J Stat Phys (2010) 138: 351–380
DOI 10.1007/s10955-009-9913-z

The McKean–Vlasov Equation in Finite Volume

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Received: 24 October 2009 / Accepted: 23 December 2009 / Published online: 8 January 2010

Abstract We study the McKean–Vlasov equation on the finite tori of length scale L in d-dimensions. We derive the necessary and sufficient conditions for the existence of a phase transition, which are based on the criteria first uncovered in Gates and Penrose (Commun. Math. Phys. 17:194–209, 1970) and Kirkwood and Monroe (J. Chem. Phys. 9:514–526, 1941). Therein and in subsequent works, one finds indications pointing to critical transitions at a particular model dependent value, $\theta^\sharp$ of the interaction parameter. We show that the uniform density (which may be interpreted as the liquid phase) is dynamically stable for $\theta < \theta^\sharp$ and prove, abstractly, that a *critical* transition must occur at $\theta = \theta^\sharp$. However for this system we show that under generic conditions—L large, $d \geq 2$ and isotropic interactions—the phase transition is in fact discontinuous and occurs at some $\theta_{\mathrm{T}} < \theta^\sharp$. Finally, for H-stable, bounded interactions with discontinuous transitions we show that, with suitable scaling, the $\theta_{\mathrm{T}}(L)$ tend to a definitive non-trivial limit as $L \to \infty$.

Keywords Phase transitions · Mean-field approximation · Kirkwood–Monroe equation · H-stability

1 Introduction

This paper concerns the McKean–Vlasov equation [26] which describes the time-evolution of a density $\rho = \rho(x,t)$,

$$\rho_t = \Delta_x \rho + \theta L^d \nabla_x \cdot \rho \nabla_x (V \star \rho). \tag{1}$$

In the above V is a real-valued function of x which has the meaning of interaction potential, we take $x \in \mathbb{T}_L^d$—the d-dimensional torus of scale L—and $\star$ denotes the convolution

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in x. It is noted that the above dynamics is positivity and L^1-norm preserving thus $\rho(x,t)$ has a probabilistic interpretation which we relate to *particle* or *fluid* density. It is hereafter assumed that ρ integrates to one. As discussed in [33], the dynamics in (1) is a gradient flow (with respect to a certain distance in the space of probability measures) for the "free energy" functional

$$\mathcal{F}_\theta(\rho) = \int_{\mathbb{T}_L^d} \rho \log \rho \, dx + \frac{1}{2}\theta L^d \int_{\mathbb{T}_L^d \times \mathbb{T}_L^d} V(x-y)\rho(x)\rho(y)\, dx\, dy. \tag{2}$$

In particular all steady state solutions of (1) must be stationary points of the functional in (2). These densities satisfy an Euler–Lagrange equation, namely

$$\rho(x) = \frac{\mathrm{e}^{-\theta L^d [\rho \star V](x)}}{\int_{\mathbb{T}_L^d} \mathrm{e}^{-\theta L^d \rho \star V} dx} \tag{3}$$

sometimes known as the Kirkwood–Monroe equation [20]. (The above follows from the fact, readily checked, that the dynamical equation can be recast into the form

$$\frac{d}{dt}\mathcal{F}_\theta(\rho) = -\int_{\mathbb{T}_L^d} \rho \left| \nabla \log \frac{\rho}{\mathrm{e}^{-\theta L^d V \star \rho}} \right|^2 dx.)$$

The volume factor, L^d, associated with the *coupling strength* in (1)–(3) may appear unfamiliar to some but it is in fact a principal subject of this note. Otherwise, θ corresponds to interaction strength: E.g., inverse temperature and, in a sense we do not make precise, the underlying density of the fluid.

We shall not digress with a detailed discussion of the motivations for the study of (1)–(2). It is sufficient to mention the following:

- Equation (1) can be realized as the large N-limit of the N-particle Fokker–Planck equation under suitable rescaling of the interaction. This goes back to the original derivation by McKean [26] and, even today, is an active topic of mathematical research. A partial list of relevant papers: [3, 5, 23, 28–30].
- Equation (1) can be realized as a diffusive limit of the standard Vlasov–Fokker–Planck equation. Cf. the derivation in [24].
- The model of chemotaxis introduced by Keller and Segel [19] is, in fact, precisely the McK–V equation in slightly disguised form with a Newtonian (logarithmic) interaction; cf. [15, 29] for a derivation from particle dynamics. For our purposes, the Keller–Segel form of the interaction is overly singular—by no means a requirement dictated by biological applications. Related models with biological applications are described in [1, 2, 7, 8, 10, 22]. The latter two are *exactly* the McK–V equation without the diffusive term.
- In a number of older works, beginning with [16] and [17] and including (but not limited to) [12, 13, 18], and [21] (cf. the article [32] for additional information and references) the van der Waals theory of interacting fluids in statistical equilibrium was elucidated as the limit of "realistic" systems under *scaling* of the interaction range. A modified version of the functional in (2), evaluated at its minimizer constitutes the free energy for these (limiting) theories. Finally, in the remarkable work [20]—predating all of the above by over two decades—the equation (3) for the equilibrium "distribution function" was inferred, under certain approximations, by direct considerations.

It should be remarked that the scaling limits achieved in the first item are not always in accord with those of the last. As such the volume factor is conspicuously absent in many modern mathematical treatments of these and related problems. However, on careful examination, the latter derivations contain the former in the static cases. Thus, for physically motivated *stable* interactions (which will be discussed in Sect. 3) with sensible thermodynamic limits, this factor indeed belongs as written in (1)–(3). For unstable interactions—which may have biological applications—the correct nature of the scaling has not been elucidated. However it appears that mathematically tractable problems in large or infinite volume emerge if the factor of L^d is omitted.

1.1 Mathematical Assumptions and Notations

Since the majority of this work takes place in fixed volume, we will omit, whenever possible, the L-dependence in our notation for the various classes of functions etc. that we employ. In particular all L^p-norms on $\mathbb{T}_L^d$ will be unadorned.

The class of potentials that we consider in this work is described as follows: Foremost we shall assume that the V are finite range, that is

$$V(x) = 0 \quad \text{if } |x| > a.$$

We will always take $L > a$ and thus we may define the remaining (minimalist) properties as though V is a function on $\mathbb{R}^d$. First, we take $V \in L^1$ and, second we assume that V is bounded below. The former is obviously required in order to make (good) sense of the uniform state. As for the latter, if $V \to -\infty$ it is unreasonable to suppose that this happens anywhere besides the origin. Even mild divergence (e.g., logarithmic in $d = 2$) can cause the functional to be unbounded below (and, in fact, just having $V < 0$ a.e. in a neighborhood of the origin leads to unphysical behavior). Finally, on physical grounds, we shall assume that V is a symmetric function of its argument: $V(x) = V(-x)$. We shall denote the class by $\mathscr{V}$:

$$\mathscr{V} = \{V \in L^1 \text{ s.t. } V^- \in L^\infty \text{ and } V \text{ symmetric with } V(x) = 0 \text{ for } |x| > a\} \tag{4}$$

where V^- denotes the negative part of V and $a < L$. Additional technical assumptions will be implemented as needed.

For the analysis of the functional $\mathcal{F}_\theta$, we shall denote by $\mathscr{P}$ the class of probability densities on $\mathbb{T}_L^d$ (although it is clear that $\mathscr{P}$ is much larger than necessary). The uniform density, will be denoted by ρ_0:

$$\rho_0 := L^{-d}. \tag{5}$$

The Fourier transform on $\mathbb{T}_L^d$ will be defined by

$$\hat{f}_k = \int_0^L f(x)\, \mathrm{e}^{-ik\cdot x}\, dx, \quad k \in \frac{2\pi}{L}\mathbb{Z}^d;$$

the inverse Fourier transform is then

$$f(x) = \frac{1}{L^d}\sum_k \hat{f}_k\, \mathrm{e}^{ik\cdot x}, \quad x \in \mathbb{T}_L^d,$$

where the summation is extended over the lattice $\frac{2\pi}{L}\mathbb{Z}^d$.

We denote the separate pieces of $\mathcal{F}_\theta(\cdot)$ by an $\mathcal{S}$ and $\mathcal{E}$: $\mathcal{F}_\theta(\cdot) =: \mathcal{S}(\cdot) + \frac{1}{2}\theta\rho_0^{-1}\mathcal{E}(\cdot,\cdot)$. For the second, we will often have occasion to regard this as the bilinear functional

$$\mathcal{E}(\rho_a, \rho_b) := \int_{\mathbb{T}_L^d \times \mathbb{T}_L^d} V(x-y)\rho_a(x)\rho_b(y)\, dx\, dy$$

which is (usually) defined regardless of the signs or normalization of its arguments. Likewise, we will have some occasion to utilize the functional $\mathcal{S}$ for arguments that, albeit non-negative, may not be normalized. For a legitimate non-negative, normalized $\rho(x)$, the quantities $\mathcal{S}(\rho)$ and $\frac{1}{2}\theta L^d \mathcal{E}(\rho,\rho)$ are (modulo signs) vaguely related to the entropy and energy of the system when the equilibrium density is ρ; the two terms will be indicated by these names.

1.2 Summary and Statement of Results

The central purpose of this note is the study of these systems as θ varies. Often enough these systems go from a quiescent (gaseous) state where no minimizers of $\mathcal{F}_\theta(\cdot)$ exist save for the uniform state to a state where this is no longer the minimizer and other minimizers are prevalent. In short, a phase transition occurs the nature of which we shall partially elucidate. The results proved and their relevant location are as follows:

In Sect. 2, the subject of phase transitions in the McK–V system will be discussed from the ground up. First, in Sect. 2.1 (which may be omitted on a preliminary reading) we establish the existence of minimizers. This allows, in Sect. 2.2 a "thermodynamic" definition of the entropic and energetic content of the system as a function of the interaction parameter θ which in turn will clarify the definition and possible nature of the (lower) transition point. In Sect. 2.3, necessary and sufficient conditions (on V) are established for the occurrence of a phase transition. The candidate transition point, much discussed in other works and here denoted by $\theta^\sharp$ is elucidated and it is shown that for $\theta < \theta^\sharp$, the uniform density is dynamically stable. In Sect. 2.4, a concise definition of a (lower) *critical* transition point is provided. First it is demonstrated (under the additional and presumably unnecessary assumption that $V \in L^2$) that if such a transition occurs, it must take place at $\theta = \theta^\sharp$. Then it is shown that the features of a non-critical transition (where at least one of the criteria for a critical transition fails) are dramatically different. The subsection ends with a principal result of this note. Namely under the majority of physically—or for that matter biologically—reasonable circumstances, it is a *non-critical* transition which occurs in the McK–V system. Moreover these occur at parameter value θ_T which is *strictly* smaller than $\theta^\sharp$. Finally in Sect. 3, the limiting behavior in large volume is discussed. In Sect. 3.1 it is shown that, for fixed interaction, the $L \to \infty$ limit of the transition points always exist. But the limit may be trivial. In Sect. 3.2, a criterion closely related to H-stability is introduced and it is shown that (with the scalings featured in (1)–(3)) for stable potentials the transition points tend to a definitive non-trivial limit. Conversely, in Sect. 3.3, the complementary—catastrophic—cases, are investigated and it is shown that the transition values tend quickly to zero.

2 Phase Transitions

2.1 Minimizing Solutions

The starting point in our analysis is to establish, for all θ, the existence of stationary solutions to (1) that minimize the free energy functional in (2). The existence of minimizers for these sorts of problems has a history: In particular [4] discuss the existence of minimizers for functionals of this form referring back to the works [12, 13]. In [6] there is an explicit construction for a related problem and, recently [9], established the desired result by methods not dissimilar to those presently employed. We shall include a proof for completeness which is succinct given the following:

Lemma 2.1 *Let $\mathcal{F}_\theta(\cdot)$ be as described. Then $\exists B_0 < \infty$ such that for all $\rho \in \mathscr{P}$ the following holds: if $\|\rho\|_\infty > B_0$ then there is another $\rho^\ddagger \in \mathscr{P}$ with $\|\rho^\ddagger\|_\infty \leq B_0$ for which*

$$\mathcal{F}_\theta(\rho) > \mathcal{F}_\theta(\rho^\ddagger).$$

Proof We start with the observation that for any ρ,

$$\mathcal{S}(\rho) \geq \mathcal{S}(\rho_0) = -\log L^d$$

and

$$\frac{1}{2}\theta L^d \mathcal{E}(\rho, \rho) \geq -\frac{1}{2}\theta L^d V_0$$

where $-V_0$ is the lower bound on $V(x)$.

For $B > 0$ and $\rho \in \mathscr{P}$, let $\mathbb{B}_B(\rho)$ denote the set

$$\mathbb{B}_B(\rho) = \{x \in \mathbb{T}_L^d \mid \rho \geq B\}$$

and $\varepsilon_B(\rho)$ the ρ-measure of $\mathbb{B}_B$:

$$\varepsilon_B = \int_{\mathbb{B}_B} \rho dx.$$

We shall (rather arbitrarily) divide into the two cases of (ρ, B)'s for which $\varepsilon_B(\rho) \geq \frac{1}{2}$ and $\varepsilon_B(\rho) < \frac{1}{2}$.

Obviously if $\varepsilon_B(\rho) \geq \frac{1}{2}$ then

$$\mathcal{S}(\rho) \geq \frac{1}{2}\log B + \int_{\mathbb{B}_B^c} \rho \log \rho.$$

The second term may be estimated from below by $(1-\varepsilon_B)\log(1-\varepsilon_B) - (1-\varepsilon_B)\log|\mathbb{B}_B^c|$ which can be bounded by quantities which do not depend on B. Since the energy term is bounded below it is clear that for some $B_1 < \infty$ if $B > B_1$ $\mathcal{F}_\theta(\rho)$ will exceed $\mathcal{F}_\theta(\rho_0)$. We turn attention to the cases $\varepsilon_B < \frac{1}{2}$.

We write $\rho = \rho_b + \rho_r$ where ρ_b is the restriction of ρ to the set $\mathbb{B}_B$ and ρ_r is the rest. Our claim is that if B is too large—and $\varepsilon_B > 0$—then

$$\mathcal{F}_\theta(\rho) > \mathcal{F}_\theta(\overline{\rho}_r)$$

where $\overline{\rho}_r = (1-\varepsilon_B)^{-1}\rho_r$ is the normalized version of ρ_r.

We write, $\mathcal{S}(\rho_r) := \int_{\mathbb{T}_L^d} \rho_r \log \rho_r dx$, notwithstanding the fact that ρ_r is not normalized, and observe (assuming $B > 1$ and $\varepsilon_B > 0$) that

$$\mathcal{S}(\rho) \geq \mathcal{S}(\rho_r) + \varepsilon_B \log B > \mathcal{S}(\rho_r).$$

Since we might as well assume that $\mathcal{F}_\theta(\rho) \leq \mathcal{F}_\theta(\rho_0)$ and the energetic components of both of these quantities are bounded above and below this implies that for some $s_\star < \infty$

$$s_\star \geq \mathcal{S}(\rho) > \mathcal{S}(\rho_r)$$

regardless of the particulars of ρ vis-à-vis B and ε_B. Similarly, we have (since $\mathcal{E}(\rho, \rho) < \mathcal{E}(\rho_0, \rho_0)$ and $\varepsilon_B < 1/2$) that $\mathcal{E}(\rho_r, \rho_r) \leq \mathcal{E}(\rho_0, \rho_0) + V_0 =: e^\star < \infty$.

Now let us estimate $\mathcal{F}_\theta(\rho) - \mathcal{F}_\theta(\overline{\rho}_r)$. First

$$\begin{aligned}\mathcal{S}(\rho) - \mathcal{S}(\overline{\rho}_r) &\geq \varepsilon_B \log B - \frac{\varepsilon_B}{1-\varepsilon_B}\mathcal{S}(\rho_r) + \log(1-\varepsilon_B) \\ &\geq \varepsilon_B \left[\log B - \frac{1+s^\star}{1-\varepsilon_B}\right] \end{aligned} \tag{6}$$

where we have used the fact that $\log(1-\varepsilon_B) \geq -\frac{\varepsilon_B}{1-\varepsilon_B}$. As for the energetics, it is seen that

$$\mathcal{E}(\rho,\rho) \geq \mathcal{E}(\rho_p,\rho_p) - \theta V_0 \varepsilon_B$$

while

$$\mathcal{E}(\overline{\rho}_p,\overline{\rho}_p) = \frac{1}{(1-\varepsilon_B)^2}\mathcal{E}(\rho_p,\rho_p),$$

so

$$\mathcal{E}(\rho,\rho) - \mathcal{E}(\overline{\rho}_r,\overline{\rho}_r) \geq \left[\frac{-2\varepsilon_B + \varepsilon_B^2}{(1-\varepsilon_B)^2}\right]\mathcal{E}(\rho_r,\rho_r) \geq -8\varepsilon_B e_\star \tag{7}$$

where we have used $\varepsilon_B < 1/2$.

The combination of (6) and (7) shows that if B exceeds some (finite) B_2 the density $\overline{\rho}_r$ represents an "improvement" (unless $\varepsilon_B = 0$). Note that, conceivably, the improvement may take values as large as *twice* B_2. Nevertheless, the theorem is completed by declaring $B_0 = \max\{B_1, 2B_2, 1\}$ and using for $\rho^\ddagger$ the uniform or above described density as appropriate. □

Theorem 2.2 *Let $\mathcal{F}_\theta(\rho)$ be as described in (2) Then there exists a $\rho_\theta \geq 0 \in \mathscr{P}$ that minimizes $\mathcal{F}_\theta(\cdot)$.*

Proof Let (ρ_j) denote a minimizing sequence for $\mathcal{F}_\theta(\cdot)$. Since, without loss of generality $\rho_j \in L^1 \cap L^\infty$, we may place the ρ_j in L^2 with $\|\rho_j\|_2^2 < B_0$. Let ρ_∞ denote a weak limit of the sequence. By standard convexity arguments, $\lim_{j\to\infty} \mathcal{S}(\rho_j) \geq \mathcal{S}(\rho_\infty)$ (where we have used (ρ_j) to denote the *sub*sequence).

We claim that

$$\lim_{j\to\infty} \mathcal{E}(\rho_j,\rho_j) = \mathcal{E}(\rho_\infty,\rho_\infty). \tag{8}$$

This follows from some elementary Fourier analysis: Since $V(x) \in L^1$, $|\hat{V}(k)| \to 0$ as $k \to \infty$. Let $\overline{w}_{k_0} = \max_{|k|>|k_0|} |\hat{V}(k)|$ where here and throughout it is assumed that all k's are legitimate wave vectors for $\mathbb{T}_L^d$. Then

$$|\mathcal{E}(\rho_j,\rho_j) - \mathcal{E}(\rho_\infty,\rho_\infty)| \leq \sum_{k:|k|\leq|k_0|} \hat{V}(k)[|\hat{\rho}_j(k)|^2 - |\hat{\rho}_\infty(k)|^2] + 2B_0\overline{w}_{k_0}. \tag{9}$$

The first term tends to zero since for each individual k, $\hat{\rho}_j(k) \to \hat{\rho}_\infty(k)$ and the second term can be made as small as desired. Thus we may conclude that ρ_∞ actually (globally) minimizes the functional. □

On the basis of the above, we may define

$$\mathscr{M}_\theta := \{\rho \in \mathscr{P} \mid \rho \text{ minimizes } \mathcal{F}_\theta(\cdot)\} \tag{10}$$

(where the above refers to *global* minimizers) with the assurance that $\forall\theta$, $\mathscr{M}_\theta \neq \emptyset$. As an obvious corollary to Lemma 2.1, we have that any $\rho \in \mathscr{M}_\theta$ is bounded above. Conversely, we have uniform lower bounds (which, strictly speaking, do not play a rôle in later developments).

Proposition 2.3 *Let $\rho \in \mathscr{M}_\theta$. Then ρ is bounded below strictly away from zero.*

Proof We appeal directly to the Kirkwood–Monroe equation (3) from which it is clear that pointwise upper and lower bounds on $V \star \rho$ are sufficient. Obviously $V \star \rho \leq \|\rho\|_\infty \|V\|_1$. Next, with more elaboration than may be necessary, let

$$P_a(\rho) = \sup_{y \in \mathbb{T}_L^d} \int_{|y-y'|\leq a} \rho(y')dy' \tag{11}$$

where it is recalled that a denotes the range of the interaction. Then $V \star \rho \geq -P_a V_0$. This provides

$$\rho(x) \geq \exp -\theta L^d [P_a V_0 + \|\rho\|_\infty \|V\|_1] > 0. \qquad \square$$

Remark It is anticipated that in physically reasonable (stable) cases, which will be discussed in Sect. 3, both terms in the square bracket appearing in the previous equation are of the order of L^{-d}. However, in catastrophic cases, it seems that $P_a(\rho)$ will indeed achieve values of order unity independent of L for $\rho \in \mathscr{M}_\theta$.

2.2 Thermodynamics for the McK–V System

We may now separately define the energetic and entropic content of the system as a function of the parameter θ; these form the basis of a thermodynamic theory.

Definition We define

$$E_\theta = \inf_{\rho \in \mathscr{M}_\theta} \frac{1}{2} \theta \rho_0^{-1} \mathcal{E}(\rho, \rho) \tag{12}$$

and

$$S_\theta = \inf_{\rho \in \mathscr{M}_\theta} \mathcal{S}(\rho). \tag{13}$$

Furthermore, defining

$$F_\theta = \inf_{\rho \in \mathscr{P}} \mathcal{F}_\theta(\rho) \tag{14}$$

we have, to within signs and constants, the energy, entropy and free energy of the system at parameter value θ. It is noted that the first two do not always add up to the third.

Proposition 2.4 *Consider the above defined thermodynamic functions. Then*

(a) *S_θ is non-decreasing*
(b) *$F_\theta - \frac{1}{2}\theta\rho_0^{-1}\mathcal{E}(\rho_0, \rho_0)$ is non-increasing and continuous while*
(c) *$\theta^{-1} E_\theta$ and $E_\theta - \frac{1}{2}\theta\rho_0^{-1}\mathcal{E}(\rho_0, \rho_0)$ are non-increasing.*

We remark that the subtractions are actually necessary: consider, e.g., the situation where $\mathcal{E}(\rho_0, \rho_0) > 0$ in the region of small values of θ where $\mathcal{F}_\theta(\cdot)$ is always minimized by ρ_0.

Proof We shall start with the energetics. Let $\theta_1, \theta_2 \geq 0$ and let $\rho_{\theta_1} \in \mathscr{M}_{\theta_1}$ and similarly for ρ_{θ_2}. Then, using ρ_{θ_2} instead of ρ_{θ_1} we have that

$$\begin{aligned} F_{\theta_1} &\leq \mathcal{F}_{\theta_1}(\rho_{\theta_2}) = \mathcal{F}_{\theta_2}(\rho_{\theta_2}) - \frac{1}{2}\rho_0^{-1}(\theta_2 - \theta_1)\mathcal{E}(\rho_{\theta_2}, \rho_{\theta_2}) \\ &\leq F_{\theta_2} - \frac{1}{2}(\theta_2 - \theta_1)\rho_0^{-1}\mathcal{E}(\rho_{\theta_2}, \rho_{\theta_2}). \end{aligned}$$

Similarly,

$$F_{\theta_2} \leq F_{\theta_1} - \frac{1}{2}(\theta_1 - \theta_2)\rho_0^{-1}\mathcal{E}(\rho_{\theta_1}, \rho_{\theta_1})$$

so that $(\theta_2 - \theta_1)\mathcal{E}(\rho_{\theta_2}, \rho_{\theta_2}) \leq (\theta_2 - \theta_1)\mathcal{E}(\rho_{\theta_1}, \rho_{\theta_1})$ which, if $\theta_2 > \theta_1$, certainly implies the first of the items in (c). However, a bit more has been shown: The energetic content of *any* $\rho_{\theta_1} \in \mathscr{M}_{\theta_1}$ is monotonically related to the energetic content of *any* $\rho_{\theta_2} \in \mathscr{M}_{\theta_2}$.

This immediately establishes monotonicity of the entropy-term. Indeed, suppose that, $\theta_2 > \theta_1$. Then, at $\theta = \theta_1$ using a ρ_{θ_2} we have:

$$F_{\theta_1} \leq \mathcal{S}(\rho_{\theta_2}) + \frac{1}{2}\theta_1\rho_0^{-1}\mathcal{E}(\rho_{\theta_2}, \rho_{\theta_2}). \tag{15}$$

The energy term is less than that associated with $\mathcal{E}(\rho_{\theta_1}, \rho_{\theta_1})$ and we arrive at

$$F_{\theta_1} \leq \mathcal{S}(\rho_{\theta_2}) + \frac{1}{2}\theta_1\rho_0^{-1}\mathcal{E}(\rho_{\theta_1}, \rho_{\theta_1}) = F_{\theta_1} + S(\rho_{\theta_2}) - S(\rho_{\theta_1}). \tag{16}$$

We again have that for *any* $\rho_{\theta_1} \in \mathscr{M}_{\theta_1}$ and $\rho_{\theta_2} \in \mathscr{M}_{\theta_2}$, with $\theta_1 < \theta_2$,

$$\mathcal{S}(\rho_{\theta_1}) \leq \mathcal{S}(\rho_{\theta_2}).$$

As for the claims about F_θ, continuity follows from the first two displays in this proof. For the monotonicity, of $E_\theta - \frac{1}{2}\theta\rho_0^{-1}\mathcal{E}(\rho_0, \rho_0)$, we first observe that for any θ and any $\rho_\theta \in \mathscr{M}_\theta$

$$\mathcal{E}(\rho_\theta, \rho_\theta) \leq \mathcal{E}(\rho_0, \rho_0)$$

with equality only if $\rho_\theta = \rho_0$ a.e. Indeed, assuming that ρ_θ is not a.e. equal to ρ_0, then $\mathcal{S}(\rho_0) < \mathcal{S}(\rho_\theta)$ so ρ_θ could not possibly be a minimizer if the opposite of the above display were to hold. Then $[\mathcal{E}(\rho_\theta, \rho_\theta) - \mathcal{E}(\rho_0, \rho_0)]$ is non-positive and non-increasing so $\theta[\mathcal{E}(\rho_\theta, \rho_\theta) - \mathcal{E}(\rho_0, \rho_0)]$ is non-increasing.

The final claim is now proved by reiteration of the previous procedures with the subtraction in place:

$$\begin{aligned} &F_{\theta_2} - \frac{1}{2}\theta_2\rho_0^{-1}\mathcal{E}(\rho_0, \rho_0) \\ &\quad\leq \mathcal{S}(\rho_{\theta_1}) + \frac{1}{2}\theta_2\rho_0^{-1}\mathcal{E}(\rho_{\theta_1}, \rho_{\theta_1}) - \frac{1}{2}\theta_2\rho_0^{-1}\mathcal{E}(\rho_0, \rho_0) \\ &\quad= F_{\theta_1} - \frac{1}{2}\theta_1\rho_0^{-1}\mathcal{E}(\rho_0, \rho_0) + \frac{1}{2}(\theta_2 - \theta_1)\rho_0^{-1}[\mathcal{E}(\rho_{\theta_1}, \rho_{\theta_1}) - \mathcal{E}(\rho_0, \rho_0)] \end{aligned}$$

where we have assumed $\theta_2 > \theta_1$. By the non-positivity of the quantity in the square brackets, the stated monotonicity is established. $\square$

With the above monotonicities in hand, the objects S_θ and E_θ can now be considered well defined functions for all θ which are continuous for a.e. θ. However at points of discontinuity, it may be more useful to focus on the range of the function rather than its value at the point. In particular S_θ is continuous iff E_θ is continuous while at points of discontinuity, the density that minimizes $\mathcal{S}$ is the one that maximizes $\mathcal{E}$ and vice versa.

2.3 Phase Transitions in the McK–V Systems (1): The Point of Linear Stability

We start this subsection with some preliminary results—most of which have appeared elsewhere in the literature (albeit by different methods)—concerning the single phase regime: The regime where ρ_0 is the unique minimizer of $\mathcal{F}_\theta(\cdot)$.

Proposition 2.5 *Let $V \in \mathscr{V}$ be bounded i.e. $|V| \le V_{\max} < \infty$. Then for θL^d sufficiently small—less than $[V_{\max}]^{-1}$—the functional $\mathcal{F}_\theta(\rho)$ is convex.*

Proof The functional $\mathcal{F}_\theta(\rho)$ is finite on the set

$$\mathscr{Q} = \{\rho \in \mathscr{P} \mid \rho \log \rho \in L^1\};$$

and there is no ambiguity to set $\mathcal{F}_\theta(\rho) = +\infty$ for $\rho \in \mathscr{P} \setminus \mathscr{Q}$.

Then, it suffices to show that for any $\rho_1, \rho_2 \in \mathscr{Q}$ the function $s \mapsto \mathcal{F}_\theta(\rho_s)$ where $\rho_s = \rho_2 s + \rho_1(1-s)$ is convex. It is straightforward to verify that $\mathcal{F}_\theta(\rho_s)$ is twice differentiable in $s \in (0,1)$. Then, we compute

$$\left(\frac{d}{ds}\right)^2 \mathcal{F}_\theta(\rho_s) = \int_{\mathbb{T}_L^d} \frac{\eta^2}{\rho_s}\, dx + \theta L^d \int_{\mathbb{T}_L^d \times \mathbb{T}_L^d} V(x-y)\eta(x)\eta(y)\, dx\, dy,$$

where $\eta = \rho_2 - \rho_1$. By Jensen's inequality we have

$$\int_{\mathbb{T}_L^d} \frac{\eta^2}{\rho_s}\, dx = \int_{\mathbb{T}_L^d} \left(\frac{\eta}{\rho_s}\right)^2 \rho_s\, dx \ge \left(\int_{\mathbb{T}_L^d} \left|\frac{\eta}{\rho_s}\right| \rho_s\, dx\right)^2 = \left(\int_{\mathbb{T}_L^d} |\eta|\, dx\right)^2.$$

On the other hand, since $|V(x-y)| \le V_{\max}$ we have

$$\left|\int_{\mathbb{T}_L^d \times \mathbb{T}_L^d} V(x-y)\eta(x)\eta(y)\, dx\, dy\right| \le V_{\max}\left(\int_{\mathbb{T}_L^d} |\eta|\, dx\right)^2.$$

This implies the inequality

$$\left(\frac{d}{ds}\right)^2 \mathcal{F}_\theta(\rho_s) \ge (1 - \theta L^d V_{\max})\left(\int_{\mathbb{T}_L^d} |\eta|\, dx\right)^2 > 0$$

if $\theta L^d V_{\max} < 1$. $\square$

This immediately implies:

Corollary 2.6 *Under the conditions of Proposition 2.5, $\rho_0 = 1/L^d$ is the unique minimizer of $\mathcal{F}_\theta(\rho)$.*

From the proof of the above Proposition we also obtain a corollary for potentials V which are of *positive type*:

Definition A potential V is said to be of *positive* type if for all functions h in some suitable class (e.g., L_∞)

$$\int_{\mathbb{T}_L^d \times \mathbb{T}_L^d} V(x-y)h(x)h(y)\,dx\,dy \geq 0,$$

which is equivalent to the condition that $\forall k$

$$\hat{V}(k) \geq 0.$$

We let $\mathscr{V}^+ \subset \mathscr{V}$ denote the set of interactions that are of positive type and, for future reference, the complementary set by $\mathscr{V}_N$:

$$\mathscr{V}_N = \mathscr{V} \setminus \mathscr{V}^+. \tag{17}$$

Corollary 2.7 *Let $V \in \mathscr{V}^+$. Then for all θ, the unique minimizer of $\mathcal{F}_\theta(\cdot)$ is the uniform density ρ_0.*

Proof For $\rho = \rho_0(1+\eta)$ in $\mathscr{P}$, we consider $f_\eta(s) := \mathcal{F}_\theta(\rho_0(1+s\eta))$. Calculating $f_\eta''(s)$ as in the proof of Proposition 2.5, the entropy term is still positive while the energy term yields

$$\rho_0\theta \int_{\mathbb{T}_L^d \times \mathbb{T}_L^d} V(x-y)\eta(x)\eta(y)\,dx\,dy \geq 0.$$

Thus $f_\eta(s)$ is always convex and, for all η always minimized at $s=0$.

Note that since all convexities are *strict*, any $\rho \in \mathscr{P}$ that is not a.e. equal to ρ_0 admits, for all θ,

$$\mathcal{F}_\theta(\rho_0) < \mathcal{F}_\theta(\rho).$$

□

Next we show that $V \in \mathscr{V}_N$ is also sufficient for the existence of a non-trivial phase. The starting point is an elementary result which, strictly speaking is a corollary to Proposition 2.4.

Proposition 2.8 *Let $V \in \mathscr{V}$ (but in $\mathscr{V}_N$ for non-triviality) and suppose that at some $\theta_d < \infty$ there is a ρ_{θ_d} which is not a.e. equal to ρ_0 such that*

$$\mathcal{F}_{\theta_d}(\rho_{\theta_d}) \leq \mathcal{F}_{\theta_d}(\rho_0).$$

Then for all $\theta > \theta_d$, ρ_0 is not the minimizer of $\mathcal{F}_\theta(\cdot)$.

Proof Indeed, since ρ_{θ_d} is not a constant it must be the case that

$$\mathcal{S}(\rho_{\theta_d}) > \mathcal{S}(\rho_0) \tag{18}$$

thence

$$\mathcal{E}(\rho_{\theta_d}, \rho_{\theta_d}) < \mathcal{E}(\rho_0, \rho_0). \tag{19}$$

Thus for $\theta > \theta_d$, it is seen that

$$\begin{aligned} F_\theta &\leq \mathcal{F}_{\theta_d}(\rho_{\theta_d}) + \frac{1}{2}\rho_0^{-1}(\theta - \theta_d)\mathcal{E}(\rho_{\theta_d}, \rho_{\theta_d}) \\ &< \mathcal{F}_{\theta_d}(\rho_{\theta_d}) + \frac{1}{2}\rho_0^{-1}(\theta - \theta_d)\mathcal{E}(\rho_0, \rho_0) \leq \mathcal{F}_\theta(\rho_0) \end{aligned}$$

which is the stated result. □

Thus beginning at $\theta = 0$ there is a non-trivial interval of θ characterized by the property that ρ_0 is the unique minimizer for $\mathcal{F}_\theta(\cdot)$. The interval "terminates" at some value of θ-possibly infinite. Assuming this value is finite, we may refer to it as the *lower transition point* and, above this point, there are non-trivial minimizers of $\mathcal{F}_\theta$ and non-trivial solutions to (3) and (1). (We shall refrain from naming this point till the possible nature of the transition at this point has been clarified.) It should be noted, by a variant of the above argument, that *at* the lower transition point ρ_0 is actually still a minimizer of the functional in (2).

We introduce some notation:

Definition For $V \in \mathscr{V}_N$, let $k^\sharp$ denote a minimizing wave vector for $\hat{V}(k)$:

$$\hat{V}(k^\sharp) \leq \hat{V}(k) \quad \forall k.$$

Note that $\hat{V}(k^\sharp) < 0$ by assumption. We define $\theta^\sharp = \theta^\sharp(V)$ via

$$\theta^\sharp := |\hat{V}(k^\sharp)|^{-1}.$$

We are finally ready for the following:

Proposition 2.9 ([13]; see also [4]) *Let $V \in \mathscr{V}_N$. If $\theta > \theta^\sharp$ then $\exists \rho \in \mathscr{P}$, $\rho \neq \rho_0$ which minimizes $\mathcal{F}_\theta(\cdot)$. In particular, for $\theta > \theta^\sharp$, ρ_0 is no longer a minimizer of $\mathcal{F}_\theta$. Thus $V \in \mathscr{V}_N$ is the necessary and sufficient condition for the existence of a non-trivial phase.*

Proof For $\theta > \theta^\sharp$ we may use as a trial minimizing function

$$\rho = \rho_0(1 + \varepsilon\eta^\sharp)$$

where $\eta^\sharp$ is a plane wave at wave number $k^\sharp$ and is itself of order unity while ε is to be regarded as a small parameter. Since all quantities are bounded, we may expand:

$$\begin{aligned} &\rho_0(1 + \varepsilon\eta^\sharp)\log\rho_0(1 + \varepsilon\eta^\sharp) \\ &\quad = \rho_0(1 + \varepsilon\eta^\sharp)\log\rho_0 + \rho_0(1 + \varepsilon\eta^\sharp)\left(\varepsilon\eta^\sharp - \frac{1}{2}[\varepsilon\eta^\sharp]^2\right) + o(\varepsilon^2). \end{aligned}$$

Since $\eta^\sharp$ integrates to zero,

$$\mathcal{S}(\rho) = \mathcal{S}(\rho_0) + \frac{1}{2}\varepsilon^2\rho_0 \int |\eta^\sharp|^2 dx + o(\varepsilon^2). \tag{20}$$

Meanwhile

$$\frac{1}{2}\theta\rho_0^{-1}\mathcal{E}(\rho,\rho) = \frac{1}{2}\theta\rho_0^{-1}\mathcal{E}(\rho_0,\rho_0) + \frac{1}{2}\varepsilon^2\theta\rho_0 \int V(x-y)\eta^\sharp(x)\eta^\sharp(y)\,dx\,dx$$
$$= \frac{1}{2}\theta\rho_0^{-1}\mathcal{E}(\rho_0,\rho_0) + \frac{1}{2}\varepsilon^2\rho_0\hat{V}(k^\sharp)\|\eta^\sharp\|_2^2[\theta^\sharp + (\theta-\theta^\sharp)].$$

By definition of $\theta^\sharp$,

$$-\frac{1}{2}\varepsilon^2\|\eta^\sharp\|_2^2 = \frac{1}{2}\theta^\sharp\varepsilon^2\hat{V}(k^\sharp)\|\eta^\sharp\|_2^2$$

so that

$$\mathcal{F}_\theta(\rho) = \mathcal{F}_\theta(\rho_0) - \frac{1}{2}\varepsilon^2\rho_0\|\eta^\sharp\|_2^2[|\hat{V}(k^\sharp)|](\theta-\theta^\sharp) + o(\varepsilon^2)$$

which is strictly less than $\mathcal{F}_\theta(\rho)$ for ε sufficiently small. (Here it is noted that the quantity $\rho_0\|\eta^\sharp\|_2^2$ is itself of order unity.) By Proposition 2.8 the above is sufficient to establish the statement of this proposition. □

Corollary 2.10 *For $V \in \mathscr{V}_N$, $\theta^\sharp(V)$ is the supremum of the set of quadratically stable parameter values for $\mathcal{F}_\theta(\rho_0)$. Furthermore, $\theta^\sharp$ marks the boundary for the linear stability of (1) with solution ρ_0. I.e. for $\theta < \theta^\sharp$, ρ_0 is linearly stable while for $\theta > \theta^\sharp$, it is not.*

Proof The first statement follows, in essence, from the above display. As for the dynamics, the linearized version of (1) reads, for $\eta = (\rho-\rho_0)\rho_0^{-1}$

$$\frac{\partial\eta}{\partial t} = \nabla^2(\eta + \theta V \star \eta). \tag{21}$$

The linear operator $\nabla^2[1+\theta V\star](\cdot)$ has, by the definition of $\theta^\sharp$, a strictly negative spectrum if and only if $\theta < \theta^\sharp$. The second statement of this corollary therefore follows from the definition of linear order stability. □

While the above statement does not necessarily have a direct implication on dynamical stability of ρ_0 for the nonlinear evolution with $\theta < \theta^\sharp$, such a result is in fact true. Here we find that ρ_0 in that case has a non-trivial *basin of stability*.

Theorem 2.11 *Under the regularity assumption*

$$G = \frac{1}{L^d}\sum_k |\hat{V}(k)||k| < \infty$$

there is a non-trivial basin of attraction for ρ_0 which contains all Borel measures that are sufficiently close to ρ_0 in the total variation distance. In particular, at positive times, any such perturbing measure regularizes and, for any particular Sobolev norm, the density converges to ρ_0 exponentially fast in this norm. The stated results hold uniformly in L for the rate of convergence and the size of the perturbation relative to ρ_0.

Remark The regularity assumption on V is for convenience; presumably a stronger result is available. In particular, it is not hard to see that with greater regularity of the perturbing density, regularity assumptions on the interaction potential can be relaxed. Moreover, with *greater* regularity assumptions on V, even more singular objects than Borel measures are contained in the basin of attraction. It is noted that the condition on V is, in essence independent of L. I.e., for fixed $V(x)$ defined on $\mathbb{R}^d$ with $\hat{V}(k)$ denoting the Fourier transform with $k \in \mathbb{R}^d$, the above amounts to the condition that

$$\int_{\mathbb{R}^d} |k|\hat{V}(k)dk < \infty.$$

Proof We write $\rho = \rho_0(1+\eta)$ with η measure valued. Let $\hat{\eta}_k(t)$ denote the dynamically evolving kth Fourier mode. We shall assume that in the initial state, each mode is small—which is certainly implied by the smallness of the total variation distance. In particular, we will assume that at $t = 0$ each $\hat{\eta}_k(0)$ is bounded by an ε_0 which satisfies the condition that for all k,

$$2|k|\theta G\varepsilon_0 < \lambda(k) \tag{22}$$

where $\lambda(k) = k^2(1 + \theta\hat{V}(k))$ is the decay rate for the kth mode in the linear approximation. It is emphasized that $\lambda(k) > ck^2$ with $c > 0$ if $\theta < \theta^\sharp$.

The $\hat{\eta}_k(t)$ satisfy the formal equation

$$\frac{\partial\hat{\eta}_k(t)}{\partial t} = -\lambda(k)\hat{\eta}_k(t) - \frac{1}{L^d}\theta k\cdot\sum_{k'} k'\hat{V}(k')\hat{\eta}_{k'}(t)\hat{\eta}_{k'-k}(t) \tag{23}$$

where, it is emphasized, all other factors of volume have canceled out. It is noted that (23) may certainly be used to formulate dynamics via an iterative scheme—provided that control is maintained under reiteration. Thus we may consider the sequence $(\hat{\eta}_k^{(\ell)}(t) \mid \ell = 0, 1, 2, \dots)$ where $\hat{\eta}_k^{(0)}(t) \equiv \hat{\eta}_k(0)$ and $\hat{\eta}_k^{(\ell+1)}(t)$ is defined as the solution of (23) with $\hat{\eta}_k^{(\ell)}(t)$ the argument of the non-linear kernel.

The form in which we will use equation (23) is with moduli; we have

$$\frac{\partial|\hat{\eta}_k(t)|}{\partial t} = -\lambda(k)|\hat{\eta}_k(t)| - \frac{\theta}{2}\frac{1}{L^d}\left[\frac{\overline{\hat{\eta}_k(t)}}{|\hat{\eta}_k(t)|}k\cdot\sum_{k'} k'\hat{V}(k')\hat{\eta}_{k'}(t)\hat{\eta}_{k'-k}(t) + \text{c.c.}\right].$$

The first claim is that for ε_0 satisfying the condition in (22) then for all k and t and ℓ,

$$|\eta_k^{(\ell)}(t)| \leq \varepsilon_0.$$

Indeed, this is certainly true for $\eta_k^{(0)}$ so, inductively,

$$\frac{\partial|\eta_k^{(\ell)}(t)|}{\partial t} \leq -\lambda(k)|\eta_k^{(\ell)}(t)| + \theta\varepsilon_0^2 G|k|. \tag{24}$$

First, let us consider modes that satisfy

$$|\eta_k(0)| > \frac{|k|\theta G\varepsilon_0^2}{\lambda(k)}. \tag{25}$$

Such modes will decrease in magnitude—at least till $|\eta_k(t)|$ reaches the right side of the inequality in (25) whereupon they may "stick". But by assumption, these modes started out smaller than ε_0. On the other hand, modes with initial conditions that satisfy the opposite inequality of (25) may actually grow till the inequality saturates but this does not get them past ε_0 since for all k,

$$\varepsilon_0 > \frac{G\theta\varepsilon_0^2|k|}{\lambda(k)} \tag{26}$$

by hypothesis. (The factor of two does not yet come into play.)

Contraction of the sequence follows an identical argument which *does* employ the factor of 2. We define $\Delta_k^\ell(t) = |\hat{\eta}^{(\ell+1)} - \hat{\eta}^{(\ell)}|$ and $\Delta_\star^\ell = \sup_{k,t} \Delta_k^\ell(t)$. It is found that $\forall k, t$,

$$\Delta_k^\ell(t) \leq \frac{2\Delta_\star^{\ell-1}\varepsilon_0|k|\theta G}{\lambda(k)} < (1-\delta)\Delta_\star^{\ell-1} \tag{27}$$

for some $\delta > 0$ by (22). Thus (23) indeed defines our dynamics and we may perform manipulations on its basis without further discussion. Our next task will be to get the η_k uniformly decaying.

By repeating the steps of (24)–(26) it is clear that for any $e_0 > \varepsilon_0$, there is a time t_0 such that for all $t > t_0$,

$$|\eta_k(t)| < \frac{G\theta e_0^2|k|}{\lambda(k)}. \tag{28}$$

Incidentally, we have now placed η in some reasonable Sobolev space—but this is not yet relevant. For the moment, the pertinent observation is that there is a maximum sized mode which is to be found at a finite value of k (which may, of course, change from time to time). Thus, for each $t > t_0$, let β_0 denote the modulus of the maximum mode and $\overline{k}$ denote the wave vector that maximizes. Then, for all $t > t_0$ we have

$$\frac{\partial\beta_0}{\partial t} \leq -\lambda(\overline{k})\beta_0 + G\theta|\overline{k}|\beta_0\varepsilon_0 \leq -\frac{1}{2}\lambda_{\min}\beta_0 \tag{29}$$

where $\lambda_{\min}$ is the minimum of $\lambda(k)$ (which is positive for $\theta < \theta^\sharp$). We conclude that all the $\eta_k(t)$ tends to zero exponentially fast with rate at least as large as $\frac{1}{2}\lambda_{\min}$.

We use a small variant of this argument to show that for any n, the maximum of $|k|^n|\eta_k(t)|$ (exists and) decays with a rate at least as large as $\frac{1}{2}\lambda_{\min}$. Focusing on $n \geq 1$ let us assume that at the $n-1$st stage of the argument, we have a t_{n-1} such that for all $t > t_{n-1}$,

$$\beta_k^{[n-1]}(t) \leq \frac{\theta|k|G}{\lambda(k)}\delta_{n-1}2^{n-1} \tag{30}$$

here $\beta_k^{[n]}(t) := |k|^n|\eta_k(t)|$ and the quantity δ_n is specified as follows: Multiplying both sides by $|k|$, since $\lambda \geq ck^2$ this puts a uniform bound on $\beta_k^{[n]}(t)$ which is stipulated to be less than one.

We now write

$$\begin{aligned}\frac{\partial\beta_k^{[n]}}{\partial t} &\leq -\lambda(k)\beta_k^{[n]} + \frac{1}{L^d}2^{n-1}|k|\theta\sum_{k'}\beta_{k'}^{[n]}|\eta_{k'-k}||\hat{V}(k')k'| \\ &\quad + \frac{1}{L^d}2^{n-1}|k|\theta\sum_{k'}\beta_{k'-k}^{[n]}|\eta_{k'}||\hat{V}(k')k'|\end{aligned}$$

where we have used $|k|^n = |k' + k - k'|^n \leq 2^{n-1}[|k|^n + |k - k'|^n]$. We now wait till a time t'_n when each $|\eta_t(k)|$ is less then some ε_n which is small and to be specified. Summing, the estimates,

$$\frac{\partial \beta_k^{[n]}}{\partial t} \leq -\lambda(k)\beta_k^{[n]} + 2^n \theta |k| \varepsilon_n \tag{31}$$

and we now wait till a time $t_n > t'_n$ so that, similar to the previous portion of the argument,

$$\beta_k^{[n]}(t) \leq \frac{\theta |k| G}{\lambda(k)} 2^n \delta_n \tag{32}$$

for any $\delta_n > \varepsilon_n$. Obviously this δ_n will be tailored to satisfy the requirements to propagate the *next* iterate of the argument—and so we stipulate. But in addition we require that $2^n \delta_n < \varepsilon_0$.

The proof is completed by noting that (32) allows us to conclude that the supremum of $\beta_k^{[n]}$ is to be found at a finite k and the rest of the argument proceeds as described in the vicinity of (29). The desired result has been proved. □

2.4 Phase Transitions in the McK–V Systems (2): First Order Transitions

In order to investigate the possibility of continuous/discontinuous transitions in this model, an appropriate definition must be provided.

Definition Consider the McK–V functional $\mathcal{F}_\theta$ with $V \in \mathscr{V}_N$. We define θ_c to be a (lower) critical point if the following criteria are satisfied:

- For $\theta \leq \theta_c$, ρ_0 is the unique minimizer of $\mathcal{F}_\theta(\cdot)$.
- For $\theta > \theta_c$, $\exists \rho_\theta \neq \rho_0$ which minimizes $\mathcal{F}_\theta(\cdot)$, (which necessarily implies that ρ_0 is no longer a minimizer of $\mathcal{F}_\theta(\cdot)$).
- If $(\rho_\theta \mid \theta > \theta_c)$ is any family of such minimizers then

$$\limsup_{\theta \downarrow \theta_c} \|\rho_0 - \rho_\theta\|_1 = 0.$$

Remark We have called this a lower critical transition since, conceivably there could be later (in θ) transitions of this type with non-trivial solutions "bifurcating" from preexisting non-trivial solutions. This would be difficult to detect—analytically or numerically—since the non-trivial solutions are anyway evolving with θ. Such a phenomenon would, presumably, have to be tied to non-analyticity in $\mathcal{E}(\cdot)$ or $\mathcal{S}(\cdot)$ notwithstanding their *continuity*. By contrast (cf. Proposition 2.13 below) for the other possible type of transition, these objects are generically *discontinuous*. In any case, the foremost possible phase transition in these systems is the lower one and will be the focus of all our attention.

Any (lower) phase transition not satisfying the above three items will be called a *discontinuous transition* and we will denote such a transition point by θ_{T}. As we shall see later, in Proposition 2.13, for a discontinuous transition the second item will hold while in the first item, we must replace $\theta \leq \theta_c$ with $\theta < \theta_{\mathrm{T}}$. But most pertinently, the third item fails in its entirety. Thus, at such a transition point, a new minimizing solution of (1) appears which, for $\theta = \theta_{\mathrm{T}}$, is degenerate (in the sense of minimizing $\mathcal{F}_\theta(\cdot)$) with ρ_0 but is markedly separated from ρ_0.

Our first result characterizes the critical transitions:

Proposition 2.12 *Let $V \in \mathscr{V}_N \cap L^2$ and suppose a (lower) critical phase transition as described above occurs in the McK–V system at some θ_c. Then, necessarily, $\theta_c = \theta^\sharp$.*

Proof The trivial cases $\theta^\sharp = 0$ or $\theta^\sharp = \infty$ are easily dispensed with. Assuming otherwise for $\theta^\sharp$, it is obvious that a (lower) critical point θ_c could not exceed $\theta^\sharp$ since non-trivial minimizers already exist at any $\theta > \theta^\sharp$. We shall therefore work with $\theta < \theta^\sharp$ and write $\theta = \theta^\sharp - \delta$ where $\delta > 0$.

As a preliminary, it should be noted that while the third item in the definition of the θ_c necessarily reflects the natural L^1-norm, it will be more convenient to work with L^2 and L^∞. We will show that, as far as $\rho_\theta - \rho_0$ is concerned, these are controlled by the L^1-norm. First, for expositional ease, let us define

$$\eta_\theta := \frac{\rho_\theta - \rho_0}{\rho_0}. \tag{33}$$

Starting with L^2, recall from the "obvious corollary" to Lemma 2.1 that since ρ_θ is a minimizer of $\mathcal{F}_\theta(\cdot)$ it is bounded uniformly (enough) in θ and thence η_θ is similarly bounded—say by ω. Then

$$\|\eta_\theta\|_2^2 \le \|\eta_\theta\|_1 \|\eta_\theta\|_\infty \le \omega \|\eta_\theta\|_1. \tag{34}$$

For the moment, we can only employ the outer inequality but at least we now have that $\|\eta_\theta\|_2$ is "small". Next we use the fact that ρ_θ satisfies the Kirkwood–Monroe equation, (3). As is not hard to see, in the language of η_θ this reads

$$1 + \eta_\theta(x) = \frac{\mathrm{e}^{-[\theta V \star \eta_\theta](x)}}{\int \mathrm{e}^{-\theta V \star \eta_\theta} \rho_0 dx}. \tag{35}$$

Now, for a.e. x

$$|[V \star \eta_\theta](x)| = \left| \int_{\mathbb{T}_L^d} V(x-y)\eta_\theta(y)\, dy \right| \le \|V\|_2 \|\eta_\theta\|_2 \tag{36}$$

thence, if $\eta_\theta(x) > 0$,

$$\eta_\theta(x) \le (\mathrm{e}^{2\theta\|V\|_2\|\eta_\theta\|_2} - 1) \tag{37}$$

while if $\eta_\theta(x) < 0$,

$$\eta_\theta(x) \ge (\mathrm{e}^{-2\theta\|V\|_2\|\eta_\theta\|_2} - 1). \tag{38}$$

Thus, for $\|\eta_\theta\|_2$ sufficiently small (which we know happens as $\theta \downarrow \theta_c$ from (34)) there is a K—which is uniform in θ near θ_c and of order unity—such that $\|\eta_\theta\|_\infty < K\|\eta_\theta\|_2$. We may now exploit the middle inequality in (34) and declare that in the vicinity of the purported θ_c all norms of any η_θ are comparably small.

Now, suppose that $\theta \gtrsim \theta_c$. We repeat the calculations performed in Proposition 2.9 with the result that

$$\mathcal{F}_\theta(\rho_\theta) = \mathcal{S}(\rho_0) + \frac{1}{2}\theta L^d \mathcal{E}(\rho_0, \rho_0) + \frac{1}{2}\rho_0 \left[\|\eta_\theta\|_2^2 + \theta \mathcal{E}(\eta_\theta, \eta_\theta)\right] + o(\|\eta_\theta\|_2^2). \tag{39}$$

The term in the square brackets is strictly positive and at least of the order $\|\eta_\theta\|_2^2$ if $\theta \approx \theta_c = \theta^\sharp - \delta$ with $\delta > 0$. Evidently, as indicated, the only possibility for a continuous transition is at $\theta^\sharp$. □

The alternative to a critical transition is a *discontinuous* transition which is also called a first order transition. For such transitions, the following holds:

Proposition 2.13 *If $V \in \mathscr{V}_N$ and at least one of the criteria given in the definition of a critical point at the beginning of this subsection fails then there is a transition at some θ_T which is characterized by the following*:

$\exists \rho_{\theta_T} \neq \rho_0$ *such that*

- $\mathcal{F}_{\theta_T}(\rho_{\theta_T}) = \mathcal{F}_{\theta_T}(\rho_0) = F_{\theta_T}$
- $\mathcal{E}(\rho_{\theta_T}, \rho_{\theta_T}) < \mathcal{E}(\rho_0, \rho_0)$
- $\mathcal{S}(\rho_{\theta_T}) > \mathcal{S}(\rho_0)$ (*and thus both E_θ and S_θ are discontinuous at $\theta = \theta_T$*).

Since two distinct minimizers exist at the same value of θ, such a point may also be described as a point of *phase coexistence*.

Proof At $\theta > \theta_{\mathrm{T}}$ we have for $\eta_\theta = (\rho_\theta - \rho_0)\rho_0^{-1}$

$$\limsup_{\theta \downarrow \theta_{\mathrm{T}}} \|\eta_\theta\|_1 \neq 0. \tag{40}$$

Since, in these matters, all norms are more or less equivalent, we will take the above statement in L^2 and extract a weakly convergent sequence which we will still denote by η_θ. Let us first rule out the possibility that $\eta_\theta \rightharpoonup 0$. Indeed, supposing this to be the case, we would certainly have

$$\lim_{\theta \to \theta_{\mathrm{T}}} \mathcal{E}(\eta_\theta, \eta_\theta) = 0,$$

e.g., as discussed in the proof of Theorem 2.2. However, we have that all along the subsequence, $\|\eta_\theta\|_2 \geq h_{\mathrm{T}}$ for some $h_{\mathrm{T}} > 0$ and, moreover, for some $b < \infty$, $\|\eta_\theta\|_\infty < b$. Thence, by the convexity properties of the $\mathcal{S}$-term we have that for s small,

$$\mathcal{S}(\rho_\theta) \geq \mathcal{S}(\rho_0) + \frac{1}{2}s^2\|\eta_\theta\|_2^2 + o(s^2).$$

This indicates that

$$\limsup_{\theta \downarrow \theta_{\mathrm{T}}} F_\theta > F_{\theta_{\mathrm{T}}}$$

in violation of the stated continuity result.

Thus, in our sequence η_θ converges to a non-trivial limit which we denote (optimistically) by $\eta_{\theta_{\mathrm{T}}}$. On the energetic side, we still have

$$\lim_{\theta \to \theta_{\mathrm{T}}} \mathcal{E}(\eta_\theta, \eta_\theta) = \mathcal{E}(\eta_{\theta_{\mathrm{T}}}, \eta_{\theta_{\mathrm{T}}})$$

and, again, by convexity properties, $\mathcal{S}(\rho_0(1 + \eta_{\theta_{\mathrm{T}}}))$ does not exceed any limit of $\mathcal{S}(\rho_\theta)$ as $\theta \downarrow \theta_{\mathrm{T}}$. Evidently this $\eta_{\theta_{\mathrm{T}}}$ provides a genuine minimizer for $\mathcal{F}_{\theta_{\mathrm{T}}}(\cdot)$ which we now denote by $\rho_{\theta_{\mathrm{T}}}$.

By hypothesis (of a *lower* transition) the uniform solution is a minimizer of $\mathcal{F}_\theta$ up to $\theta = \theta_{\mathrm{T}}$ and thus by continuity is also a minimizer *at* θ_{T}: $\mathcal{F}_{\theta_{\mathrm{T}}}(\rho_0) = \mathcal{F}_{\theta_{\mathrm{T}}}(\rho_{\theta_{\mathrm{T}}})$ (see Proposition 2.4). Moreover, we reiterate, $\mathcal{S}(\rho_0) < \mathcal{S}(\rho_{\theta_{\mathrm{T}}})$ necessarily implying $\mathcal{E}(\rho_{\theta_{\mathrm{T}}}, \rho_{\theta_{\mathrm{T}}}) < \mathcal{E}(\rho_0, \rho_0)$. All of the stated results have now been proven. □

The two preceding results—concerning (i) the purported critical behavior at $\theta = \theta^\sharp$ and (ii) the characteristics of systems with purported non-critical lower transitions—allow for the following:

Theorem 2.14 *Consider, in dimension $d \geq 2$ a fixed $V \in \mathscr{V}_N$ which is isotropic. Then, if the volume is sufficiently large there is never a (lower) critical transition. In particular under the above stated conditions there is a discontinuous transition at some θ_T satisfying $\theta_T < \theta^\sharp$ where there is phase coexistence and various other properties all of which has been described in the context of Proposition 2.13.*

Proof We will consider disturbances of the form

$$\rho = \rho_0(1 + \varepsilon\eta)$$

with $\eta(x)$ a function (with L^∞-norm) of order unity which integrates to zero, and ε a small (pure) number of order unity. Then

$$\mathcal{S}(\rho) = \mathcal{S}(\rho_0) + \int_{\mathbb{T}_L^d} \rho_0\left[\frac{1}{2}\varepsilon^2\eta^2 - \frac{1}{6}\varepsilon^3\eta^3\right]dx + o(\varepsilon^3) \tag{41}$$

where it is slightly important to observe that $o(\varepsilon^3)$ is independent of the volume. Of course the above expansion also contained a *linear* odd term which vanishes since η has zero mean. Similarly, we have $\mathcal{E}(\rho, \rho) - \mathcal{E}(\rho_0, \rho_0) = \varepsilon^2\mathcal{E}(\rho_0\eta, \rho_0\eta)$.

We set $\theta = \theta^\sharp$ where, as we recall, the minimizing wave vector satisfies $-\hat{V}(k^\sharp)\theta^\sharp = 1$. Now, we invoke the assumption that $V(x)$ depends only on $|x|$,—so that $\hat{V}(k)$ depends only on $|k|$. Then, under the auspices of continuous wave numbers ("the infinite volume limit") we could find $\tilde{k}_1$ and $\tilde{k}_2$ with $|k^\sharp| = |\tilde{k}_1| = |\tilde{k}_2|$ necessarily satisfying

$$\hat{V}(k^\sharp) = \hat{V}(\tilde{k}_1) = \hat{V}(\tilde{k}_2) \tag{42}$$

such that

$$k^\sharp + \tilde{k}_1 + \tilde{k}_2 = 0. \tag{43}$$

Thus, in finite volume, we can find approximating $k_1 \approx \tilde{k}_1$ and $k_2 \approx \tilde{k}_2$ with, e.g., $|k_1 - \tilde{k}_1| = O(L^{-1})$ that are appropriate to $\mathbb{T}_L^d$ such that (43) is true and (42) is approximately true. We now use

$$\eta = \eta^\sharp + \eta_1 + \eta_2$$

with η_1 and η_2 plane waves at wavenumbers k_1 and k_2 respectively. We have, e.g.,

$$\hat{V}(k_1)\theta^\sharp\rho_0\|\eta_1\|_2^2 + \rho_0\|\eta_1\|_2^2 \leq \sigma(L) \tag{44}$$

with $\sigma \to 0$ as $L \to \infty$. (We reiterate that each term in the above display is separately of order unity.) Thus, we may declare that, essentially, up through second order $\mathcal{F}_{\theta^\sharp}(\rho_0(1+\varepsilon\eta))$ equals $\mathcal{F}_{\theta^\sharp}(\rho_0)$. But now, since $k^\sharp + \tilde{k}_1 + \tilde{k}_2 = 0$, then unlike a plane wave which, even cubed, would integrate to zero, it is in general the case that

$$\int_{\mathbb{T}_L^d} (\eta^3)dx \neq 0. \tag{45}$$

Moreover by adjusting the phases of the constituents, the corresponding term in the expansion of $\mathcal{F}_{\theta^\sharp}(\rho)$ can be made to be negative.

It is thus evident that for all L large enough, ρ_0 is not the global minimizer for $\mathcal{F}_{\theta^\sharp}(\cdot)$. Thus, by the continuity result of Proposition 2.8, ρ_0 is not the global minimizer for a *range* of θ which lies strictly below $\theta^\sharp$ (although by Theorem 2.11, it is evidently still a local minimum). Thus the transition takes place at some $\theta_{\mathrm{T}} < \theta^\sharp$ and is (therefore) not continuous. □

We conclude this section with an (abbreviated) spectrum of remarks.

Remark For the vast majority of physically motivated single component systems, the above theorem precludes, in the general context, the possibility of continuous transitions. (Cf. the third remark in this sequence for additional discussion.) This is in apparent contradiction with a number of results for these system—some of which receive additional discussion in the subsequent remark—the most pertinent of which have been the subject of [6] and, recently, discussed in [4]. In these works, a continuous transition was indeed found at the analog of $\theta^\sharp$. The important distinction between the present work and [4, 6] is in the nature of the entropy functional that was employed. Indeed, therein the prototypical entropy functional was of the form

$$\mathcal{A}_0(\rho) = \int [\rho \log \rho + (1-\rho)\log(1-\rho)]\, dx. \tag{46}$$

Thus, in the expansion which uses $\rho = \rho_0(1+\eta)$, all the odd terms in η vanish identically; from this perspective, $\mathcal{A}_0(\rho)$ is simply the symmetrized version of $\mathcal{S}(\rho)$. Of course this preempts the term(s) driving the conclusion of Theorem 2.14 and thus allows for a continuous transition at $\theta = \theta^\sharp$.

However, $\mathcal{A}_0(\rho)$ is not a natural entropy form for a one-component system and, as argued in [4], is in fact an *effective* entropy term for a two component Ising-type system. The first principles version of these sorts of Ising systems is currently a subject of intensive investigation; e.g. the works [6] and [11] and some work in progress by R. Esposito and R. Marra in conjunction with the authors. The present set of models under consideration appear to undergo a transition that is, at least sometimes, "weakly first-order" at some $\theta_{\mathrm{T}} \lesssim \theta^\sharp$. However, it may well be the case that the consideration of more general interactions leads, in the two–component cases, to generic circumstances where there are continuous transitions.

Remark In a variety of contexts, e.g. [14, 25, 31], various workers have claimed that non-trivial solutions to (3) appear—continuously or otherwise—only after $\theta \geq \theta^\sharp$. Since this attitude seems prevalent, perhaps some comments are in order. As is typical—by definition—for discontinuous transitions the new minimizing solutions or *states* are *not* continuously connected to the old. This and, especially, Theorem 2.11 accounts for some of the difficulties attempting to generate stable solutions dynamically as described in [25]. It may, perhaps, prove useful to attempt to generate the stable solutions by a nucleation technique (e.g., based on the solution for small systems) at parameter values *below* $\theta^\sharp$ where, perhaps, fewer interfering solutions exist. Indeed, the basin of attraction provided by Theorem 2.11 may itself, for $L \gg 1$, be arguably small from a certain perspective.

The results in [14] and [31] both rely on standard fixed point/bifurcation analyses. In [14], it was simply *assumed* that the non-trivial solutions were periodic with period $k^\sharp$. Of course, as was noted in [14] the Kirkwood–Monroe equation is "closed" under periodic functions with *any* period. (By this it is meant that if we write (3) in the form $\rho = \Xi(\rho)$ then, if σ is periodic so is $\Xi(\sigma)$ with the same period.) Thus, using this equation as the basis for a fixed point argument (with the help of the Krasnoselskii fixed point theorem) one *is* able to manufacture a solution of sorts. Moreover, this scheme indeed requires $\theta \geq \theta^\sharp$ for the solution of period $2\pi[k^\sharp]^{-1}$ to be non-trivial. However it is also clear that these solutions have no stability under the dynamics of (1) and, even, the discrete time dynamics which produced these solutions in the first place. In particular it is almost certain that these solutions do not minimize the free energy functional. (Although, no doubt, they have a lower free energy than the uniform solution.) Indeed while it is not impossible that the stable solutions appearing at $\theta = \theta_{\mathrm{T}}$ are periodic with *some* period, as is typical in non-linear phenomena, there is no reason for the period to exactly match that of the unstable mode which appears at $\theta = \theta^\sharp$.

Finally, we wish to comment on the careful analysis in [31]. Here, standard results in the theory of bifurcations were brought to bear under the explicitly stated assumption that the relevant hypotheses for the theorem actually apply. In this context, the most important of these ingredients is that the kernel and co-kernel of the linear operator are one-dimensional. Under the required symmetry $V(x-y) = V(y-x)$—without which the model does not make sense as a description of identical interacting constituents—this condition is obviously violated. And it may or may not be a "technical" violation, cf. the next remark. Notwithstanding, even if the conditions for the bifurcation results are satisfied, provided that $\hat{V}(k)$ is continuous, there are always modes near $k^\sharp$ which are nearly unstable at $\theta = \theta^\sharp$. Thus any basin of stability and domain of validity will be vanishingly small with increasing volume.

Remark It is remarked that full isotropy of $V(x)$ and/or $d > 1$ is not strictly required. The condition used in the preceding proof was the existence of three wave vectors adding up to zero each of which (nearly) minimize $\hat{V}(k)$. Obviously this can be achieved in $d > 1$ if $V(x)$ has an appropriate 3-fold symmetry. Moreover, a detailed analysis will yield alternative sufficient conditions: (I) If $\hat{V}(0)$ (assumed positive) is not too large. (II) if $\hat{V}(2k^\sharp)$ is negative and, in magnitude, an appreciable fraction of $\hat{V}(k^\sharp)$; etc. However, full isotropy is not an unreasonable assumption for fluid systems—as well as other applications—and, in fact, $d > 1$ is required for actual statistical mechanics systems with short-range interactions to exhibit changes of state. Thus we are content with the present result and will not pursue these alternative specialized circumstances.

Remark In the language of equilibrium statistical mechanics, θ_{T} is, of course, classified as a point of first order transition while the point $\theta^\sharp$ is not recognized. From the perspective of dynamical systems, $\theta^\sharp$ is a subcritical pitchfork bifurcation. It may be presumed that solutions of the type which minimize at and above θ_{T} are present even before θ_{T}. The point at which they first appear—temporarily denoted by θ_{R}—would then represent a *saddle node bifurcation* while, from this perspective, the point θ_{T} is not recognized.

3 The Large Volume Limit

In this final section, we shall investigate the behavior of our systems—with fixed $V(x)$—as L tends to infinity. The upshot, roughly speaking, is that for interaction potentials which are appropriate for physical problems the energy/temperature scaling is viable and not so otherwise. Since the L-dependence of these problems will now be our focus, all relevant quantities will adorned with superscript $[L]$.

3.1 The Limit of the Transition Points

If the interaction violates the conditions of Theorem 2.14 and has a (sequence of) continuous transitions then, by Proposition 2.12, these all take place at the relevant $\theta^\sharp$ which is only weakly dependent on system size. Thus the interesting questions concern the discontinuous transitions. Notwithstanding, the forthcoming makes no explicit use of the discontinuity other than the convenience of label.

Theorem 3.1 *For fixed $V \in \mathscr{V}_N$ consider the system on $\mathbb{T}_L^d$ with discontinuous transition at $\theta_T^{[L]}$. Then these transition points tend to a definitive limit.*

Proof We shall start with the statement that for any L and any integer n,

$$\theta_{\mathrm{T}}^{[L]} \geq \theta_{\mathrm{T}}^{[nL]}. \tag{47}$$

To see this, we patch together n^d copies of a non-trivial minimizer of $\mathbb{T}_L^d$ at $\theta_{\mathrm{T}}^{[L]}$ to cover $\mathbb{T}_{nL}^d$ (which is facilitated by the fact that, anyway, these solutions are periodic). First, letting

$$v = \int_{\mathbb{R}^d} V(x)\, dx \tag{48}$$

it is noted that for any L_a,

$$\mathcal{F}_\theta^{[L_a]}(\rho_0^{[L_a]}) = -\log L_a^d + \frac{1}{2}\theta\, v. \tag{49}$$

Now let L denote any scale with transition temperature θ_{T}^{L} and let $\rho_\star^{[L]}$ denote the non-trivial minimizer for $\mathbb{T}_L^d$ at this value of the parameter. Let $\tilde{\rho}_\star^{[nL]}$ denote the periodic extension of this function to $\mathbb{T}_{nL}^d$ rescaled by a factor of n^{-d} so that it is properly normalized. It is seen that

$$\begin{aligned}
\mathcal{S}^{nL}(\tilde{\rho}_\star^{[nL]}) &= \int_{\mathbb{T}_{nL}^d} \tilde{\rho}_\star^{[nL]} \log \tilde{\rho}_\star^{[nL]} dx \\
&= -\log n^d + n^d \times \frac{1}{n^d} \int_{\mathbb{T}_L^d} \rho_\star^{[L]} \log \rho_\star^{[L]} dx \\
&= -\log n^d + \mathcal{S}^{[L]}(\rho_\star^{[L]}).
\end{aligned}$$

Making use of the underlying periodic structure, we have that for fixed L-periodic $g(y)$, the integral $\int_{\mathbb{T}_{nL}^d} V(x-y)g(y)dy$ is equal to the periodic extension of the corresponding integral on $\mathbb{T}_L^d$. Thus, the energetics will come out the same. In particular, if we define

$$\tilde{N}(x) = \int_{\mathbb{T}_{nL}^d} \tilde{\rho}_\star^{[nL]}(y) V(x-y) [nL]^d\, dy \tag{50}$$

then $\tilde{N}$ is the periodic extension of the function $N(x)$ given by

$$N(x) = \int_{\mathbb{T}_L^d} \rho_\star^{[L]}(y) V(x-y) L^d\, dy \tag{51}$$

(Note that in (50)–(51) the factors of $(nL)^d$ and L^d have been brought inside so that the *integrands* are both ostensibly of order unity and therefore the "same" function.)

Thus, again,

$$\frac{1}{2}\theta[nL]^d\mathcal{E}^{[nL]}(\tilde{\rho}_\star^{[nL]},\tilde{\rho}_\star^{[nL]})=\frac{1}{2}\theta n^d\times\frac{1}{n^d}L^d\mathcal{E}^{[L]}(\rho_\star^{[L]},\rho_\star^{[L]}). \tag{52}$$

Altogether, we find

$$\mathcal{F}_\theta^{[nL]}(\tilde{\rho}_\star^{[nL]})=-\log n^d+F_\theta^{[L]}(\rho_\star^{[L]}) \tag{53}$$

while, from (49) with $L_a=nL$

$$\mathcal{F}_\theta^{[nL]}(\rho_0^{nL})=-\log n^d+F_\theta^{[L]}(\rho_0^{[L]}). \tag{54}$$

From the above two equations, we may conclude that $\theta_{\mathrm{T}}^{[L]}\geq\theta_{\mathrm{T}}^{[nL]}$.

Now consider L, K with $K\gg L$ when K is not an integer multiple of L. We will use almost exactly the above argument except that we will acquire an error due to "boundary terms". Let us find n such that

$$nL<K<(n+1)L. \tag{55}$$

We shall treat $\mathbb{T}_K^d$ like the hypercube $[0,K]^d$ which is divided into n^d hypercubes of scale L which occupy $[0,nL]^d$. For future reference, we refer to boxes that share a face with the region $\mathbb{T}_K^d\setminus[0,nL]^d$ as *boundary* boxes. It is noted that there are $B(n,d)=n^d-(n-2)^d$ such boxes. In the region $[0,nL]^d$, we define, similar to before, the density $\tilde{\rho}_\star^{[K]}$ which is the rescaled periodic extension of $\rho_\star^{[L]}$, the non-trivial density which minimizes the free energy at $\theta_{\mathrm{T}}^{[L]}$ on $\mathbb{T}_L^d$. In the complimentary region, we set $\tilde{\rho}_\star^{[K]}$ to zero.

The entropic calculation proceeds exactly as before with the same result namely $-\log n^d+\mathcal{S}^{[L]}(\rho_\star^{[L]})$. However, for the energy integrals, we cannot simply use (52) because, e.g., if both x and y are in boundary cubes (on opposite sides) the formula may be in error because $V(x-y)$ no longer "reaches around". However for present purposes, it is sufficient to use the results of (52) and subtract the maximum possible gain from these cubes—which would be $-V_0$. The result is

$$\begin{aligned}K^d\mathcal{E}(\tilde{\rho}_\star^{[K]},\tilde{\rho}_\star^{[K]})\leq\left(\frac{K}{nL}\right)^d&[L^d\mathcal{E}(\rho_\star^{[L]},\rho_\star^{[L]})]\\&+V_0\cdot[nL]^d\int_{\mathbf{H}(n,d)^2}\tilde{\rho}_\star^{[K]}(x)\tilde{\rho}_\star^{[K]}(y)\,dx\,dy\end{aligned}$$

where $\mathbf{H}(n,d)$ is standing notation for the above described region of boundary cubes. Note that the $\tilde{\rho}_\star^{[K]}$'s are normalized to n^{-d} in each such cube and the order of $B(n,d)$ is n^{d-1}. As a result,

$$K^d\mathcal{E}(\tilde{\rho}_\star^{[K]},\tilde{\rho}_\star^{[K]})\leq[L^d\mathcal{E}(\rho_\star^{[L]},\rho_\star^{[L]})](1+O(K/L)). \tag{56}$$

Consequently, for any $\epsilon>0$,

$$\theta_{\mathrm{T}}^{[L]}+\epsilon>\theta_{\mathrm{T}}^{[K]} \tag{57}$$

for all K sufficiently large which implies the desired result. □

3.2 Stable Behavior

Since $\theta_{\mathrm{T}}^{[L]}$ tends to a definitive limit which (for $V \in \mathscr{V}_N$) is not infinite, it is important to establish the criterion for when this limit is not zero. As it turns out, the correct condition is closely related to thermodynamic stability.

For two body interactions, the condition of *H-stability* (see [27], p. 34) is as follows: $\exists b > -\infty$ such that for any N points, $x_1, \ldots, x_N$ in $\mathbb{R}^d$,

$$\sum_{i \neq j} V(x_i - x_j) \geq -bN. \tag{58}$$

This condition is regarded as necessary and sufficient for the existence of thermodynamics—although the early proofs usually assume continuity properties of the interaction. Provided that V is bounded and continuous, H-stability is equivalent to the condition that for all probability measures described by a density $\rho(x)$,

$$\int_{\mathbb{R}^d \times \mathbb{R}^d} V(x-y)\rho(x)\rho(y)\,dx\,dy \geq 0 \tag{59}$$

(cf. [27]) as is easily seen by utilizing sums of point masses to approximate probability measures. This will be our working hypotheses for the benefit of the next result along with the technical assumption that V is bounded:

Definition An interaction $V \in \mathscr{V}$ is said to satisfy *condition-K* if $|V(x)| \leq V_{\max} < \infty$ for all $x \in \mathbb{R}^d$ and if for all L sufficiently large, the inequality

$$\int_{\mathbb{T}_L^d \times \mathbb{T}_L^d} V(x-y)\rho(x)\rho(y)\,dx\,dy \geq 0 \tag{60}$$

holds for all $\rho \in \mathscr{P}^{[L]}$.

The principal result of this section is as follows:

Theorem 3.2 *Let $V \in \mathscr{V}_N$ denote an interaction that satisfies condition-K and has (for all L sufficiently large) discontinuous lower transitions at $\theta_T^{[L]}$ on $\mathbb{T}_L^d$. Then the $\theta_T^{[L]}$ tends to a limit that is strictly positive.*

Proof For convenience in the up and coming we shall streamline notation—e.g., revert to the omission of all L's in the superscripts, etc. We start by assuming $\theta \geq \theta_{\mathrm{T}}$ and write, for this value of θ, a non-trivial minimizer and its deviation

$$\rho = \rho_0(1+\eta).$$

Further, we define the positive and negative parts of η as η^+ and, η^- respectively and, finally,

$$h = \|\rho_0\eta\|_1.$$

The aim is to show that if θ is small than, regardless of L, h must be zero.

The first step will be an estimate on the free energetics. We have

$$0 \leq \mathcal{F}_\theta(\rho_0) - \mathcal{F}_\theta(\rho) = S(\rho_0) - S(\rho) + \frac{1}{2}\theta L^d[\mathcal{E}(\rho_0, \rho_0) - \mathcal{E}(\rho, \rho)]. \tag{61}$$

As has been stated before, we have $\frac{1}{2}\theta L^d\mathcal{E}(\rho_0,\rho_0)=\frac{1}{2}\theta v$ while

$$\frac{1}{2}\theta L^d\mathcal{E}(\rho,\rho)=\frac{1}{2}\theta v+\frac{1}{2}\theta L^d\mathcal{E}(\rho_0\eta,\rho_0\eta). \tag{62}$$

Let us decompose:

$$\begin{aligned}\frac{1}{2}\theta L^d\mathcal{E}(\rho_0\eta,\rho_0\eta)=\frac{1}{2}\theta L^d[&\mathcal{E}(\rho_0\eta^+,\rho_0\eta^+)+\mathcal{E}(\rho_0\eta^-,\rho_0\eta^-)\\&-2\mathcal{E}(\rho_0\eta^+,\rho_0\eta^-)].\end{aligned}$$

The first two terms are positive by the hypothesis that V satisfies the condition-K thus

$$\begin{aligned}\frac{1}{2}\theta L^d\mathcal{E}(\rho,\rho)&\geq\frac{1}{2}\theta v-\theta\int_{\mathbb{T}_L^d\times\mathbb{T}_L^d}V(x-y)\eta^-(y)\rho_0\eta^+(x)\,dx\,dy\\&\geq\frac{1}{2}\theta v-\frac{1}{2}\theta\|V\|_1 h\end{aligned}$$

where we have used $\|\eta^-\|_\infty\leq 1$ and $\|\rho_0\eta^+\|_1=\frac{1}{2}h$.

Putting these together we have

$$\mathcal{S}(\rho)-\mathcal{S}(\rho_0)\leq\frac{1}{2}\theta L^d[\mathcal{E}(\rho_0,\rho_0)-\mathcal{E}(\rho,\rho)]\leq\frac{1}{2}\theta\|V\|_1 h. \tag{63}$$

Incidentally we may use the *lower* bound (see, [33], p. 271) $\mathcal{S}(\rho)-\mathcal{S}(\rho_0)\geq\frac{1}{2}h^2$ to learn that the assumption that θ is "small" necessarily implies that h is small but the particulars of this bound does not play a major rôle.

Now, let us write the mean-field equation, (3), in a form useful for the present purposes:

$$\log\rho+\theta L^d\int_{\mathbb{T}_L^d}V(x-y)\rho(y)\,dy=C_{\mathrm{KM}} \tag{64}$$

with C_{KM} a constant that we are now prepared to "evaluate"

$$C_{\mathrm{KM}}=\mathcal{S}(\rho)+\theta L^d\mathcal{E}(\rho,\rho). \tag{65}$$

Expressing (64)–(65) for the benefit of η we have

$$\log\rho_0+\log(1+\eta)+\theta v+\theta\int_{\mathbb{T}_L^d}V(x-y)\eta(y)dy=\mathcal{S}(\rho)+\theta L^d\mathcal{E}(\rho,\rho) \tag{66}$$

so

$$\begin{aligned}&\log(1+\eta)+\theta\int_{\mathbb{T}_L^d}V(x-y)\eta(y)\,dy\\&\quad=:-\kappa=\mathcal{F}_\theta(\rho)-\mathcal{F}_\theta(\rho_0)+\frac{1}{2}\theta L^d[\mathcal{E}(\rho,\rho)-\mathcal{E}(\rho_0,\rho_0)]\end{aligned}$$

where it is noted that the sign of κ is pertinent. Indeed by the display just prior to (63) we have

$$0\leq\kappa\leq\frac{1}{2}\theta\|V\|_1 h. \tag{67}$$

(Thus, in addition, κ is small.) Note that all the above holds formally even if $\eta = 0$ so in the future, we need not insert provisos.

For use in the remainder of this proof, we shall divide $\mathbb{T}_L^d$ into disjoint cubes $C_1, \dots C_j, \dots$ (half open/closed etc.) of diameter a. Since we are only pursuing the limit of $\theta_{\mathrm{T}}^{[L]}$, it may just as well be assumed that $2a$ divides L. We use the notation

$$\|f\|_{L^1(C_j)} := \int_{C_j} |f(x)|\,dx$$

and similarly for other local norms.

Our first substantive claim is as follows:
Let ϵ denote a small number which is of order unity independent of L (the nature of which is not so important and will, to some extent, be clarified below) and suppose that for all j,

$$\|\eta\|_{L^1(C_j)} \le \frac{\epsilon}{\theta}. \tag{68}$$

Then, for all θ is sufficiently small, for all L under discussion, we have that $\eta \equiv 0$.

To see this we let $x \in C_j$ be in the support of η^+ so, ostensibly, we have

$$1 + \eta^+(x) = \mathrm{e}^{-\kappa}\mathrm{e}^{-\theta \int_{\mathbb{T}_L^d} V(x-y)\eta(y)dy}. \tag{69}$$

However, due to the finite range of V, the integration actually takes place on only the cubes in the immediate vicinity of C_j so that

$$1 + \eta^+(x) \le \exp\left[\theta V_{\max} \sum_{j' \sim j} \|\eta\|_{L^1(C_{j'})}\right] \le \mathrm{e}^{\epsilon V_{\max} D_1} \tag{70}$$

where $j' \sim j$ means that $\overline{C}_{j'} \cap \overline{C}_j \neq \emptyset$ and $D_1 = D_1(d)$ is the number of j' such that $j' \sim j$. This implies an L^∞-bound on η^+ which is (a small number) of order unity. We run a similar argument for η^-—only now we have to contend with κ:

$$1 - \eta^- \ge \mathrm{e}^{-\kappa}\mathrm{e}^{-\epsilon V_{\max} D_1} \tag{71}$$

i.e.,

$$\eta^- \le \kappa + \epsilon V_{\max} D_1. \tag{72}$$

Thus we have an L^∞ bound on the full η which implies, at this stage—since h and θ are supposed to be small—an improved bound on $\|\eta\|_{L^1(C_j)}$ in all cubes C_j. Let us continue the process. Suppose that for all j

$$\|\eta\|_{L^1(C_j)} \le \phi \tag{73}$$

where $\phi = \phi(\theta, h)$ represents the latest improvement. Then

$$1 + \|\eta^+\|_\infty \le \exp[D_1 V_{\max} \phi\theta] \tag{74}$$

—so that $\|\eta^+\|_\infty \lesssim D_1 V_{\max}\phi\theta$—and

$$\|\eta\|_\infty \le D_1 V_{\max}\phi\theta + \kappa \tag{75}$$

which, at least for a while, represents an improvement on the various L^1-norms.

The procedure is no longer beneficial if ϕ is on the order of κ. E.g. we may stop when $\kappa \geq \phi[[2a]^{-d} - \theta V_{\max} D_1]$—where it is assumed that θ is small enough so that the coefficient of ϕ is positive. We arrive at an overall bound:

$$\|\eta\|_\infty \leq c_a \kappa \leq c_b \theta h$$

where the c's are constants of order unity independent of L and θ (provided that the latter is sufficiently small). Clearly, for θ small enough, this cannot be consistent with $\|\eta\rho_0\|_1 = h$ unless $h = 0$.

Thus, we are done with the proof unless there are bad blocks where the local L^1-norm of η is in excess of $\epsilon\theta^{-1}$. In fact, we will present an additional hierarchy of bad blocks. The above blocks will be the *core blocks* which will be denoted by $\mathbf{C}$. We shall define blocks $\mathbf{B}_n$, $n = 0, 1, \ldots s$ by

$$\mathbf{B}_n = \{C_j \mid \epsilon\theta^n < \|\eta\|_{L^1(C_j)} \leq \theta^n\} \tag{76}$$

and (unfortunately) other bad blocks

$$\mathbf{B}'_n = \{C_j \mid \epsilon\theta^{n-1} \geq \|\eta\|_{L^1(C_j)} > \theta^n\}. \tag{77}$$

Thus it is seen that our ϵ should be small enough to absorb various constants which crop up but large compared to the assumed value of θ. The hierarchy of these sets stops when the L^1-norm is comparable to κ—pretty much as in the previous argument. Here we shall say that s is defined so that blocks outside the hierarchy have local L^1-norm of η less than a constant Q_0 times κ with Q_0 to be described shortly. Such blocks will be informally referred to as *background* blocks.

We order the hierarchy in the obvious fashion:

$$\cdots\ \mathbf{B}'_n \succ \mathbf{B}_n \succ \mathbf{B}'_{n+1} \succ \cdots \tag{78}$$

with every element of the hierarchy considered to be above the background blocks and below the core blocks.

Our next claim is that for any block in the hierarchy there must be a neighboring block which is further up the hierarchy. Indeed suppose not and that, e.g., $C_j \in B_n$. If all neighbors—that is to say all blocks $C_{j'}$ with $j' \sim j$—were only at the level $\mathbf{B}_n$ or below, we would have, for $x \in C_j$

$$1 + \eta^+(x) \leq \mathrm{e}^{\theta D_1 V_{\max} \theta^n} \tag{79}$$

and

$$\eta^-(x) \leq \theta D_1 V_{\max} \theta^n + \kappa. \tag{80}$$

This, for most cases, implies that $\|\eta\|_{L^\infty(C_j)}$ is of the order θ^{n+1} which precludes $C_j \in \mathbf{B}_n$; a similar derivation applies to the $\mathbf{B}'_n$. At the very bottom of the hierarchy, the same situation holds with any reasonable choice of Q_0 which is of the order of unity.

The implication of the preceding claim is that each block in the hierarchy is connected to the core by a path whose length does not exceed the order of its the hierarchal index.

Our next claim is that (under the hypothesis of non-triviality) the vast majority of the L^1-norm of η is carried by the core and its immediate vicinity. First, let us estimate $|\mathbf{C}|$, the volume of the core. We argue that

$$|\mathbf{C}| \cdot \epsilon \cdot \frac{1}{\theta} \leq h L^d \tag{81}$$

since the right side is the full L^1-norm of η and the left side represents the minimal contribution to this effort on the part of the core. Thus the core volume fraction is the order of θh which, we remind the reader is supposed small.

Now, by the connectivity property of the hierarchy, (81) can be translated into an estimate on the volume of the sets $\mathbf{B}_n$, $\mathbf{B}'_n$. Indeed, we may write

$$|\mathbf{B}_n| \le |\mathbf{C}| D_2 n^d \tag{82}$$

where $D_2 = D_2(d)$ is another constant.

The above two estimates are sufficient to vindicate the claim at the beginning of the paragraph containing (81). We denote by $\mathbf{C}^\star = \mathbf{C} \cup \mathbf{B}_0 \cup \mathbf{B}'_0$ which we call the extended core. Turning attention to the complimentary set we have, for $\mathbf{B}_n$:

$$\int_{\mathbf{B}_n} |\eta| dx \le \theta^n |\mathbf{C}| D_2 n^d [2a]^{-d} \le h\theta L^d \frac{1}{\epsilon} \cdot \theta^n n^d D_2 [2a]^{-d}. \tag{83}$$

Summing this over *all* n starting from $n = 1$ we get a contribution (for all θ sufficiently small) which is bounded by $K\epsilon^{-1}\theta^2 h L^d$ for some constant K. Similarly

$$\int_{\mathbf{B}'_n} |\eta| dx \le \epsilon\theta^{n-1} |\mathbf{C}| D_2 n^d [2a]^{-d} \tag{84}$$

whence the total contribution from the primed portion of the hierarchy on the compliment of the extended core to $\|\eta\|_1$ is no more than $K'\theta h L^d$ for some constant K'. Note that these are small compared to the purported total of hL^d. Finally, the contribution from all the background blocks is surely no more than $Q_0[2a]^{-d}\kappa[L/a]^d$ and we recall that κ itself is bounded above by the order of θh. So, in summary, we arrive at

$$\int_{\mathbf{C}^\star} \eta^+ dx \ge (1 - g\theta) h L^d \tag{85}$$

for some constant g which is independent of L and θ (for θ sufficiently small).

With the preceding constraint in mind, let us bound from *below* the relative entropy

$$\mathcal{S}(\rho) - \mathcal{S}(\rho_0) = \int_{\mathbb{T}_L^d} \rho_0 (1 + \eta^+) \log(1 + \eta^+) + \int_{\mathbb{T}_L^d} \rho_0 (1 - \eta^-) \log(1 - \eta^-). \tag{86}$$

The second term may be bounded below by $-\frac{1}{2}h$. As for the former, since the function is always positive, we may restrict attention to the set $\mathbf{C}^\star$. As is not hard to show, the contribution from $\mathbf{C}^\star$ is larger than that of the function which is uniform on $\mathbf{C}^\star$ and has the same total mass. As a result:

$$\mathcal{S}(\rho) - \mathcal{S}(\rho_0) \ge -\frac{1}{2}h + \frac{|\mathbf{C}^\star|}{L^d} \left(1 + \frac{1}{|\mathbf{C}^\star|}(1 - g\theta) h L^d\right) \log\left(1 + \frac{1}{|\mathbf{C}^\star|}(1 - g\theta) h L^d\right). \tag{87}$$

As is not hard to see (and is intuitively clear) this is decreasing in $|\mathbf{C}^\star|$—meaning we may substitute the upper bound based on (81): $|\mathbf{C}^\star| \le L^d G\theta h$ with G ($\propto \epsilon^{-1}$) another constant of order unity independent of L and θ. All in all,

$$\mathcal{S}(\rho) - \mathcal{S}(\rho_0) \ge -\frac{1}{2}h + G\theta h \left(1 + \frac{(1 - g\theta)}{G}\frac{1}{\theta}\right) \log\left(1 + \frac{(1 - g\theta)}{G}\frac{1}{\theta}\right). \tag{88}$$

By contrast we have, from (63), that $\mathcal{S}(\rho) - \mathcal{S}(\rho_0)$ is *less* than a constant times θh. This along with (88) implies that $h = 0$ or, assuming that $h \neq 0$ a strict lower bound on θ. Either of these conclusions allows us to infer the desired result. □

3.3 Catastrophic Behavior

We conclude with some examples of what can go "wrong" if the criterion of thermodynamic stability is violated. For the benefit of these final results we shall violate condition-K by assuming the existence of a compactly supported probability density $\rho_{\odot}(x)$ such that

$$\int_{\mathbb{R}^d \times \mathbb{R}^d} V(x-y)\rho_{\odot}(x)\rho_{\odot}(y)\,dx\,dy = -u_0 \tag{89}$$

with $u_0 > 0$. First, some specific instances:

Proposition 3.3 *If V satisfies either of the following then it violates condition-K*

(a) *The interaction V satisfies $\int_{\mathbb{R}^d} V(x)dx = -v_0 < 0$*
(b) *For some $\lambda < 1$, in a λa_0 neighborhood of the origin, V integrates to $+c_0$ while for $\lambda a_0 \leq |x| \leq 2a_0$, $V(x)$ is bounded above by $-v_0$ where*

$$v_0(1-\lambda^d) > c_0.$$

Proof In the first case, we choose

$$\rho_{\ell,\odot}(x) = \chi_{|x|\leq \ell a}\frac{1}{\gamma[\ell a]^d}$$

where γ is a geometric constant. It is noted that

$$\lim_{\ell\to\infty} g(a\ell)^d \int_{\mathbb{R}^d} V(x-y)\rho_{\ell,\odot}(x)\rho_{\ell,\odot}(y)\,dx\,dy = -v_0 \tag{90}$$

so the result follows for ℓ sufficiently large.

As for the second case, we simply use $\rho_{\odot}(x) = \frac{1}{\gamma[a_0]^d}\chi_{|x|\leq a_0}$. In performing the integration

$$\int_{\mathbb{R}^d \times \mathbb{R}^d} V(x-y)\rho_{\odot}(x)\rho_{\odot}(y)\,dx\,dy$$

and ignoring the positive contribution from $|x-y| < \lambda a_0$ the result would be not more than $-v_0$. For each x we must cut out a ball of radius (no more than) λa_0 around each point of the integration and insert a corresponding factor of (no more than) c_0. The result is no more than $-(v_0(1-\lambda^d) - c_0)$ and we are done. It is noted that this latter result applies immediately to the case where V is negative in a deleted neighborhood of the origin. □

Theorem 3.4 *For potentials that violate condition-K via (89), the McK–V system exhibits non-physical scaling. In particular, for L sufficiently large,*

$$\theta_T(L) \leq rL^{-d}$$

for some $r > 0$.

Proof Recalling (49) we have for any L

$$\mathcal{F}_\theta^{[L]}(\rho_0^{[L]}) = -\log L^d + \frac{1}{2}\theta v.$$

By contrast, if we abide by the recommended density we obtain:

$$\mathcal{F}_\theta^{[L]}(\rho_\odot) = \mathcal{S}(\rho_\odot) - \frac{1}{2}\theta\rho_0^{-1}u_0$$

where it is noted that $\mathcal{S}(\rho_\odot) < \infty$ by hypothesis and by the restrictive nature of the support of $\rho_\odot$, it is independent of L. But then, as soon as $-\frac{1}{2}\theta u_0 L^d + \mathcal{S}(\rho_\odot) < \log L^d + \frac{1}{2}\theta g_0$ it must be that $\theta \le \theta_T$. This implies the stated bound. □

Acknowledgements L. Chayes is supported by the NSF under the grant DMS-0805486. Both L. Chayes and V. Panferov gratefully acknowledge support of the Institute of Pure and Applied Mathematics at UCLA where, under the *Kinetic Transport* program, this work initiated.

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