Supplementary information

Phase diagram of self-assembled rigid rods on two-dimensional lattices: Theory and Monte Carlo simulations

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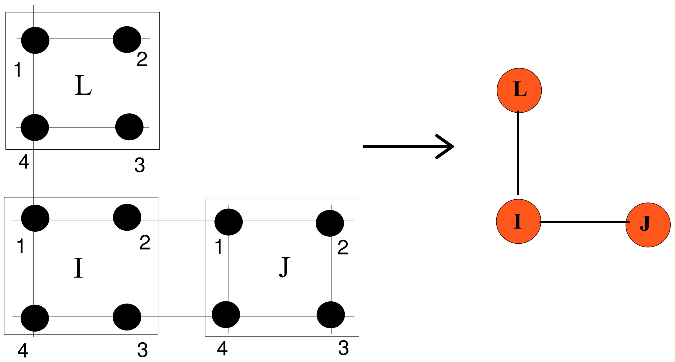
Here we provide the details of the RSRG calculations presented in the manuscript.

I. RSRG METHOD

Consider the Kadanoff blocks of size $N_b = b^2 = 4$ shown in Fig. S1.



Lopez et al, Supplementary figure S1: Kadanoff blocks of size $b = 2$ for the square lattice.

Let's denote by S'_I the block spin associated to the block I and s_I the set of lattice spins belonging to the block I: $s_I \equiv \{s_i\}$ with $i \in I$. Let's also denote by S' and s the complete sets of block and lattice spins respectively. We can express $\mathcal{H} = \mathcal{H}_0 + \mathcal{V}$, where $\mathcal{H}_0 = \sum_I \mathcal{H}_I(s_I)$ contains all the interactions between spins belonging to the block I and $\mathcal{V}$ all the interblock interactions. Introducing an RG projection matrix $P(S', s) = \prod_I P_I(S'_I, s_I)$, an average of an arbitrary function $X(S', s)$ as

$$\langle X \rangle_0 (S') \equiv \frac{1}{Z_0} \sum_s P(S', s) e^{\mathcal{H}_0(s)} X(S', s) \tag{1}$$

where $Z_0 = \prod_I Z_0^I$ with

$$Z_0^I(S_I) = \sum_{s_I} P_I(S'_I, s_I) e^{\mathcal{H}_I(s_I)}$$

The simplest RG approach within Niemeijer and van Leeuwen[1] scheme consist into the identification

$$\mathcal{H}'(S') + \mathcal{C} = \ln Z_0 + \langle V \rangle_0 \,, \tag{2}$$

where $\mathcal{H}'(S')$ is the block Hamiltonian and $\mathcal{C}$ is a spin-independent constant. This uncontrolled approximation results from the truncation to the first-order cumulant[1] of $\langle \exp(V) \rangle_0$. Using then of the double majority rule RG projection matrix $P_I(S'_I, s_I)$ introduced by Berker and Wortis for the pure isotropic Blume-Emery-Griffiths (BEG) model[2], it is easy to see that $\langle S_{iI} \rangle_0 = a_1\, S'_I$, $\left\langle S_{iI}^2 \right\rangle_0 = a_2\, S_I'^2 + a_3$, and $\ln Z_0^I = a_4 S_I'^2 + a_5$, where

$$
\begin{aligned}
a_1 &= \left.\langle S_{iI} \rangle_0\right|_{S'_I=1} && (3)\\
a_2 &= \left.\left\langle S_{iI}^2 \right\rangle_0\right|_{S'_I=1} - \left.\left\langle S_{iI}^2 \right\rangle_0\right|_{S'_I=0} && (4)\\
a_3 &= \left.\left\langle S_{iI}^2 \right\rangle_0\right|_{S'_I=0} && (5)\\
a_4 &= \left.\ln Z_0^I\right|_{S'_I=1} - \left.\ln Z_0^I\right|_{S'_I=0} && (6)\\
a_5 &= \left.\ln Z_0^I\right|_{S'_I=0} . && (7)
\end{aligned}
$$

Applying this scheme to the Hamiltonian

$$\mathcal{H}_{RG} = h \sum_i S_i^2 + \sum_{<i,j>} \left[L\, S_i S_i + M\, S_i^2 S_j^2 + U\, (S_i^2 S_j + S_j^2 S_i)\, (\hat{y}.\vec{r}_{ij} - \hat{x}.\vec{r}_{ij}) \right] , \tag{8}$$

we obtain the closed RG recursion relations

$$
\begin{aligned}
L' &= 2L\, a_1^2 && (9)\\
M' &= 2M\, a_2^2 && (10)\\
U' &= 2U\, a_1 a_2 && (11)\\
h' &= 8M\, a_2\, a_3 + a_4, && (12)
\end{aligned}
$$

together with

$$g = \mathcal{C}/N = (M\, a_3^2 + a_5/4). \tag{13}$$

Defining

$$
\begin{aligned}
B_1(L,M,U,h) &= Z_0^I\big|_{S_I'=0} \\
B_2(L,M,U,h) &= Z_0^I\big|_{S_I'=1}
\end{aligned}
$$

we obtain

$$
\begin{aligned}
a_3 &= \frac{2\,e^{h}+2\,e^{2h}+2\,e^{2h+M-L}+2\,e^{2h+M+L}\cosh(2U)}{B_1(L,M,U,h)} \\
a_4 &= \ln\frac{B_2(L,M,U,h)}{B_1(L,M,U,h)} \\
a_5 &= \ln B_1(L,M,U,h)
\end{aligned}
$$

and

$$
\begin{aligned}
a_1 &= \frac{1}{B_2(L,M,U,h)}\left[\frac{1}{2}\,e^{2h}+2\,e^{4(h+M)}+e^{3h+2(M-L)}+3\,e^{3h+2(M+L)}+e^{4(h+M+L)}+\right. \\
&+ \left. e^{2h+M+L}\,\cosh(2U)+2\,e^{3h+2M}\,\cosh(2U)\right] \\
a_2 &= \frac{1}{B_2(L,M,U,h)}\left[e^{2h}+6\,e^{4(M+h)}+e^{2h+M-L}+6\,e^{3h+2M}\,\cosh(2L)+2\,e^{4(M+h)}\,\cosh(4L)+\right. \\
&+ \left. e^{2h+M+L}\,\cosh(2U)+6\,e^{2M+3h}\,\cosh(2U)\right]-a_3(L,M,U,h) \\
a_3 &= \frac{2\,e^{h}+2\,e^{2h}+2\,e^{2h+M-L}+2\,e^{2h+M+L}\cosh(2U)}{B_1(L,M,U,h)}
\end{aligned}
$$

$$
\begin{aligned}
B_1 &= 1+8\,e^{h}+4\,e^{2h}+4\,e^{2h+M-L}+4\,e^{2h+M+L}\,\cosh(2U) \\
B_2 &= 2\,e^{2h}+6\,e^{4(M+h)}+2\,e^{2h+M-L}+8\,e^{3h+2M}\,\cosh(2L)+2\,e^{4(M+h)}\,\cosh(4L)+ \\
&+ 2\,e^{2h+M+L}\,\cosh(2U)+8\,e^{3h+2M}\,\cosh(2U).
\end{aligned}
$$

II. RSRG FLOW AND FIXED POINTS STRUCTURE

We found that all the relevant fixed points of the recursion equations lie in the BEG subspace $U=0$. The RG flow and the fixed points structure in the $U=0$ subspace is qualitatively similar to that obtained in Ref. [2], including first and second-order surfaces, as well as tricritical and critical endpoint lines[2].

We focused only on those fixed points relevant to the present problem namely, those which govern the RG flow starting from the subspace $(L, M, U, h) = (K/4, K/4, K/4, h)$, with $K \equiv \beta w$. The whole flow starting from that subspace is attracted by two subspaces invariant under RG: $L = M = U = 0$ and $(M, h) = (0, +\infty)$.

A. Flow in the $L = M = U = 0$ subspace

The recursion relations in this case reduce to $h' = a_4(0, 0, 0, h)$. This RG equation presents three fixed points: two attractors at $h = \pm\infty$, which are the loci of the high ($h = \infty$) and low ($h = -\infty$) density isotropic phases respectively and one unstable high temperature fixed point at $h = -\ln 2$. The first two fixed points are attractors in the complete (L, M, U, h) space and we will call them I_+ and I_-. They represent the high ($\langle S_i^2 \rangle \approx 1$) and the low ($\langle S_i^2 \rangle \ll 1$) density isotropic phases respectively. The fixed point $T_1 \equiv (0, 0, 0, -\ln 2)$ is the locus of a surface in the (L, M, U, h) space that corresponds to a smooth continuation at high temperatures between both phases.

B. Flow in the $(M, h) = (0, +\infty)$ subspace

This subspace corresponds to an anisotropic Ising model, since in this limit the $S_i = 0$ state has zero probability. The recursion relations reduce in this case to

$$L' = 2L\, d(L)^2 \tag{14}$$

$$U' = U d(L) \tag{15}$$

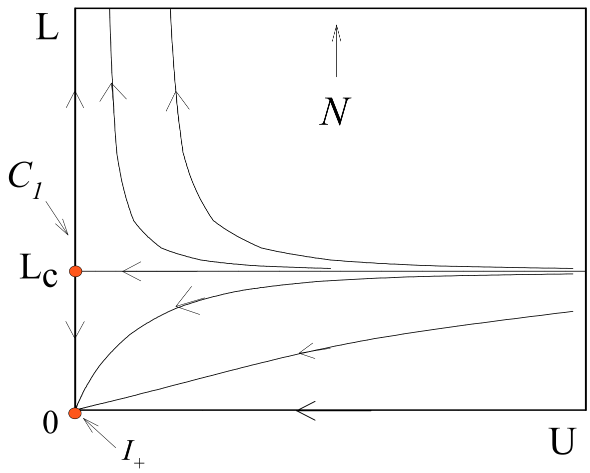
with

$$d(L) = \lim_{h\to\infty} a_1(L, 0, U, h) = \frac{2 + e^{4L}}{6 + 2\,\cosh(4L)}. \tag{16}$$

Since $L' = L'(L)$, independently of the parameter U, the whole flow is governed by the RG equation corresponding to the isotropic Ising model. This equation has a non trivial fixed point at $d(L) = 1/\sqrt{2}$, whose solution is $L_c = \frac{1}{4}\,\ln\left[1 + 2\sqrt{2} + \sqrt{10 + 5\sqrt{2}}\right] \approx 0.518612$, corresponding to the critical point of the Ising model in the square lattice under the present approximation (compare with exact Onsager result $L_c = \frac{1}{2}\ln(1+\sqrt{2}) \approx 0.44069$). We will call this fixed point C_1. The critical exponent ν is given by

$$\nu = \frac{\ln b}{\ln \lambda} \quad \lambda = \left.\frac{\partial L'}{\partial L}\right|_{L_c} .$$

We obtain $\nu = 1.0013...$, in excellent agreement with the exact result $\nu = 1$. The RG recursion equation also has two attractors: I_+ ($L = 0$) and the isotropic ferromagnetic fixed point $L = \infty$ ($T = 0$). At $L = L_c$ we have another invariant line at the (L, U) space, whose RG equation is $U' = U'/\sqrt{2}$. This recursion relation has only trivial fixed points: one attractor at $U = 0$ and one unstable at $U = +\infty$. The line $L = 0$ is also invariant and have the same fixed points. Finally, we have that $\lim_{L\to\infty} d(L) = 1$ Hence, $U' = U$ and the whole line $L = +\infty$ is a line of fixed points. This is the locus of the ferromagnetic phase in the whole (L, M, U, h) space and we will call it the N attractor. In Fig. S2 we show the flow diagram in the complete (U, L) space.



Lopez et al, Supplementary figure S2: RG flow in the $(L, 0, U, +\infty)$ invariant subspace.

III. RSRG COVERAGE CALCULATION

The coverage can be expressed as

$$\theta(K, h) = -\beta \frac{\partial f(K, h)}{\partial h}. \tag{17}$$

Let $\vec{K} \equiv (L, M, U, h)$ be the parameters vector of Hamiltonian (8). From the renormalization group transformation we have the following relation after n applications of the RG transformation[1]

$$f(\vec{K}_0) = -\frac{1}{\beta}\sum_{m=0}^{n} b^{-md} g(\vec{K}_m) + b^{-nd} f(\vec{K}_n), \tag{18}$$

where $\vec{K}_m$ is the parameters vector after m applications of the RG transformation, $\vec{K}_0$ is the initial value and $g(\vec{K}) = \mathcal{C}/N$ is given by Eq. (13). Since θ is not singular at the critical line, we can assume that the singular part of the free energy will make no contribution to Eq. (18) and therefore the derivative of the second term in the right hand of the previous expression vanishes when $n \to \infty$. Therefore, we can express

$$\theta(K, h) = \frac{\partial}{\partial h}\left[\sum_{m=0}^{\infty} b^{-md} g(\vec{K}_m)\right]_{\vec{K}_0=(K/4, K/4, K, 4, h)}. \tag{19}$$

Computing numerically the above sum and taking the numerical derivative we obtain the critical line T^* vs. θ shown in Fig. 8 of the manuscript.

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[1] T. Niemeijer and J. M. J. van Leeuwen, *Phase Transition and Critical Phenomena*, **6**, C. Domb and M. S. Green (eds.) (Springer-Verlag, New York, 1982).

[2] A. N. Berker and M. Wortis, Phys. Rev. B **14**, 4946 (1976).