Rod magnets inscribed in an elastic cuboid

Interpreting single-domain ferroics in Onsager's spirit

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A toy model for ferroic orders through entropy. As the rod/spin concentration (or the volume enclos-
ing the ferroic rods) is variable by a tunable force conjugate to the order parameter, the model exhibits hysteresis associated to some discontinuous isotropic-nematic transitions explained essentially by On-
sager's hard-rod model. The uniaxial anisotropy and nonperiodicity by construction is reminiscent of Stoner-Wohlfarth's single-domain magnet, and the toy model may ultimately be seen as a minimal-
istic for hard ferroics with some possible self-averaging disorders. Spin toggling shall be reliable due to the
clean two-well energy landscapes in the athermal transition theory.

I. QUANTUM FLUCTUATIONS

THE PHILOSOPHY IN A THERMAL TRANSITIONS

Onsager’s model [1] of athermal transition through rival en-
tropies consists of rigid rods (referred to as Onsager’s rods hereafter) of infinite length-diameter ratio \( e^{-1} := l/d \). The system shall be isotropic (with \( [1 + j] \) different axes along which the rods tend to align) and nematic (all rods align uniaxially) re-
spectively at two extremum concentrations \( c := C/V \) or equivalently, packing fractions [2] \( \varphi := \frac{2d^2c}{\varepsilon} \approx e^{1.2} \). To locate the transition point \( \varphi^* \) between the least and the most concentrated phases, one may refer to the energy/entropy difference [3]

\[
\ln \left\{ V - 2\pi d^2lC \right\} + \ln 1 - \left( \ln \left\{ V - 2d^2C \right\} + \ln (1 + j) \right) =: \delta S_{\text{trans}} = \delta S_{\text{fr} \varphi} = \delta S_{\text{iso}} \quad \varphi^* = \frac{1}{1 + j}, \quad \varphi = \frac{0}{1 + j}, \quad \left\{ \begin{array}{l}
\delta S_{\text{trans}} \xrightarrow{\varphi \rightarrow \varphi^*} 0, \\
\delta S_{\text{fr} \varphi} \xrightarrow{\varphi \rightarrow \varphi^*} 1/2, \\
\delta S_{\text{iso}} \xrightarrow{\varphi \rightarrow \varphi^*} 1,
\end{array} \right.
\]

where (i) \( \left( V - 2\pi d^2lC \right) \) is the explorable space for rods in a nematic single phase, and \( \left( V - 2d^2C \right) \) the one in an isotropic case (ii) \( (1 + j) \) is interpreted as number of component species of a self-assembly in [3b] (iii) we shall call a \( \varphi \sim \varphi^* \) semidilute [4], and the transition depends trivially on the exact value of \( \left[ \frac{s}{(1 + j)} \right] \) if it remains some finite constant.

Summaries of the essence and pedagogical practices have been abundant [3]-[6] since Onsager’s first insight. Three basic facts about the model are

Athermality as Mayer’s function used to polynomial/Virial expand a partition function depends trivially on temperatures (footnote 21); this shall be rephrased in the language of quantum fluctuations in a moment

Discontinuous phase transition whose many links to the ferroic hystereses4 are in evidence

Two-well potential as higher-than-second-order Virial’s terms are greatly suppressed by \( \varepsilon \), the free energy \( f[\varphi] \) shall have a two-well landscape by Landau’s mean-field (m.f.) idea in the close vicinity of the semidilute transition point; if the isotropic minima are pinned, then any errors in desired micro-state pattern can only concern the nematic ones.

The essay’s goal is to encapsulate ultimately Onsager’s spirit into ferroics, with the trial prototype here Stoner-Wohlfarth’s (S-W’s) macro-spin [7, 8]. Viz., to fashion a ferroic switch triggered by a variable field with the usual outcome of polarisation reversals, but the internal mechanism governed by Onsager’s entropy competitions—hence athermal, and a reli-
able two-state toggling free from pitfalls of some muddled energy landscapes.

Before continuing the main thread of narration, I shall give a few more legitimacy checks on the aforementioned model features and some philosophies involved.

Quantum phase transition stands out typically when phasing out the ‘internal energy-entropy’ tradeoff in eq (B1) at zero temperature, with frozen particles and proliferating quantum fluctuations by Heisenberg’s uncertainty principle.6 In Onsager’s model, the rod exploration space or positional uncertainty is abruptly reduced when \( \varphi \) drops across \( \varphi^* \), leading to multi-

1 I shall stick to the notational conventions in apps. A and B, in which some elements of statistical physics are ‘popularised’ for interested audiences.
2 Imagine two perpendicular rods excluding each other’s geometrical centres from occupying a certain volume, the average excluded volume produced by a single rod \( \sim 2d^2l \); cf. fig. 1a of [4b]. Other examples of excluded volumes could be (i) \( 4\pi r^3/3 \) for a radius-\( l \) sphere (ii) \( 2d^2l \) for a cylinder of length \( 2l \) and diameter \( 2d \), with packing fractions \( \sim (2 \pm 1)/4 \pi \) respectively.
3 Cf. app.B; app.C shall elaborate somewhat the sketch of the model here.
4 Below some critical/“order disruption” temperatures of Curie’s, Néel’s etc. [98].
5 Strictly speaking, of some \( 1/f \) [order parameter \( \sigma \) ] now for different m.f. solutions \( \varphi \); but the m.f. constraint/saddle-point equation sets some relations between \( \sigma \) and its conjugate force \( \varphi \), so everything could eventually be expressed as a function of \( \varphi \) (or \( \sigma \)). Cf. app.C.
6 Some Schwarz’s/triangle inequality, [11] such that a vanishing root-mean-square deviation \( \Delta x \) of the position operator \( x \) evaluated at a given system state \( \Psi \) would pick some momentum root-mean-square \( \Delta p \rightarrow \infty \).
plication of the quantised rotational degrees of freedom, and thus some athermal 'quantum phase transition' like those of quantum Ising/rotor models etc. in [10].

**Mean-field theory**\(^8\) (i) coarse-grains fractions of a statistical system into self-equilibrial 'molecules'

\[ m^i := \left\{ \sigma^i = \delta \sigma^i + \left( m \equiv \sum_{j=1}^{C} m^j / C \right) \right\}, \]

with \( \sigma^i \) a variable (named spin) representative of fraction \( i \) (ii) approximates the partition functions/statistic \( Z \) by a series of the local means. Such m.f. predictions may break down by Ginzburg’s criterion [9] for a low-dimensional system, with finite-range interactions, at a *continuous* phase transition where the correlation length \( \xi \) (characteristic size of fluctuations \( \langle \delta \sigma^1 \delta \sigma^2 \rangle \)) explodes.\(^{10}\) As for a *discontinuous* transition like ONSAGER’s athermal one, an instability of the continuation from one coexisting phase to another shall yield some hysteresis/memory effect. I.e., the system needs time to readjust between single phases, with \( \xi \) finite at such transitions in general. Note the expected transitions in the toy model to be proposed are *abrupt*. As we are not concerned anyway with the asymptotic exponents of critical behaviours during the abrupt periods, a first qualitatively m.f. treatment seems adequate.

One more thing to stress is that a uniform \( m \equiv m^i \) is not a necessity for optimising a m.f. free energy. The implicit homogeneity from a m.f. idea is explicitly lost in a disorder system. Parissi’s remedy [2] is to (i) replicate the statistics \( Z \) \( s \) times and allow '\( \sigma^i_j \cdot \sigma^j_i \)' interactions, but every \((1+s)\) replicas \( \sigma^i_{s+1} \in \{1, \ldots, C\} \) form a 'molecule' bound by a strong-localisation constraint,\(^9\) with \( \{ \sigma^i_{s+1} = \sigma^i \} \) the reference *quenched* disorder, such molecular liquid shall recover some translational and rotational invariance, and one could use again methods like Virial’s expansion etc. generalised from theories of conventional atomic/molecular liquids (ii) *conflate* dissenting statistics into a full average/integral \( Z \equiv \int Z_{s} \) \( \sigma \) and, the final desired *glass free energy* is an analytic continuation of

\[ \left( \frac{\partial \ln Z_{\sigma}}{\partial \ln Z} \right) \left. \right|_{Z,C} \overset{\rightarrow}{\to} \left. \frac{(- \ln Z)}{C} \right|_{C = f_{\text{gth}}}. \]

\( ^{7} \) Sending centres of all rods to a fixed \( \mathbb{R}^3 \)-origin, \( \mathbb{R}^3 \)-rotations of the directional unit vectors \( \mathbf{n} \) are then typified by group elements \( \mathcal{B} \in \text{SO}_3 \). Note some \( \mathbb{C}^2 \)-'spin rotations' in quantum mechanics can be represented by \( \gamma_{s} = e^{i \pi \sigma / 2 \mathbf{n}} \in \text{SU}_2 \) generated by Pauli’s matrices \( \sigma_{x,y,z} \), such that \( \text{SU}_2(\pm 1) \) 3-sphere \( S^2 \), topologically acts locally like \( \text{SO}_3 \) (quotient group \( S^3 / \{ \pm 1 \} \)).

\( ^{8} \) Cf. chaps. 1-2 of [9], and [1] etc.

\( ^{9} \) In 1st derivatives of the free energy with respect to applied forces.

\( ^{10} \) I.e., nonnegligible fluctuations over all distances force the entire system to form a unique critical phase; the properly compatible ideas of scaling and renormalisation are then needed for quantitative descriptions.

\( ^{11} \) Reminiscent of the extra rotational degrees of freedom for each ONSAGER’s rod in an isotropic phase than in a nematic one.

## II. PHENOMENOLOGIES FOR HYSTERESIS

### A. A thought experiment

The task is simply to well encapsulate \( C \) magnetised ONSAGER’s rods in an elastic cuboid\(^{12}\) of height \( L \sim l \) and volume \( D^2L \sim l^3 \). Small variations of the cuboid volume/occupied volume of the rods allow variations of packing fractions \( \varphi \) around the critical \( \varphi^* \) (1/2 for simplicity) in eq (i).\(^{13}\) Label the three axes through the centres of the opposite cuboid faces as \( x, y \) and \( z \); let the vertical axis be \( z \), so that the principal facade and the aerial view are respectively in the \( x-z \) and \( x-y \) planes.

1. **Initial configuration**

   **Introduction of a mechanism for protecting rods’ impenetrability**

   (i) all north poles \( \mathbb{Q} \) are perfectly up in a strong applied force \( \mathbf{B} \equiv \mathbf{B}^z \) (table I), inducing naturally a unique *nematic axis* as the \( z \)-axis

   (ii) the horizontal \( \mathbb{Q} \leftrightarrow \mathbb{O} \) and \( \mathbb{Q} \leftrightarrow \mathbb{W} \) repulsions keep the confined rods from collapsing together but aligning at equal spacings \( a \leq 2 \sqrt{D} \ll D \), as the preset \( L \equiv l \) \( \{D/l\} \) finite \( \varphi = \left| 2d^2(D/a)^2 \right| / D^2L \geq \varphi^* \) for now; note that \( a \approx d = \epsilon l \), \( \mathbb{Q} \leftrightarrow \mathbb{Q} \) is hence morphologically nothing more than a bundle of fibres/lines of induction

   (iii) dipolar interactions \( \left( 1 / \left| r^{i, j} \right| \right) \) for parallel dipoles \( i \) and \( j \) at a distance \( r^{i, j} \)\(^{14}\) are assumed to be so weak and well screened \([13]\), say the characteristic length of damping is \( \sim a \) that they compare minorly with the prescribed two-well potential in the system free energy \( F \); cf. discussions of the non-local forces etc. in some Langevin’s equation \( \dot{\varphi} = ( - \beta / \beta \dot{\varphi}) \) of \([14]\), with \( \varphi(x,t) \) a scalar variable forming the phenomenological \( F [\varphi] \).

### Table I: Ferroic dipoles \( \mathbf{M} \) subject to their conjugate force \( \mathbf{B} \)

| \( \mathbf{B} \)     | \( \mathbb{Q} \) | \( \mathbb{O} \) | \( \mathbb{W} \) | \( \mathbb{I} \) | \( \mathbb{O} \) |
|-----------------|---|---|---|---|---|
| \( \uparrow \)   | + | + | - | - | + |
| \( \downarrow \)  | - | - | + | + | - |

\( ^{12} \) Or any similar geometry like a cylinder of length \( L \) and diameter \( D \), for negligible boundary effects.

\( ^{13} \) The average nematic excluded volume for rods in the cramped box is now a cylinder \( \pi a^2 l \) of length \( l \) (rather than \( 2l \)) and diameter \( 2a \), but this will not change the final \( \varphi^* \) anyway.

\( ^{14} \) Cf. prob.6.21 in [12] for a general potential between angled dipoles.
Assuming that the above protection for impenetrability remains effective, \( \mathbf{b}@\rightarrow\mathbf{b}@: \) the same reduction continues until a breakdown in \( @ \), where \( \varphi \) touches the transition \( \varphi^* \), and all rods flip in ONSAGER’s spirit at once to the configuration \( \varnothing \) with \( \mathbf{m} \)’s direction the same as \( \mathbf{b} \’s \) again. The configuration \( \varnothing \) during the flip could be a superposition (i) \( \approx (\varnothing + \mathbf{O})/2 \), of swapping spins, or (ii) \( \approx (\mathbf{O} + \varnothing)/2 \), of rotating spins, but is not much of our concern as mentioned in the m.f. discussions in sec.1.

The next half ‘\( \varnothing \rightarrow @ \)’ of the loop in fig.1 shall be symmetric with the first half. Note the number of ONSAGER’s order transitions in a loop is four, twice the one of ferroic reversals, which is reminiscent of SU_2’s double covering of SO_3 in a simple group theory.

3. An effective single-domain ferroic
Duality to Stoner–Wohlfarth’s model in a static case

The hysteresis-loop squareness and the rod-bundle morphology are immediate reminiscences of S-W’s model for single-domain magnets [7, 8], with S-W’s (i) macro-spin \( \mathcal{F} \) identified here as projection (at the first configuration) of the sum \( \mathbf{m}_{\text{tot}} \) of dipolar rods on the anisotropy (indicated by a unit vector \( \mathbf{a} \)) axis (ii) ‘anisotropy-ZEEMAN’ energy \( (E_{\text{an}}, Z_{\text{an}}) \propto |\mathbf{a} \cdot \mathcal{F}|/|\mathcal{F}|^2 \),

\[ -\mathcal{F} \cdot \mathbf{b} \] competition a mutant of the ‘nematic-isotropic’ entropy competition. Note the above transition properties are implicitly quasistatic, which is relevant at zero temperature or infinite frequency of \( \mathbf{b} \), viz., increasing/decreasing the temperature/frequency may soften the hardness of a ferroic material of strong anisotropy (cf. the numerical results in fig.3 of [8]).

B. Recapture of boundary conditions & some final remarks

The ideal case is the cuboid immersed in a reservoir of \( \mathbf{b} \) absorption, with uniform \( \mathbf{b} \equiv \mathbf{b}_z \) inside and \( \equiv \varnothing \) outside the cuboid. To explain any real [16] and numerical [14, 17] experiments on strongly anisotropic materials, we shall consider some more realistic conditions. E.g.,

(i) rather than the effectively infinite rods through the entire thickness of my model, [17] simulated much shorter ONSAGER’s rods, and defined some power-law two-body potential (eq (i) of [17]) to (a) soften the rods’ hardness or (b) provide bondings between neighbouring ends from different rods, leading to a high-density columnar crystal state (an enhanced nematic state; cf. fig.2 etc. of [17])

(ii) [14] models the \( \mathbf{m} \) of thin films with easy perpendicular (z) axis anisotropy upon change of \( \mathbf{b} \) along \( z \), with the widths of domain walls much smaller than those of the uniform domains. The system may jump abruptly between \( \mathbf{m} \) of opposite signs in the hysteresis loops for weak enough exchange/dipolar interactions and Gaussian disorders (introduced to the anisotropy; cf. figs.2.6(9) and 5 etc. of [14]).

The toy model can thus be seen as a sample (with a finite ‘height L-width D’ ratio, and \( \mathbf{b} \’s \) effective applied area \( \sim D^2) \) cropped
from a uniform domain (say of which the zero-force configuration $\sim \bullet \circ \bullet$ of such a film (whose $L/D_{B1}$ → 0), where the (more or less fixed) boundary conditions at $\mathbb{C}$ and $\mathbb{G}$ might yield some asymmetry $\bullet \bullet \circ$ and $\bullet \circ \bullet$, but a constant kink $[5]$ energy difference shall not affect significantly the transition physics etc.

A last word to mention is that the nonperiodic ferroic model here seems different from the conventional ones of lengthless Ising’s spins (separated by a few crystalline spacings). Viz., some multi-ferroics may be yielded if one could mathematically impose some abstract ‘infinitely long’ ferroic verticals, between which the horizontal impenetrabilities are well protected, compatibly on other periodic ferroic models.

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Appendix A: Bohr-van Leeuwen’s theorem

The following concepts and derivations are rather general and routine;\(^{16}\) one may refer to, e.g., [18, 19] or Tong’s online lectures on classical dynamics (2005) and statistical physics (2012).

Classical dynamics specifies a gas of C identical particles (of mass) $\mu$ in a three-dimensional volume $V$ (at a given $\beta := 1/\text{temperature } T$) by a Lagrangian (as a function on a parameterised tangent bundle of a differentiable manifold), $L : \mathcal{T}M \times \mathbb{R} \rightarrow \mathbb{R}$, or its LEGENDRE counterpart—a Hamiltonian/energy

$$E\left[\{\mathbf{x}_i\}, \{\dot{\mathbf{x}}_i\}; \mathcal{E}\right] = \sum_i \left(\frac{p_i^2}{2m} - L\right) \mathbf{x}_i$$

with $\mathbf{x}_i$, $\mathbf{p}_i$ and time derivatives $\dot{\mathbf{x}}_i$ respectively the (generalised) coordinates, momenta and velocities of $\mu_i$. If $\mu_i$ are charge-\(e\) electrons, then an applied magnetic field $\mathbf{B} = (\mathbf{A} \times \text{vector potential } \mathbf{A})$ induces some current densities $\mathbf{j} = \epsilon \mathbf{A} \times \mathbf{A}'$, and some magnetic moments $\mathbf{m}_i = (\mathbf{x}_i \times \mathbf{j}_i)/2$ whose sum of \(a\)-directional magnitudes is

[HAMILTON’S equation]

$$M_a \propto \sum_i a^{(a)} \partial_t \mathbf{x}_i^{(a)}, \quad \text{with } \partial_t \mathbf{x}_i = \frac{\partial}{\partial t} E \implies \mathbf{F}_i^{(a)} \mathbf{X}_i^{(a)}$$

and $a^{(a)}$ some coefficients of the linear combination.

Statistical physics measures the ensemble\(^{16}\) mean

$$\langle O \rangle = \frac{1}{Z_\beta} \sum_{\beta} \mathcal{Z}_\beta \left(= \frac{1}{Z_\beta} \exp \left(-\beta \langle E \rangle \right) \right) \prod_{i=1}^C \mathbf{F}_i$$

of an observable $O$ with BOLTZMANN’S weights $\mathbf{p}_\beta \propto e^{-\beta E_\beta}$, and the normaliser $Z_\beta$ called partition function a folded rack for displaying statistics. If $E$ is the one in eq (A2) with no explicit ZEEKMAN’s perturbations $-\mathbf{m}_i \mathbf{B}$,\(^{17}\) then $Z_\beta$ depends trivially on $\mathbf{B}$, and any $B\text{-directional } M^B$ (not necessarily $M^a$ along the basis directions) vanishes averages eq.\(^{18}\)

Appendix B: Statistical preference for maximum entropy & minimum free energy

SHANNON’s entropy (a vogue synonym for disorder)

$$S := -\ln \left\{ \frac{Z_\beta}{Z}\right\} \left(= -\beta F_\beta \langle 1 \rangle Z_\beta + \beta \langle E \rangle Z_\beta \right), \tag{Bi}$$

with HELMHOLTZ’S free energy (multiplied by $\beta$)

$$\beta F_\beta := \langle -\ln Z_\beta \rangle \text{ a mathematical equivalent to } Z_\beta, \tag{B2}$$

and 0 $\equiv \langle 1 \rangle Z_\beta - 1 =: \phi_1$ a natural constant of probability. Since

$$\left\{ \begin{array}{l} \partial_{\mathbf{p}_\beta} S \equiv \partial_{\mathbf{p}_\beta} \left( S - \sum_{\omega=1}^\omega \gamma_\omega \phi_\omega \right) = \lambda_1 + \lambda_2 S = 0, \\
\partial_{\mathbf{p}_\beta} \mathbf{P}_\omega \cdot \mathbf{p}_\beta \leq 0,
\end{array} \right.$$

$S$ shall maximise (or equivalently $\beta F_\beta$ tends to minimise) itself for an imposed expectation $\mathbb{E}$ set by the constraint $\phi_1 := \langle E \rangle Z_\beta = \mathbb{E} \equiv 0$, with the so-called LAGRANGE’s multipliers $\lambda_{a=1,2} = -\beta \phi_1, \mathbf{B}$. As we only care for energy differences in physics, the sign of $\phi_1$ in eq (Bi) may serve as an indicator of some temperature-driven order-disorder transitions. A typical example is PIERL’S argument [20] that the paramagnetic disorder overwhelms the ferromagnetic order in ISING’s model if $T$ exceeds a critical temperature $T_c$ (viz., thermal fluctuations go wild).\(^{20}\) Subject to some tunable forces (e.g., a magnetic field $\mathbf{B}$) other than $T$, Ising’s magnets may see some athermal/$T_f$-fixed transitions.

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16. A virtual collection of many replicas of the statistical system.
17. Quantum effects, as classical electrons cannot whirl forever without collapsing into the nuclei. I.e., quantum mechanics gives $m$ as prior to $\mathbf{B}$.
18. Viz., $\langle M^B \rangle$ is a sum of terms, each of which $\sim \int dp \exp[-\beta F_\beta / 2] \sim 0$, as the integrand is odd in $p$; cf. [18]. Adding a ZEEMAN term to $\mathbb{E}$, one might expect $(m) \sim \langle p \rangle \sim \int dp \exp[-(p^2 / 2 - \beta B)] p - \exp[-(B^2 / 2) - \beta] \not\equiv 0$.
19. Summations sometimes present data clearer than multiplications.
20. Cf. the simplified description on pp. 44 of BERNARDO & JACOBSEN’s online lecture manuscript Statistical field theory and applications: an introduction for (and by) amateurs (29 June 2020).
Appendix C: Miscellaneous of Onsager's model

This section is based on [2, 4 etc.] and a tutorial of nematic liquid crystals (given by profs. van Wijland, Lenz & Trizac) I took at l’ENS de Paris in 2019. Consider

\[ \mathcal{E} = \sum_{i \neq j} \frac{|\vec{p}_i - \vec{p}_j|^2}{2\mu} + \sum_{i, j} \left( u_{i, j} = \nu |x_i - x_j|^{-1} \right) \]

as a simplest form of eq (A4) for interacting \( \mu' \equiv \mu \) at a finite concentration \( c = \frac{\mu}{V} \). From eq (A3),

\[ \beta \Pi := -\partial_c (\beta f_c V) \approx \beta \frac{\partial^2 e_{\text{che}}}{\partial c^2} + \int \frac{dn}{n} \beta f_c \ln (c/n_0) \approx \beta \frac{\partial^2 e_{\text{che}}}{\partial c^2} + \beta f_c \]

by STIRLING’s formula.

where (i) MAIER’s function \( \mathcal{M}_{i, j} \equiv \mathcal{M}_{x_{i, j}} := \left( e^{-\beta_0 e_{\text{che}}(x_{i, j})} - 1 \right) \) is assumed to be mostly small [21] (ii) \( n_0 \) and DE BROGLIE’s wavelength \( \lambda = \frac{2\pi \beta}{\mu} \) are irrelevant reference constants (iii) we would like to express everything as a function of \( c \) up to \( O(c^2) \). E.g.,

\[ \beta \Pi = -\partial_c (\beta f_c V) \approx \beta \frac{\partial^2 e_{\text{che}}}{\partial c^2} + \beta f_c \ln (c/n_0) \approx \beta \frac{\partial^2 e_{\text{che}}}{\partial c^2} + \beta f_c \]

If \( \mu' \) are now Onsager’s rods pointing in directions (of some unit vectors) \( \mathbf{n}' \), one might promote the scalar \( c = c(\Psi_n) \) by adding a factor of orientational probability distribution \( \Psi_n \) constrained by

\[ 1 = \int \! dn \, \Psi_n \]

and reformulate eq (C2b) directly into

\[ \beta f_c = \beta f_{che} + c \int \frac{dn}{n} \frac{\partial^2 e_{\text{che}}}{\partial c^2} + \beta f_c \ln (c/n_0) \frac{\partial^2 e_{\text{che}}}{\partial c^2} + \beta f_c \]

with the tildes simply dropped hereafter; (i) saddle-point con-

\[ 0 = \lambda + \beta \left( 1 + \ln \frac{\Psi_n}{\Psi_n^{\text{ref}}} + \int \frac{dn}{n} \frac{\partial^2 e_{\text{che}}}{\partial c^2} \right) \]

Onsager proposed a trial distribution

\[ \Psi_n^{\text{ref}} \propto \cos \frac{\phi \cos \theta}{4\pi} \sinh \frac{\phi}{\theta} \]

and with \( j \) chose (by the system) to minimise eq (C4b) (i.e., to reach \( \beta f_{che, \text{saddle}} \) by seeking solutions to the m.f. condition/saddle-point eq (C4c)) and to parameterise the order: isotropic \( \rightarrow \) nematic \( \Rightarrow \) flat \( \Psi_n^{\text{che}} \) peaks as Dirac’s \( \delta \) at \( \theta = \pi \) and vanishes elsewhere \( \Rightarrow \) 0 \( \rightarrow \) \( \infty \). Substituting further some hypothetical 2B_{n,m} \( c \) \( \phi \) \( \sim \{ \mathbf{n} \} \) into eq (C4b), one could read off useful m.f. information about the preferable single phase from the diagrams of the energy differences \( \beta f_{\phi} [\phi] \) \( \sim \beta f_{\phi} [\phi \equiv 0 \text{rem}] \) \(- \beta f_{\phi} [\phi \equiv \pi \text{rem}] \). Since (i) all we need here is a simple illustration (ii) the direct analytical/numerical computations for the m.f. energies in Onsager’s model could be quite involved [6], try some makeup series (at the request of a minimal description for discontinuous transitions like ‘gas condensation to liquid’)

\[ \beta f_{\phi} [\sigma] = g_0^2 \sigma^2 - g_2^3 \sigma^3 + g_4^3 \sigma^4 + O(\sigma^5) \]

of Landau’s to mimic the one schematically shown in fig.10.1 of [4], with \( \sigma, \) some makeup order parameter [44] equivalent to \( \phi \). To capture physics in the vicinity of a transition point, assume a linear form \( g_0^2 = \sigma^0 - \sigma^0 \frac{\partial^2 \sigma}{\partial \sigma^0} \) (as we expect some sign changes of the \( \sigma^2 \)-term due to the variations of \( \phi \)), with \( \sigma^0,1 \) as well as the higher-order coefficients \( \sigma^3 \) (with the prefixed minus sign to induce a local maximum) and \( \sigma^4 \) constants. Up to some rescaling (to have some desired form \( \{ \sigma_{1/2}^0, \sigma_{1/2}^0 \equiv [\sigma^0, 0], [0, 1] \) etc.,

\[ \beta f_{\phi} [\sigma] = \frac{1}{\sqrt{2}} \left( \frac{1-\sigma}{2} - \frac{3}{2} \right) \frac{\sigma^2}{\sigma^2} + \frac{1}{4} \frac{\sigma^4}{\sigma^4} \]

with \( \beta \) and \( \phi \) dropped hereafter; (i) saddle-point con-

\[ NB \] (i) the so-called Virial’s expansion (C4) or (C4b). (C4b) is formally only reliable at \( \epsilon, \epsilon \to 0 \). (ii) for perfectly hard particles with \( u_{x_{i, j}} \equiv \infty \) and \( u_{x_{i, j}} \equiv 0 \) (say \( x_i \)’s the excluded volume of \( x_i \) when \( x_{i, j} \leq \infty \), \( x_{i, j} \) is really some HEAVISIDE’s step function \( \delta_{x_{i, j}} \) and independent of \( \beta \).

\[ \text{Lagrange’s multiplier } \lambda \] for the normalisation (C4b) of \( \Psi_n \) is redundant once an explicit form (C3) of \( \Psi_n \) is given.
\[ 0 = \frac{\partial^2}{\partial \varphi^2} \delta f_\sigma \quad \text{two local-minimum solutions} \]

\[ \delta f_\sigma[\sigma = 0] = 0, \quad \delta f_\sigma[\sigma = 1 + \sqrt{\varphi}] = \frac{1}{12} - \left( \frac{1}{3} + \frac{2}{\sqrt{3}} + \frac{2}{3} \right) \varphi, \]

and a local-maximum one \( \sigma = 1 - \sqrt{\varphi} \) (ii) \( 0 = \delta^2 \delta f_\varphi = \delta^2 \delta f_c \Rightarrow \) two reflective points \((\sigma_{1,2}, \varphi_{1,2}^*) = (1,0), (0,1)\), where the metastable nematic/isotropic state appears respectively when increasing/decreasing \( \varphi \) (iii) \( 0 \equiv \delta f_\varphi[0] = \delta f_\varphi[\sigma \neq 0] \Rightarrow \) a transition point \((\sigma_*^*, \varphi_*^*) = (4/3, 1/9)\). In short, (i) the isotropic/nematic state is more stable respectively for \( \varphi \in (\varphi_*^*, \varphi_*^*) \) or \( (\varphi_*^*, \varphi_*^*) \) (ii) \( \delta f_\varphi \) has a unique minimum dubbed isotropic/nematic respectively for \( \varphi < \varphi_*^* \) or \( \varphi > \varphi_*^* \).

REFERENCES

[1] Onsager, L. The effects of shape on the interaction of colloidal particles. Ann. N. Y. Acad. Sci. 51, 627–659 (1949).
[2] Parisi, G., Urbani, P. & Zamponi, F. Theory of simple glasses: exact solutions in infinite dimensions (Cambridge University Press, 2020).
[3] Frenkel, D. a, in Theor. Chem. Acc. (eds Cramer, C. J. & Truhlar, D. G.) 212–213 (Springer, 2001).
[4] Doi, M. & Edwards, S. F. The theory of polymer dynamics (Clarendon Press, 1988).
[5] Chaikin, P. M. & Lubensky, T. C. Principles of condensed matter physics (Cambridge University Press, 1995).

[6] a, Vroege, G. J. & Lekkerkerker, H. N. Phase transitions in lyotropic colloidal and polymer liquid crystals. Rep. Prog. Phys. 55, 124 (1992).
[7] Tannous, C. & Gieraltowski, J. The Stoner-Wohlfarth model of Ferromagnetism: Static properties. https://arxiv.org/abs/physics/0607117 (2006).
[8] Carrey, J., Mehdouaib, B. & Respaud, M. Simple models for dynamic hysteretic loop calculations of magnetic single-domain nanoparticles: Application to magnetic hyperthermia optimization. J. Appl. Phys. 109, 083921 (2011).
[9] Cardy, J. Scaling and renormalization in statistical physics (Cambridge University Press, 1997).
[10] Sachdev, S. a, in Encyclopedia of Mathematical Physics (eds Francoise, J.-P., Naber, G. L. & Tsou, S. T.) 289–295 (Elsevier, 2006).
[11] Weibeberg, S. Lectures on quantum mechanics (Cambridge University Press, 2015).
[12] Griffiths, D. J. Introduction to Electrodynamics 4th ed. (Cambridge University Press, 2017).
[13] Altland, A. & Simons, B. D. Condensed Matter Field Theory 2nd ed. (Cambridge University Press, 2010).
[14] Jagla, E. A. Hysteresis loops of magnetic thin films with perpendicular anisotropy. Phys. Rev. B 72, 094406 (9 2005).
[15] Wiese, K. J. Theory and Experiments for Disordered Elastic Manifolds, Depinning, Avalanches, and Sandpiles https://arxiv.org/abs/1112.8121 (2022).
[16] Speliotis, D., Bate, G., Alstad, J. & Morrison, J. Hard magnetic films of iron, cobalt, and nickel. J. Appl. Phys. 36, 972–974 (1967).
[17] Kuriabova, T., Betterton, M. & Glaser, M. A. Linear aggregation and liquid-crystalline order: comparison of Monte Carlo simulation and analytic theory. J. Mater. Chem. 20, 10366–10383 (2010).
[18] Aharoni, A. Introduction to the Theory of Ferromagnetism 2nd ed. (Clarendon Press, 2000).
[19] Pathria, R. K. & Beale D. P. Statistical mechanics 4th ed. (Elsevier, 2011).
[20] Peierls, R. On Ising’s model of ferromagnetism in Math. Proc. Camb. Philos. Soc. 32 (1936), 477–481.
[21] Porter, D. A. & Easterling, K. E. Phase transformations in metals and alloys 3rd ed. (CRC press, 2009).