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Dynamics and geometric properties of the k -trigonometric model

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Abstract

We analyse the dynamics and the geometric properties of the potential energy surfaces (PES) of the k -trigonometric model (k TM), defined by a fully connected k -body interaction. This model has no thermodynamic transition for $k = 1$, a second-order one for $k = 2$, and a first-order one for $k > 2$. In this paper we (i) show that the single-particle dynamics can be traced back to an effective dynamical system (with only one degree of freedom), (ii) compute the diffusion constant analytically, (iii) determine analytically several properties of the self-correlation functions apart from the relaxation times which we calculate numerically, (iv) relate the collective correlation functions to those of the effective degree of freedom using an exact Dyson-like equation, (v) using two analytical methods, calculate the saddles of the PES that are visited by the system evolving at fixed temperature. On the one hand we minimize $|\nabla V|^2$, as usually done in the numerical study of supercooled liquids and, on the other hand, we compute the saddles with minimum distance (in configuration space) from initial equilibrium configurations. We find the same result from the two calculations and we speculate that the coincidence might go beyond the specific model investigated here.

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1. Introduction

In the last few years there has been an intensive study [1–7] concerning the connection between the slow dynamics of complex systems and the extrema of the potential energy surface (PES), defined through the potential energy function $V(q)$, following the seminal work of Stillinger and Weber [8].

Two ways of studying the dynamics of supercooled liquids and glasses that are based on the analysis of the PES have been of particular importance in the recent past. The first one concerns the analysis of the properties (energy location, number, curvature, and so on) of the minima of the PES that are visited by the system during its evolution at fixed temperature. Assigning to each minimum its zero-temperature basin of attraction, one obtains a partition of the phase space allowing to define a configurational entropy for the supercooled and the out-of-equilibrium glassy regime [9]. The properties of the minima of the PES have also been connected to several features of supercooled liquids and glasses. We can mention their relation to the *fragility* of the glass former [3], the diffusion processes in supercooled liquids [4, 10–12] and the effective fluctuation–dissipation temperature [14–16] in the out-of-equilibrium glassy phase [13]. This method is closely related to Edwards’ proposal [18] to describe the main properties of granular matter with a *flat* measure over blocked configurations that correspond to the minima of the PES. Note that granular matter is an effectively zero-temperature system for which the study of the energy landscape is fully justified.

The second approach, which corresponds to the study of the *instantaneous normal modes*, is based on the study of the eigenvalues of the Hessian at the instantaneous configurations along the trajectory (in configurational space) that the system follows during its dynamical evolution [19, 20]. This approach allowed one to relate the diffusion process to the local curvature of the landscape.

More recently a third approach has been proposed [21, 22] and applied [23–28] to study the slow dynamics in supercooled liquids. Within this approach, the *saddles* of the potential energy surface play a central role. It has been found numerically that the order of the saddles (number of negative eigenvalues of the Hessian matrix) visited during the equilibrium dynamics at temperature T extrapolates to zero when T reaches the dynamic transition temperature T_{MCT} (or mode-coupling temperature [29]).

The role of the stationary points of the PES (saddles and minima) has been also pointed out in a different context. Indeed, studies aiming to clarifying the microscopic origin of phase transitions suggest that the presence and the order of such transitions are related to changes in the topology of the manifold of the PES sampled by the system when crossing the (thermodynamic) critical point [30, 31]. This has been observed by counting the number and the order of the stationary points of $V(q)$ and building up the Euler characteristic of the manifold. The latter is a genuine topological property of the energy surface defined by $V(q) = \text{constant}$, and, in particular, it does not depend on the statistical measure defined on it (i.e., on temperature).

Disordered mean-field spin models have been proposed to mimic the behaviour of supercooled liquids and glasses. Their statics and dynamics, as well as the properties of their free-energy and energy landscapes, are amenable to analytical studies [16]. The main features mentioned in the previous paragraphs are realized by these models where, at finite temperature, the geometry of the free-energy landscape replaces the PES. In particular, the importance of saddles in the free-energy landscape for the evolution of these systems has been elucidated in the past and a comparison between the roles played by free-energy and energy landscapes has also been discussed in this and more general contexts [32, 33].

If one wishes to relate the equilibrium dynamics of a complex system to the properties of the saddles of its PES, an unambiguous definition of *saddle visited during the equilibrium dynamics* is mandatory. Until now, two different definitions have been used. (1) In the numerical simulations of simple models—but still too hard to study analytically—such as Lennard-Jones systems, a partitioning of the configuration space in basins of attraction of saddles is obtained via an appropriate function W (usually $W = |\nabla V|^2$) that has a local minimum on each stationary point of V , and the saddles are then obtained via a minimization of W starting from an equilibrium configuration obtained from a molecular dynamics simulation at temperature T . (2) In the analytic computations applied to disordered mean-field spin models one looks to the saddles that are closest, with respect to some distance in the configuration space, to a reference configuration extracted from the Gibbs distribution at temperature T [34]. Unfortunately, until now the two methods have been applied to different models so the comparison between them is still qualitative.

In this paper, we study a very simple mean-field model without quenched disorder, the k -trigonometric model (k TM), for which one can calculate analytically all the relevant quantities that have been previously studied numerically for more realistic models. In spite of its simplicity, the thermodynamic behaviour of this model is quite rich, and its PES shows some of the features that have been observed in the PES of Lennard-Jones systems [21–27]. Unfortunately, the model is too simple to show interesting dynamics. The dynamical behaviour is closely related to the thermodynamics and, due to the absence of frustration or disorder, no dynamical arrest is observed. Still, on the one hand we have been able to check analytically the validity of some ideas that had been proposed in the literature and, on the other hand, to elaborate a method for the minimization of $W = |\nabla V|^2$ that will be of use for a larger class of mean-field models including the disordered ones. This method allowed us to compare analytically the two definitions of closest saddles to equilibrium configurations, and to show that they coincide in our model.

The paper is organized as follows. In section 2 we introduce the model and present its main features. Then we analyse its static properties: in section 3 we discuss its thermodynamical behaviour, in section 4 we study the topological properties of the PES and relate them to the results of section 3. In sections 5 and 6 we present a detailed study of the dynamical behaviour of the model. Then, in section 7 we discuss the definition of the closest saddles to equilibrium configurations, their properties and their relation with the dynamics of the system. Many of the calculations require the introduction of a formalism that may not be familiar to all the readers and is not really necessary to follow the relevant part of the presentation; they are then presented in detail in the appendices.

2. The model

The k -trigonometric model (k TM) has been introduced in [31] with the aim of studying the relation between phase transitions and topological properties of the PES. The model is defined by the Hamiltonian

$$H = \frac{\Delta}{N^{k-1}} \sum_{i_1, \dots, i_k} [1 - \cos(\varphi_{i_1} + \dots + \varphi_{i_k})] = N \Delta (1 - \text{Re } z^k) \quad (1)$$

having introduced the ‘magnetization’

$$z = \frac{1}{N} \sum_i e^{i\varphi_i} = \xi e^{i\psi}. \quad (2)$$

Here $\varphi_i \in [0, 2\pi)$, $i = 1, \dots, N$, are angular variables and Δ is the energy scale. It is easy to see that the model is not invariant under continuous transformations of φ_i but only under the

discrete group C_{kv} generated by

$$\varphi_i \rightarrow \varphi_i + \frac{2\pi}{k} \quad \varphi_i \rightarrow -\varphi_i. \quad (3)$$

If one interprets the variable φ_i as the angle between a two-dimensional unitary vector and a fixed axis, the transformations in equation (3) are rotations by an angle $2\pi/k$ of the vector and the reflection with respect to the fixed axis. In the low temperature phase this symmetry is broken, and a spontaneous magnetization is generated in a direction $\psi_n = 2\pi n/k$. We will often choose $\psi = 0$ without loss of generality, in order to keep unbroken the symmetry $\varphi_i \rightarrow -\varphi_i$.⁶

The system is subject to a dynamics generated by a Langevin equation [35],

$$\gamma \dot{\varphi}_i = -\frac{\partial H}{\partial \varphi_i} + \eta_i \quad (4)$$

where γ/Δ is the time scale and η_i is a Gaussian noise with

$$\langle \eta_i(t) \rangle = 0 \quad \langle \eta_i(t) \eta_j(t') \rangle = 2T\gamma \delta_{ij} \delta(t - t'). \quad (5)$$

We will consider averages of a generic observable $A(\{\varphi\})$ over the noise distribution, and we choose random initial data (that correspond to a quench from infinite temperature). Eventually, we will consider the $t \rightarrow \infty$ limit, in which the system equilibrates and is described by the Gibbs ensemble at temperature T .

3. Thermodynamics

The thermodynamics of mean-field models is exactly solved neglecting the correlations between different degrees of freedom and obtaining an effective Hamiltonian that contains a parameter to be determined self-consistently. For example, in the fully connected Ising model, with Hamiltonian $H = -(2N)^{-1} \sum_{ij} s_i s_j$, the substitution reads $s_i s_j \rightarrow \langle s_i \rangle s_j + s_i \langle s_j \rangle - \langle s_i \rangle \langle s_j \rangle$. Defining $m = \langle s_i \rangle$, one obtains the effective Hamiltonian $\mathcal{H}(s) = ms + c(m)$ for a single degree of freedom s ($c(m)$ is an irrelevant constant that depends only on m). The self-consistency equation is finally obtained calculating $m = \langle s \rangle$ on this effective Hamiltonian. In fact, one can show that this procedure is equivalent to the evaluation of the free energy at the saddle point in the $N \rightarrow \infty$ limit.

The generalization of this procedure to the k TM is obtained substituting in equation (1) the expression

$$e^{i\varphi_{i_1}} \dots e^{i\varphi_{i_k}} \rightarrow k e^{i\varphi_{i_1}} \langle e^{i\varphi_{i_2}} \rangle \dots \langle e^{i\varphi_{i_k}} \rangle - (k-1) \langle e^{i\varphi_{i_1}} \rangle \dots \langle e^{i\varphi_{i_k}} \rangle \quad (6)$$

and introducing the mean (complex) ‘magnetization’ $\zeta = \langle e^{i\varphi} \rangle$, that has to be determined self-consistently on the mean-field effective Hamiltonian \mathcal{H} . As we always choose $\psi = 0$, ζ is real and the effective Hamiltonian reads

$$\mathcal{H} = \Delta[1 + (k-1)\zeta^k - k\zeta^{k-1} \cos \varphi]. \quad (7)$$

The self-consistency equation for ζ turns out to be

$$\zeta = \langle \cos \varphi \rangle_{\mathcal{H}} = \frac{I_1(\beta \Delta k \zeta^{k-1})}{I_0(\beta \Delta k \zeta^{k-1})} \quad (8)$$

where $\beta = 1/T$, $I_0(\alpha) = (2\pi)^{-1} \int_0^{2\pi} d\varphi e^{\alpha \cos \varphi}$ and $I_1(\alpha) = I_0'(\alpha)$ are the modified Bessel functions of order 0 and 1 respectively. For each β equation (8) gives the thermodynamic value of the mean magnetization $\zeta(T)$. The value $\zeta = 0$ always solves equation (8), but is a stable

⁶ Obviously, if $\psi = 2\pi n/k \neq 0$, the unbroken symmetry is $\varphi \rightarrow 2\psi - \varphi$.

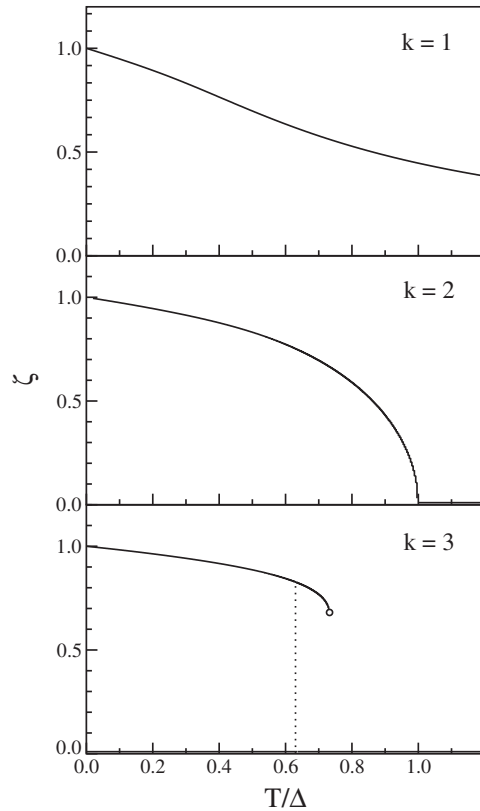


Figure 1. Mean magnetization ζ as a function of temperature for $k = 1, 2, 3$. For $k = 3$ the value of the canonical transition temperature $T_0 = 0.63$ is indicated by a dotted vertical line, while the temperature $T_c = 0.72$ at which the magnetic solution disappears is marked by a white dot. The magnetic solution is metastable for $T_0 < T < T_c$; the same happens to the $\zeta = 0$ solution for $T < T_0$.

solution only at low β (high temperature). As β is increased other solutions may appear, and one has to consider the one that minimizes the free energy as the stable one, while the other solutions can be either unstable or metastable. In figure 1 we report the function $\zeta(T)$ for $k = 1, 2, 3$. For $k = 1$ the curve is smooth, no phase transition occurs and the magnetization approaches zero at high temperature. For $k = 2$ a second-order phase transition takes place at $T_c = \Delta$, separating a high temperature paramagnetic phase, where only the solution $\zeta = 0$ exists, and a low temperature ordered phase, where $\zeta = 0$ becomes a maximum of the free energy separating two minima with $\zeta \neq 0$ corresponding to $\psi = 0$ and $\psi = \pi$. From this symmetry structure one sees that for $k = 2$ the model is in the universality class of the Ising model; the (scalar) order parameter is the real part of the magnetization, while the imaginary part is never different from zero. The critical exponents are then the classical mean-field exponents of the Ising model; in particular we have $\zeta \sim |T - T_c|^{1/2}$ close to T_c and, if a perturbation $\delta\mathcal{H} = -h \cos \varphi$ is added, $\zeta \sim h^{1/3}$ at $T = T_c$. For $k = 3$ (and also for $k > 3$, not reported in the figure) the system undergoes a first-order phase transition. At high T only the paramagnetic solution $\zeta = 0$ exists, but on lowering T two other solutions appear at $T = T_c$: the magnetic one with $\zeta > 0$ and degeneration k (i.e. k different possible values of ψ) and the one corresponding to the maximum of the free energy separating the magnetic and

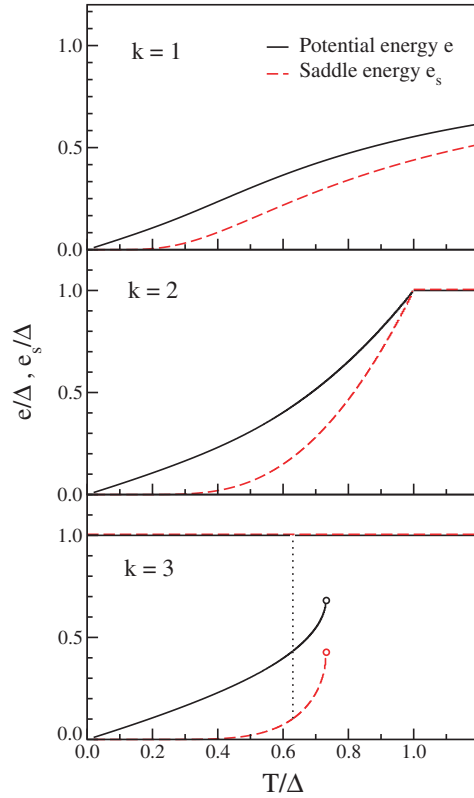


Figure 2. Potential energy e (full lines) and saddle energy e_s (dashed lines, see section 7) as a function of temperature for $k = 1, 2, 3$. The notation is the same as in figure 1.

paramagnetic solutions. The magnetic minimum becomes stable at $T = T_0 < T_c$. In figure 1, for the $k = 3$ case, we show the evolution of the two minima as a function of temperature. The second minimum appears at $T_c = 0.72$ (white dot in the figure) and the transition temperature $T_0 = 0.63$ is indicated by a dotted vertical line. In figure 2 the temperature dependence of the potential energy $e = \langle \mathcal{H} \rangle = \Delta(1 - \zeta^k)$ (full lines in the figures) is shown for $k = 1, 2, 3$. The first-order phase transition also manifests itself in a discontinuity of the potential energy as a function of temperature.

4. Topological properties of the energy surface

In this section we will study the properties of the stationary points (saddles) of the potential energy surface (PES) of the system, defined by the Hamiltonian (1). We will now focus only on the *topological* properties of the saddles, while in section 7 we will study the properties of the saddles sampled by the system equilibrated at temperature T . We will now follow the derivation in [31], while in appendix A we present a different derivation that will be useful in the following. The stationary points $\bar{\varphi}$ are defined by the condition $dH(\bar{\varphi}) = 0$, and their order ν is defined as the number of negative eigenvalues of the Hessian matrix

$H_{ij}(\bar{\varphi}) = (\partial^2 H / \partial \varphi_i \partial \varphi_j) |_{\bar{\varphi}}$. To determine the location of the stationary points we have to solve the system

$$\frac{\partial H}{\partial \varphi_j} = -\Delta k \operatorname{Re}[iz^{k-1} e^{i\varphi_j}] = \Delta k \xi^{k-1} \sin[(k-1)\psi + \varphi_j] = 0 \quad \forall j \quad (9)$$

where we have used the definition $z \equiv \xi e^{i\psi}$ given in equation (2). A first group of solutions arises for $\xi = 0$; from equation (1) we have $H(\varphi) = N\Delta[1 - \xi^k \cos(k\psi)]$, and then the stationary points with $\xi(\bar{\varphi}) = 0$ are all located at the energy $e = H(\bar{\varphi})/N = \Delta$. We will now restrict ourselves to the region $e \neq \Delta$ because, as we will see at the end, the quantities in which we are interested are singular when $e = \Delta$. The presence of this singularity seems to be related, as we discussed elsewhere [31], to the presence (and the order) of a phase transition. For $e \neq \Delta$, equation (9) becomes

$$\sin[(k-1)\psi + \varphi_j] = 0 \quad \forall j \quad (10)$$

and its solutions are

$$\bar{\varphi}_j^{\mathbf{m}} = [m_j \pi - (k-1)\psi]_{\text{mod } 2\pi} \quad (11)$$

where $m_j \in \{0, 1\}$ and $\mathbf{m} \equiv \{m_j\}$. Therefore, besides the different possible values of ψ , each stationary point $\bar{\varphi}^{\mathbf{m}}$ is characterized by the set \mathbf{m} . To determine the unknown constant ψ we have to substitute equation (11) in the self-consistency equation

$$z = \xi e^{i\psi} = N^{-1} \sum_j e^{i\varphi_j} = N^{-1} e^{-i\psi(k-1)} \sum_j (-1)^{m_j}. \quad (12)$$

If we introduce the quantity $n(\bar{\varphi})$ defined by

$$n = N^{-1} \sum_j m_j \quad 1 - 2n = N^{-1} \sum_j (-1)^{m_j} \quad (13)$$

and we have from equation (12)

$$\xi = |1 - 2n| \quad \psi_l = \begin{cases} 2l\pi/k & \text{for } n < 1/2 \\ (2l+1)\pi/k & \text{for } n > 1/2 \end{cases} \quad (14)$$

where $l \in \mathbb{Z}$, then the choice of the set \mathbf{m} is not sufficient to specify the set $\{\varphi_j\}$ because the constant ψ can assume some different values. This fact is connected with the symmetry structure of the potential energy surface (the different values of ψ_l generate the multiplets of stationary points). We have then obtained that all the stationary points of energy $e \neq \Delta$ have the form

$$\bar{\varphi}_j^{\mathbf{m},l} = [m_j \pi - (k-1)\psi_l]_{\text{mod } 2\pi}. \quad (15)$$

The Hessian matrix is given by

$$H_{ij} = \Delta k \operatorname{Re}[N^{-1}(k-1)z^{k-2} e^{i(\varphi_i+\varphi_j)} + \delta_{ij}z^{k-1} e^{i\varphi_i}]. \quad (16)$$

In the thermodynamic limit it becomes diagonal,

$$H_{ij} = \delta_{ij} \Delta k \xi^{k-1} \cos(\psi(k-1) + \varphi_i). \quad (17)$$

One cannot *a priori* neglect the contribution of the off-diagonal terms to the eigenvalues of H , but we have numerically checked that their contribution changes the sign of at most one eigenvalue out of N . Neglecting the off-diagonal contributions, the eigenvalues λ_j of the Hessian calculated at the stationary point $\bar{\varphi}$ are obtained substituting equation (15) in (17),

$$\lambda_j = (-1)^{m_j} \Delta k \xi^{k-1} \quad (18)$$

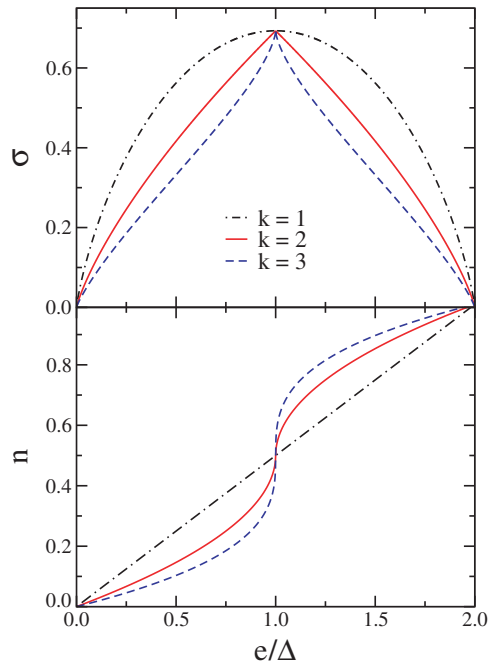


Figure 3. The logarithm σ of the number of saddles and the saddle order n as a function of the energy level e for $k = 1, 2, 3$.

so the stationary point order $\nu(\bar{\varphi})$, defined as the number of negative eigenvalues of the Hessian matrix, is simply the number of $m_j = 1$ in the set \mathbf{m} associated with $\bar{\varphi}$; we can identify the quantity $n(\bar{\varphi})$ given by equation (13) with the fractional order $\nu(\bar{\varphi})/N$ of $\bar{\varphi}$. Then, from equations (1) and (14) we get a relation between the fractional order $n(\bar{\varphi})$ and the potential energy $e(\bar{\varphi}) = H(\bar{\varphi})/N$ at each stationary point $\bar{\varphi}$. It reads

$$n(e) = \frac{1}{2} \left[1 - \operatorname{sgn} \left(1 - \frac{e}{\Delta} \right) \left| 1 - \frac{e}{\Delta} \right|^{1/k} \right]. \quad (19)$$

Moreover, the number of stationary points of given order ν is simply the number of ways in which one can choose ν times 1 among the $\{m_j\}$, see equation (15), multiplied by a constant C_k that does not depend on N and takes into account the degeneracy introduced by equation (14). Therefore, (i) the fractional order $n = \nu/N$ of the stationary points is a well-defined monotonic function of their potential energy e , given by equation (19), and (ii) the number of stationary points of a given order ν is $C_k \binom{N}{\nu}$. We can define the quantity

$$\sigma(e) = \lim_{N \rightarrow \infty} \frac{1}{N} \log \left(\frac{N}{Nn(e)} \right) = -n(e) \log n(e) - (1 - n(e)) \log(1 - n(e)) \quad (20)$$

that represents the ‘configurational entropy’ of the saddles. In [31] we have shown that this quantity is related to the Euler characteristic of the manifolds $M_e = \{\varphi | H(\varphi) \leq Ne\}$ and that its singular behaviour around the point $e = \Delta$ is related to both the presence and the order of the phase transitions that occur for $k \geq 2$. In figure 3 the quantities $\sigma(e)$ and $n(e)$ are reported for $k = 1, 2, 3$ for all values of $e \neq \Delta$: one can see that the presence of a phase transition for $k \geq 2$ is signalled by a singularity in the first derivative of $\sigma(e)$. The order of the transition seems to be related to the sign of the second derivative of $\sigma(e)$ around the transition point, that is negative for second-order phase transitions and positive for first-order ones.

5. Single-particle dynamics

The single-particle dynamics can be studied by means of observables of the form

$$A(\{\varphi\}) = \frac{1}{N} \sum_i \mathcal{A}(\varphi_i). \quad (21)$$

Some interesting quantities are, for example, the diffusion constant $D(T)$, defined as

$$D(T) = \lim_{t \rightarrow \infty} \frac{1}{2Nt} \sum_i \langle |\varphi_i(t) - \varphi_i(0)|^2 \rangle \quad (22)$$

(where obviously the angular variables have to be considered as variables defined on the whole real axis without introducing the periodic condition $\varphi_i + 2\pi = \varphi_i$) and the self-correlation function, defined as

$$F(t, t') = \frac{1}{N} \sum_i [\langle e^{i\varphi_i(t) - \varphi_i(t')} \rangle - \langle e^{i\varphi_i(t)} \rangle \langle e^{-i\varphi_i(t')} \rangle]. \quad (23)$$

To study the single-particle dynamics, we introduce an effective dynamical system for a single degree of freedom φ , defined by

$$\begin{cases} \mathcal{H}(\varphi, t) = -\Delta \operatorname{Re}[k\zeta(t)^{k-1} e^{i\varphi}] \\ \gamma \dot{\varphi}(t) = -\frac{\partial \mathcal{H}}{\partial \varphi}(\varphi(t), t) + \eta(t) \\ \zeta(t) = \langle e^{i\varphi(t)} \rangle \end{cases} \quad (24)$$

where again η is a δ -correlated Gaussian noise with variance $2\gamma T$ and the averages are calculated on its distribution. Note that the derivative of the effective Hamiltonian $\mathcal{H}(\varphi, t)$ is performed with respect to φ at fixed time t (the time dependence of \mathcal{H} is encoded in $\zeta(t)$). The last equation is, as in the static case, a self-consistency equation. In appendix B we show that the averages of observables of type (21) on the dynamics defined by equation (4) can be calculated using this effective single-variable dynamical system:

$$\langle A(\{\varphi\}) \rangle = \langle \mathcal{A}(\varphi) \rangle_{\mathcal{H}}. \quad (25)$$

We will consider the limit $t \rightarrow \infty$ in which the system is in equilibrium, and ζ does not depend on t and is equal to its equilibrium value $\zeta(\beta)$ given by equation (8). In this limit the correlation function (23) depends only on the time difference, $F(t, t') = F(t - t')$, and the dynamical system (24) reduces to

$$\gamma \dot{\varphi}(t) + k\Delta \zeta(\beta)^{k-1} \sin \varphi(t) = \eta(t). \quad (26)$$

If $\zeta \neq 0$, we can define the reduced variables $\tilde{t} \equiv \frac{k\Delta \zeta^{k-1}}{\gamma} t$ and $\tilde{\eta}(\tilde{t}) \equiv \frac{1}{k\Delta \zeta^{k-1}} \eta(t)$, and equation (26) can be rewritten as

$$\frac{d\varphi}{d\tilde{t}} + \sin \varphi(\tilde{t}) = \tilde{\eta}(\tilde{t}) \quad (27)$$

with $\langle \tilde{\eta}(\tilde{t}) \tilde{\eta}(0) \rangle = \frac{2T}{k\Delta \zeta^{k-1}} \delta(\tilde{t}) \equiv 2\tilde{T} \delta(\tilde{t})$. The k dependence is then encoded in \tilde{t} and \tilde{T} .

5.1. The diffusion constant

The analytical expression for the diffusion constant of equation (27) is found, for example, in [36] and is given by

$$\tilde{D}(\tilde{T}) = \lim_{\tilde{t} \rightarrow \infty} \frac{1}{2\tilde{t}} \langle |\varphi(\tilde{t}) - \varphi(0)|^2 \rangle = \frac{\tilde{T}}{I_0(\tilde{T}^{-1})^2}. \quad (28)$$

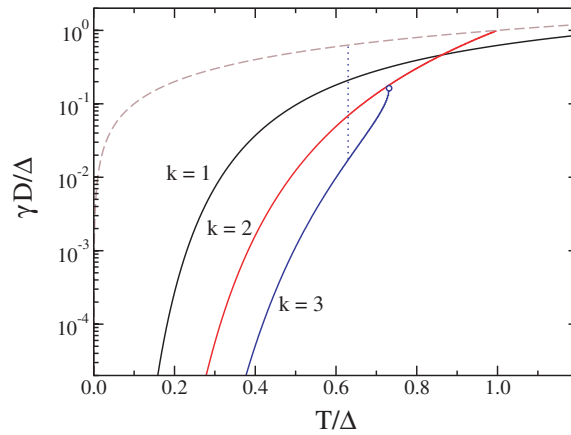


Figure 4. Logarithm of the diffusivity D as a function of the temperature T for $k = 1, 2, 3$. For $k = 3$ the notation is the same as in figure 1. The dashed line is the value of D in the paramagnetic phase, $D = T/\gamma$.

Then, from the definition of D given by equation (22) and from equation (25) one gets

$$D(T) = \frac{k\Delta\zeta^{k-1}}{\gamma} \tilde{D}(T) = \frac{T}{\gamma} I_0(k\beta\Delta\zeta(T)^{k-1})^{-2}. \quad (29)$$

In figure 4 we report D as a function of temperature T in a semilogarithmic scale. At low temperature equation (29) predicts an Arrhenius behaviour:

$$D(T \ll \Delta) \simeq \frac{2\pi\Delta k e^{k-1}}{\gamma} e^{-\beta 2\Delta k}. \quad (30)$$

In the high temperature paramagnetic phase one has $\zeta \equiv 0$ so that equation (27) reduces to a free Brownian motion and the diffusion constant is simply given by $D = T/\gamma$.⁷ It is worth noting that for $k = 1$ the paramagnetic phase does not exist and $D = T/\gamma$ is only the asymptotic limit of equation (29) for $T \rightarrow \infty$.

5.2. The self-correlation function

As we have already discussed, the model is not rotationally invariant, and when the C_{kv} symmetry is broken a spontaneous magnetization appears, whose phase can be an integer multiple of $2\pi/k$. We will choose the phase to be zero in order not to break the $\varphi_i \rightarrow -\varphi_i$ symmetry. In this situation, it is expected that even and odd functions of φ have different behaviour. Therefore, it is convenient to separate the contributions in $F(t)$ given by the real and imaginary parts of $e^{i\varphi_i}$. Using the relations $\langle \cos(\varphi_i(t)) \sin(\varphi_i(0)) \rangle = 0$ and $\langle \sin(\varphi_i(t)) \rangle = 0$, due to the unbroken symmetry $\varphi_i \rightarrow -\varphi_i$, we can define from equation (23) (setting $t' = 0$

⁷ While for $\zeta = 0$ equation (27) makes no sense (\tilde{T} is infinite), we obtain the correct result for the diffusion constant in the paramagnetic phase substituting $\zeta = 0$ in the expression obtained in the magnetic phase. This will not be the case for the relaxation times of the correlation functions.

because of the time translation invariance)

$$\begin{aligned}
 F(t) &= F_c(t) + F_s(t) \\
 F_c(t) &= \frac{1}{N} \sum_i [\langle \cos \varphi_i(t) \cos \varphi_i(0) \rangle - \langle \cos \varphi_i(t) \rangle \langle \cos \varphi_i(0) \rangle] \\
 F_s(t) &= \frac{1}{N} \sum_i \langle \sin \varphi_i(t) \sin \varphi_i(0) \rangle.
 \end{aligned} \tag{31}$$

As previously discussed, see appendix B or equation (25), the above correlations are equal to those calculated using the effective dynamical system (24); at equilibrium they are given by

$$F(t) = \mathcal{F}(t) \equiv \langle e^{i[\varphi(t) - \varphi(0)]} \rangle_{\mathcal{H}} - \langle e^{i\varphi(t)} \rangle_{\mathcal{H}} \langle e^{-i\varphi(0)} \rangle_{\mathcal{H}}. \tag{32}$$

We will use for $\mathcal{F}(t)$ the same notation used for $F(t)$, see equations (31).

5.2.1. The reduced system. To compute the correlation functions, it is useful to use again the reduced variables and equation (27). Unfortunately, we have not been able to derive an analytic expression for the correlations in the whole \tilde{T} range, but only in the high and low temperature limits. In these limits, the correlation functions turn out to be exponentials:

$$\begin{aligned}
 \mathcal{F}_c(\tilde{t}) &= \langle \cos \varphi(\tilde{t}) \cos \varphi(0) \rangle - \langle \cos \varphi \rangle^2 = A_c \exp \left[-\frac{\tilde{t}}{\tilde{\tau}_c} \right] \\
 \mathcal{F}_s(\tilde{t}) &= \langle \sin \varphi(\tilde{t}) \sin \varphi(0) \rangle = A_s \exp \left[-\frac{\tilde{t}}{\tilde{\tau}_s} \right].
 \end{aligned} \tag{33}$$

It is important to note that the amplitudes of these correlations (which are equal to those of the original system as the variables φ are not rescaled) are analytically computable at each temperature and are given by

$$\begin{aligned}
 A_c &= \langle \cos^2 \varphi \rangle - \langle \cos \varphi \rangle^2 = 1 - \tilde{T} \zeta(\tilde{T}) - \zeta(\tilde{T})^2 \\
 A_s &= \langle \sin^2 \varphi \rangle = \tilde{T} \zeta(\tilde{T})
 \end{aligned} \tag{34}$$

where $\zeta(\tilde{T})$ is the magnetization expressed as a function of \tilde{T} and determined self-consistently by equation (8). The relaxation times are related to the real ones by $\tau_{c,s} = \frac{\gamma}{k\Delta\epsilon^{k-1}} \tilde{\tau}_{c,s}$. The limits in which equations (33) are analytically obtained are as follows:

- *High \tilde{T} limit:* if $\tilde{T} \rightarrow \infty$ one can neglect in equation (26) the term proportional to $\sin \varphi$. In this case the dynamics is close to a free Brownian motion and the correlation functions are exponentials with $\tilde{\tau}_c \sim \tilde{\tau}_s \sim 1/\tilde{T}$ and $A_s \sim A_c \sim 1/2$.
- *Low \tilde{T} limit:* the low temperature limit is obtained by considering $\varphi(\tilde{T}) \ll \pi/2$ and (i) by expanding $\sin \varphi \sim \varphi$ in equation (27) and (ii) by approximating $\mathcal{F}_s(\tilde{t}) \sim \langle \varphi(\tilde{t}) \varphi(0) \rangle$ and $\mathcal{F}_c(\tilde{t}) \sim \frac{1}{4} [\langle \varphi^2(\tilde{t}) \varphi^2(0) \rangle - \langle \varphi^2 \rangle^2]$. In approximation (i) the equation of motion (27) is easily solved, the correlation functions are exponentials and one obtains

$$A_c = \frac{\tilde{T}^2}{2} \quad \tilde{\tau}_c = \frac{1}{2} \quad A_s = \tilde{T} \quad \tilde{\tau}_s = 1. \tag{35}$$

The expressions for the amplitudes are consistent with equation (34) observing that in this limit $\zeta \sim 1 - \frac{\tilde{T}}{2} - \frac{\tilde{T}^2}{8}$.

The complete \tilde{T} dependence is obtained by solving equation (27) numerically: the numerical solution has been performed using (i) the true dynamical system (defined through equations (1) and (4)), and (ii) the effective one defined by equation (27). In both cases the reduced variables (\tilde{t} and $\tilde{\eta}$) have been used. The integration of the true dynamical system allowed

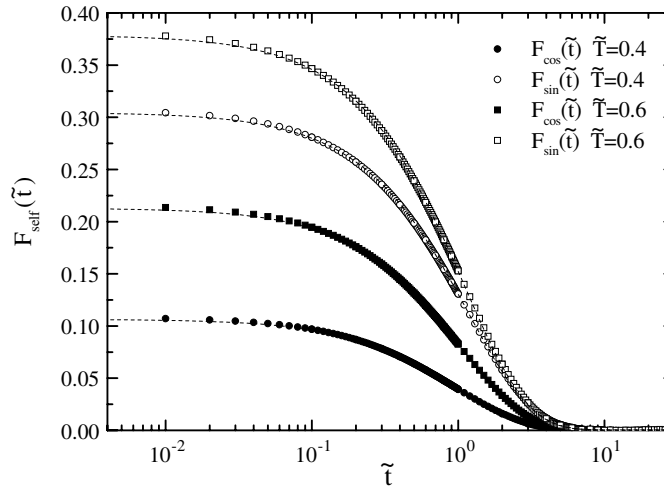


Figure 5. The correlation functions of $\cos \varphi$ and $\sin \varphi$ calculated using equation (27) for two different values of \tilde{T} . They are well fitted by an exponential form.

the self-correlation and the collective correlation functions to be derived numerically (in each case for both the $\sin \varphi$ and $\cos \varphi$ variables). The self-correlation functions, that for a check have been compared to those obtained through the integration of the effective dynamical systems, were fitted to an exponential decay to derive the parameters A_c , A_s , τ_c and τ_s . The simulated system is composed of $N = 1000$ degrees of freedom (in the case of the effective dynamical systems, the N independent degrees of freedom have been used to collect a statistical average over the initial conditions). The equation of motion has been integrated by a simple constant step size ($d\tilde{t} = 0.001$) Runge–Kutta method, and the RAND [37] Fortran routine has been used to generate the Gaussian noise $\tilde{\eta}$. At each temperature we performed an equilibration of 5×10^6 integration steps followed by 5×10^6 steps of data collection. The time history of the variables φ has been stored and a multi-step circular buffer scheme has been employed to calculate the appropriate correlation functions. We found that for any \tilde{T} the correlations are well (but not exactly) described by equation (33); in figure 5 we report some correlations calculated numerically for intermediate \tilde{T} values, together with an exponential fit. The relaxation times obtained numerically are reported in figure 6. They have been fitted for simplicity with a polynomial function,

$$\tilde{\tau}(\tilde{T}) = \frac{\tilde{\tau}(0)(1 + P_1\tilde{T}) + P_3\tilde{T}^2}{1 + P_1\tilde{T} + P_2\tilde{T}^2 + P_3\tilde{T}^3} \quad (36)$$

where $\tilde{\tau}(0)$ is given by equation (35). The previous expression reproduces the correct high and low \tilde{T} limits. The values of the parameters P_i are

$$\begin{aligned} \tilde{\tau}_c: & P_1 = 0 & P_2 = 0.90 & P_3 = 6.28 \\ \tilde{\tau}_s: & P_1 = 1 & P_2 = 1.66 & P_3 = 6.28. \end{aligned}$$

The relaxation times obtained by the numerical calculations are reported in figure 6 together with the corresponding fit and the high and low temperature expansions. Having an (exact) expression for the amplitudes (equation (34)) and another for the relaxation times (equation (36), extrapolated from numerical data) we can discuss the behaviour of the correlation functions for any value of k by substituting in these expressions $\tilde{T} = \frac{T}{k\Delta\zeta^{k-1}}$.

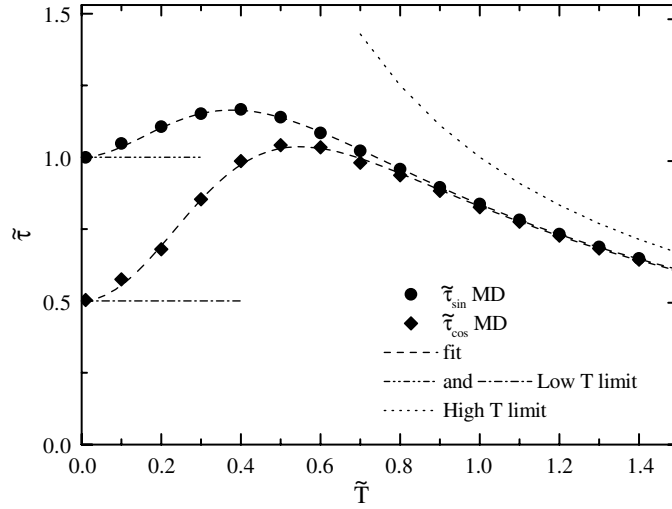


Figure 6. Relaxation times of the correlation functions of equation (27). The symbols are the result of the numerical calculation, while the dashed lines are the fits and the dot (dot-dashed) line is the high (low) temperature expansion.

5.2.2. $k = 1$. For $k = 1$ we have $T = \Delta \tilde{T}$ and $\tau_{c,s} = \frac{\gamma}{\Delta} \tilde{\tau}_{c,s}$, so that the behaviour of the relaxation times is obviously the same as in figure 6. The amplitudes, that we do not report, are analytic functions of the temperature.

5.2.3. $k = 2$. As reported before, for $k = 2$ a second-order phase transition takes place at $T_c = \Delta$. The parameters A and τ for this case are reported in figure 7. We have that $\tilde{T} \rightarrow \infty$ by approaching the phase transition from the magnetic phase, so $A_{c,s} \rightarrow \frac{1}{2}$ and $\tau_{c,s} \rightarrow \gamma/T_c = \gamma/\Delta$ at the transition. In the paramagnetic phase one has $\zeta \equiv 0$, so that equation (26) reduces to a free Brownian motion; then $A_c = A_s = 1/2$ and $\tau_c = \tau_s = \gamma/T$ exactly for all temperatures above T_c . We obtain then that A and τ are continuous functions of temperature but their derivatives have a discontinuity at T_c .

5.2.4. $k \geq 3$. For $k \geq 3$ a first-order phase transition takes place. The parameters A and τ are reported in figure 8. In this case \tilde{T} does not diverge approaching the transition temperature, while the behaviour in the high temperature paramagnetic phase is the same as for $k = 2$. Then, obviously, A and τ are discontinuous at the transition.

6. Collective dynamics

To study the collective behaviour of the system we introduce the correlation function of the magnetization z . It is defined by

$$\begin{aligned} G(t, t') &= \frac{1}{N} \sum_{ij} [\langle e^{i\varphi_i(t) - \varphi_j(t')} \rangle] - \langle e^{i\varphi_i(t)} \rangle \langle e^{-i\varphi_j(t')} \rangle \\ &= N[\langle z(t)z^*(t') \rangle - \langle z(t) \rangle \langle z^*(t') \rangle]. \end{aligned} \quad (37)$$

Again, with the aim of obtaining simple exponential behaviour of the correlation functions, it is convenient to separate the contributions coming from the real and imaginary parts of the

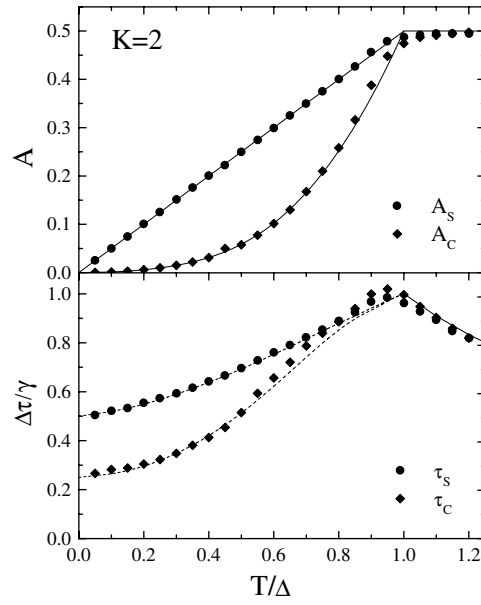


Figure 7. The parameters of the self-correlations for $k = 2$. The symbols are the result of the numerical calculation. The full lines are obtained from analytic computation, while the dashed lines are obtained from the polynomial fit (equation (36)) on the reduced system and the substitution of \bar{T} with its value for $k = 2$ (see text). The agreement is not perfect around T_c due to finite size effects.

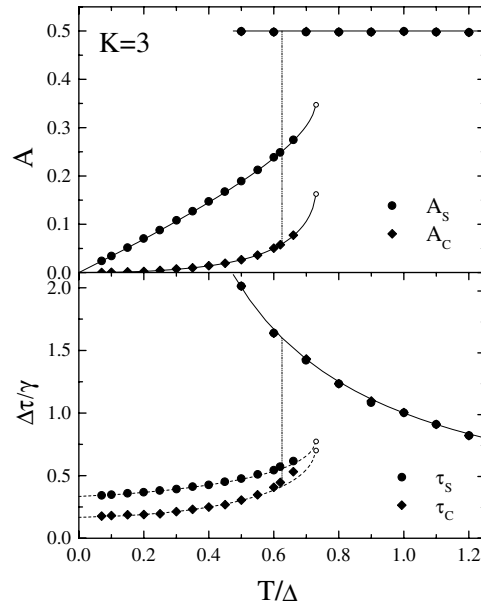


Figure 8. The parameters of the self-correlations for $k = 3$ (with the same notation used in figure 7). The vertical lines mark the transition temperature T_0 ; the numerical calculations can be done also in the metastable phases around T_0 . The white dots mark the points at which the two solutions with $\zeta \neq 0$ disappear.

magnetization, defining

$$\begin{aligned} G_c(t, t') &= \frac{1}{N} \sum_{ij} [\langle \cos \varphi_i(t) \cos \varphi_j(t') \rangle - \langle \cos \varphi_i(t) \rangle \langle \cos \varphi_j(t') \rangle] \\ G_s(t, t') &= \frac{1}{N} \sum_{ij} \langle \sin \varphi_i(t) \sin \varphi_j(t') \rangle. \end{aligned} \quad (38)$$

These correlations are related to the Gaussian correction around the thermodynamic limit, i.e. the leading correction in $1/N$ for $N \rightarrow \infty$. In appendix C we derive a general expression (equation (C.19)) that relates $G(t)$ to the self-correlation function $F(t)$ defined in the previous section. Using this expression and assuming that (i) the magnetization is always real and (ii) $F_{c,s}(t)$ are given by equation (33), $G_{c,s}(t)$ turn out to be also exponentials and are given by

$$G_c(t) = Z_c A_c \exp\left[-\frac{t}{Z_c \tau_c}\right] \quad G_s(t) = Z_s A_s \exp\left[-\frac{t}{Z_s \tau_s}\right] \quad (39)$$

where

$$Z_c = \frac{1}{1 - \beta \Delta k(k-1) \zeta(\beta)^{k-2} A_c} \quad Z_s = \frac{1}{1 + \beta \Delta k(k-1) \zeta(\beta)^{k-2} A_s}. \quad (40)$$

As expected in the absence of interactions, for $k = 1$ we have $Z_c = Z_s = 1$, so that $G(t) = F(t)$ at all temperatures. In order to treat the $k \geq 2$ case we define

$$G_{c,s}(t) = A_{c,s}^G \exp\left[-\frac{t}{\tau_{c,s}^G}\right] \quad (41)$$

with

$$A_{c,s}^G = Z_{c,s} A_{c,s} \quad \tau_{c,s}^G = Z_{c,s} \tau_{c,s}. \quad (42)$$

From the analytic expression for $A_{c,s}$, given by equation (34), we get an analytic expression for the constants $Z_{c,s}$. The exact expressions for the parameters $A_{c,s}^G$, that are connected by the fluctuation–dissipation theorem to the susceptibilities of the magnetization, can then be derived. The relaxation times of $G(t)$ are obtained from those of $F(t)$, that we studied in the previous section, using equation (36). Then, their expression is not exact but derives from the numerical data on the reduced system that we defined in the previous section. To emphasize this, in figures 9 and 10 we report as a full line the exact expressions and with a dashed line the expressions derived using the numerical solution of the reduced system and equation (42).

6.1. $k = 2$

The parameters A^G and τ^G given by equation (42) for $k = 2$ are reported in figure 9. From the symmetry structure of the model, we know that it can acquire a spontaneous magnetization in the directions $\psi = 0$ and $\psi = \pi$, but not in the orthogonal direction. Then we expect a divergence in the amplitude and in the relaxation time of $G_c(t)$ but not in the same parameters of $G_s(t)$. In the high temperature paramagnetic phase we have $A_c = A_s = 1/2$ and $\tau_c = \tau_s = \gamma/T$ (see the discussion of the $k = 2$ case in the previous section); then $Z_c = 1/(1 - \beta \Delta)$ and $Z_s = 1/(1 + \beta \Delta)$. From these expressions and equation (42) we get an expression for A^G and τ^G in the paramagnetic phase (full lines in figure 9). It is easy to see that close to T_c one has $A_c^G \sim |T - T_c|^{-1}$ and $\tau_c^G \sim |T - T_c|^{-1}$. The same behaviour is obtained approaching the transition temperature from below, as one can easily check remembering that for $T \rightarrow T_c^-$ one has $\tilde{T} \rightarrow \infty$, $A_{c,s} \rightarrow 1/2$, $\tau_{c,s} \rightarrow \gamma/T$. We obtain again the classical mean-field critical exponents for the universality class of our model. In the low temperature phase, as previously discussed, the expression for the relaxation times is not exact, and is reported as a dashed line in figure 9.

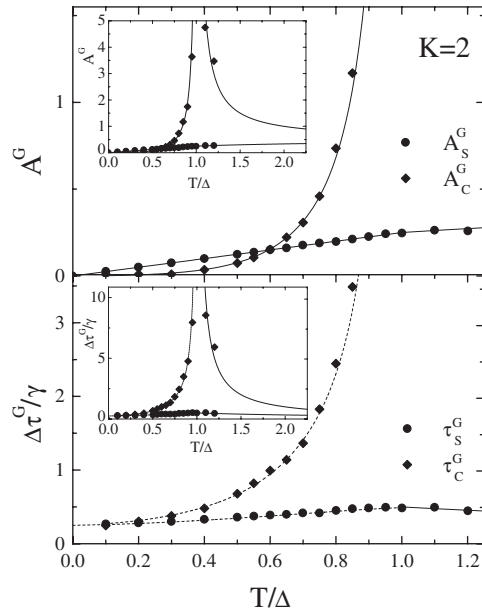


Figure 9. The parameters of the collective correlations for $k = 2$. As in the previous figures, the symbols are from numerical computation, the full lines are obtained analytically, while the dashed lines are obtained using the fitted expression (equation (36)) in equation (42). In the inset the divergence at T_c of the susceptibility and of the relaxation time related to the real part of the magnetization is evidenced.

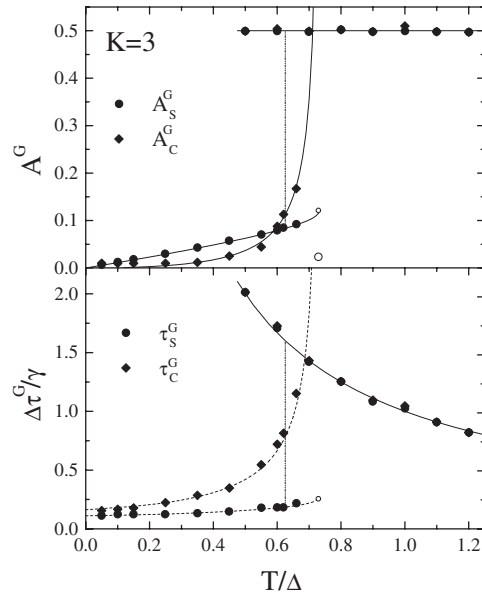


Figure 10. The parameters of the collective correlations for $k = 3$ (with the same notation used in figure 9). In this case A_c^G and τ_c^G diverge in the metastable phase when the metastable solution disappears (white dot in the figure).

6.2. $k \geq 3$

The parameters A^G and τ^G given by equation (42) for $k = 3$ are reported in figure 10. As previously shown, for $k \geq 3$ the model undergoes a first-order transition at T_0 . The low temperature phase is metastable up to a certain temperature T_c (see figure 1) where it disappears, while the high temperature phase is metastable down to $T = 0$. In the high temperature phase we have, as in the $k = 2$ case, $A_c = A_s = 1/2$ and $\tau_c = \tau_s = \gamma/T$. But for $k \geq 3$ we have $Z_c = Z_s = 1$, so that $G(t) = F(t)$. We note that $A_{c,s}^G$ does not diverge in this phase, and the same happens to $\tau_{c,s}^G$ that diverge only for $T \rightarrow 0$. In the low temperature phase, it is easy to see (substituting equation (34) in (40)) that $Z_s = 1/k$; this happens for all k if $\zeta \neq 0$. Then, A_s^G and τ_s^G are simply proportional to A_s and τ_s respectively, and do not show any anomaly. The behaviour of Z_c is more interesting: using its definition given in equation (40), equations (8) and (34), one can show that $Z_c \rightarrow \infty$ when $T \rightarrow T_c^-$. Thus, A_c^G and τ_c^G diverge in the metastable region of the paramagnetic phase approaching the temperature at which the paramagnetic phase itself disappears. Again, the expression for τ^G is obtained using equation (36), and is reported as a dashed line in figure 10.

7. Closest saddles to equilibrium configurations

The important role that stationary points (saddles) of the potential energy surface (PES) play in the dynamics of various systems has been clarified recently [21–28, 34]. From previous works it seems that, in order to describe the equilibrium dynamics at a given temperature T , it is sufficient to know the properties of some of them, that have often been called the ‘closest saddles to the equilibrium configurations at temperature T ’.⁸ To locate these particular stationary points, two main strategies have been adopted: (1) defining in a proper way a ‘distance’ in phase space and, given an equilibrium configuration, looking at the stationary point that has minimum distance from this configuration; (2) partitioning the phase space in ‘basins of attraction’ of stationary points via an appropriate function that has a local minimum on each stationary point. While the first approach has been exploited analytically on some disordered spin models [34], the second one has been extensively used in numerical simulations of simple model liquids [21–27].

The problem with definition (2) is that one has to define a function W such that *each stationary point of H is a local minimum of W and each local minimum of W is a stationary point of H* . Otherwise, while looking for the closest saddle starting from a reference configuration one can remain trapped in some local minimum of W that is not a stationary point of H . It has been shown in [24] that this possibility effectively arises in the majority of the cases if one chooses, as usual in simple liquids, $W = |\nabla H|^2$.

To compare the two methods avoiding the difficulties of the numerical computations, we tried to find some models in which the minimization of a function W with the desired property could be analytically performed. In the k -trigonometric model this function can correctly be chosen as $W = |\nabla H|^2$, as we will show that all the minima of W correspond to stationary points of H . In this section we present a general method for the minimization of $W = |\nabla H|^2$, that can probably be extended to treat a large class of mean-field systems without quenched disorder. We apply this technique to our model and we show that definitions (1) and (2) give in this case *exactly* the same result. Note that the idea on which the method is constructed can also be used with W functions different from that chosen here, even if the practical calculation might be difficult depending on the particular form chosen for W . Future work will be devoted

⁸ Another denomination is ‘generalized inherent structures’, see [28].

to applying our method, if possible, to disordered systems such as the p -spin disordered model studied in [34].

7.1. Definition of the relevant quantities

In section 4 we studied the properties of the stationary points of the PES that are independent of the statistical measure that describes the system at temperature T (i.e. they are independent of temperature). From this study, we were able to find a relation between the energy of a saddle and its order and to compute the number of saddles, $\exp(N\sigma(e))$, located at a given energy e . Now we want to calculate the energy of the ‘closest saddles to equilibrium configurations at temperature T ’. The procedure used to calculate this quantity is the same used *numerically* in [21, 22]: we consider an initial configuration extracted from the Gibbs distribution at temperature T , and we perform a minimization of

$$W = |\nabla H|^2 = \frac{N\Delta^2 k^2}{2} [(z z^*)^{k-1} - \text{Re}(z^{2k-2} z_2)] \quad (43)$$

(where $z_2 \equiv N^{-1} \sum_i e^{2i\varphi_i}$) that leads to a stationary point of the PES that we associate with the initial configuration. Finally, we average the energy of the stationary point over the equilibrium distribution of initial data. The minimization of W is performed using the dynamical system

$$\gamma \dot{\varphi}_i = -\frac{\partial W}{\partial \varphi_i} \quad (44)$$

that is completely analogous to (4) with $H \rightarrow W$ and $T = 0$. We want to calculate the energy of the configurations in the limit of infinite time starting from a Gibbs ensemble, i.e.

$$e_s(T) = \frac{1}{N} \lim_{t \rightarrow \infty} \langle H(t) \rangle_W. \quad (45)$$

From this quantity, we obtain the order of the saddles as a function of temperature using equation (19) and the ‘configurational entropy’ of the saddles that is given by $\sigma(T) = \sigma(e_s(T))$.

7.2. Effective dynamical system

Using the same argument presented in appendix B for the real dynamics, it is possible to show that the dynamical system (44) is equivalent to the single-particle one given by

$$\begin{cases} \mathcal{W}(\varphi, t) = \Delta^2 k^2 (k-1) \text{Re}\{[\zeta^*(t)(\zeta(t)\zeta^*(t))^{k-2} - \zeta_2(t)\zeta(t)^{2k-3}] e^{i\varphi}\} \\ \quad - \frac{1}{2} \Delta^2 k^2 \text{Re}\{\zeta(t)^{2k-2} e^{2i\varphi}\} \\ \gamma \dot{\varphi}(t) = -\frac{\partial \mathcal{W}}{\partial \varphi}(\varphi(t), t) \\ \zeta(t) = \langle e^{i\varphi(t)} \rangle \\ \zeta_2(t) = \langle e^{2i\varphi(t)} \rangle. \end{cases} \quad (46)$$

The derivation is sketched in appendix D; note that an irrelevant constant term has been neglected in \mathcal{W} , so that \mathcal{W} is not always positive, while $W = |\nabla V|^2 \geq 0$. In this case, we will calculate the averages over the distribution of initial data setting the noise to zero. As the system is mean field, the correlations between different degrees of freedom vanish in the thermodynamic limit and the Gibbs distribution can be written in the form

$$P(\{\varphi\}) = \prod_i \mathcal{P}(\varphi_i) = \prod_i \frac{e^{-\beta \mathcal{H}(\varphi_i)}}{\mathcal{Z}_i} = \prod_i \frac{e^{\beta \Delta k \text{Re}[\zeta(\beta)^{k-1} e^{i\varphi_i}]} }{\mathcal{Z}_i} \quad (47)$$

where $\zeta(\beta) = \zeta(t = 0)$ is as usual the equilibrium average magnetization. The problem is then reduced to the calculation of

$$e_s(T) = \lim_{t \rightarrow \infty} \langle \mathcal{H}(\varphi) \rangle_{\mathcal{W}} \tag{48}$$

using the dynamical system (46) and averaging over the distribution (47) of initial data.

7.3. Calculation of the energy of the closest saddles

Again we assume that the system is not magnetized or that the mean magnetization has zero phase. So, we assume that $\zeta(t)$ and $\zeta_2(t)$ are real functions of time. In this case the system (46) becomes

$$\begin{cases} \mathcal{W}(\varphi, t) = \Delta^2 k^2 \zeta(t)^{2k-3} [(k-1)(1-\zeta_2(t)) \cos \varphi - \frac{1}{2} \zeta(t) \cos 2\varphi] \\ \gamma \dot{\varphi}(t) = -\frac{\partial \mathcal{W}}{\partial \varphi}(\varphi(t), t) \\ \zeta(t) = \langle \cos \varphi(t) \rangle \\ \zeta_2(t) = \langle \cos 2\varphi(t) \rangle. \end{cases} \tag{49}$$

We want now to show that the first term in \mathcal{W} can be neglected, at least in some limits. For $k = 1$ the first term disappears and one simply has $\mathcal{W} = -\frac{\Delta^2}{2} \cos 2\varphi$. For $k \geq 2$, in the paramagnetic phase one has $\zeta(0) = \zeta_2(0) = 0$, then $\mathcal{W} = 0$ and the closest saddle is the starting configuration itself. In the low temperature phase we know that at the initial time $1 - \zeta_2(0) = 2 \langle \sin^2 \varphi \rangle = \frac{2T}{k \Delta \zeta(0)^{k-2}}$. Then we can neglect the first term with respect to the second one (at $t = 0$) if

$$(k-1) \frac{2T}{k \Delta \zeta(0)^{k-2}} \ll 4 \frac{1}{2} \zeta(0) \Leftrightarrow \frac{T}{\Delta} \frac{k-1}{k} \ll \zeta(0)^{k-1} \tag{50}$$

where the 4 on the right-hand side comes from the fact that the derivative of the second term is proportional to $2 \sin 2\varphi \sim 4\varphi$ while the derivative of the first term is proportional to $\sin \varphi \sim \varphi$. This condition is clearly satisfied for low enough temperature because $\zeta(T = 0) = 1$. It is easy to check (see figure 1) that for $k = 3$ the inequality is satisfied up to the transition temperature T_0 . Obviously, for $k = 2$ it cannot be satisfied close to T_c where $\zeta \sim 0$.

If one can neglect the first term at $t = 0$, it can be neglected at all subsequent times, because during the minimization of \mathcal{W} both $\zeta(t)$ and $\zeta_2(t)$ increase, and $\zeta_2 \rightarrow 1$ rapidly. To give an argument, let us neglect again the first term in \mathcal{W} ; then the minima of the pseudopotential are such that $\cos 2\varphi = 1$, so that increasing time $\zeta_2(t)$ will move towards 1, that is its infinite time limit. ζ will increase due to the fact that the final energy is lower than the initial one, as we will show below. Surprisingly, while we expect all these approximations to work only at low enough temperature, they give the correct result in the whole temperature range, as we checked numerically.

In the approximations discussed before, the system (49) becomes of the form

$$\begin{cases} \dot{\varphi} = -\nabla \mathcal{W} = -\Delta^2 k^2 \zeta(t)^{2k-2} \sin 2\varphi \\ \zeta(t) = \langle \cos \varphi(t) \rangle. \end{cases} \tag{51}$$

We are interested in the infinite time solutions of equation (51), $\varphi(t \rightarrow \infty | \varphi_0)$, as a function of the initial conditions $\varphi_0 \equiv \varphi(t = 0)$. Without explicitly solving equation (51), we observe that the sign of $\nabla \mathcal{W}$ at fixed φ does not change with time, due to the fact that the time-dependent factor in equation (51) is always positive. This implies that the specific time dependence of ζ does not affect the final point $\varphi(t \rightarrow \infty | \varphi_0)$ reached from a given initial condition, rather it controls the rapidity of approaching this final point. It is easy to see that the solutions are

$$\varphi(t \rightarrow \infty | \varphi_0) = \begin{cases} 0 & \text{if } \varphi_0 \notin \left(\frac{\pi}{2}, \frac{3\pi}{2}\right) \\ \pi & \text{if } \varphi_0 \in \left(\frac{\pi}{2}, \frac{3\pi}{2}\right). \end{cases} \tag{52}$$

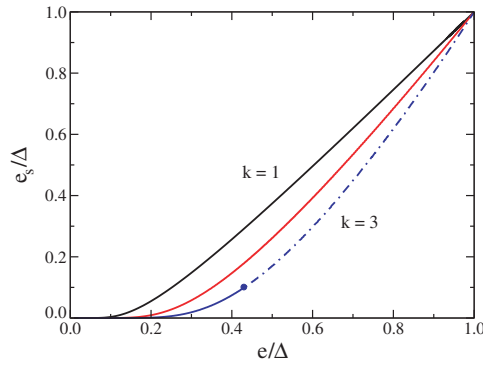


Figure 11. Saddle energy e_s versus the thermodynamic energy e for $k = 1, 2, 3$. The dashed line is the unstable region that corresponds to the solution of equation (8) that is a maximum of the free energy.

The solution $\varphi = 0$ is a minimum of \mathcal{W} corresponding to a minimum of the effective potential energy (equation (7)), while the solution $\varphi = \pi$ is a minimum of \mathcal{W} that corresponds to a maximum of the effective potential. From equation (52) one can see that at the final point $\zeta_2 = 1$ and $|\zeta| = 1$; then, substituting in equation (43), where ζ and ζ_2 have to be considered as the mean values of z and z_2 respectively, one gets $W = 0$ at the final point. This means that the final point is a real saddle of the original system, because from the definition of W it is obvious that $W = 0$ implies $\nabla H = 0$. Then, in our system it is not possible to remain trapped in a local minimum of W with $W > 0$, at variance with what happens in simple liquids [24]. Note that the same argument cannot be made using \mathcal{W} as defined, for example, in equation (46) because, as already stated, a constant term has been neglected in its definition.

The energy e_s of the saddle is then obtained as $e_s(T) = \Delta(1 - \zeta(\infty)^k)$, where $\zeta(\infty)$ is the average of $\cos \varphi(t \rightarrow \infty | \varphi_0)$ over the distribution (47) of initial data,

$$\begin{aligned} \zeta(\infty) &= \int_0^{2\pi} d\varphi_0 \mathcal{P}(\varphi_0) \cos \varphi(t \rightarrow \infty | \varphi_0) \\ &= \int_0^{2\pi} d\varphi_0 \mathcal{P}(\varphi_0) \operatorname{sgn}(\cos \varphi_0) = \frac{L_0(\beta \Delta k \zeta^{k-1})}{I_0(\beta \Delta k \zeta^{k-1})} \end{aligned} \quad (53)$$

where we have introduced the modified Struve function of order 0: $L_0(\alpha) = 2\pi^{-1} \int_0^{\pi/2} d\varphi \sinh(\alpha \cos \varphi)$. In figure 2 the saddle energies e_s (dashed lines) are reported as a function of temperature for $k = 1, 2, 3$: qualitatively e_s reproduces the shape of the potential energy e , and it is always below e , but coincides with e in the paramagnetic region for $k \geq 2$, as previously discussed. The map e_s versus e is shown in figure 11, where one observes that, when the parameter k increases, the energy difference between instantaneous configurations and saddles becomes more and more pronounced. From equation (19) we obtain the saddle order n as a function of temperature:

$$n(T) = \frac{1}{2} \left[1 - \frac{L_0(\beta \Delta k \zeta^{k-1})}{I_0(\beta \Delta k \zeta^{k-1})} \right]. \quad (54)$$

This function is reported in figure 12 for $k = 1, 2, 3$. At low temperature (high β) equation (54) is approximated by

$$n(\beta \gg 1) \simeq \sqrt{\frac{2 e^{k-1}}{\pi k \beta \Delta}} e^{-\beta \Delta k} \quad (55)$$

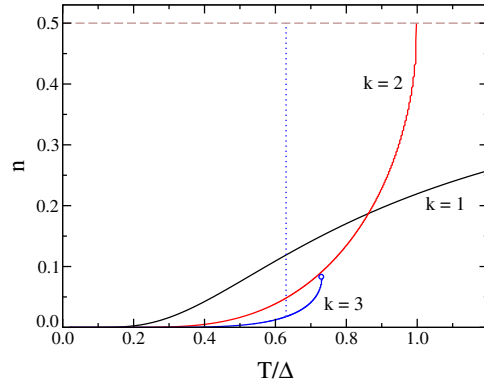


Figure 12. Saddle order as a function of temperature for $k = 1, 2, 3$.

which corresponds to an Arrhenius behaviour. We have shown in [38] that the behaviour of $n(T)$ is related to that of the diffusion constant $D(T)$, as previously found numerically in simple model liquids [21], and that the energy barrier appearing in the Arrhenius low temperature expansion of $D(T)$ is exactly the energy difference between saddles of order 1 and the underlying minima.

7.4. Distance of the closest saddle to the reference configuration

In this section, we show that the two possible definitions of ‘closest saddles to equilibrium configurations’ that we discussed above coincide in our model. To this end, we apply the method introduced in [34] to our model. We compute the quantity

$$\sigma(T; e_s, d) = \frac{1}{N} \int d\varphi_i \frac{e^{-\beta H(\varphi)}}{Z(T)} \times \log \int d\psi_i \delta(H(\psi) - Ne_s) \delta(\partial_i H(\psi)) \det H(\psi) \delta(d - d(\varphi, \psi)) \quad (56)$$

where $H_{ij} = \partial_i \partial_j H$ is the Hessian matrix and $d(\varphi, \psi)$ is some distance function between the two configurations φ_i and ψ_i . The argument of the logarithm is the number of stationary points of energy e_s and distance d from the reference configuration φ (see appendix A or [34] for a detailed discussion). Then the logarithm of this number (divided by N) is averaged over the equilibrium distribution at temperature T of the reference configuration.

Using this quantity we can provide a definition of ‘closest saddles to equilibrium configurations’ [34]: in fact, let the temperature be fixed (and neglect the explicit dependence on it of all the quantities) and consider $\sigma(e_s, d)$ as a function of d at fixed e_s . This is the number of saddles of energy e_s and average distance d from the typical configurations at temperature T . We expect that for too small distances this quantity will be zero, because there will be no saddles of energy e_s at too small distance from the equilibrium configurations. So we can define $\bar{d}(e_s)$ as the value of d at which $\sigma(e_s, d)$ goes to zero: $\sigma(e_s, \bar{d}(e_s)) \equiv 0$. Then $\bar{d}(e_s)$ is the minimum distance at which one can find saddles of energy e_s . Now we can minimize $\bar{d}(e_s)$ with respect to e_s : the value \bar{e}_s of e_s such that $\bar{d}(e_s)$ minimum will be the energy of the closest saddles to the equilibrium configurations, while $\bar{d}(\bar{e}_s)$ will be the average distance from these saddles and the equilibrium configuration themselves.

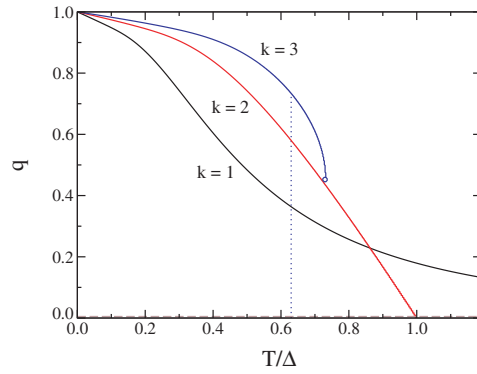


Figure 13. Mean overlap between instantaneous configuration and the closest saddles (see text) as a function of temperature for $k = 1, 2, 3$.

In our model the distance function can be defined as

$$d^2(\varphi, \psi) = 1 - q(\varphi, \psi) = 1 - \frac{1}{N} \sum_i \cos(\varphi_i - \psi_i). \quad (57)$$

In fact $\cos(\varphi_i - \psi_i)$ can be interpreted as the scalar product of the unitary spins represented by the angles φ_i and ψ_i , so that $q(\varphi, \psi)$ is the overlap between the two configurations. The calculations are reported in appendix E; the result is that the energy of the saddles is given by the same expression derived in the previous section,

$$\bar{e}_s = e_s(T) = \Delta \left[1 - \left(\frac{L_0(\beta \Delta k \zeta^{k-1})}{I_0(\beta \Delta k \zeta^{k-1})} \right)^k \right] \quad (58)$$

where ζ is given by the thermodynamics, see equation (8), while the mean overlap is given by

$$\bar{q} = \int_0^{2\pi} d\varphi \mathcal{P}(\varphi) |\cos \varphi| = \langle |\cos \varphi| \rangle_{\mathcal{H}} = \frac{L_1(\beta \Delta k \zeta^{k-1})}{I_0(\beta \Delta k \zeta^{k-1})} \quad (59)$$

where \mathcal{P} has been defined in equation (47) and $L_1(\alpha) = L'_0(\alpha)$. Note that this result could also be derived using the method of the previous section: in fact, we would have, in analogy to equation (48),

$$\begin{aligned} q_s(T) &= \lim_{t \rightarrow \infty} \langle \cos(\varphi(t) - \varphi_0) \rangle_{\mathcal{W}} \\ &= \langle \cos(\varphi(t \rightarrow \infty | \varphi_0) - \varphi_0) \rangle_{\mathcal{H}(\varphi_0)} = \langle |\cos(\varphi)| \rangle_{\mathcal{H}} = \bar{q}(T). \end{aligned} \quad (60)$$

Then, we can conclude that in our model the minimization of W starting from an instantaneous configuration equilibrated at temperature T leads, on average, to that stationary point of the PES which has maximum overlap with the starting configuration itself. Moreover, we can calculate the average overlap (or distance) between the equilibrium configurations and the associated stationary points, that is reported in figure 13 as a function of temperature for $k = 1, 2, 3$.

8. Conclusions

In this paper, we presented a study of the thermodynamics and the dynamics of a very simple mean-field model of N variables interacting through a fully connected k -body trigonometric term. In spite of its simplicity this model shows interesting behaviour undergoing

second- or first-order phase transitions depending on the value of k . All the results that we present here have been obtained analytically (except for the computation of the relaxation times of the self-correlation function which has been done numerically). In particular, the dynamics is analysed in detail, and we find a relation between the single-particle dynamics and the collective one in terms of a Dyson-like equation that links the self-correlation and collective correlation functions. Using this relation we studied, among other dynamical properties, the critical slowing down around the second-order phase transition or close to the stability limit in the case of the first-order phase transition. A rather complete characterization of the geometry of the potential energy surface (PES) has been achieved. This allowed us to relate some of the macroscopic properties of the model to the PES characteristics: the thermodynamic singularities (phase transitions) are located at the same energy as the geometrical ones, and, in the dynamics, the low temperature behaviour of the diffusion constant is similar to the behaviour of the order of the saddles visited during the equilibrium dynamics. The concept of ‘saddles visited during the equilibrium dynamics’ (or ‘generalized inherent structures’) has been widely used in the literature, even if an unambiguous definition of them has not yet been found. In this respect, we compared two definitions that have been used in the past, and we found that they give exactly the same result when applied to the k TM. This result supports the use of PES to analyse the behaviour of interacting systems and suggests that the present analysis could be applied to other interesting systems.

Acknowledgments

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Appendix A. Topological properties of the saddles in mean-field models

In this appendix, we will calculate the number of stationary points of energy $e = E/N$ and their order using a general method that works well for all mean-field models. Although this method is well known [34, 39] and in our model the same results can be obtained in a simpler way, it is useful to recall it here because it will be generalized in appendix E to calculate the number of saddles of energy e located at a given distance from a reference configuration equilibrated at a given temperature T .

We introduce the quantity

$$\chi'(E) \equiv \int d\varphi_i \delta(H - E) \delta(\partial_i H) \det H = \sum_{\nu=0}^N (-1)^\nu \mathcal{N}_\nu(E) \quad (\text{A.1})$$

where H is the Hessian matrix ($H_{ij} = \partial_i \partial_j H$), $\mathcal{N}_\nu(E)$ is the number of stationary points of H of order ν and energy E , and a product over the index i is omitted. The last equality is easily checked by noting that the function $\det H \prod_i \delta(\partial_i H)$ is equal to $(-1)^\nu$ if integrated in a small volume around a stationary point of order ν . According to Morse theory, $\chi'(E)$ is the derivative with respect to E of the Euler characteristic of the manifolds $M_E \equiv \{\varphi | H(\varphi) \leq E\}$ [30]. Using the relations

$$\det H = \int d\bar{\eta}_i d\eta_i e^{\sum_{ij} \eta_i H_{ij} \bar{\eta}_j} \quad \delta(\partial_i H) = \int d\lambda_i e^{2\pi i \lambda_i \partial_i H} \quad (\text{A.2})$$

where $\{\eta, \bar{\eta}\}$ are Grassman variables [35] we have

$$\chi'(E) = \int \frac{d\beta}{2\pi} e^{\beta E} \int d\varphi_i d\bar{\eta}_i d\eta_i d\lambda_i \exp[-\beta H + \eta_i \partial_i \partial_j H \bar{\eta}_j + 2\pi i \lambda_i \partial_i H]. \quad (\text{A.3})$$

Introducing the superfield

$$\phi_i(\theta, \bar{\theta}) = \varphi_i + \eta_i \bar{\theta} + \bar{\eta}_i \theta + 2\pi i \lambda_i \theta \bar{\theta} \quad (\text{A.4})$$

where θ and $\bar{\theta}$ are two other Grassman variables we have

$$\chi'(E) = \int \frac{d\beta}{2\pi} e^{\beta E} \int \mathcal{D}\phi_i \exp \left[\int d\bar{\theta} d\theta (1 - \beta \theta \bar{\theta}) H(\phi) \right]. \quad (\text{A.5})$$

The last equality is easily checked remembering that

$$H(\phi) = H(\varphi) + (\eta_i \bar{\theta} + \bar{\eta}_i \theta + i \lambda_i \theta \bar{\theta}) \partial_i H(\varphi) + (\eta_i \bar{\eta}_j \theta \bar{\theta}) \partial_i \partial_j H(\varphi) \quad (\text{A.6})$$

due to the fact that $\theta^2 = \bar{\theta}^2 = 0$. In mean-field models we can evaluate the integral (A.5) at the saddle point; from equation (A.1) we see that the integral will be dominated by a particular value of ν ,

$$\chi'(E) \sim_{N \rightarrow \infty} (-1)^{\bar{\nu}(E)} \mathcal{N}_{\bar{\nu}(E)}(E) \equiv e^{N\sigma(e)} \quad (\text{A.7})$$

so that

$$\lim_{N \rightarrow \infty} \frac{1}{N} \log \chi'(E) = \lim_{N \rightarrow \infty} \frac{1}{N} (\log \mathcal{N}_{\bar{\nu}(E)}(E) + i\pi \bar{\nu}(E)). \quad (\text{A.8})$$

Then we expect that at the saddle point the real part of $\sigma(e)$ will be the logarithm of the number of saddles located at energy e , while its imaginary part will be the order of these saddles [34]. We will now calculate explicitly all this quantities in our model. The Hamiltonian of the k -trigonometric model is written in terms of the variable $z = N^{-1} \sum_i e^{i\varphi_i}$ in equation (1). This variable has a real and an imaginary part. As we want to evaluate equation (A.5) at the saddle point in z , we will need to consider the real and imaginary parts of z as complex variables themselves. To avoid confusion, it is convenient to use another imaginary unit I and define $z = N^{-1} \sum_i e^{I\varphi_i} = \text{Re } z + I \text{Im } z$. When we consider $\text{Re } z$ and $\text{Im } z$ as complex numbers themselves, we will use the notation $\text{Re } z = \text{Re } \text{Re } z + i \text{Im } \text{Re } z$. Setting $\Delta = 1$ we have (neglecting all the constant prefactors)

$$\begin{aligned} \chi'(e) &= \int d\beta e^{N\beta e} \int \mathcal{D}z \delta \left(Nz - \sum_i e^{I\varphi_i} \right) \int \mathcal{D}\phi_i \exp \left[\int d\bar{\theta} d\theta (1 - \beta \theta \bar{\theta}) N (1 - \text{Re } z^k) \right] \\ &= \int d\beta e^{N\beta e} \int \mathcal{D}z \mathcal{D}\hat{z} \exp N \left\{ \int d\bar{\theta} d\theta [(1 - \beta \theta \bar{\theta})(1 - \text{Re } z^k) + \text{Re}(z i\hat{z})] + \log \mathcal{X}(i\hat{z}) \right\} \\ \mathcal{X}(i\hat{z}) &= \int \mathcal{D}\phi \exp \left[- \int d\bar{\theta} d\theta \text{Re}(e^{I\phi} i\hat{z}) \right] \end{aligned} \quad (\text{A.9})$$

where we introduced the supervariables z and \hat{z} ($z = z_0 + z_1\theta + z_2\bar{\theta} + z_3\theta\bar{\theta}$) and the superdelta-function

$$\delta(z) = \int \mathcal{D}\hat{z} \exp \left[\int d\bar{\theta} d\theta \text{Re}(z i\hat{z}) \right]. \quad (\text{A.10})$$

In the definition of $\delta(z)$ and $\mathcal{X}(i\hat{z})$ we note that both imaginary units appear: I serves to select only the component $\text{Re } \hat{z} \cos \phi - \text{Im } \hat{z} \sin \phi$ in the product $e^{I\phi} \hat{z}$, but $\text{Re } \hat{z}$, $\text{Im } \hat{z}$ and ϕ are themselves complex superfunctions with respect to i . We will also rotate the integration path on $\text{Re } \hat{z}$ and $\text{Im } \hat{z}$ in the complex (i) plane (that is equivalent to the substitution $i\hat{z} \rightarrow \hat{z}$); this is

irrelevant because at the end we will look for the saddle point in the whole complex (i) plane. We obtain then

$$\chi'(e) = \int d\beta \mathcal{D}z \mathcal{D}\hat{z} \exp N\sigma(z, \hat{z}, \beta | e) \tag{A.11}$$

$$\sigma(z, \hat{z}, \beta | e) = \beta e + \int d\bar{\theta} d\theta [(1 - \beta\theta\bar{\theta})(1 - \operatorname{Re} z^k) + \operatorname{Re} z\hat{z}] + \log \mathcal{X}(\hat{z}).$$

To solve the saddle point equations we will assume that at the saddle point, (i) all the fermionic components vanish ($z_1 = z_2 = \hat{z}_1 = \hat{z}_2 = 0$) and (ii) the Im part of the bosonic components is always 0 ($\operatorname{Im} z_0 = \operatorname{Im} z_3 = \operatorname{Im} \hat{z}_0 = \operatorname{Im} \hat{z}_3 = 0$). The first assumption is standard in this kind of computation. The second one is a consequence of the symmetry structure of the model: one can always choose the magnetization $z = N^{-1} \sum_i e^{i\varphi_i}$ such that its imaginary (in the I plane) component is zero. Firstly, we will evaluate $\mathcal{X}(\hat{z})$ in the case in which \hat{z} has the form that we have assumed above. We get

$$\begin{aligned} \mathcal{X}(\hat{z}) &= \int \mathcal{D}\phi \exp\left(-\int d\bar{\theta} d\theta (\hat{z}_0 + \hat{z}_3\theta\bar{\theta}) \cos \phi\right) \\ &= \int d\varphi d\bar{\eta} d\eta d\lambda \exp(\hat{z}_0(2\pi i\lambda \sin \varphi + \eta\bar{\eta} \cos \varphi) - \hat{z}_3 \cos \varphi) \\ &= \int_0^{2\pi} d\varphi e^{-\hat{z}_3 \cos \varphi} \delta(\hat{z}_0 \sin \varphi) \hat{z}_0 \cos \varphi. \end{aligned} \tag{A.12}$$

If \hat{z}_0 is real and different from 0 we get

$$\mathcal{X}(\hat{z}) = -2 \operatorname{sgn} \hat{z}_0 \sinh \hat{z}_3. \tag{A.13}$$

Then we obtain

$$\sigma(z, \hat{z}, \beta | e) = \beta e + z_0\hat{z}_3 + z_3\hat{z}_0 - \beta(1 - z_0^k) - kz_0^{k-1}z_3 + \log(-2 \operatorname{sgn} \hat{z}_0 \sinh \hat{z}_3). \tag{A.14}$$

The saddle point equations are

$$\begin{cases} e = 1 - z_0^k \\ \hat{z}_0 = kz_0^{k-1} \\ \hat{z}_3 = -\beta kz_0^{k-1} \\ z_0 = -\frac{1}{\tanh \hat{z}_3} \\ z_3 = 0. \end{cases} \tag{A.15}$$

Substituting in σ we obtain

$$\sigma(e) = z_0\hat{z}_3 + \log 2 \sinh \hat{z}_3 + \log \operatorname{sgn} \hat{z}_0. \tag{A.16}$$

Now, if k is odd or if k is even and $e < 1$, z_0 is real and given by $z_0 = (1 - e)^{1/k}$. Then \hat{z}_0 is real and equation (A.13) is correct. Note also that \hat{z}_0 is positive so that the last term in σ is 0. Recalling that $\tanh^{-1} x = \frac{1}{2} \log \frac{1+x}{1-x}$ one has

$$\hat{z}_3 = \tanh^{-1}\left(-\frac{1}{z_0}\right) = \frac{1}{2} \log \frac{1 - z_0}{1 + z_0} + \frac{i\pi}{2}. \tag{A.17}$$

It is interesting to note that as \hat{z}_3 is complex while z_0 is real, from the third of the saddle point equations one obtains that β is complex at the saddle point; this is a consequence of the strongly oscillating behaviour of $\chi'(e)$. Using the relation $\sinh x = \frac{\tanh x}{\sqrt{1 - \tanh^2 x}}$ we get

$$\begin{aligned} \sinh \hat{z}_3 &= \frac{i}{\sqrt{1 - z_0^2}} \text{ and introducing the variable} \\ n(e) &= \frac{1}{2}(1 - z_0(e)) = \frac{1}{2}[1 - (1 - e)^{1/k}] \end{aligned} \tag{A.18}$$

we finally obtain

$$\sigma(n) = -n \log n - (1-n) \log(1-n) - i\pi n \quad (\text{A.19})$$

and

$$\chi'(n(e)) \sim (-1)^{Nn(e)} e^{N\text{Re}\sigma(n(e))}. \quad (\text{A.20})$$

This result is consistent with that obtained in section 4 and with the discussion at the beginning of this appendix. The case in which k is even and $e > 1$ is a little more involved and we will not discuss it here.

Appendix B. Single-particle dynamics

In this appendix we will show that one can use the effective dynamical system (24) to compute one-particle quantities (defined in equation (21)). We will restrict to the observable $e^{i\varphi(t)}$ and its n -times correlations; the other observables are linear combinations of this one (via a Fourier expansion). We will use the formalism of the generating functional in its supersymmetric formulation as presented in [16, 17, 35], and a notation similar to that of appendix A.

B.1. The generating functional

The generating functional of the correlation functions can be written as [16, 17, 35]

$$Z[h(t)] = \int \mathcal{D}\phi_i \exp \left[\frac{1}{2} \sum_i \int da \phi_i(a) \Delta^{(2)} \phi_i(a) - \int da H(\phi) + \text{Re} \int da h(a) e^{I\phi_i} \right] \quad (\text{B.1})$$

where $\theta, \bar{\theta}$ are Grassman variables, $\phi_i(\theta, \bar{\theta}, t)$ is a time-dependent superfield, see equation (A.4), $da = d\bar{\theta} d\theta dt$, $h(a) = h(t)\theta\bar{\theta}$, $h(t) = \text{Re} h(t) + I \text{Im} h(t)$ and

$$\Delta^{(2)} = 2T \frac{\partial^2}{\partial \bar{\theta} \partial \theta} - 2\gamma\theta \frac{\partial}{\partial \theta} \frac{\partial}{\partial t} + 4\gamma\theta\bar{\theta} \frac{\partial^2}{\partial \bar{\theta} \partial \theta} \frac{\partial}{\partial t}. \quad (\text{B.2})$$

In fact it is easy to check that the self-correlation functions (31) can be written as

$$F(t, t') = \left[\frac{\delta^2 Z}{\delta \text{Re} h(t) \delta \text{Re} h(t')} + \frac{\delta^2 Z}{\delta \text{Im} h(t) \delta \text{Im} h(t')} - \frac{\delta Z}{\delta \text{Re} h(t)} \frac{\delta Z}{\delta \text{Re} h(t')} - \frac{\delta Z}{\delta \text{Im} h(t)} \frac{\delta Z}{\delta \text{Im} h(t')} \right]_{h=0} \quad (\text{B.3})$$

using the symmetry under permutations of the φ_i . Defining formally the operators

$$\frac{\delta}{\delta h(t)} = \frac{\delta}{\delta \text{Re} h(t)} + I \frac{\delta}{\delta \text{Im} h(t)} \quad \frac{\delta}{\delta h^*(t)} = \left(\frac{\delta}{\delta h(t)} \right)^* \quad (\text{B.4})$$

one can see that

$$F(t, t') = \left[\frac{\delta^2 Z}{\delta h(t) \delta h^*(t')} - \frac{\delta Z}{\delta h(t)} \frac{\delta Z}{\delta h^*(t')} \right]_{h=0} \quad (\text{B.5})$$

using $\langle \sin(\varphi_i(t)) \cos(\varphi_i(t')) \rangle \equiv 0$ and $\langle \sin(\varphi_i(t)) \rangle \equiv 0$ because of the symmetry $\varphi \rightarrow -\varphi$, as we have already discussed before equation (31). We can generalize this relation defining the supercorrelator

$$F(a, b) = \frac{1}{N} \sum_i [\langle e^{I(\phi_i(a) - \phi_i(b))} \rangle - \langle e^{I\phi_i(a)} \rangle \langle e^{-I\phi_i(b)} \rangle] \\ = \left[\frac{\delta^2 Z}{\delta h(a) \delta h^*(b)} - \frac{\delta Z}{\delta h(a)} \frac{\delta Z}{\delta h^*(b)} \right]_{h=0}. \quad (\text{B.6})$$

B.2. The saddle point equations

Substituting equation (1) in (B.1) and introducing the supervariable

$$z(a) = \frac{1}{N} \sum_i e^{I\phi_i(a)} \tag{B.7}$$

we get

$$Z[0] = 1 = \int \mathcal{D}\phi_i \mathcal{D}z \delta \left(Nz(a) - \sum_i e^{i\phi_i(a)} \right) \exp \left[\sum_i T(\phi_i) - N\Delta \int da (1 - \text{Re } z(a)^k) \right] \tag{B.8}$$

where $T(\phi) = \frac{1}{2} \int da \phi \Delta^{(2)} \phi$. Using the integral representation of the δ -function

$$\delta(z) = \int \mathcal{D}\hat{z} \exp \left[\int da \text{Re}(z(a) i\hat{z}(a)) \right] \tag{B.9}$$

we get, rotating as usual the integration path in the \hat{z} plane,

$$\begin{aligned} Z[0] &= \int \mathcal{D}\phi_i \mathcal{D}z \mathcal{D}\hat{z} \exp \left[N \text{Re} \int da \hat{z}(a) z(a) - \sum_i \text{Re} \int da \hat{z}(a) e^{I\phi_i(a)} \right. \\ &\quad \left. + \sum_i T(\phi_i) - N\Delta \text{Re} \int da (1 - z(a)^k) \right] \\ &= \int \mathcal{D}z \mathcal{D}\hat{z} \exp N \left[\text{Re} \int da \hat{z}(a) z(a) - \Delta \text{Re} \int da (1 - z(a)^k) + \log \mathcal{Z}[\hat{z}] \right] \\ &= \int \mathcal{D}z \mathcal{D}\hat{z} \exp NL(z, \hat{z}) \end{aligned} \tag{B.10}$$

where we defined

$$\mathcal{Z}[\hat{z}] = \int \mathcal{D}\phi \exp [T(\phi) - \text{Re} \int da \hat{z}(a) e^{I\phi(a)}]. \tag{B.11}$$

By comparison with equation (B.1) we see that $\mathcal{Z}[\hat{z}]$ is the generating functional for the dynamics of a single degree of freedom with energy

$$\mathcal{H}(\phi, \hat{z}) = \text{Re} \hat{z}(a) e^{I\phi}. \tag{B.12}$$

We can evaluate the integral in equation (B.10) by a saddle point, as usual in mean-field models; we get, using again the formal operators (B.4)

$$\begin{aligned} \frac{\delta L}{\delta z^*(a)} &= \hat{z}(a) + \Delta k z(a)^{k-1} = 0 \implies \hat{\zeta}(a) = -\Delta k \zeta(a)^{k-1} \\ \frac{\delta L}{\delta \hat{z}^*(a)} &= z(a) + \frac{\delta}{\delta \hat{z}^*(a)} \log \mathcal{Z}[\hat{z}] = 0 \implies \zeta(a) = \langle e^{I\phi(a)} \rangle_{\mathcal{H}(\hat{z})} \end{aligned} \tag{B.13}$$

where we defined ζ and $\hat{\zeta}$ as the saddle point values of z and \hat{z} respectively. So, in the thermodynamic limit the dynamics of the system is equivalent to that of a single degree of freedom with Hamiltonian

$$\begin{cases} \mathcal{H}(\phi, a) = -\Delta \text{Re}[k\zeta(a)^{k-1} e^{I\phi}] \\ \zeta(a) = \langle e^{I\phi(a)} \rangle. \end{cases} \tag{B.14}$$

Setting $\theta = \bar{\theta} = 0$, we get the effective dynamical system for the variable φ :

$$\begin{cases} \mathcal{H}(\varphi, t) = -\Delta \text{Re}[k\zeta(t)^{k-1} e^{I\varphi}] \\ \zeta(t) = \langle e^{I\varphi(t)} \rangle. \end{cases} \tag{B.15}$$

B.3. Self-correlation functions

We want now to show that it is possible to use the effective Hamiltonian, equation (B.15), to calculate the self-correlation function given by equation (B.6). In fact we obtain in the same way as we obtained equation (B.10)

$$\begin{aligned} Z &= \int \mathcal{D}z \mathcal{D}\hat{z} \exp \left[N \operatorname{Re} \int da \hat{z}(a) z(a) - N \Delta \operatorname{Re} \int da (1 - z(a)^k) \right. \\ &\quad \left. + (N - 1) \log \mathcal{Z}[\hat{z}] + \log \mathcal{Z}[\hat{z} + h] \right] \\ &= \int \mathcal{D}z \mathcal{D}\hat{z} \exp [NL(z, \hat{z}) + \log \mathcal{Z}[\hat{z} + h] - \log \mathcal{Z}[\hat{z}]] \end{aligned} \quad (\text{B.16})$$

so that

$$F(a, b) = \int \mathcal{D}z \mathcal{D}\hat{z} \frac{\delta^2 \log \mathcal{Z}[\hat{z}]}{\delta \hat{z}(a) \delta \hat{z}^*(b)} \exp [NL(z, \hat{z})]. \quad (\text{B.17})$$

In the thermodynamic limit we know from the saddle point equations that the integral is dominated by $z = \zeta$, $\hat{z} = \hat{\zeta}$, and that

$$\exp NL(\zeta, \hat{\zeta}) \sim Z[0] \sim 1 \quad (\text{B.18})$$

so that

$$F(a, b) = \left[\frac{\delta^2 \log \mathcal{Z}[\hat{z}]}{\delta \hat{z}(a) \delta \hat{z}^*(b)} \right]_{\hat{z}=\hat{\zeta}} = \langle e^{I(\phi(a)-\phi(b))} \rangle_{\mathcal{H}(\hat{\zeta})} - \langle e^{I\phi(a)} \rangle_{\mathcal{H}(\hat{\zeta})} \langle e^{-I\phi(b)} \rangle_{\mathcal{H}(\hat{\zeta})} \equiv \mathcal{F}(a, b). \quad (\text{B.19})$$

The self-correlation function is then equal to that calculated for a single degree of freedom using the effective Hamiltonian (B.15). The same argument is extended to n -times correlations by differentiating n -times.

Appendix C. Collective dynamics

In this appendix, we will derive a general relation between the self-correlation functions and the collective ones. The latter vanish in the thermodynamic limit, and are related to the Gaussian corrections around the mean-field saddle point that we studied in appendix B.

C.1. Gaussian corrections to mean field

We want now to calculate the correlation function of the ‘magnetization’ (multiplied by N in order to have a well-defined thermodynamic limit)

$$G(a, b) = N[\langle z(a)z^*(b) \rangle - \langle z(a) \rangle \langle z^*(b) \rangle] \quad (\text{C.1})$$

by expanding L at second order around the saddle point; to do this, it is not possible to use the operators (B.4). We have to separate the real and imaginary parts of z and \hat{z} . We get, calling $\Delta z_\sigma = [\operatorname{Re}(z - \zeta), \operatorname{Im}(z - \zeta), \operatorname{Re}(\hat{z} - \hat{\zeta}), \operatorname{Im}(\hat{z} - \hat{\zeta})]$ with $\sigma = 1, 2, 3, 4$,

$$L(z, \hat{z}) = L(\zeta, \hat{\zeta}) + \frac{1}{2} \left[\sum_{\sigma, \sigma'} \int da db \Delta z_\sigma(a) \frac{\delta^2 L}{\delta z_\sigma(a) \delta z_{\sigma'}(b)} \Delta z_{\sigma'}(b) \right]. \quad (\text{C.2})$$

Then, at second order around the saddle point,

$$P(\Delta z) \propto \exp \left[-\frac{N}{2} \sum_{\sigma, \sigma'} \int da db \Delta z_\sigma(a) J_{\sigma\sigma'}(a, b) \Delta z_{\sigma'}(b) \right] \quad (\text{C.3})$$

where the matrix $J(a, b)$ is given by

$$J(a, b) = - \begin{pmatrix} \operatorname{Re} w(a)\delta(a-b) & -\operatorname{Im} w(a)\delta(a-b) & \delta(a-b) & 0 \\ -\operatorname{Im} w(a)\delta(a-b) & -\operatorname{Re} w(a)\delta(a-b) & 0 & -\delta(a-b) \\ \delta(a-b) & 0 & \mathcal{F}_c(a, b) & 0 \\ 0 & -\delta(a-b) & 0 & \mathcal{F}_s(a, b) \end{pmatrix} \quad (\text{C.4})$$

where

$$\begin{aligned} \mathcal{F}_c(a, b) &= \langle \cos(\phi(a)) \cos(\phi(b)) \rangle_{\mathcal{H}(\hat{\zeta})} - \langle \cos(\phi(a)) \rangle_{\mathcal{H}(\hat{\zeta})} \langle \cos(\phi(b)) \rangle_{\mathcal{H}(\hat{\zeta})} \\ &\quad \langle \cos(\phi(a)) \sin(\phi(b)) \rangle_{\mathcal{H}(\hat{\zeta})} = 0 \\ \mathcal{F}_s(a, b) &= \langle \sin(\phi(a)) \sin(\phi(b)) \rangle_{\mathcal{H}(\hat{\zeta})} - \langle \sin(\phi(a)) \rangle_{\mathcal{H}(\hat{\zeta})} \langle \sin(\phi(b)) \rangle_{\mathcal{H}(\hat{\zeta})} \\ &\quad w(a) = k(k-1)\zeta(a)^{k-2} \end{aligned} \quad (\text{C.5})$$

are calculated on the effective Hamiltonian (B.14). We have also

$$J_{\sigma\sigma'}(a, b) = J_{\sigma'\sigma}(b, a). \quad (\text{C.6})$$

Then defining

$$G_{\sigma\sigma'}(a, b) = N \langle \Delta z_\sigma(a) \Delta z_{\sigma'}(b) \rangle \quad (\text{C.7})$$

one has

$$\sum_{\sigma'} \int db J_{\sigma\sigma'}(a, b) G_{\sigma'\sigma''}(b, c) = \delta_{\sigma\sigma''} \delta(a-c). \quad (\text{C.8})$$

We are interested in calculating

$$\begin{aligned} G(a, b) &= N[\langle z(a)z^*(b) \rangle - \langle z(a) \rangle \langle z^*(b) \rangle] = N \langle \Delta z_1(a) \Delta z_1(b) \rangle + N \langle \Delta z_2(a) \Delta z_2(b) \rangle \\ &= G_{11}(a, b) + G_{22}(a, b). \end{aligned} \quad (\text{C.9})$$

By writing explicitly some of equations (C.8) and making some substitutions one gets

$$\begin{aligned} G_{11}(a, c) &= \mathcal{F}_c(a, c) + \int db \mathcal{F}_c(a, b) [\operatorname{Re} w(b)G_{11}(b, c) - \operatorname{Im} w(b)G_{21}(b, c)] \\ G_{12}(a, c) &= \int db \mathcal{F}_c(a, b) [\operatorname{Re} w(b)G_{12}(b, c) - \operatorname{Im} w(b)G_{22}(b, c)] \\ G_{21}(a, c) &= - \int db \mathcal{F}_s(a, b) [\operatorname{Im} w(b)G_{11}(b, c) + \operatorname{Re} w(b)G_{21}(b, c)] \\ G_{22}(a, c) &= \mathcal{F}_s(a, c) - \int db \mathcal{F}_s(a, b) [\operatorname{Im} w(b)G_{12}(b, c) + \operatorname{Re} w(b)G_{22}(b, c)]. \end{aligned} \quad (\text{C.10})$$

These equations give the collective correlation functions in terms of the self-correlations evaluated on the effective Hamiltonian; but using equation (B.19) we can replace the effective self-correlations with the original ones, and obtain a relation between self-correlation and collective correlations of the original system.

C.2. Solution in the equilibrium case

Probability conservation and causality imply that [16, 17]

$$\begin{aligned} G_{\sigma\sigma'}(a, b) &= C_{\sigma\sigma'}(t, t') + (\bar{\theta}' - \bar{\theta})(\theta' R_{\sigma\sigma'}(t, t') + \theta \bar{R}_{\sigma\sigma'}(t, t')) \\ \mathcal{F}_{c,s}(a, b) &= \mathcal{C}_{c,s}(t, t') + (\bar{\theta}' - \bar{\theta})(\theta' \mathcal{R}_{c,s}(t, t') + \theta \bar{\mathcal{R}}_{c,s}(t, t')) \end{aligned} \quad (\text{C.11})$$

where

$$\bar{R}(t, t') = R(t', t). \quad (\text{C.12})$$

In the $t \rightarrow \infty$ limit the system reaches equilibrium, so that the correlation functions depend only on the time difference, the response functions are related to the correlations by the fluctuation–dissipation theorem, and w does not depend on time and is equal to its equilibrium value. From the solution of the thermodynamics we know that the equilibrium magnetization does not depend on θ and $\bar{\theta}$, so that

$$\lim_{t \rightarrow \infty} w(a) = w = k(k - 1)\zeta(\beta)^{k-2} \tag{C.13}$$

is independent on a and

$$\lim_{t, t' \rightarrow \infty} G_{\sigma\sigma'}(a, b) = C_{\sigma\sigma'}(t - t') + (\bar{\theta}' - \bar{\theta})(\theta' R_{\sigma\sigma'}(t - t') + \theta R_{\sigma\sigma'}(t' - t)) \tag{C.14}$$

where the limit is obtained at fixed $t - t' = \tau$. If we suppose that the correlations decay fast (exponentially) for $\tau \rightarrow \infty$, the values of t_b in the integrals in equation (C.10) must stay close to t_a, t_c . Then in the limit in which t_a, t_c go to infinity, t_b also must go to infinity, and w becomes a constant also with respect to the fermionic variables. Then we can rewrite equations (C.10) as

$$\begin{aligned} G_{11} &= \mathcal{F}_c + \text{Re } w\mathcal{F}_c \otimes G_{11} - \text{Im } w\mathcal{F}_c \otimes G_{21} \\ G_{12} &= \text{Re } w\mathcal{F}_c \otimes G_{12} - \text{Im } w\mathcal{F}_c \otimes G_{22} \\ G_{21} &= -\text{Im } w\mathcal{F}_s \otimes G_{11} - \text{Re } w\mathcal{F}_s \otimes G_{21} \\ G_{22} &= \mathcal{F}_s - \text{Im } w\mathcal{F}_s \otimes G_{12} - \text{Re } w\mathcal{F}_s \otimes G_{22} \end{aligned} \tag{C.15}$$

where

$$(G_1 \otimes G_2)(a, c) = \int db G_1(a, b)G_2(b, c). \tag{C.16}$$

If G_1 and G_2 are of the form (C.11), $G_1 \otimes G_2$ has the same form [16, 17],

$$\begin{aligned} (G_1 \otimes G_2)(a, c) &= (C_1 \otimes \bar{R}_2 + R_1 \otimes C_2)(t, t') \\ &+ (\bar{\theta}' - \bar{\theta})(\theta'(R_1 \otimes R_2)(t, t') + \theta(\bar{R}_2 \otimes \bar{R}_1)(t, t')) \end{aligned} \tag{C.17}$$

where \otimes is the time convolution product. Equating (for example) the $\theta'\bar{\theta}'$ component of equation (C.15) and moving to the frequency domain, we finally get

$$\begin{aligned} R_{11}(\omega) &= \mathcal{R}_c(\omega) + \text{Re } w\mathcal{R}_c(\omega)R_{11}(\omega) - \text{Im } w\mathcal{R}_c(\omega)R_{21}(\omega) \\ R_{12}(\omega) &= \text{Re } w\mathcal{R}_c(\omega)R_{12}(\omega) - \text{Im } w\mathcal{R}_c(\omega)R_{22}(\omega) \\ R_{21}(\omega) &= -\text{Im } w\mathcal{R}_s(\omega)R_{11}(\omega) - \text{Re } w\mathcal{R}_s(\omega)R_{21}(\omega) \\ R_{22}(\omega) &= \mathcal{R}_s(\omega) - \text{Im } w\mathcal{R}_s(\omega)R_{12}(\omega) - \text{Re } w\mathcal{R}_s(\omega)R_{22}(\omega) \end{aligned} \tag{C.18}$$

and

$$\begin{aligned} R_{11}(\omega) &= \frac{\mathcal{R}_c(\omega)}{1 - \text{Re } w\mathcal{R}_c(\omega) + \frac{(\text{Im } w)^2 \mathcal{R}_c(\omega)\mathcal{R}_s(\omega)}{1 + \text{Re } w\mathcal{R}_s(\omega)}} \\ R_{22}(\omega) &= \frac{\mathcal{R}_s(\omega)}{1 + \text{Re } w\mathcal{R}_s(\omega) - \frac{(\text{Im } w)^2 \mathcal{R}_c(\omega)\mathcal{R}_s(\omega)}{1 - \text{Re } w\mathcal{R}_c(\omega)}}. \end{aligned} \tag{C.19}$$

Using the fluctuation–dissipation theorem, one can transform this relation into a relation between the correlation functions.

C.3. Other simplifications

In our model one can always choose the magnetization such that $\text{Im } w = 0$. In this case one has

$$R_{11}(w) = \frac{\mathcal{R}_c(w)}{1 - w\mathcal{R}_c(w)} \quad R_{22}(w) = \frac{\mathcal{R}_s(w)}{1 + w\mathcal{R}_s(w)}. \quad (\text{C.20})$$

Moreover, we can assume that the self-correlation functions are exponentials, so that

$$\mathcal{R}_{c,s}(w) = \frac{\beta A_{c,s}}{1 - i\omega\tau_{c,s}}. \quad (\text{C.21})$$

We get easily

$$R_{11}(w) = \frac{\beta Z_c A_c}{1 - i\omega Z_c \tau_c} \quad Z_c = (1 - \beta w A_c)^{-1}. \quad (\text{C.22})$$

The same relation holds for R_{22} with the substitution $w \rightarrow -w$. From this relation, using the fluctuation–dissipation theorem and moving back to the time domain, one gets equations (39).

Appendix D. Effective dynamical system for the minimization of W

The calculation of the effective potential \mathcal{W} used in equation (46) is carried out on the same lines as that presented in appendix B.2. We start from the generating functional

$$Z[0] = \int \mathcal{D}\phi_i \exp \left[\frac{1}{2} \sum_i \int da \phi_i(a) \Delta^{(2)} \phi_i(a) - \int da W(\phi) \right] \quad (\text{D.1})$$

where $W(\phi)$ is given by equation (43). Now we introduce δ -functions for the variables $z(a)$ and $z_2(a)$, and we get

$$Z[0] = \int \mathcal{D}z \mathcal{D}\hat{z} \mathcal{D}z_2 \mathcal{D}\hat{z}_2 \exp N \left[\text{Re} \int da (z(a)\hat{z}(a) + z_2(a)\hat{z}_2(a)) - \int da \frac{W(z, z_2)}{N} + \log \mathcal{Z}(\hat{z}, \hat{z}_2) \right] \quad (\text{D.2})$$

where now

$$\mathcal{Z}(\hat{z}, \hat{z}_2) = \int \mathcal{D}\phi \exp \left[T(\phi) - \text{Re} \int da (\hat{z}(a) e^{I\phi(a)} + \hat{z}_2(a) e^{2I\phi(a)}) \right]. \quad (\text{D.3})$$

We find then

$$\mathcal{W}(\phi, a) = \text{Re}[\hat{z}(a) e^{I\phi} + \hat{z}_2(a) e^{2I\phi}]. \quad (\text{D.4})$$

The saddle point equations are

$$\begin{aligned} \frac{\delta L}{\delta z^*(a)} &= \hat{z}(a) - \frac{1}{N} \frac{\delta W}{\delta z^*(a)} = 0 \implies \hat{z}(a) = \Delta^2 k^2 (k-1) [\zeta^*(a) (\zeta(a) \zeta^*(a))^{k-2} - \zeta_2(a) \zeta(a)^{2k-3}] \\ \frac{\delta L}{\delta \hat{z}^*(a)} &= z(a) + \frac{\delta}{\delta \hat{z}^*(a)} \log \mathcal{Z}[\hat{z}, \hat{z}_2] = 0 \implies \zeta(a) = \langle e^{I\phi(a)} \rangle_{\mathcal{W}(\hat{z}, \hat{z}_2)} \\ \frac{\delta L}{\delta z_2^*(a)} &= \hat{z}_2(a) - \frac{1}{N} \frac{\delta W}{\delta z_2^*(a)} = 0 \implies \hat{z}_2(a) = -\frac{1}{2} \Delta^2 k^2 \zeta(a)^{2k-2} \\ \frac{\delta L}{\delta \hat{z}_2^*(a)} &= z_2(a) + \frac{\delta}{\delta \hat{z}_2^*(a)} \log \mathcal{Z}[\hat{z}, \hat{z}_2] = 0 \implies \zeta_2(a) = \langle e^{2I\phi(a)} \rangle_{\mathcal{W}(\hat{z}, \hat{z}_2)} \end{aligned} \quad (\text{D.5})$$

and finally we obtain

$$\begin{cases} \mathcal{W}(\phi, a) = \Delta^2 k^2 (k-1) \operatorname{Re}\{[\zeta^*(a)(\zeta(a)\zeta^*(a))^{k-2} - \zeta_2(a)\zeta(a)^{2k-3}] e^{I\phi}\} \\ \quad - \frac{1}{2} \Delta^2 k^2 \operatorname{Re}\{\zeta(a)^{2k-2} e^{2I\phi}\} \\ \zeta(a) = \langle e^{I\phi(a)} \rangle \\ \zeta_2(a) = \langle e^{2I\phi(a)} \rangle \end{cases} \quad (\text{D.6})$$

that after setting $\theta = \bar{\theta} = 0$ reduces to equation (46). Note that an irrelevant constant term in \mathcal{W} has been neglected in this derivation.

Appendix E. Closest saddles to equilibrium configurations

In this section we will derive the result presented in section 7.4. We have to compute the quantity

$$\begin{aligned} \sigma(T; e_s, q) &= \frac{1}{N} \int d\varphi_i \frac{e^{-\beta H(\varphi)}}{Z(T)} \\ &\quad \times \log \int d\psi_i \delta(H(\psi) - Ne_s) \delta(\partial_i H(\psi)) \det H(\psi) \delta(q - q(\varphi, \psi)) \end{aligned} \quad (\text{E.1})$$

where $q(\varphi, \psi) = N^{-1} \sum_i \cos(\varphi_i - \psi_i)$. To do that, we need to prove a general relation. Suppose we want to calculate at the saddle point a quantity Q of the form

$$\begin{aligned} Q &= \frac{1}{N} \int d\varphi_i \frac{e^{-\beta H(\varphi)}}{Z(T)} \log A(\varphi) = \lim_{n \rightarrow 0} \frac{1}{Nn} \left[\int d\varphi_i \frac{e^{-\beta H(\varphi)}}{Z(T)} A^n(\varphi) - 1 \right] \\ &= \lim_{n \rightarrow 0} \frac{1}{Nn} \log \int d\varphi_i \frac{e^{-\beta H(\varphi)}}{Z(T)} A^n(\varphi) \end{aligned} \quad (\text{E.2})$$

where we used the relations $\log x = \lim_{n \rightarrow 0} \frac{x^n - 1}{n}$ and $\lim_{n \rightarrow 0} (f(n) - 1) = \lim_{n \rightarrow 0} \log f(n)$ if $f(n) \rightarrow_{n \rightarrow 0} 1$. Suppose also that the energy depends only on some collective parameter as in mean-field models: $H(\varphi) = Ne(z(\varphi))$, where $Nz(\varphi) = \sum_i z(\varphi_i)$ (in our model, $z(\varphi_i) = \exp(I\varphi_i)$). Then we have

$$\begin{aligned} Q &= \lim_{n \rightarrow 0} \frac{1}{Nn} \log \int dz \frac{e^{-\beta Ne(z)}}{Z(T)} \int d\varphi_i \delta(z - z(\varphi)) A^n(\varphi) \\ &= \lim_{n \rightarrow 0} \frac{1}{Nn} \log \int dz d\hat{z} \frac{e^{-\beta Ne(z)}}{Z(T)} \int d\varphi_i \exp\left(i\hat{z} \left(Nz - \sum_i z(\varphi_i)\right)\right) A^n(\varphi) \\ &= \lim_{n \rightarrow 0} \frac{1}{Nn} \log \frac{1}{Z(T)} \int dz d\hat{z} \exp(-\beta N(e(z) - Ts(n; z, i\hat{z}))) \end{aligned} \quad (\text{E.3})$$

where we defined

$$s(n; z, i\hat{z}) = z i\hat{z} + \frac{1}{N} \log \int d\varphi_i \exp\left(-i\hat{z} \sum_i z(\varphi_i)\right) A^n(\varphi). \quad (\text{E.4})$$

Clearly $s(0; z, i\hat{z})$ is the entropic contribution to the free energy as a function of z, \hat{z} that we obtain in the calculation of the partition function $Z(T)$, so that

$$f(T) = -\frac{1}{\beta N} \log Z(T) = \min_{z, \hat{z}} [e(z) - Ts(0; z, i\hat{z})] = e(\zeta) - Ts(0; \zeta, \hat{\zeta}) = f(0; \zeta, \hat{\zeta}) \quad (\text{E.5})$$

where $(\zeta(T), \hat{\zeta}(T))$ is the (T -dependent) thermodynamic minimum of the free energy (note that at the saddle point $i\hat{z} = \hat{\zeta}$). Then we have

$$Q = \lim_{n \rightarrow 0} \frac{1}{Nn} \log \int dz \exp(-\beta N[f(n; z, i\hat{z}) - f(0; \zeta, \hat{\zeta})]). \tag{E.6}$$

We can now expand $z = \zeta + n\zeta^{(1)} + o(n^2)$, $i\hat{z} = \hat{\zeta} + n\hat{\zeta}^{(1)} + o(n^2)$ and

$$\begin{aligned} f(n; z, i\hat{z}) - f(0; \zeta, \hat{\zeta}) &= \frac{\partial f}{\partial z}(0; \zeta, \hat{\zeta})n\zeta^{(1)} + \frac{\partial f}{\partial i\hat{z}}(0; \zeta, \hat{\zeta})n\hat{\zeta}^{(1)} + \frac{\partial f}{\partial n}(0; \zeta, \hat{\zeta})n + o(n^2) \\ &= \frac{\partial f}{\partial n}(0; \zeta, \hat{\zeta})n + o(n^2) \end{aligned} \tag{E.7}$$

because by definition of $(\zeta, \hat{\zeta})$ we have $\frac{\partial f}{\partial z}(0; \zeta, \hat{\zeta}) = 0$, $\frac{\partial f}{\partial i\hat{z}}(0; \zeta, \hat{\zeta}) = 0$. We then get the final result:

$$Q = -\beta \frac{\partial f}{\partial n}(0; \zeta, \hat{\zeta}) = \frac{\partial s}{\partial n}(0; \zeta, \hat{\zeta}). \tag{E.8}$$

We have then to calculate (neglecting the term $\zeta\hat{\zeta}$ that vanishes on taking the derivative with respect to n),

$$\begin{aligned} s(n; \hat{\zeta}, e_s, q) &= \frac{1}{N} \log \int d\varphi_i \exp\left(-\sum_i \hat{\zeta} \cos \varphi_i\right) \\ &\times \prod_{a=1}^n \int d\psi_i^a \delta(H(\psi^a) - Ne_s) \delta(\partial_i H(\psi^a)) \det H(\psi^a) \delta(q - q(\varphi, \psi^a)) \end{aligned} \tag{E.9}$$

where from the thermodynamic calculation $\hat{\zeta}(T) = -\beta k \zeta^{k-1}$ and ζ is given by equation (8). Using a representation analogous to equation (A.5) we get

$$\begin{aligned} s(n; \hat{\zeta}, e_s, q) &= \frac{1}{N} \log \int d\varphi_i \exp\left(-\sum_i \hat{\zeta} \cos \varphi_i\right) \prod_{a=1}^n \int \frac{d\beta_a}{2\pi} e^{N\beta_a e_s} \\ &\times \int \mathcal{D}\Psi_i^a \exp\left[\int d\bar{\theta} d\theta (1 - \beta_a \theta \bar{\theta}) H(\Psi^a)\right] \delta\left(Nq - \sum_i \cos(\varphi_i - \psi_i^a)\right). \end{aligned} \tag{E.10}$$

We will now (i) substitute the expression $H(\Psi^a) = N(1 - \text{Re } y_a^k)$, using y instead of z to avoid confusion with the thermodynamic variable ζ , (ii) insert some δ -functions for y_a and the corresponding integral representation with a multiplier \hat{y}_a , (iii) neglect all the product and sum signs related to the index a , (iv) use the integral representation for the δ -function of q with a multiplier λ_a . Then we get an expression that has to be maximized with respect to all the parameters to get the saddle point value of $s(n; \hat{\zeta}, e_s, q)$:

$$\begin{aligned} s(n; \hat{\zeta}, e_s, q) &= \max_{\text{all par}} \left[\sum_a \beta_a e_s + \sum_a \int d\bar{\theta} d\theta [(1 - \beta_a \theta \bar{\theta})(1 - \text{Re } y_a^k) + \text{Re } y_a \hat{y}_a] \right. \\ &\quad \left. + \sum_a \lambda_a q + \log \mathcal{S}(\hat{\zeta}, \hat{y}_a, \lambda_a) \right] \\ \mathcal{S}(\hat{\zeta}, \hat{y}_a, \lambda_a) &= \int d\varphi \mathcal{D}\Psi^a \exp\left[-\hat{\zeta} \cos \varphi - \sum_a \int d\bar{\theta} d\theta \text{Re } \hat{y}_a e^{i\Psi^a} - \sum_a \lambda_a \cos(\varphi - \psi^a)\right]. \end{aligned} \tag{E.11}$$

As usual, we will assume that (i) there is symmetry between the replicas ($y_a = y$, etc), (ii) y and \hat{y} are real, (iii) all the fermionic components are 0. Then we get

$$s(n; \hat{\zeta}, e_s, q) = \max_{\text{allpar}} \left[n(\beta(e_s - 1 + y_0^k) - ky_0^{k-1}y_3 + \hat{y}_0y_3 + \hat{y}_3y_0 + \lambda q) + \log \mathcal{S}(\hat{\zeta}, \hat{y}, \lambda) \right]$$

$$\mathcal{S}(\hat{\zeta}, \hat{y}, \lambda) = \int d\varphi e^{-\hat{\zeta} \cos \varphi} \left[\int \mathcal{D}\Psi \exp \left(- \int d\bar{\theta} d\theta (\hat{y}_0 + \hat{y}_3\theta\bar{\theta}) \cos \Psi - \lambda \cos(\varphi - \psi) \right) \right]^n.$$

Now we have to take the derivative of s with respect to n at $n = 0$. By direct computation

$$\sigma(\hat{\zeta}; e_s, q) = \max_{\text{allpar}} \frac{\partial s}{\partial n}(0; \hat{\zeta}, e_s, q) = \max_{\text{allpar}} \left[\beta(e_s - 1 + y_0^k) - y_3(ky_0^{k-1} - \hat{y}_0) + \hat{y}_3y_0 + \lambda q \right. \\ \left. + \int d\varphi \frac{e^{-\hat{\zeta} \cos \varphi}}{2\pi I_0(\hat{\zeta})} \log \int \mathcal{D}\Psi \exp \left(- \int d\bar{\theta} d\theta (\hat{y}_0 + \hat{y}_3\theta\bar{\theta}) \cos \Psi - \lambda \cos(\varphi - \psi) \right) \right]. \quad (\text{E.12})$$

The interpretation of this expression is straightforward by comparison with equation (A.14): in fact if we put $\lambda = 0$ we get exactly equation (A.14). This corresponds to integrating σ over q , so the dependence on the reference configuration (and hence on the temperature) disappears and we get the number of saddles of energy e_s . When λ is different from 0 the last term of the previous expression represents the single-particle version of σ . Now we can proceed exactly in the same way as we proceeded after equation (A.14): we take the derivatives with respect to β and y_3 . This fixes $y_0 = (1 - e_s)^{1/k}$ and $\hat{y}_0 = ky_0^{k-1}$ and makes the first two terms of σ equal to zero. As we are looking for saddles of energy $e_s < 1$, we then have $\hat{y}_0 > 0$, and the dependence on \hat{y}_0 in the last term disappears. We get

$$\sigma(\hat{\zeta}; e_s, q) = \max_{\lambda, \hat{y}_3} \left[\hat{y}_3y_0 + \lambda q + \int d\varphi \mathcal{P}(\varphi) \log(-2 \sinh(\hat{y}_3 + \lambda \cos \varphi)) \right] \quad (\text{E.13})$$

where $\mathcal{P}(\varphi)$ is given by equation (47). From the equation $y_0 = (1 - e_s)^{1/k}$ we see that y_0 is the average of $\cos \varphi$ on the saddles; then we will change the notation calling $y_0 = \zeta_s$. Taking the derivatives of σ with respect to λ and \hat{y}_3 we get

$$\zeta_s = - \int d\varphi \mathcal{P}(\varphi) [\tanh u(\varphi)]^{-1} \quad q = - \int d\varphi \mathcal{P}(\varphi) \cos \varphi [\tanh u(\varphi)]^{-1} \quad (\text{E.14})$$

where $u(\varphi) = \hat{y}_3 + \lambda \cos \varphi$. Now if we want $\zeta_s \in [0, 1]$, $u(\varphi)$ must have an imaginary part; but if we want ζ_s to be real, this imaginary part must be constant and equal to $\pi/2$. We will then assume that $\hat{y}_3 = y + i\frac{\pi}{2}$; note that this is the correct solution for $\lambda = 0$ (see equation (A.17)). We obtain easily the parametric relation for $\sigma(T; \zeta_s, q)$,

$$\zeta_s(y, \lambda) = - \int d\varphi \mathcal{P}(\varphi) f(t(\varphi))$$

$$q(y, \lambda) = - \int d\varphi \mathcal{P}(\varphi) \cos \varphi f(t(\varphi)) \quad (\text{E.15})$$

$$\sigma(y, \lambda) = \int d\varphi \mathcal{P}(\varphi) [\log 2 \cosh t(\varphi) - t(\varphi) f(t(\varphi))] - i\pi \frac{1 - \zeta_s(y, \lambda)}{2}$$

where $t(\varphi) = y + \lambda \cos \varphi$ and $f(t) = \frac{\cosh t - 1}{\sinh t}$. We see that the imaginary part of σ is, as expected, equal to $i\pi n(e_s)$, remembering the relation between energy and order of each stationary point. In the following we will neglect the imaginary part of σ . Now we have to maximize q on the curve $\sigma = 0$ (see section 7.4). To do that, we start with a simple argument: as λ is the field conjugated to q (the relation between λ and q is the same as the relation between

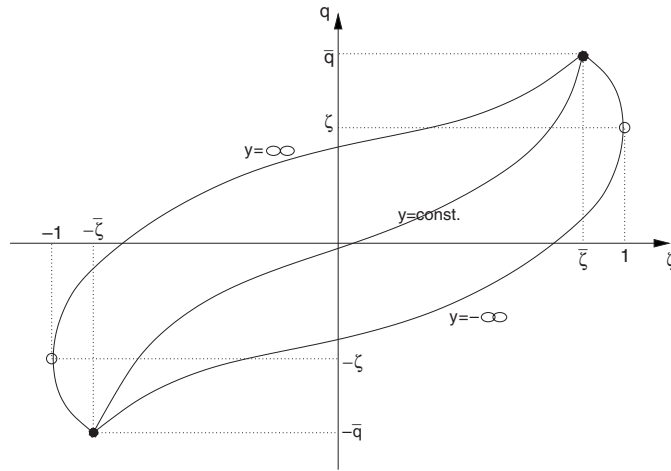


Figure 14. Schematic diagram of the constant y paths in the (q, ζ_s) plane. $\sigma(q, \zeta_s)$ is equal to 0 on the border of the domain, and is greater than 0 inside the domain. The black dots are the point for which q is maximum in the $\sigma > 0$ domain.

magnetization and magnetic field in a ferromagnet) we expect that the maximum overlap will be obtained in the $|\lambda| \rightarrow \infty$ limit. In fact, for $\lambda \rightarrow \pm\infty$, we have $t(\varphi) \rightarrow \pm\text{sgn}(\cos \varphi)\infty$ and $f(t(\varphi)) \rightarrow \pm\text{sgn}(\cos \varphi)$, so that

$$\lim_{\lambda \rightarrow \pm\infty} q(y, \lambda) = \mp \int d\varphi \mathcal{P}(\varphi) |\cos \varphi|. \tag{E.16}$$

As we want q to be positive, we have to choose $\lambda \rightarrow -\infty$. We have then

$$\begin{aligned} \lim_{\lambda \rightarrow -\infty} q(y, \lambda) &= \int d\varphi \mathcal{P}(\varphi) |\cos \varphi| = \bar{q} \\ \lim_{\lambda \rightarrow -\infty} \zeta(y, \lambda) &= \int d\varphi \mathcal{P}(\varphi) \text{sgn}(\cos \varphi) = \bar{\zeta}_s \\ \lim_{\lambda \rightarrow -\infty} \sigma(y, \lambda) &= 0. \end{aligned} \tag{E.17}$$

Then we have a consistency check of our assumption, that the point reached in the limit $\lambda \rightarrow -\infty$ belongs to the curve $\sigma = 0$.

A more accurate argument can be given in this way: one can look numerically at the curve $q(\zeta_s)$, parametrically in λ at fixed y . The curve looks like the one given in figure 14, and as λ moves from $-\infty$ to ∞ the point in the (ζ_s, q) plane moves from $(\bar{\zeta}_s, \bar{q})$ to $(-\bar{\zeta}_s, -\bar{q})$ (black dots in figure 14) as predicted by equation (E.17). Now it is easy to show that

$$\lim_{y \rightarrow \pm\infty} q(y, \lambda) = \mp \zeta \quad \lim_{y \rightarrow \pm\infty} \zeta_s(y, \lambda) = \mp 1 \quad \lim_{y \rightarrow \pm\infty} \sigma(y, \lambda) = 0. \tag{E.18}$$

Then for $|y| \rightarrow \infty$ and λ fixed all the curves collapse on the white dots in figure 14. But it is also easy to show that for $y \rightarrow \infty$ and $\lambda = -y(1 + \delta) \rightarrow -\infty$ the point goes on the upper border of the domain given in figure 14, and moves from the left white dot to the upper black dot as δ moves from 0 to ∞ (the other branch, from the left white dot to the lower black dot, is obtained for δ going from -2 to $-\infty$). On the whole border of the domain we have $\sigma = 0$ from equation (E.18); then $(\bar{\zeta}_s, \bar{q})$ is exactly the point at which q is maximum on the curve $\sigma = 0$.

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