorem 1. ■

The variational problem to find the minimum of  $F(\rho)$  can be somewhat rephrased. Taking the functional derivative of (2.31) one finds that  $\rho \in \mathfrak{N}_f$  has to satisfy

$$\rho(x) = \exp \left[ - \int dy \rho(y) V(x, y) \right] / \int dx \exp \left[ - \int dy \rho(y) V(x, y) \right] \tag{2.32}$$

$\rho \in \mathfrak{N}_a$ . (2.32) can have solutions which do not minimize  $F(\rho)$ . (Solutions of (2.32) are stationary points of  $F$ .) Therefore in addition one has to require that

$$\tilde{F}(\rho) = - \frac{1}{2} \int dx dy \rho(x)\rho(y) V(x, y) - \log \int dx \exp \left[ - \int dy \rho(y) V(x, y) \right] \tag{2.33}$$

with  $\rho$  solution of (2.32) takes its global minimum.

We will refer to (2.32) *together* with the minimizing condition (2.33) as the Lane–Emden equation (LE equation).

*Remark.* Our proof uses very little of the structure of  $(\Lambda, dx)$ . Theorem 2 remains valid, if  $\Lambda$  is replaced by a complete, separable metric space  $X$  and  $dx$  by a probability measure  $m(dx)$  on  $X$  and provided the potential  $V$  satisfies certain growth conditions. The measure  $\mu^{(N)}$  on  $X^N$  is then given by

$$\mu^{(N)} = Z(N)^{-1} \prod_{j=1}^N m(dx_j) \exp \left[ -\frac{1}{2N} \sum_{i \neq j=1}^N V(x_i, x_j) \right]$$

and  $\rho(x)$  is a density with respect to  $m(dx)$ .

### 3. GLOBAL AND LOCAL STRUCTURE OF THE RANDOM FIELD OF PARTICLES

Physically it is more natural and more transparent to think of particle configurations as a random field over  $\mathbb{R}^d$ .

We facilitate the description by introducing some notation. Let  $\mathcal{S}(\mathbb{R}^d)$  be the space of rapidly decreasing functions and let  $\mathcal{S}'(\mathbb{R}^d)$  be the space of tempered distributions. We equip  $\mathcal{S}'(\mathbb{R}^d)$  with the weak\*-topology. For  $n \in \mathcal{S}'(\mathbb{R}^d)$  and  $g \in \mathcal{S}(\mathbb{R}^d)$  let  $n(g)$  be the linear functional  $n$  evaluated at  $g$ . The functions  $n \mapsto n(g)$  are continuous by definition. To each configuration  $(x_1, \dots, x_N) \in \Lambda^N$  we associate an element of  $\mathcal{S}'(\mathbb{R}^d)$  by

$$S : (x_1, \dots, x_N) \mapsto \frac{1}{N} \sum_{j=1}^N \delta_{x_j} \tag{3.1}$$

where  $\delta_x$  is the Dirac delta distribution at  $x$ . Then  $\mu^{(N)}$  induces a probability measure  $\langle \cdot \rangle_N$  on  $\mathcal{S}'(\mathbb{R}^d)$  by

$$\langle \cdot \rangle_N = \mu^{(N)} \circ S^{-1} \tag{3.2}$$

By definition there are no particles outside  $\Lambda$ , i.e.,  $n(g) = 0 \langle \cdot \rangle_N$ -a.s. for  $g$ 's with support in  $\mathbb{R}^d \setminus \Lambda$ . If necessary we extend functions originally defined only on  $\Lambda$  by zero outside  $\Lambda$ . Note that now all  $N$  dependence is in the measure  $\langle \cdot \rangle_N$ .

We say that  $\langle \cdot \rangle_N$  converges in the sense of moments, if for all  $m, g_1, \dots, g_m \in \mathcal{S}(\mathbb{R}^d)$

$$\lim_{N \rightarrow \infty} \langle n(g_1) \dots n(g_m) \rangle_N = \langle n(g_1) \dots n(g_m) \rangle \tag{3.3}$$

**Proposition 1.** Any limit point of  $\{ \langle \cdot \rangle_N, N = 1, 2, \dots \}$  in the sense of moments is concentrated on  $\mathfrak{M}_f$  considered as a subset of  $\mathcal{S}'(\mathbb{R}^d)$ .

Of interest is also the *local* structure of the random field  $(n(g), \langle \cdot \rangle_N)$ . Let  $q \in \Lambda^0$ . Then we want to consider the particle distribution locally in a

neighborhood of size  $N^{-1/d}$  around  $q$ . The size of this neighborhood shrinks in such a way that its density of particles remains finite. Let  $g \in \mathcal{S}(\mathbb{R}^d)$ . Then we define

$$(\tau_{q,Ng})(x) = Ng(N^{1/d}(x - q)) \tag{3.4}$$

The local measure at  $q$  is defined by

$$\left\langle \prod_{j=1}^m n(g_j) \right\rangle_N(q) = \left\langle \prod_{j=1}^m n(\tau_{q,Ng_j}) \right\rangle_N \tag{3.5}$$

$\langle \cdot \rangle_N(q)$  just describes the local distribution of particles around  $q$ .

**Proposition 2.** Any limit point of  $\{\langle \cdot \rangle_N(q), N = 1, 2, \dots\}$  in the sense of moments is a superposition of Poisson fields with constant density  $\rho(q)$  and weight  $\nu(d\rho | \mu)$ .

*Proof.* One computes that for  $g$ 's with disjoint support

$$\begin{aligned} & \left\langle \prod_{j=1}^m n(g_j) \right\rangle_N(q) \\ &= \int dx_1 \dots dx_m \prod_{j=1}^m \{g_j(x_j)\} \\ & \quad \times f_m^{(N)}(q + N^{-1/d}x_1, \dots, q + N^{-1/d}x_m) + O(1/N) \end{aligned} \tag{3.6}$$

Let  $N(k)$  be a subsequence such that  $\mu^{(N(k))} \rightarrow \mu$  weakly as  $k \rightarrow \infty$ . Then by Lipschitz continuity

$$\begin{aligned} & \lim_{k \rightarrow \infty} f_m^{(N(k))}(q + N(k)^{-1/d}x_1, \dots, q + N(k)^{-1/d}x_m) \\ &= f_m(q, \dots, q) = \int \nu(d\rho | \mu) \rho(q)^m \end{aligned} \tag{3.7}$$

Therefore  $\langle \cdot \rangle_{N(k)}(q) \rightarrow \langle \cdot \rangle(q)$  in the sense of moments and  $\langle \cdot \rangle(q)$  is a superposition of Poisson fields. ■

We have obtained the usual physical picture. As  $N \rightarrow \infty$  the discrete field tends to a continuous field concentrated on such mass distributions which minimize the free energy functional (2.31). Locally the system looks like a superposition of ideal gases with uniform density.

#### 4. UNIQUENESS OF SOLUTIONS

We show that the free energy functional  $F$  [cf. (2.31)] has a unique minimum if either  $V$  is sufficiently small or if  $V$  is of positive type. In the following section we discuss an example where  $F$  has two distinct global minima.

**Theorem 3.** If  $\sup_{x,y}|V(x, y)| < 1/2$ , then (2.32) admits a unique solution  $\rho$ . In this case

$$\text{weak - } \lim_{N \rightarrow \infty} \mu^{(N)} = \mu_\rho \tag{4.1}$$

*Proof.* Let  $K : \mathcal{L}_{+,1}^1(\Lambda) \rightarrow \mathcal{L}_{+,1}^1(\Lambda) = \{\rho \in \mathcal{L}_1(\Lambda) / \rho \geq 0, \|\rho\|_1 = 1\}$  be defined by

$$K(\rho)(x) = Z^{-1} \exp \left[ - \int dy \rho(y) V(x, y) \right] \tag{4.2}$$

We show that, if  $\|V\|_\infty < 1/2$ , then  $K$  is a contraction. Let  $(V\rho)(x) = \int dy \rho(y) V(x, y)$ . Then

$$\begin{aligned} & \|K(\rho_1) - K(\rho_2)\|_1 \\ &= \|\exp(-V\rho_1 - \log Z_1) - \exp(-V\rho_2 - \log Z_2)\|_1 \\ &= \left\| \int_0^1 dt \exp\{ - [(1-t)(V\rho_1 + \log Z_1) + t(V\rho_2 + \log Z_2)] \} \right. \\ &\quad \times (V\rho_1 - V\rho_2 + \log Z_1 - \log Z_2) \Big\|_1 \\ &\leq \int_0^1 dt \left\| [Z_1^{-1} \exp(-V\rho_1)]^{1-t} [Z_2^{-1} \exp(-V\rho_2)]^t \right\|_1 \\ &\quad \times [\|V(\rho_1 - \rho_2)\|_\infty + |\log Z_1 - \log Z_2|] \end{aligned} \tag{4.3}$$

By Hölder inequality

$$\int dx [\varphi_1(x)]^t [\varphi_2(x)]^{1-t} \leq 1 \tag{4.4}$$

for any  $\varphi_1, \varphi_2 \in \mathcal{L}_{+,1}^1(\Lambda)$ . Furthermore

$$\begin{aligned} |\log Z_1 - \log Z_2| &= \left| \log \int dx \exp[-(V\rho_1)(x)] - \log \int dx \exp[-(V\rho_2)(x)] \right| \\ &\leq \|V(\rho_1 - \rho_2)\|_\infty \end{aligned} \tag{4.5}$$

Therefore

$$\|K(\rho_1) - K(\rho_2)\|_1 \leq 2\|V\|_\infty \|\rho_1 - \rho_2\|_1 \tag{4.6}$$

If  $2\|V\|_\infty < 1$ , then  $K$  is a contraction, and  $K(\rho) = \rho$  has a unique solution by the contraction mapping principle. ■

**Theorem 4.** If  $V$  is of positive type, i.e., for each  $f \in \mathcal{L}_2(\Lambda)$

$$\int \overline{f(x)} V(x, y) f(y) dx dy \geq 0 \tag{4.7}$$

then (2.32) admits a unique solution  $\rho$  and (4.1) holds.

*Proof.* With the condition stated, the free energy functional (2.31) is convex. This follows, with (4.7), from the equality

$$\begin{aligned} & \int \rho_\alpha(x)\rho_\alpha(y)V(x,y) dx dy \\ &= \alpha \int \rho_1(x)\rho_1(y)V(x,y) dx dy + (1-\alpha) \int \rho_2(x)\rho_2(y)V(x,y) dx dy \\ & \quad - \alpha(1-\alpha) \int [\rho_2(x) - \rho_1(x)] V(x,y) [\rho_2(y) - \rho_1(y)] dx dy \end{aligned} \tag{4.8}$$

with

$$\rho_\alpha = \alpha\rho_1 + (1-\alpha)\rho_2, \quad \alpha \in [0, 1]$$

and from the concavity of the entropy functional. On  $\mathcal{E}_{+,1}^1$  the free energy functional is even strictly convex, proving uniqueness of extrema. A second proof follows by considering the second functional derivative of  $F(\rho)$ , which is a functional of positive type, by (4.7), for all  $\rho \geq 0$ . This contradicts the existence of a local maximum in case of two global minima of  $F(\rho)$ .

### 5. THE COSINE MODEL

We investigate the LE equation for particles in the interval  $[-\pi L, \pi L] = \Lambda$  interacting through the pair potential

$$V(x,y) = -\beta \cos(x-y) \tag{5.1}$$

This “cosine model” was suggested in Ref. 14. It seems to be one of the simplest models with a *continuous* potential which exhibits a phase transition. The thermodynamic parameters are  $L > 0$  and  $\beta \in \mathbb{R}$ . For  $\beta < 0$  the potential (5.1) is of positive type and therefore, by Theorem 4, the LE equation has a unique solution. Despite the fact that the potential does not decay at infinity, the usual thermodynamic limit exists. The thermodynamic functions are identical to those of the ideal gas.<sup>(18)</sup> Henceforth we assume  $\beta > 0$ . Then the potential is unstable and the usual thermodynamic limit does not exist. As pointed out by the referee for  $L = 1$  our model interpreted as a spin model is equivalent to a Curie–Weiss  $X$ – $Y$  model.

**Lemma 6.** (i) If  $L$  is not integer, then any solution of the self-consistency equation (2.32) is given by

$$\rho(x) = Z^{-1} \exp(a\beta \cos x) \tag{5.2}$$

with

$$a = Z^{-1} \int_{-\pi L}^{\pi L} dx \cos x \exp(a\beta \cos x) \tag{5.3}$$

$$Z = \int_{-\pi L}^{\pi L} dx \exp(a\beta \cos x) \tag{5.4}$$

(ii) If  $L$  is integer, then any solution of the self-consistency equation (2.32) is of the form

$$\rho_\alpha(x) = Z^{-1} \exp[a\beta \cos(x - \alpha)] \quad (5.2a)$$

with  $\alpha \in [0, 2\pi]$  and a solution of (5.3), (5.4).

*Proof.* Inserting (5.1) in (2.32) we obtain

$$\rho(x) = \tilde{Z}^{-1} \exp(a\beta \cos x) \exp(b\beta \sin x) \quad (5.5)$$

with

$$a = \tilde{Z}^{-1} \int dx \cos x \exp[\beta(a \cos x + b \sin x)] \quad (5.6)$$

$$b = \tilde{Z}^{-1} \int dx \sin x \exp[\beta(a \cos x + b \sin x)] \quad (5.7)$$

$$\tilde{Z} = \int dx \exp[\beta(a \cos x + b \sin x)] \quad (5.8)$$

We distinguish three cases. (i)  $a \neq 0$  and  $\sin \pi L \neq 0$ . From

$$b = \frac{-1}{a\beta\tilde{Z}} \int dx \exp(b\beta \sin x) \frac{d}{dx} \exp(a\beta \cos x) \quad (5.9)$$

we obtain by partial integration and with (5.6)

$$\frac{1}{a\beta\tilde{Z}} \exp(a\beta \cos \pi L) [\exp(b\beta \sin \pi L) - \exp(-b\beta \sin \pi L)] = 0 \quad (5.10)$$

thus  $b = 0$ . (ii)  $a = 0$  and  $\sin \pi L \neq 0$ . From (5.6)

$$0 = \int dx \cos x \exp(b\beta \sin x) \quad (5.11)$$

thus  $b = 0$ . (iii) If  $\sin \pi L = 0$ , then we set in (5.6) and (5.7)  $a = \bar{a} \cos \alpha$ ,  $b = \bar{b} \sin \alpha$ . Adding (5.6) and (5.7) and using the periodicity of the cosine in  $[-\pi L, \pi L]$  it follows that  $\bar{a}$  satisfies (5.3). ■

By Lemma 6 we only have to determine the parameter  $a \in \mathbb{R}$ . The free energy as a function of  $a$  is

$$F(a) = \frac{1}{2} \beta a^2 - \log Z \quad (5.12)$$

We have to find the global minima of  $F$ . Let

$$f(a) = Z^{-1} \int dx \cos x \exp(a\beta \cos x) \quad (5.13)$$

Then stationary points of  $F$  satisfy

$$a = f(a) \quad (5.14)$$

**Lemma 7.** Let  $0 < L \leq 1$  and let  $a > 0$  be a solution of (5.14). Then

$$f'(a) < 1 \quad (5.15)$$

*Proof.* We expand

$$\begin{aligned}
 f(a) &= Z^{-1} \sum_{n=0}^{\infty} \frac{(a\beta)^n}{n!} \int dx (\cos x)^{n+1} \\
 &= Z^{-1} \sum_{n=0}^{\infty} \frac{(a\beta)^n}{n!} \left[ \frac{2}{n+1} (\cos \pi L)^n \sin \pi L + \frac{a\beta}{n+2} \int dx (\cos x)^n \right]
 \end{aligned}
 \tag{5.16}$$

We also expand

$$Z = \sum_{n=0}^{\infty} \frac{(a\beta)^n}{n!} \int dx (\cos x)^n
 \tag{5.17}$$

Since each term in this sum is positive, Jensen’s inequality applied to the second term of (5.16) gives

$$\begin{aligned}
 a = f(a) &> \frac{2 \sin \pi L}{Z a \beta \cos \pi L} [\exp(a\beta \cos \pi L) - 1] \\
 &+ a\beta \left[ 2 + Z^{-1} \sum_{n=0}^{\infty} \frac{(a\beta)^n}{n!} n \int dx (\cos x)^n \right]^{-1}
 \end{aligned}
 \tag{5.18}$$

The sum equals  $a\beta f(a) = a^2\beta$ . Therefore

$$\beta \frac{1}{2 + a^2\beta} < 1 + \frac{2 \sin \pi L}{Z a^2 \beta \cos \pi L} [1 - \exp(a\beta \cos \pi L)]
 \tag{5.19}$$

We have

$$\begin{aligned}
 f'(a) &= \frac{\beta}{Z} \int dx (\cos x)^2 \exp(a\beta \cos x) - a^2\beta \\
 &= \frac{\beta}{Z} \sum_{n=0}^{\infty} \frac{(a\beta)^n}{n!} \int dx (\cos x)^{n+2} - a^2\beta \\
 &= \frac{\beta}{Z} \sum_{n=0}^{\infty} \frac{(a\beta)^n}{n!} \left[ \frac{2}{n+2} (\cos \pi L)^{n+1} \sin \pi L \right. \\
 &\quad \left. + \frac{n+1}{n+2} \int dx (\cos x)^n \right] - a^2\beta
 \end{aligned}
 \tag{5.20}$$

Again by Jensen’s inequality

$$\begin{aligned}
 f'(a) &< \frac{2 \sin \pi L}{Z a^2 \beta \cos \pi L} [1 - \exp(a\beta \cos \pi L)] + \frac{2 \sin \pi L}{aZ} \exp(a\beta \cos \pi L) \\
 &+ \beta \frac{1 + a^2\beta}{2 + a^2\beta} - a^2\beta
 \end{aligned}
 \tag{5.21}$$

Inserting (5.19) we arrive at

$$f'(a) < 1 + \frac{2 \sin \pi L}{aZ} \exp(a\beta \cos \pi L) \times \left[ \frac{2 + a^2\beta}{a\beta \cos \pi L} [\exp(-a\beta \cos \pi L) - 1] + 1 \right] \tag{5.22}$$

To show that the term in the square brackets is negative, we distinguish two cases. (i) If  $\cos \pi L < 0$ , then

$$\frac{2 + a^2\beta}{a\beta \cos \pi L} \left[ \exp(-a\beta \cos \pi L) - 1 + \frac{a\beta \cos \pi L}{2 + a^2\beta} \right] \leq 0 \tag{5.23}$$

since  $e^x - 1 - x/(2 + a^2\beta) \geq 0$  for  $x \geq 0$ . (ii) If  $\cos \pi L > 0$ , then (5.13) and (5.14) implies the bound

$$a \geq \cos \pi L \tag{5.24}$$

Inserting in (5.22) we have, since  $[\exp(-a\beta \cos \pi L) - 1] \leq 0$ ,

$$\begin{aligned} & \frac{2 + a^2\beta}{a\beta \cos \pi L} [\exp(-a\beta \cos \pi L) - 1] + 1 \\ & \leq \frac{2 + a\beta \cos \pi L}{a\beta \cos \pi L} [\exp(-a\beta \cos \pi L) - 1] + 1 \leq 0 \end{aligned} \tag{5.25}$$

since  $(2 + x)(1/x)(e^{-x} - 1) + 1 \leq 0$  for  $x \geq 0$ . ■

**Theorem 5.** Let  $V(x, y) = -\beta \cos(x - y)$  and let  $\Lambda = [-\pi L, \pi L]$  with  $\beta, L > 0$ . Then for  $L$  noninteger the LE equation has a unique solution. For  $L$  integer and  $\beta \leq 2$  the LE equation has a unique solution. For  $L$  integer and  $\beta > 2$  the LE equation has the solutions

$$\rho_\alpha(x) = Z^{-1} \exp[a_0 \beta \cos(x - \alpha)], \quad \alpha \in [0, 2\pi] \tag{5.26}$$

with  $a_0 > 0$  the unique solution of (5.14) restricted to  $a > 0$ .

*Proof.* We discuss only the case  $0 < L \leq 1$ . The remainder of the phase diagram follows by symmetry.

Let  $0 < L < 1$ . With  $Z = Z(a)$ , for  $a > 0$   $Z(a) > Z(-a)$  and therefore  $F(a) < F(-a)$ . Hence the minimum of  $F$  has to occur for  $a > 0$ . Now  $f(0) > 0$ . Since  $f(a) \rightarrow 1$  as  $a \rightarrow \infty$ , there is at least one  $a_0 > 0$  which satisfies  $f(a_0) = a_0$ . Since by Lemma 7  $f'(a_0) < 1$ , it follows that  $a_0$  is the only solution of  $a = f(a)$  for  $a > 0$ .

Let  $L = 1$ . Then  $f(0) = 0$  and therefore  $a = 0$  is always a solution of (5.14). Since  $f(-a) = -f(a)$ , if  $a_0$  is a solution of (5.14), so is  $-a_0$ . Since  $F(a) = F(-a)$ , to every global minimum of  $F$  for  $a \geq 0$  there is one with  $a \leq 0$ . If  $\beta < 2$ , then  $f'(0) < 1$ . The existence of an  $a_0 > 0$  such that  $a_0 = f(a_0)$  contradicts Lemma 7. If  $\beta > 2$ , then  $f'(0) > 1$  and  $F''(0) < 0$ .



Since  $f(a) \rightarrow 1$  as  $a \rightarrow \infty$  there exists at least one further  $a_0 > 0$  satisfying  $a_0 = f(a_0)$ . Since by Lemma 7  $f'(a_0) < 1$ , there can be at most one. ■

Since for the cosine model we have a complete solution of the LE equation, Theorem 5 can be strengthened to the following:

**Proposition 3.** Let  $V(x, y) = -\beta \cos(x - y)$  and let  $\Lambda = [-\pi L, \pi L]$  with  $\beta, L > 0$ . Then  $\lim_{N \rightarrow \infty} \mu^{(N)}$  exists. If either  $L$  is noninteger or  $L$  integer with  $\beta \leq 2$ , then  $\nu(d\rho | \mu)$  is concentrated on a single  $\rho$ . If  $L$  is integer and  $\beta > 2$ , then  $\nu(\{\rho_\alpha / \alpha \in B\} | \mu) = (1/2\pi) \int_B d\alpha$  with  $B \subset [0, 2\pi]$ .

*Proof.* The superposition with equal weight follows from symmetry under the shift by  $\alpha$ . ■

The free energy is given by

$$F(\beta, L) = \min_a F(a) \quad (5.27)$$

The internal energy

$$u(\beta, L) = \left( \frac{\partial \beta F(\beta, L)}{\partial \beta} \right)_L \quad (5.28)$$

is continuous, whereas the mechanical pressure

$$p(\beta, L) = -\beta^{-1} \left( \frac{\partial \beta F(\beta, L)}{\partial L} \right)_\beta \quad (5.29)$$

is discontinuous at phase coexistence points. In this sense the phase transition is of first order.

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