Phase transitions and coarse-graining for a system of particles in the continuum

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Abstract

We revisit the proof of the liquid-vapor phase transition for systems with finite-range interaction by Lebowitz, Mazel and Presutti [1] and extend it to the case where we additionally include a hard-core interaction to the Hamiltonian. We establish the phase transition for the mean field limit and then we also prove it when the interaction range is long but finite, by perturbing around the mean-field theory. A key step in this procedure is the construction of a density (coarse-grained) model via cluster expansion. In this note we present the overall result but we mainly focus on this last issue.

Key words and phrases. Continuum particle system, mean field theory, phase transition, coarse-graining, Pirogov-Sinai Theory, Cluster expansion.

1 Introduction

One of the main open problems in equilibrium statistical mechanics is to prove the validity of a liquid-vapour phase transition in a continuum particle system. Although this is well observed in experiments as well as in continuum theories, a rigorous proof for particle systems is still lacking. Intermolecular forces are often described by Lennard-Jones interactions, however the difficulty of handling such (or more realistic) systems has promoted the introduction of several simplified models. A good compromise between realistic models of fluids and mathematically treatable systems may consist of particles interacting via a combination of hard spheres (for repulsion) and an attractive long-range Kac interaction. However, the free energy of hard spheres can be studied for very small values of the density, far from the value at which a transition occurs. Hence, we still need to use a long range 4-body repulsive term as in [1] to determine the phase transition point. Then, the hard-core interaction acts just as a perturbation to the mean-field case. In fact, we show that the liquid-vapour transition persists if the volume of the hard spheres is sufficiently small, but finite. Nevertheless, our model presents a richer behaviour and if one manages to deal with a higher density regime, the hard-core interaction will become relevant and responsible for another transition of the gas-solid type.

Our proof will follow Pirogov-Sinai theory in the version proposed by Zahradník, [8]. The analysis requires first of all the notions of *coarse-graining* and *contours* which are introduced in Section 3 and subsequently, with an argument á la Peierls, one has to prove that contours are improbable which we do in Section 4. In this scenario we are able to compute the effective Hamiltonian for the coarse-grained system with a multi-canonical constraint (given by the fixed density in each cell). This computation

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involves an integration over the positions of the particles in each cell leading to a new measure on the density at the cells. The computations which lead to the effective Hamiltonian are in general very complicated, nevertheless due to the choice of the interaction they can be carried out. The crucial point here is to show convergence of a cluster expansion in the canonical ensemble with hard-core, Kac interaction and contour weights. This is done in Section 5.2 by extending the results in [5].

For more details on the proofs we refer to [7], from which the present paper is a follow-up, to [6] and to the monograph of Presutti [4].

2   Model

We consider a system of identical point particles in $\mathbb{R}^d$, $d \geq 2$, and call *particle configuration* a countable, locally finite collection of points in $\mathbb{R}^d$. The *phase space* $\mathcal{Q}^\Lambda$ is the collection of all particle configurations in a bounded region Λ. We use the notation $\mathcal{Q}$ when $\Lambda \equiv \mathbb{R}^d$. We write $q = (q_1, ... q_n)$ to indicate a configuration of n particles positioned at points $q_1, ..., q_n$ (the order is not important) of $\mathbb{R}^d$, while we write q_Λ when we want to specify that the particles are in $\mathcal{Q}^\Lambda$.

We consider a mean field model with an energy density given by:

$$e_\lambda(\rho) = -\lambda\rho - \frac{\rho^2}{2} + \frac{\rho^4}{4!}, \tag{2.1}$$

where λ is the chemical potential. Here, the density $\rho = n/|\Lambda|$ is set equal to the total density and it is therefore constant. We further define the LMP model, [1], by relaxing to a local mean field: the Hamiltonian (for configurations with finitely many particles) is given by the following function

$$H_{\lambda,\gamma}^{\text{LMP}}(q) = \int_{\mathbb{R}^d} e_\lambda(\rho_\gamma(r; q))\, dr, \tag{2.2}$$

where

$$\rho_\gamma(r; q) := \sum_{q_i \in q} J_\gamma(r, q_i) \tag{2.3}$$

is the local particle density at $r \in \mathbb{R}^d$. The local density is defined through Kac potentials, $J_\gamma(r, r') = \gamma^d J(\gamma r, \gamma r')$, where $J(s, t)$ is a symmetric, translation invariant ($J(s,t) = J(, t-s)$) smooth function which vanishes for $|t - s| \geq 1$. Thus, the range of the interaction has order γ^{-1} (for both repulsive and attractive potentials) and the "Kac scaling parameter" γ is assumed to be small. This choice of the potentials makes the LMP model a perturbation of the mean-field, in the sense that when taking the thermodynamic limit followed by the limit $\gamma \to 0$ the free energy is equivalent to the free energy in the mean-field description (2.1).

Note that the LMP interaction is the sum of a repulsive four body potential and an attractive two body potential, which can be written in the following way

$$H_{\lambda,\gamma}^{\text{LMP}}(q) = -\lambda|q| - \frac{1}{2!} \sum_{i \neq j} J_\gamma^{(2)}(q_i, q_j) + \frac{1}{4!} \sum_{i_1 \neq ... \neq i_4} J_\gamma^{(4)}(q_{i_1}, ..., q_{i_4}), \tag{2.4}$$

where $|\cdot|$ denotes the cardinality of a set and

$$J_\gamma^{(2)}(q_i, q_j) = \int J_\gamma(r, q_i) J_\gamma(r, q_j)\, dr \tag{2.5}$$

$$J_\gamma^{(4)}(q_{i_1}, ..., q_{i_4}) = \int J_\gamma(r, q_{i_1}) \cdots J_\gamma(r, q_{i_4})\, dr.$$

To this model we add an extra hard-core interaction described by a potential $V^R : \mathbb{R}^d \to \mathbb{R}$ such that

$$V^R(q_i, q_j) = \begin{cases} +\infty & \text{if } |q_i - q_j| \leq R \\ 0 & \text{if } |q_i - q_j| > R \end{cases} \tag{2.6}$$

where $|q_i - q_j|$ denotes the euclidean distance between the two particles in q_i and q_j. R is the radius of the hard spheres and their volume is $\epsilon = V_d(R)$, i.e., the volume of the d-dimensional sphere of radius R. Note also that the hard-core potential depends on q_i, q_j only through their distance.

Hence, the Hamiltonian of the model (LMP-hc) we consider is the following

$$H_{\gamma,R,\lambda}(q) = \int e_\lambda(J_\gamma * q(r)) \, dr + H_R^{\text{hc}}(q), \tag{2.7}$$

where

$$H_R^{\text{hc}}(q) := \sum_{i<j} V^R(q_i, q_j). \tag{2.8}$$

Given two configurations q and $\bar{q}$, we will use the following two notations to represent the energy of the particle configuration q in the field generated by $\bar{q}$ and the interaction energy between the particle configuration q and $\bar{q}$

$$H_{\gamma,R,\lambda}(q|\bar{q}) = H_{\gamma,R,\lambda}(q + \bar{q}) - H_{\gamma,R,\lambda}(\bar{q}) \tag{2.9}$$

$$U_{\gamma,R,\lambda}(q,\bar{q}) = H_{\gamma,R,\lambda}(q + \bar{q}) - H_{\gamma,R,\lambda}(q) - H_{\gamma,R,\lambda}(\bar{q}). \tag{2.10}$$

respectively, both for configurations with finitely many particles.

The grand-canonical Gibbs measure in the bounded measurable region Λ in $\mathbb{R}^d$ and boundary conditions $\bar{q} \in \mathcal{Q}^{\Lambda^c}$ is the probability measure on $\mathcal{Q}^\Lambda$ defined by

$$\mu^\Lambda_{\gamma,\beta,R,\lambda,\bar{q}}(dq) = Z^{-1}_{\gamma,\beta,R,\lambda,\bar{q}}(\Lambda) e^{-\beta H_{\gamma,R,\lambda}(q|\bar{q})} \nu^\Lambda(dq), \tag{2.11}$$

where β is the inverse temperature, $\nu^\Lambda(dq)$ is the Poisson point process of intensity 1 and $Z_{\gamma,\beta,R,\lambda,\bar{q}}(\Lambda)$ is the grand canonical partition function (defined as the normalization factor for $\mu^\Lambda_{\gamma,\beta,R,\lambda,\bar{q}}(dq)$ to be a probability).

2.1 Mean-field model

The model introduced above is a perturbation of a mean-field model, which is defined as follows. We consider the space of configurations with hard-core constraint

$$\mathcal{X}^R_{n,\Lambda} = \{(q_1, ...q_n) \in \Lambda^n : \min_{i \neq j} |q_i - q_j| > R\}. \tag{2.12}$$

Given a configuration $q \equiv (q_1, ..., q_n)$ in $\mathcal{X}^R_{n,\Lambda}$, the mean-field Hamiltonian is

$$H^{\text{mf}}_{\Lambda,R,\lambda}(q) = |\Lambda| e_\lambda(\rho) \tag{2.13}$$

where $\rho = n/|\Lambda|$ and $e_\lambda(\cdot)$ is given in (2.1). The mean-field canonical partition function is

$$Z^{\text{mf}}_{n,\Lambda,R} = \frac{1}{n!} \int_{\mathcal{X}^R_{n,\Lambda}} e^{-\beta H^{\text{mf}}_{\Lambda,R,0}(q)} dq_1 \cdots dq_n \tag{2.14}$$

$$= \exp\left\{ -\beta\left(-\frac{n^2}{2|\Lambda|} + \frac{n^4}{4!|\Lambda|^3} \right) \right\} \frac{1}{n!} \int_{\mathcal{X}^R_{n,\Lambda}} dq_1 \cdots dq_n. \tag{2.15}$$

The existence of its thermodynamic limit follows from general arguments and the canonical mean-field free energy is

$$\phi_{\beta,R}(\rho) = \lim_{|\Lambda|,n\to\infty: \frac{n}{|\Lambda|} \to \infty} -\frac{1}{|\Lambda|\beta} \log Z^{\text{mf}}_{n,\Lambda,R} = e_0(\rho) + f^{\text{hc}}_{\beta,R}(\rho) \tag{2.16}$$

where

$$f^{\text{hc}}_{\beta,R}(\rho) := \lim_{|\Lambda|,n\to\infty: \frac{n}{|\Lambda|} \to \infty} -\frac{1}{|\Lambda|\beta} \log Z^{\text{hc}}_{n,\Lambda,R}, \qquad Z^{\text{hc}}_{n,\Lambda,R} := \frac{1}{n!} \int_{\mathcal{X}^R_{n,\Lambda}} dq_1 \cdots dq_n \tag{2.17}$$

is a convex function of ρ.

The mean-field model shows a phase transition for β large enough, which is reflected in a loss of convexity of $\phi_{\beta,R}(\rho)$. The critical points of $\phi_{\beta,R,\lambda}(\rho) = \phi_{\beta,R}(\rho) - \lambda\rho$, as a function of ρ, are the solutions of the mean-field equation

$$\frac{d}{d\rho}\Big\{e_\lambda(\rho) + f_{\beta,R}^{\mathrm{hc}}(\rho)\Big\} = 0 \tag{2.18}$$

and have the form

$$\rho = \exp\Big\{-\beta e_\lambda'(\rho) - \psi_{\beta,R}'(\rho)\Big\} := K_{\beta,\lambda,R}(\rho), \tag{2.19}$$

where $\psi_{\beta,R}(\rho)$ is the free energy minus the entropy of the free system, i.e.,

$$f_{\beta,R}^{\mathrm{hc}}(\rho) - \frac{1}{\beta}\rho(\log\rho - 1). \tag{2.20}$$

We have the following properties

- There is a critical inverse temperature $\beta_{c,R}$, such that $\phi_{\beta,R}(\rho)$ is convex for $\beta \le \beta_{c,R}$, while for $\beta > \beta_{c,R}$ it has two inflection points $0 < s_-(\beta) < s_+(\beta)$, being concave for $\rho \in (s_-(\beta), s_+(\beta))$ and convex for $\rho \notin (s_-(\beta), s_+(\beta))$.

- For any $\beta > \beta_{c,R}$, there is $\lambda(\beta, R)$ so that $\phi_{\beta,\lambda(\beta,R),R}(\cdot)$ has two global minimizers, $\rho_{\beta,R,-} < \rho_{\beta,R,+}$ (and a local maximum at $\rho_{\beta,R,0}$). For $\lambda \ne \lambda(\beta, R)$ and for $\beta \le \beta_{c,R}$ the minimizer is unique.

- For any $\beta > \beta_{c,R}$ there is an interval $(\lambda_-(\beta, R), \lambda_+(\beta, R))$ containing $\lambda(\beta, R)$ and for any λ in the interval $\phi_{\beta,\lambda,R}(\cdot)$ it has two local minima $\rho_{\beta,\lambda,R,\pm}$ which are differentiable functions of λ and $\frac{d}{d\lambda}(\phi_{\beta,\lambda,R}(\rho_{\beta,\lambda,R,+}) - \phi_{\beta,\lambda,R}(\rho_{\beta,\lambda,R,-})) = \rho_{\beta,\lambda,R,-} - \rho_{\beta,\lambda,R,+} < 0$. For all $\beta > \beta_{c,R}$,

$$\frac{d}{d\rho}K_{\beta,\lambda(\beta,R),R}(\rho)\Big|_{\rho=\rho_{\beta,R,\pm}} \equiv K_{\beta,\lambda(\beta,R),R}'(\rho_{\beta,R,\pm}) < 1, \tag{2.21}$$

the condition (2.21) being equivalent to $\phi_{\beta,\lambda(\beta),R}''(\rho_{\beta,R,\pm}) > 0$. Moreover, there exists $\beta_{0,R} > \beta_{c,R}$ such that

$$K_{\beta,\lambda(\beta,R),R}'(\rho_{\beta,R,\pm}) > -1, \qquad \text{for all } \beta \in (\beta_{c,R}, \beta_{0,R}). \tag{2.22}$$

- We have an expansion for $\beta_{c,R}$ in powers of $\epsilon = V_d(R)$

$$\beta_{c,R} = \beta_c^{\mathrm{LMP}} - \epsilon\,(\beta_c^{\mathrm{LMP}})^{2/3} + O(\epsilon^2),$$

$\beta_c^{\mathrm{LMP}} = \frac{3}{2}^{\frac{3}{2}}$ being the critical inverse temperature for the LMP mean-field model. Note that while $\beta_{c,R}$ has the meaning of critical inverse temperature, $\beta_{0,R}$ has no physical meaning, but it is introduced for technical reasons. In fact $\beta_{0,R}$ is necessary for (2.22) to be true and depends on the choice of the mean-field Hamiltonian (2.13).

3 Contour model

To prove the phase transition in the LMP-hc model we study perturbations of the homogeneous states with densities $\rho_{\beta,R,\pm}$ which appear in the limit $\gamma \to 0$. We follow an argument à la Peierls, which relies (as for the Ising model) on the possibility to rewrite the partition function of the model as the partition function of an "abstract contour model". To implement this strategy we need to introduce several scaling parameters and phase indicators. Namely, we introduce two scales $\ell_\pm = \gamma^{-(1\pm\alpha)}$ and an accuracy parameter $\zeta = \gamma^a$, with $1 \gg \alpha \gg a > 0$. We define $\mathcal{D}^{(\ell)}$ a partition of $\mathbb{R}^d$ into cubes of side ℓ and we denote $C_r^{(\ell)}$ the cube of $\mathcal{D}^{(\ell)}$ which contains r.

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The first phase indicator is defined as

$$\eta^{(\varsigma,\ell_-)}(q;r) = \begin{cases} \pm 1 & \text{if } \left|\rho^{(\ell_-)}(q;r) - \rho_{\beta,R,\pm}\right| \leq \varsigma \\ 0 & \text{otherwise} \end{cases}$$

where $\rho^{(\ell)}(q;r) = |C_r^{(\ell)} \cap q|\ell^{-d}$ is the empirical densiy in a cube of side ℓ containing r given a configuration q.

Thus $\eta^{(\varsigma,\ell_-)}(q;r)$ indicates the phase (or its absence) on the small scale ℓ_-. Because of statistical fluctuations, we must allow for deviations from the ideal plus configurations $\eta^{(\varsigma,\ell_-)}(q;r) = 1$. We thus need to define which regions are still in the plus phase and which are those destroyed by the fluctuations. The fact that $\eta^{(\varsigma,\ell_-)}(q;r) = 1$ does not qualify r being in the $+$ phase, implies that we need a stronger condition which is defined in terms of two more phase indicators which describe the local phase of the system in increasing degree of accuracy. We have

$$\theta^{(\varsigma,\ell_-,\ell_+)}(q;r) = \begin{cases} \pm 1 & \text{if } \eta^{(\varsigma,\ell_-)}(q;r') = \pm 1 \quad \forall r' \in C_r^{(\ell_+)} \\ 0 & \text{otherwise} \end{cases}$$

$$\Theta^{(\varsigma,\ell_-,\ell_+)}(q;r) = \begin{cases} \pm 1 & \text{if } \eta^{(\varsigma,\ell_-)}(q;r') = \pm 1 \quad \forall r' \in C_r^{(\ell_+)} \cup \delta_{\text{out}}^{\ell_+}[C_r^{(\ell_+)}] \\ 0 & \text{otherwise} \end{cases}$$

where $\delta_{\text{out}}^{\ell}[\Lambda]$ of a $\mathcal{D}^{(\ell)}$-measurable region Λ is the union of all the cubes $C \in \mathcal{D}^{(\ell)}$ next to Λ. For simplicity, from now on we drop the superscript from the notation of $\eta^{(\varsigma,\ell_-)}, \theta^{(\varsigma,\ell_-,\ell_+)}, \Theta^{(\varsigma,\ell_-,\ell_+)}$.

With these definitions, given a configuration q, the "plus phase" is the region $\{r : \Theta(q;r) = 1\}$ while the "minus phase" is the region $\{r : \Theta(q;r) = -1\}$. We call $q^{\pm}$ a $\pm$ boundary conditions relative to a region Λ, if it belongs to the ensemble $\eta(q;r) = \pm 1$ for r on the frame of width $2\gamma^{-1}$ around Λ.

Two sets are connected if their closures have non empty intersection; hence, two cubes with a common vertex are connected. In this way, the plus and the minus regions are separated by zero-phase regions $\{r : \Theta(q;r) = 0\}$.

Definition 3.1 *A contour is a pair $\Gamma = \big(sp(\Gamma), \eta_\Gamma\big)$, where $sp(\Gamma)$ is a maximal connected component of the "incorrect set" $\{r \in \mathbb{R}^d : \Theta(q;r) = 0\}$ and η_Γ is the restriction to $sp(\Gamma)$ of $\eta(q;\cdot)$.*

The exterior, $\text{ext}(\Gamma)$, of Γ is the unbounded, maximal connected component of $sp(\Gamma)^c$. The interior is the set $\text{int}(\Gamma) = sp(\Gamma)^c \setminus \text{ext}(\Gamma)$; we denote by $\text{int}_i(\Gamma)$ the maximal connected components of $\text{int}(\Gamma)$. Let $c(\Gamma) = sp(\Gamma) \cup \text{int}(\Gamma)$ and note that $\text{int}_i(\Gamma)$ and $c(\Gamma)$ are both simply connected. The outer boundaries of Γ are the sets

$$A(\Gamma) := \delta_{\text{out}}^{\ell_+}[sp(\Gamma)] \cap \text{int}(\Gamma), \quad A_{\text{ext}}(\Gamma) := \delta_{\text{out}}^{\ell_+}[c(\Gamma)]. \tag{3.1}$$

We will also call $A_i(\Gamma) = A(\Gamma) \cap \text{int}_i(\Gamma)$.

Definition 3.2 *Γ is a plus/minus, contour if $\Theta(q;r) = \pm 1$ on $A_{\text{ext}}(\Gamma)$.*

We add a superscript $\pm$ to $A_i(\Gamma)$ to indicate the sign of Θ and we write $\text{int}_i^{\pm}(\Gamma)$ if $\text{int}_i(\Gamma)$ contains $A_i^{\pm}(\Gamma)$. Note that Θ is constant on $A_{\text{ext}}(\Gamma)$ and $A_i(\Gamma)$ and its value is determined by η.

Definition 3.3 *Given a plus contour Γ and a plus boundary condition q^+ for $c(\Gamma)$, we define the weight $W_{\gamma,R,\lambda}^+(\Gamma; \bar{q})$ of Γ as equal to*

$$\frac{\mu_{\gamma,\beta,R,\lambda,q^+}^{c(\Gamma)}\Big(\eta(q_{c(\Gamma)};r) = \eta_\Gamma(r), r \in sp(\Gamma); \; \Theta(q_{c(\Gamma)};r) = \pm 1, r \in A^{\pm}(\Gamma)\Big)}{\mu_{\gamma,\beta,R,\lambda,q^+}^{c(\Gamma)}\Big(\eta(q_{c(\Gamma)};r) = 1, r \in sp(\Gamma); \; \Theta(q_{c(\Gamma)};r) = 1, r \in A^{\pm}(\Gamma)\Big)} \tag{3.2}$$

where the measure $\mu_{\gamma,\beta,R,\lambda,q^+}^{c(\Gamma)}$ has been defined in (2.11). Analogously, we can define the weight of a minus contour.

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Thus, the numerator is the probability of the contour Γ conditioned to the outside of $\mathrm{sp}(\Gamma)$ while the denominator is the probability that the contour Γ is absent and replaced by the plus configurations (with the same conditioning to the outside).

The weight $W^-_{\gamma,R,\lambda}(\Gamma; q^-)$ of a minus contour Γ is defined analogously. The weight $W^\pm_{\gamma,R,\lambda}(\Gamma; q^\pm)$ depends only on q^D, i.e., the restriction of $q^\pm$ to $D \equiv \{r \in c(\Gamma)^c : \mathrm{dist}(r, c(\Gamma)) \leq 2\gamma^{-1}\}$.

Definition 3.4 *The plus diluted Gibbs measure in a bounded $\mathcal{D}^{(\ell_+)}$-measurable region Λ with plus boundary conditions $\bar{q}$ is*

$$\mu^{\Lambda,+}_{\gamma,\beta,R,\lambda,\bar{q}}(dq_\Lambda) := \frac{1}{Z^+_{\gamma,\beta,R,\lambda,\bar{q}}(\Lambda)} e^{-\beta H_{\gamma,R,\lambda}(q_\Lambda|\bar{q}_{\Lambda^c})} \mathbf{1}_{\Theta((q_\Lambda + q^+_{\Lambda^c});r)=1\ r\in\delta^{\ell_+}_{\mathrm{out}}[\Lambda^c]} \nu^\Lambda(dq_\Lambda) \qquad (3.3)$$

where $q^+ \in \mathcal{Q}^+ = \{q : \eta(q;r) = 1, r \in \mathbb{R}^d\}$ and $Z^+_{\gamma,\beta,R,\lambda,\bar{q}}(\Lambda)$ is the normalization, also called the plus diluted partition function. A similar definition holds for the minus diluted Gibbs measure.

We end this section by writing the ratio (3.2) of probabilities in the definition of the weight of a contour as a ratio of two partition functions. By writing explicitly the contributions coming from the support of a contour and those coming from the interior, we have for a plus contour Γ

$$W^+_{\gamma,R,\lambda}(\Gamma; q^+) = \frac{\mathcal{N}^+_{\gamma,R,\lambda}(\Gamma, q^+)}{\mathcal{D}^+_{\gamma,R,\lambda}(\Gamma, q^+)} \qquad (3.4)$$

where:

$$\begin{aligned}
\mathcal{N}^+_{\gamma,R,\lambda}(\Gamma, q^+) &= \int_{q_{\mathrm{sp}(\Gamma)}:\eta(q_{\mathrm{sp}(\Gamma)};r)=\eta_\Gamma(r),r\in\mathrm{sp}(\Gamma)} e^{-\beta H_{\gamma,R,\lambda,\mathrm{sp}(\Gamma)}(q_{\mathrm{sp}(\Gamma)}|q^+_{A_{\mathrm{ext}}})} \\
&\times\ Z^-_{\gamma,\beta,R,\lambda,q_{\mathrm{sp}(\Gamma)}}(\mathrm{int}^-(\Gamma))\, Z^+_{\gamma,\beta,R,\lambda,q_{\mathrm{sp}(\Gamma)}}(\mathrm{int}^+(\Gamma))
\end{aligned} \qquad (3.5)$$

$$\begin{aligned}
\mathcal{D}^+_{\gamma,R,\lambda}(\Gamma, q^+) &= \int_{q_{\mathrm{sp}(\Gamma)}:\eta(q_{\mathrm{sp}(\Gamma)};r)=1,r\in\mathrm{sp}(\Gamma)} e^{-\beta H_{\gamma,R,\lambda,\mathrm{sp}(\Gamma)}(q_{\mathrm{sp}(\Gamma)}|q^+_{A_{\mathrm{ext}}})} \\
&\times\ Z^+_{\gamma,\beta,R,\lambda,q_{\mathrm{sp}(\Gamma)}}(\mathrm{int}^-(\Gamma))\, Z^+_{\gamma,\beta,R,\lambda,q_{\mathrm{sp}(\Gamma)}}(\mathrm{int}^+(\Gamma)).
\end{aligned} \qquad (3.6)$$

4 The main results

Our main theorem states that the system undergoes a first-order phase transition. This means that for β large enough the Gibbs state at the thermodynamic limit, i.e. $\Lambda \to \mathbb{R}^d$, is not unique. It is possible to fix plus/minus boundary conditions such that, if R and γ are small and for some values of β, λ, uniformly in Λ, the typical configurations of the corresponding diluted Gibbs measures are close to the plus/minus phase. This is quantified in the following theorem.

Theorem 4.1 (Liquid-vapor phase transition) *Consider the LMP-hc model in dimensions $d \geq 2$. For such a model there are R_0, $\beta_{c,R}, \beta_{0,R}$ and for any $0 < R \leq R_0$ and $\beta \in (\beta_{c,R}, \beta_{0,R})$ there is $\gamma_{\beta,R} > 0$ so that for any $\gamma \leq \gamma_{\beta,R}$ there is $\lambda_{\beta,\gamma,R}$ such that:*

There are two distinct infinite-volume measures $\mu^\pm_{\beta,\gamma,R}$ with chemical potential $\lambda_{\beta,\gamma,R}$ and inverse temperature β and two different densities: $0 < \rho_{\beta,\gamma,R,-} < \rho_{\beta,\gamma,R,+}$.

In the theorem, $\mu^\pm_{\beta,\gamma,R}$ are the infinite-volume limits of (3.3), while $\beta_{c,R}, \beta_{0,R}$ are the two inverse temperatures introduced in Section 2.1.

We prove the existence of two distinct states, which are interpreted as the two pure phases of the system: $\mu^+_{\beta,\gamma,R}$ describes the liquid phase with density $\rho_{\beta,\gamma,R,+}$ while $\mu^-_{\beta,\gamma,R}$ describes the vapor phase, with the smaller density $\rho_{\beta,\gamma,R,-}$. Furthermore we have

$$\lim_{\gamma\to 0}\rho_{\beta,\gamma,R,\pm} = \rho_{\beta,R,\pm}, \quad \rho_{\beta,R,-} < \rho_{\beta,R,+}, \qquad \lim_{\gamma\to 0}\lambda_{\beta,\gamma,R} = \lambda(\beta, R)$$

which are the densities and the chemical potential for which there is a phase transition in the mean-field model (see again Section 2.1).

The main technical point in the proof of Theorem 4.1 is to prove that contours are improbable. In particular, they satisfy Peierls estimates which proves that the probability of a contour decays exponentially with its volume.

Theorem 4.2 *There exists R_0 such that for any $R \leq R_0$ and any $\beta \in (\beta_{c,R}, \beta_{0,R})$ there exist $c > 0$, $\gamma_{\beta,R} > 0$, so that for any $\gamma \leq \gamma_{\beta,R}$, $\pm$ contour Γ and any $\pm$ boundary condition $q^\pm$ relative to $c(\Gamma)$,*

$$W^\pm_{\gamma,R,\lambda}(\Gamma; q^\pm) \leq \exp\left\{ - \beta c \left(\zeta^2 \ell^d_-\right) N_\Gamma \right\} \tag{4.1}$$

where $\lambda = \lambda_{\beta,\gamma,R}$ and

$$N_\Gamma = \frac{|\mathrm{sp}(\Gamma)|}{\ell^d_+} \tag{4.2}$$

is the number of cubes of the partition $\mathcal{D}^{(\ell_+)}$ contained in $\mathrm{sp}(\Gamma)$.

As a corollary of Theorem 4.2 we have

Corollary 4.3 *There exists R_0 such that for any $R \leq R_0$, any $\beta \in (\beta_c, \beta_0)$ and letting c, $\gamma_{\beta,R}$, γ and $\lambda_{\beta,\gamma,R}$ as in Theorem 4.2, we have that for any bounded, simply connected, $\mathcal{D}^{(\ell_+)}$ measurable region Λ, any $\pm$ boundary condition $q^\pm$ and any $r \in \Lambda$, the following holds*

$$\mu^{\Lambda,\pm}_{\gamma,\beta,R,\lambda_{\beta,\gamma,R},q^\pm}(\{\Theta(q; r) = \pm 1\}) \geq 1 - \exp\left\{ - \beta \frac{c}{2} \left(\zeta^2 \ell^d_-\right)\right\}. \tag{4.3}$$

Theorem 4.3 implies that for any $R \leq R_0$ and γ small enough (chosen according to R) the difference between the diluted Gibbs measures $\mu^{\Lambda,+}_{\gamma,\beta,R,\lambda_{\beta,\gamma,R},q^+}(dq)$ and $\mu^{\Lambda,-}_{\gamma,\beta,R,\lambda_{\beta,\gamma,R},q^-}(dq)$ survives in the thermodynamic limit $\Lambda \nearrow \mathbb{R}^d$ and a phase transition occurs.

The main difficulty in proving (4.1) is that both numerator and denominator in (3.2) are defined in terms of expressions which involve not only the support of Γ but also its whole interior. They are therefore "bulk quantities" while the desired bound involves only the volume of the support of Γ, which for some contours, at least, is a "surface quantity". The main issue here is to find cancellations of the bulk terms between the numerator and the denominator. This is easy when special symmetries allow to relate the $+$ and $-$ ensembles, as in the ferromagnetic Ising model. Such simplifications are not present here and this is one of the issues which makes continuum models difficult to study. We overcome this difficulty using the Pirogov-Sinai theory [3] which covers cases where this symmetry is broken.

A central point of the Pirogov-Sinai theory is a change of measure. The idea is to introduce a new Gibbs measure (simpler than the original one), but which gives the same properties. The diluted partition function in a region Λ can be written as a partition function in $\mathcal{Q}^\Lambda_+ = \{q \in \mathcal{Q}_\Lambda : \eta(q, r) = 1, r \in \Lambda\}$. Namely, for any bounded $\mathcal{D}^{(\ell_+)}$-measurable region Λ and any plus b.c. q^+, we have that

$$Z^+_{\gamma,\beta,R,\lambda,q^+}(\Lambda) = \sum_{\underline{\Gamma} \in \mathcal{B}^+_\Lambda} \int_{q_\Lambda \in \mathcal{Q}^\Lambda_+} W^+_{\gamma,R,\lambda}(\underline{\Gamma}, q_\Lambda)\, e^{-\beta H_{\gamma,R,\lambda}(q_\Lambda | q^+_{\Lambda^c})}, \tag{4.4}$$

where $q_{\Lambda^c}^+$ is made of all particles of q^+ which are in Λ^c. $\mathcal{B}_\Lambda^+$ is the space of all finite subsets of collection of plus contours made of elements which are mutually disconnected and with spatial support not connected to Λ^c. Furthermore if $\underline{\Gamma} = (\Gamma_1, .., \Gamma_n)$, we use the notation

$$W_{\gamma,R,\lambda}^\pm(\underline{\Gamma}, q) = \prod_{i=1}^n W_{\gamma,R,\lambda}^\pm(\Gamma_i, q). \tag{4.5}$$

A similar expression holds for the diluted minus partition function.

In order to prove Peierls bounds, we follow the version of the Pirogov-Sinai theory proposed by Zahradnik [8]. In this picture large contours are less likely to be observed and this is implemented by fixing a constraint which literally forbids contours larger than some given value. We introduce therefore a new class of systems, where the contour weights are modified, their values depending on some "cutoff" parameter. In the stable phase the cutoff (if properly chosen) is not reached and the state is not modified by this procedure.

Therefore we choose $\hat{W}_{\gamma,R,\lambda}^\pm(\Gamma; q^\pm)$, positive numbers which depend only on the restriction of $q^\pm$ to $\{r \in c(\Gamma)^c : \mathrm{dist}(r, c(\Gamma)) \leq 2\gamma^{-1}\}$ and such that for any $\pm$ contour Γ and any $q^\pm$,

$$\hat{W}_{\gamma,R,\lambda}^\pm(\Gamma; q^\pm) = \min\left\{ \frac{\hat{\mathcal{N}}_{\gamma,R,\lambda}^\pm(\Gamma, q)}{\hat{\mathcal{D}}_{\gamma,R,\lambda}^\pm(\Gamma, q)}, e^{-\beta \frac{c}{100}(\zeta^2 \ell_-^d) N_\Gamma} \right\}. \tag{4.6}$$

Here, $\hat{\mathcal{N}}_{\gamma,R,\lambda}^\pm(\Gamma, q)$ and $\hat{\mathcal{D}}_{\gamma,R,\lambda}^\pm(\Gamma, q)$ are as in (3.5)-(3.6) but depend uniquely on the weights $\hat{W}_{\gamma,R,\lambda}^\pm(\cdot; \cdot)$. With this new choice of contours weights, if we prove Peierls bounds, i.e., (4.1) on definition (4.6), we have Peierls bounds also on the "true" weights defined in (3.4). We write $\hat{Z}_{\gamma,\beta,R,\lambda,q^+}^+(\Lambda)$ to denote the new diluted partition function. For more details one can see in [4].

5 Outline of the proof

In this section we want to give a sketch of the proof of (4.1) for the case of the cutoff contours as defined above. For the complete proof of the argument see [4].

The first step is to prove that it is possible to separate in (3.5)-(3.6) the estimate in $\mathrm{int}(\Gamma)$ from the one in $\mathrm{sp}(\Gamma)$ with "negligible error". Then one needs to bound a constrained partition function in $\mathrm{sp}(\Gamma)$, which yields the gain factor $e^{-\beta(c\zeta^2 - c'\gamma^{1/2-2\alpha d})\ell_2^d N_\Gamma}$. Hence, we prove that there are $c, c' > 0$ so that given γ small enough, for $R < R_0$,

$$\frac{\hat{\mathcal{N}}_{\gamma,R,\lambda_{\beta,R,\gamma}}^+(\Gamma, q^+)}{\hat{\mathcal{D}}_{\gamma,R,\lambda_{\beta,R,\gamma}}^+(\Gamma, q^+)} \leq e^{-\beta(c\zeta^2 - c'\gamma^{1/2-2\alpha d})\ell_2^d N_\Gamma} \frac{e^{\beta I_{\gamma,\lambda(\beta,R)}^-(\mathrm{int}^-(\Gamma))} \hat{Z}_{\gamma,R,\lambda_{\beta,\gamma,R},\chi^-}^-(\mathrm{int}^-(\Gamma))}{e^{\beta I_{\gamma,\lambda(\beta,R)}^+(\mathrm{int}^-(\Gamma))} \hat{Z}_{\gamma,R,\lambda_{\beta,\gamma,R},\chi^+}^+(\mathrm{int}^-(\Gamma))} \tag{5.1}$$

where we use the shorthand notation

$$\chi_\Delta^\pm(r) = \rho_{\beta,\pm} \mathbf{1}_{r \in \Delta}, \quad \chi^\pm = \chi_{\mathbb{R}^d}^\pm \tag{5.2}$$

and where $I_{\gamma,\lambda(\beta,R)}^\pm(\Lambda)$ is a surface term

$$I_{\gamma,\lambda(\beta,R)}^\pm(\Lambda) = \int_{\Lambda^c} \left\{ e_{\lambda(\beta,R)}(\rho_{\beta,R,\pm}) - e_{\lambda(\beta,R)}(J_\gamma * \rho_{\beta,R,\pm} \mathbf{1}_{\Lambda^c}) \right\} \tag{5.3}$$

$$- \int_\Lambda e_{\lambda(\beta,R)}(J_\gamma * \rho_{\beta,R,\pm} \mathbf{1}_{\Lambda^c}). \tag{5.4}$$

The main tool used in this part of the proof is a coarse-graining argument and an analysis à la Lebowitz and Penrose, [2]. The error in doing a coarse-graining is bounded by $e^{\beta c\gamma^{1/2}|\mathrm{sp}(\Gamma)|} =$

$e^{\beta c \gamma^{1/2-2\alpha d} \ell_2^d N_\Gamma}$, which is the "negligible factor" mentioned above, as it is a small fraction of the gain term in the Peierls bounds. Thus, in this step we have a reduction, after coarse-graining, to variational problems with the LMP free energy functional. They involve two different regions, one is at the boundary between $\text{int}(\Gamma)$ and $\text{sp}(\Gamma)$, the other is in the bulk of the spatial support. In the former we exploit the definition of contours which implies that the boundary of $\text{int}^\pm(\Gamma)$ is in the middle of a "large region" (of size ℓ_+) where $\eta(\cdot;\cdot)$ is identically equal to ± 1, respectively. By the strong stability properties of the LMP free energy functional, the minimizers are then proved to converge exponentially to $\rho_{\beta,R,\pm}$ with the distance from the boundaries. Here we use the assumption that $\beta \in (\beta_{c,R}, \beta_{0,R})$, i.e., where the mean-field operator $K_{\beta,\lambda(\beta,R),R}$ is a contraction, see (2.21)-(2.22). We then conclude that with a negligible error we have "thick corridors" where the minimizers are equal to $\rho_{\beta,R,\pm}$ thus separating the regions outside and inside the corridors.

After this step we have plus/minus partition functions in $\text{int}^\pm(\Gamma)$ with boundary conditions $\rho_{\beta,R,\pm}$ and still a variational problem in the region $\text{sp}(\Gamma)$ with the constraint that profiles should be compatible with the presence of the contour Γ. The analysis of such a minimization problem leads to the gain factor in the Peierls bounds.

To complete the proof for Peierls bounds we then need to prove the following theorem.

Theorem 5.1 *There exists R_0 such that for any $R \leq R_0$ and any $\beta \in (\beta_{c,R}, \beta_{0,R})$ there are $c > 0$, $\gamma_{\beta,R} > 0$ and $\lambda_{\beta,\gamma,R}$, such that for all $\gamma \leq \gamma_\beta$, $|\lambda(\beta,R) - \lambda_{\beta,R,\gamma}| \leq c\gamma^{1/2}$, and any bounded $\mathcal{D}^{(\ell_+)}$-measurable region Λ, the following bound holds*

$$\frac{e^{\beta I_{\gamma,\lambda(\beta,R)}^-(\Lambda)} \hat{Z}_{\gamma,R,\lambda_{\beta,\gamma,R},\chi_{\Lambda^c}^-}^-(\Lambda)}{e^{\beta I_{\gamma,\lambda(\beta,R)}^+(\Lambda)} \hat{Z}_{\gamma,R,\lambda_{\beta,\gamma,R},\chi_{\Lambda^c}^+}^+(\Lambda)} \leq e^{c\gamma^{1/2}|\delta_{\text{out}}^{\ell_+}[\Lambda]|}. \tag{5.5}$$

The idea in the proof of (5.5) is that the leading term in the partition function is

$$\hat{Z}_{\gamma,\beta,R,\lambda,q_{\text{sp}(\Gamma)}}^\pm(\text{int}^\pm(\Gamma)) \approx e^{\beta P_{\gamma,R,\lambda}^\pm |\text{int}^\pm(\Gamma)|}, \tag{5.6}$$

where $P_{\gamma,R,\lambda}^\pm$ is the thermodynamic pressure given, for any van Hove sequence of $\mathcal{D}^{(\ell_+)}$-measurable regions Λ_n and any $\pm$ Λ_n-boundary conditions $q_n^\pm$, by the following limit

$$\lim_{n \to \infty} \frac{1}{\beta|\Lambda_n|} \log \hat{Z}_{\gamma,R,\lambda,q_n^\pm}^\pm(\Lambda_n) = P_{\gamma,R,\lambda}^\pm. \tag{5.7}$$

Although (5.6) is a rough approximation, we need to prove equality of $\pm$ pressures in the bulk terms in $\hat{W}_{\gamma,R,\lambda}^\pm(\Gamma;q^\pm)$ to allow for the numerator and the denominator to cancel. Again for more details we refer the reader to [4].

We now prove that the next term, i.e., the surface corrections to the pressure, are small as $e^{c''\gamma^{1/2}\ell_+^d N_\Gamma}$ at least when the boundary conditions "are perfect", i.e., given by $\chi^\pm$. The most difficult step in the proof of Theorem 5.1 are estimates involving terms which are localized in the bulk of the interior. These rely on a more delicate property of decay of correlations (Theorem 5.2), whose proof requires a whole new set of ideas.

Theorem 5.2 (Exponential decay of correlations) *Let Λ be a bounded $\mathcal{D}^{(\ell_+)}$ measurable region. Let x_i be the centers of the cubes $C^{(\ell_-)} \in \mathcal{D}^{(\ell_-)}$; then we define*

$$f_{x_1,..,x_n} = \int_{\{r_i \in C_{x_i}^{(\ell_-)}, 1 \leq i \leq n\}} q^{\otimes n}(dr_1..dr_n) J_\gamma^{(n)}(r_1,..,r_n) \tag{5.8}$$

where we use the notation

$$q^{\otimes n}(dr_1...dr_n) = \frac{1}{n!} \sum_{i_1 \neq .. \neq i_n} \delta_{q_{i_1}}(r_1)\, dr_1 \cdots \delta_{q_{i_n}}(r_n)\, dr_n. \tag{5.9}$$

There are positive constants δ, c' and c so that for all $f_{x_1,..,x_n}$

$$\left| E_{\mu^1}\left(f_{x_1,..,x_n}\right) - E_{\mu^2}\left(f_{x_1,..,x_n}\right)\right| \le c'e^{-c[\gamma^{-\delta}\ell_+^{-1}\,dist(C_{x_1}^{(\ell-)},\Lambda^c)]} \tag{5.10}$$

where E_{μ^i}, $i = 1,2$, are the expectations with respect to the following two measures: μ^1 is the finite-volume Gibbs measure in Λ with b.c. $\bar{q}$ and μ^2 the finite-volume Gibbs measure on a torus $\mathcal{T}$ much larger than Λ.

We compute the expectations in (5.10) in two steps. We first do a coarse-graining by fixing the number of particles in the cubes $C^{(\ell-)}$ and integrate over their positions; then, in the second step, we sum over the particle numbers. By its very nature, the Kac assumption makes the first step simple: in fact, to first order the energy is independent of the positions of the particles inside each cube. Neglecting the higher order terms, the energy drops out of the integrals (with fixed particle numbers) which can then be computed explicitly. The result is the phase space volume of the set of configurations with the given particle numbers: this is an entropy factor which, together with the energy, reconstructs the mesoscopic energy functional.

By using cluster expansion techniques, we will show here that it is possible to compute exactly the correction due to the dependence of the energy on the actual positions of the particles in each cube. For the hard-core part of the interaction we can use again a cluster expansion technique, using the result [5] obtained for a system with a single canonical constraint and therefore extending it to the present case of multi-canonical constraints.

Once we are left with an "effective Hamiltonian" we still have to sum over the particle numbers. Since we work in a contour model, the particle densities are close to the mean-field values $\rho_{\beta,R,\pm}$ so that the marginal of the Gibbs measure over the coarse-grained model is Gibbsian and it is a small perturbation of a Hamiltonian given by the mean-field free energy functional restricted to a neighborhood of the mean-field equilibrium density. In such a setup we manage to prove the validity of the Dobrushin uniqueness condition, where we take into account the contribution of the hard-core as a cluster expansion sum.

5.1 Coarse-graining

To carry out this plan, we need to prove that $\hat{Z}_{\gamma,\beta,R,\lambda,\bar{q}}^+(\Lambda)$ can be written as the partition function of a Hamiltonian which depends on variables ρ_x, $x \in X_\Lambda^{(\ell-)}$, $X_\Lambda^{(\ell-)}$ the set of centers of cubes $C^{(\ell-)}$ in Λ. The new energy of a density configuration $\rho = \{\rho_x\}_{x \in X_\Lambda^{(\ell-)}}$ is defined as

$$h(\rho|\bar{q}) = -\log \sum_{\underline{\Gamma} \in \mathcal{B}_\Lambda^+} \int_{\mathcal{Q}_+^\Lambda} \nu^\Lambda(dq)\mathbf{1}_{\rho^{(\ell-)}(q)=\rho}\, e^{-\beta H_{\gamma,R,\lambda}(q|\bar{q})}\hat{W}(\underline{\Gamma}|q) \tag{5.11}$$

so that

$$\hat{Z}_{\gamma,\beta,R,\bar{q}}^+(\Lambda) = \sum_\rho e^{-h(\rho|\bar{q})}.$$

Setting $n_x = \ell_-^d \rho_x$, we multiply and divide, inside the argument of the log in (5.11), by

$$\prod_{x \in X_\Lambda} \frac{\ell_-^{dn_x}}{n_x!}.$$

We denote by $\{q_{x,i},\ i = 1,..,n_x,\ x \in X_\Lambda\}$, the particles in $C_x^{(\ell-)}$. Thus particles are now labelled by the pair (x,i), x specifies the cube $C_x^{(\ell-)}$ to which the particle "belongs", i distinguishes among the particles in $C_x^{(\ell-)}$. The corresponding free measure, whose expectation is denoted by E_ρ^0, is the product of the probabilities which give uniform distribution to the positions $q_{x,i}$ in their boxes $C_x^{(\ell-)}$

divided by $n_x!$ since the particles in each box $C_x^{(\ell-)}$ are indistinguishable. Note that when we change from labeling of all particles in Λ to labeling separately the particles in each box we have to multiply by $\frac{N!}{\prod_{x \in X_\Lambda^{(\ell-)}} n_x!}$ for all such possibilities.

We define a new a priori measure for the particles in a given box $C_x^{(\ell-)}$, $x \in X_\Lambda$, as

$$\frac{dq_{x,1} \cdots dq_{x,n_x} e^{-\beta U^{\mathrm{hc}}(q^{(C_x)}, \bar{q})}}{\int dq_{x,1} \cdots dq_{x,n_x} e^{-\beta U^{\mathrm{hc}}(q^{(C_x)}, \bar{q})}} Z_{x,\bar{q}}(\rho_x) \tag{5.12}$$

where $q^{(C_x)}$ denotes the configuration of the particles in $C_x^{(\ell-)}$, each integral in the denominator is over $C_x^{(\ell-)}$ with the constraint $\mathcal{Q}_+^\Lambda$ and where

$$Z_{x,\bar{q}}(\rho_x) = \int_{\mathcal{Q}_+^\Lambda} \frac{dq_{x,1}}{\ell_-^d} \cdots \frac{dq_{x,n_x}}{\ell_-^d} e^{-\beta U^{\mathrm{hc}}(q^{(C_x)}, \bar{q})} \tag{5.13}$$

is the extra factor coming from the change of measure and contributing for each cube with

$$U^{\mathrm{hc}}(q^{(C_x)}, \bar{q}) := \sum_{i=1}^{n_x} \sum_{j=1}^{|\bar{q}|} V^R(q_{x,i} - \bar{q}_j). \tag{5.14}$$

The corresponding expectation will be denoted by $E_{\rho,\bar{q}}^0$. We then have

$$h(\rho|\bar{q}) = -\sum_x \log \frac{\ell_-^{dn_x}}{n_x!} - \sum_{x: C_x^{(\ell-)} \in \partial\Lambda^{\mathrm{int}}} \log Z_{x,\bar{q}}(\rho_x) \tag{5.15}$$
$$- \log E_{\rho,\bar{q}}^0 \left(e^{-\beta H_\gamma(q|\bar{q})} e^{-\beta H_R^{\mathrm{hc}}(q)} \sum_{\mathrm{sp}(\Gamma) \subseteq \Lambda^0} W(\Gamma|q) \right)$$

where $\partial\Lambda^{\mathrm{int}}$ is the set of the $\mathcal{D}^{(\ell-)}$ boxes adjacent to Λ^c (i.e., the interior boxes of Λ). Note that the total normalization is a product of the normalizations in each cube and that, because of the hard-core interaction, $Z_{x,\bar{q}}(\rho_x)$ for a given box C_x gives the following contribution:

$$Z_{x,\bar{q}}(\rho_x) = \left(\int_{C_x} \frac{dq}{\ell_-^d} \mathbf{1}_{q \in C_x^{\bar{q}}} \right)^{n_x} = \frac{|C_x^{\bar{q}}|^{n_x}}{\ell_-^{dn_x}} \tag{5.16}$$

where: $C_x^{\bar{q}} = \{r \in C_x : \mathrm{dist}(r, \bar{q}_i) > R, \forall i\}$. This means that, because of the presence of the hard-core, the new measure "reduces" the admissible volume for the particles in each box.

Let $H^{(\ell-)}(q|\bar{q})$ be the coarse-grained Hamiltonian on scale ℓ_-. It is obtained by replacing $J_\gamma^{(n)}$ by $\tilde{J}_\gamma^{(n)}$, where

$$\tilde{J}_\gamma^{(n)}(r_1, ..., r_n) = \frac{1}{|C^{(\ell-)}|^n} \int_{C_{r_1}^{(\ell-)}} dq_1 \cdots \int_{C_{r_n}^{(\ell-)}} dq_n J_\gamma^{(n)}(q_1, ..., q_n) \tag{5.17}$$

are the coarse-grained potentials.

It depends only on the particle numbers n_x (or the densities ρ_x) and we can thus write

$$h^0(\rho|\bar{\rho}) = H^{(\ell-)}(q|\bar{q}), \qquad \rho_x = \rho_x^{(\ell-)}(q), \ \bar{\rho}_x = \rho_x^{(\ell-)}(\bar{q}). \tag{5.18}$$

Setting

$$\Delta H(q|\bar{q}) = H_\gamma(q|\bar{q}) - H^{(\ell-)}(q|\bar{q}) \tag{5.19}$$

we have

$$h(\rho|\bar{q}) = -\sum_x \log \frac{\ell_-^{dn_x}}{n_x!} - \sum_{x: C_x^{(\ell-)} \in \partial\Lambda^{\mathrm{int}}} \log Z_{x,\bar{q}} + \beta h^0(\rho|\bar{\rho}) + \delta h(\rho|\bar{q}) \tag{5.20}$$

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where

$$\delta h(\rho|\bar{q}) = -\log E^0_{\rho,\bar{q}}\Big(e^{-\beta\Delta H(q|\bar{q})}e^{-\beta H^{\mathrm{hc}}_R(q)}\sum_{\mathrm{sp}(\Gamma)\subseteq\Lambda^0}\hat{W}(\Gamma|q)\Big). \tag{5.21}$$

It is convenient to split $\delta h(\rho|\bar{q})$ in three parts

$$\delta h(\rho|\bar{q}) = h^p(\rho|\bar{q}) + h^c(\rho|\bar{q}) \tag{5.22}$$

where

$$h^p(\rho|\bar{q}) = -\log E^0_{\rho,\bar{q}}\big(e^{-\beta\Delta H(q|\bar{q})}e^{-\beta H^{\mathrm{hc}}_R(q)}\big) \tag{5.23}$$

$$h^c(\rho|\bar{q}) = -\log E_{\rho,\bar{q}}\big(\sum_{\mathrm{sp}(\Gamma)\subseteq\Lambda^0}\hat{W}(\Gamma|q)\big) \tag{5.24}$$

$$E_{\rho,\bar{q}}(f) = \frac{E^0_{\rho,\bar{q}}\big(e^{-\beta\Delta H(q|\bar{q})}e^{-\beta H^{\mathrm{hc}}_R(q)}f\big)}{E^0_\rho\big(e^{-\beta\Delta H(q|\bar{q})}e^{-\beta H^{\mathrm{hc}}_R(q)}\big)}. \tag{5.25}$$

In words, $h^p(\rho|\bar{q})$ is the contribution to the effective Hamiltonian coming from the average over the measure (5.12) of the hard-core interaction $H^{\mathrm{hc}}_R(q)$ and the coarse-grained correction $\Delta H(q|\bar{q})$ (defined in (5.19)). It will have an expansion in polymers as we will show in Section 5.2. $h^c(\rho|\bar{q})$ is the same average to which is also added the contribution of the contours and it can also be expressed in terms of another class of polymers.

5.2   Cluster expansion

In order to find an expression for h^p and h^c we perform a cluster expansion which involves both hard-core, Kac interaction and contours. Let us start from h^p, which is easier since there are no contours. We define diagrams which will be the *polymers* of the cluster expansion. Let $L^{(2)} = (i_1, i_2)$ and $L^{(4)} = (i_1, i_2, i_3, i_4)$ denote a pair (resp. a quadruple) of mutually distinct particle labels. They will be called 2-links and 4-links. We will refer to the two types of 2-links by calling them respectively γ-links and R-links.

Definition 5.3 *A diagram θ is a collection of* 2- *and* 4-*links, i.e., an ordered triple*

$$\theta \equiv \Big(\mathcal{L}^{(2)}_R(\theta), \mathcal{L}^{(2)}_\gamma(\theta), \mathcal{L}^{(4)}(\theta)\Big), \tag{5.26}$$

where we denote by $\mathcal{L}^{(2)}_R(\theta)$, $\mathcal{L}^{(2)}_\gamma(\theta)$ and $\mathcal{L}^{(4)}(\theta)$ the set of 2-*links (of type R and γ) and of* 4-*links in θ. Note that one can have a repetition of links, i.e., the same link $L^{(2)}$ can belong to both sets $\mathcal{L}^{(2)}_\gamma(\theta)$ and $\mathcal{L}^{(2)}_R(\theta)$. We use $\mathcal{L}^{(2)}(\theta)$ for the set of* 2-*links (which eventually contains twice a link when it is both a γ-link and a R-link) and Θ for the set of all such diagrams.*

We construct the set of polymers starting from the diagrams defined above, but eliminating some of their links. Indeed, to work with cluster expansion an "a priori" estimate of some links is needed in order to reduce the complexity of the diagrams that we consider. This is an essential step to assure convergence of the cluster expansion. To this scope, we are going to define a new set of diagrams. The procedure is the following: We first get rid of all the R-links which appear over γ-links and we extract a subdiagram $\hat{\theta}$. Let $\hat{\Theta} \subset \Theta$ be the set of all the diagrams which do not have double 2-links, i.e., $\hat{\Theta} := \{\hat{\theta} : \mathcal{L}^{(2)}_\gamma(\hat{\theta}) \cap \mathcal{L}^{(2)}_R(\hat{\theta}) = \emptyset\}$.

The next step is to obtain a diagram which is at most a tree in R.

Definition 5.4 *(Partial ordering relation $\prec$ on a diagram θ). For $L^{(2)}_1, L^{(2)}_2 \in \mathcal{L}^{(2)}_R(\theta)$ we have that $L^{(2)}_1 \prec L^{(2)}_2$ according to lexicographic ordering (i.e., we start by comparing the first index and if the same we compare the next etc.). We say that a diagram is ordered if the set of its R-links is ordered according to this definition. We can endow an ordered diagram with the usual notion of distance. We will write $d(v)$ to indicate the distance of a vertex v to the first vertex in the previous order relation.*

Definition 5.5 (*Redundant link*). *Given an ordered diagram θ, we say that a link $L^{(2)} \in \mathcal{L}_R^{(2)}(\theta)$ is redundant in the following two cases:*

- *If $L^{(2)} = \{i, j\}$ with $d(i) = d(j)$;*

- *If $L_1^{(2)} = \{i_1, j\}$ with $d(i_1) = d(j) - 1$ and it exists $L_2^{(2)} = \{i_2, j\} \in \mathcal{L}_R^{(2)}(\theta)$, with $d(i_2) = d(j) - 1$, such that: $L_2^{(2)} \prec L_1^{(2)}$ (i.e., $i_2 < i_1$).*

We denote the set of the redundant links of a diagram θ by: $\mathcal{R}_R^{(2)}(\theta)$.

We call $\bar{\Theta} \subset \hat{\Theta}$ the set of diagrams with no double 2-links and with no redundant links. In formulas: $\bar{\Theta} := \{\bar{\theta} : \bar{\theta} \in \hat{\Theta}, \mathcal{R}_R^{(2)}(\bar{\theta}) = \emptyset\}$.

Two diagrams θ and θ' are *compatible* ($\theta \sim \theta'$) if the set of their common labels is empty.

Theorem 5.6 *For all γ and R small enough, there exist functions $z_{\gamma,R}^T(\pi; \rho; \bar{q})$ such that*

$$h^p(\rho|\bar{q}) = -\sum_{\pi} z_{\gamma,R}^T(\pi; \rho; \bar{q}), \tag{5.27}$$

where π is a collection of non-compatible diagrams in the space $\bar{\Theta}$.

Let us now find an expansion for h^c defined in (5.24). Let us fix a collection $\underline{\Gamma} = \{\Gamma_i\}_{i=1}^n$, where $\Gamma_i \equiv (\mathrm{sp}(\Gamma_i), \eta_{\Gamma_i})$. As said after (3.2), the weights $W_{\gamma,R,\lambda}^{\pm}(\Gamma_i; q^{\pm})$ depend only on q^{D_i}, i.e., the restriction of $q^{\pm}$ to $D_i = \{r \in c(\Gamma)^c : \mathrm{dist}(r, c(\Gamma)) \le 2\gamma^{-1}\}$. We also let $D := \cup_{i=1}^n D_i$. We then have, for the numerator of (5.24),

$$E_{\rho^D, \bar{q}}^0\Big(W(\Gamma|q) e^{-h^p(\rho^{\Lambda \setminus D}|\bar{q} \cup q^D)}\Big). \tag{5.28}$$

We write h^p as a sum of clusters using (5.27). Due to the dependence of the a priori measure on $\bar{q}$ (now on both $\bar{q}$ and q^D), the clusters involving a particle in a neighboring ℓ_--cell to D will also depend on q^D. We denote the union of the set D with the frame consisting of the neighboring ℓ_--cells by $D^* \in \mathcal{D}^{(\ell_2)}$.

To distinguish between clusters we introduce $\bar{D}_i := D_i \cup \{r : \mathrm{dist}(r, D_i) \le \ell_+/4\} \in \mathcal{D}^{(\ell_-)}$ and we call $\mathcal{B}_i$ the set of all clusters π whose points are all in $\bar{D}_i$. As the distance between contours is $\ge \ell_+$, the sets $\mathcal{B}_i$ are mutually disjoint; we call $\mathcal{B}$ their union. Note that they depend on $\underline{\Gamma}$ through the domain where they are constructed. By $\mathcal{R}_i$ we denote the set of π which have points both in D_i^* (so that they depend on q^D) and in the complement of $\bar{D}_i$ (such π are therefore not in $\mathcal{B}_i$). There may be points of $\pi \in \mathcal{R}_i$ which are in D_j^*, $j \ne i$, hence also $\pi \in \mathcal{R}_j$, so that the sets $\mathcal{R}_i$ are not disjoint. We call $\mathcal{R}$ their union.

For any given $\underline{\Gamma}$ we do analogous splitting on the polymers appearing when developing the denominator of (5.25) thus defining the sets $\mathcal{B}_i'$, $\mathcal{B}'$, $\mathcal{R}_i'$, $\mathcal{R}'$. The clusters that appear in the numerator and denominator of (5.25) are different, however those not in $\mathcal{B} \cup \mathcal{R}$ (i.e., those that do not involve q^D) are common to the corresponding ones in the denominator of (5.25) (i.e., those not in $\mathcal{B}' \cup \mathcal{R}'$) and have same statistical weights, hence they cancel.

The clusters $\pi \in \mathcal{B}$ can be grouped together and absorbed by a renormalization of the measure in $E_{\rho^D, \bar{q}}^0$, since they do not involve interactions between different contours. Thus, they will be part of the *activities* in the expansion, while the *polymers* will be defined in terms of elements of $\mathcal{R}$ and $\mathcal{R}'$.

Hence, to formulate the problem into the general context of the abstract polymer model we define as *connected* polymer P a set of contours with "connections" consisting of elements of $\mathcal{R} \cup \mathcal{R}'$ which necessarily "connect" all contours in the given set and "decorations" consisting of clusters in $\mathcal{R} \cup \mathcal{R}'$ not necessarily connecting contours. We denote by $\mathcal{P}$ the space of all such elements

$$\begin{aligned}
\mathcal{P} \quad := \quad &\{P \equiv (\underline{\Gamma}(P), R(P)), \forall \Gamma_i, \Gamma_j \in \underline{\Gamma}(P), \exists \pi \in R(P) \subset \mathcal{R} \cup \mathcal{R}' \\
&\text{connecting } D_i^*, D_j^* \in D^*(\underline{\Gamma})\}.
\end{aligned} \tag{5.29}$$

We use $D(P), D^*(P)$ to denote the set of frames corresponding to the contours in P and $R(P)$ to denote the set of clusters. We also introduce $A(\pi)$ to denote the union of the $C^{(\ell_2)}$ cells which correspond to the labels of π. Similarly, let $A(P) := \cup_{\Gamma \in \underline{\Gamma}(P)} D^*(\Gamma) \cup_{\pi \in R(P)} A(\pi)$. A compatible collection of polymers consists of mutually compatible polymers.

Theorem 5.7 *For all γ and R small enough, there exist functions $\zeta^T_{\gamma,R}(C; \rho)$ such that*

$$h^c(\rho|\bar{q}) = -\sum_C \zeta^T_{\gamma,R}(C; \rho), \qquad (5.30)$$

where C is a collection of non-compatible polymers P in the space $\mathcal{P}$.

With these two theorems we can define a new measure on the space of the density configurations $\rho = \{\rho_x\}_{x \in X_\Lambda^{(\ell_-)}}$, where the new Hamiltonian is

$$h(\rho|\bar{q}) = -\sum_x \log \frac{\ell_2^{dn_x}}{n_x!} - \sum_{x: C_x^{(\ell_2)} \in \partial \Lambda^{\text{int}}} \log Z_{x,\bar{q}} + \beta h^0(\rho|\bar{\rho}) + h^p(\rho|\bar{q}) + h^c(\rho|\bar{q}). \qquad (5.31)$$

We then use the notation $\mathbb{E}$ for the expectation w.r.t. this new coarse-grained measure ν.

To estimate the difference $E_{\mu^1}(f_{x_1,..,x_n}) - E_{\mu^2}(f_{x_1,..,x_n})$ in Theorem 5.2, we split $E_{\mu^i}(f_{x_1,..,x_n})$ into two parts, one which is of order one and one which is exponentially small. However the order one parts will be small when we consider their difference. The main idea is the following.

Given $x_1, ..., x_n$, for $n = 1, 2, 4$, and such that each x_i, x_j are not more distant than γ^{-1}, we choose a box of side $2\ell_+$ that contains all of them and is far enough from the boundary. The contribution of clusters attached to any subset of $x_1, ..., x_n$ inside the box will be denoted by g and the ones attached to any subset of $x_1, ..., x_n$ inside the box and going out of it will be denoted by R. This latter contribution is exponentially small, as a corollary of the above theorems.

We first prove this splitting in the following Lemma:

Lemma 5.8 *Let $f_{x_1,..,x_n}$ be as in (5.8), then*

$$E_{\mu^i}(f_{x_1,..,x_n}) = \mathbb{E}_{\nu^i}(g) + R_i, \qquad i = 1, 2 \qquad (5.32)$$

where g is a function of $\{\rho_x\}$ with $x \in X_\Lambda$ contained in the cube of side $2\ell_+$ and R_i are remainder terms. Moreover, there are $\delta > 0$ and constants c_1, c_2, c so that

$$\|g\|_\infty \le c_1, \qquad \|R_i\|_\infty \le c_2 e^{-c\gamma^{-\delta}}. \qquad (5.33)$$

To conclude the proof of Theorem 5.2 we need to estimate the difference $\mathbb{E}_1(g) - \mathbb{E}_2(g)$. In order to do this, we work in the coarse-grained model, i.e., in the space

$$\mathcal{X}^\Lambda = \left\{ \underline{n} = (n_x)_{x \in X_\Lambda} \in \mathbb{N}^{X_\Lambda} : |\ell_-^{-d} n_x - \rho_{\beta,+}| \le \zeta, \text{ for all } x \in X_\Lambda \right\}, \quad n_x = \ell_- \rho_x. \qquad (5.34)$$

The goal is to prove that there exists a joint representation $\mathcal{P}(\underline{n}^1, \underline{n}^2 | \bar{q}^1, \bar{q}^2)$ of the measures ν^1 and ν^2 on $\mathcal{X}^\Lambda$ such that, for any $x \in X_\Lambda$, and denoting by $\mathcal{E}$ the expectation w.r.t. to $\mathcal{P}$, we can bound the difference $\mathbb{E}_{\nu^1}(g) - \mathbb{E}_{\nu^2}(g)$ with $\mathcal{E}[d(n_x^1, n_x^2)]$, where $d(n_x^1, n_x^2)$ is an appropriate distance that we have to define and where $\mathcal{E}[d(n_x^1, n_x^2)]$ has the desired exponential decay property.

To complete the proof we then need to find a bound for $\mathcal{E}[d(n_x^1, n_x^2)]$. This comes from a Dobrushin uniqueness condition. We want to bound the Vaserstein distance between two Gibbs measures with the same Hamiltonian (5.31) but with different b.c. $\bar{q}^i$, $i = 1, 2$. It is convenient to define the Vaserstein distance in terms of the following cost functions

$$d(\underline{n}^1, \underline{n}^2) = \sum_{x \in X_\Lambda} d(n_x^1, n_x^2), \qquad d(n_x^1, n_x^2) = |n_x^1 - \underline{n}_x^2| \qquad (5.35)$$

and if we suppose $\bar{q}^1 = (\bar{q}_1^1, ..., \bar{q}_n^1)$ and $\bar{q}^2 = (\bar{q}_1^2, ..., \bar{q}_{n+p}^2)$,

$$D_z(\bar{q}^1, \bar{q}^2) := p + \min_{\{j_\ell\}} \sum_{\ell=1}^n \mathbf{1}_{\bar{q}_\ell^1 \neq \bar{q}_{j_\ell}^2}, \tag{5.36}$$

the min being over all the subsets $\{j_\ell\}$ of $\{1, ..., n+p\}$ which have cardinality n. Following Dobrushin, we need to estimate the Vaserstein distance between conditional probabilities at a single site. We thus fix arbitrarily $x \in \Lambda$, $\underline{n}^i$, $i = 1, 2$, in $\mathcal{X}^{\Lambda \setminus x}$, call $\rho^i := \ell_2^{-d} \underline{n}^i$; $\bar{q}^i$ are the b.c. outside Λ. The energy in x plus the interaction with the outside is, as usual,

$$h(\rho_x | \rho^i, \bar{q}^i) = h\big(\{\rho_x, \rho^i\}|\bar{q}^i\big) - h(\rho^i | \bar{q}^i), \tag{5.37}$$

where the first term on the r.h.s. is the energy of the configuration $\{\rho_x, \rho^i\}$ (with $\bar{q}^i$ outside Λ). The second term is the energy in $\Lambda \setminus x$ of ρ^i with nothing in x and $\bar{q}^i$ outside Λ. The conditional Gibbs measures are then the following probabilities on $\mathcal{X}^x$ (for $i = 1, 2$)

$$p(n_x | \rho^i, \bar{q}^i) = \frac{1}{Z_x(\rho^i, \bar{q}^i)} \exp\big\{ - h(\rho_x | \rho^i, \bar{q}^i)\big\}, \tag{5.38}$$

and their Vaserstein distance is

$$R\Big(p(\cdot|\rho^1, \bar{q}^1), p(\cdot|\rho^2, \bar{q}^2)\Big) := \inf_Q \sum_{n_x^1, n_x^2} Q(n_x^1, n_x^2) d(n_x^1, n_x^2), \tag{5.39}$$

where the inf is over all the joint representations Q of $p(\rho_x | \rho^i, \bar{q}^i)$, $i = 1, 2$. The key bound for the Dobrushin scheme to work is the following theorem.

Theorem 5.9 *There are $u, c_1, c_2 > 0$ s.t. $\forall x \in \Lambda$*

$$R\Big(p^1(\cdot), p^2(\cdot)\Big) \leq \sum_{z \in X_\Lambda, z \neq x} r_{\gamma, R}(x, z) d(n_z^1, n_z^2) + \sum_{z \in X_{\Lambda^c}} r_{\gamma, R}(x, z) D_z(\bar{q}^1, \bar{q}^2)$$

with

$$\sum_z r_{\gamma, R}(x, z) \leq u < 1$$

$$r_{\gamma, R}(x, z) \leq c_1 e^{-c_2 \gamma |z-x|}, \quad |z - x| \geq \ell_+.$$

Remark 5.10 The reduction to an abstract contour model allows us to deal with a coarse-grained system in which the configurations we look at are those chosen in the restricted ensembles, roughly speaking those which should be seen under the effects of a double-well potential once we restrict to its minima. In this scenario, after we compute the effective hamiltonian for the coarse-grained system, we have a new Gibbs measure which depends only on the cells variables. But now these variables are close to the mean-field value and in such a setup it is possible to prove the validity of the Dobrushin uniqueness theory.

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