The XY model

Alessandro Vindigni

28/11/2022

Low-temperature correlations in the XY model

The Hamiltonian of the classical XY model with $S = 1$ can be expressed in terms of the angle φ formed by each spin with some defined lattice direction:

$$\mathcal{H} = -\frac{1}{2}J \sum_{|\underline{n}-\underline{n}'|=1} \vec{S}(\underline{n}) \cdot \vec{S}(\underline{n}') = -\frac{1}{2}J \sum_{|\underline{n}-\underline{n}'|=1} \cos(\varphi(\underline{n}) - \varphi(\underline{n}'))\,.$$

For small variations of the $\varphi(\underline{n})$ angle between neighboring sites, this Hamiltonian can be rewritten in the continuum-limit formalism

$$\mathcal{H} = \frac{1}{2}J \int (\nabla\varphi)^2 d^{\mathrm{d}} r\,. \qquad (1)$$

The Hamiltonian (1) can be decoupled passing to the Fourier space

$$\mathcal{H} = \frac{1}{2}J \frac{1}{(2\pi)^d} \int q^2 |\tilde{\varphi}(q)|^2 \, d^{\mathrm{d}} q$$

in such a way that the *equipartition theorem* can be applied.

Q1 Evaluate the thermal averages of the Fourier amplitudes $\langle|\tilde{\varphi}(q)|^2\rangle$}:

$$\frac{1}{2}Jq^2\langle|\tilde{\varphi}(q)|^2\rangle = \frac{1}{2}k_{\mathbf{B}}T \qquad \Rightarrow \qquad \langle|\tilde{\varphi}(q)|^2\rangle = \frac{k_{\mathbf{B}}T}{Jq^2}$$

Within the linear (elastic) approximation and the continuum formalism, the following equations hold for spatial correlations

$$\langle\vec{S}(\underline{r}) \cdot \vec{S}(\underline{0})\rangle = \exp\left[-\frac{1}{2}\langle(\varphi(\underline{r}) - \varphi(\underline{0}))^2\rangle\right], \qquad (2)$$

with

$$\frac{1}{2}\langle(\varphi(\underline{r}) - \varphi(\underline{0}))^2\rangle = \frac{1}{(2\pi)^d} \int \left[1 - \cos(\underline{q} \cdot \underline{r})\right] \langle|\tilde{\varphi}(q)|^2\rangle \, d^{\mathrm{d}} q$$

Q2 Using the expression of the thermal averages $\langle|\tilde{\varphi}(q)|^2\rangle$ determined above and the Fourier transformations

$$\text{D=1} \qquad \frac{1}{2\pi}\int \frac{1-\cos(qr)}{q^2}dq \simeq \frac{r}{2}$$
$$\text{D=2} \qquad \frac{1}{(2\pi)^2}\int \frac{1-\cos(\underline{q}\cdot\underline{r})}{q^2}d^2q \simeq \frac{1}{2\pi}\ln\left(\frac{r}{a}\right),$$

compute the spatial correlations given in Eq. (2) for the one-dimensional (1D) and two-dimensional (2D) case.

$$\text{D=1} \qquad \frac{1}{2\pi}\frac{k_{\mathbf{B}}T}{J}\int \frac{1-\cos(qr)}{q^2}dq \simeq \frac{k_{\mathbf{B}}Tr}{2J} \qquad \Rightarrow \qquad \langle\vec{S}(\underline{r})\cdot\vec{S}(\underline{0})\rangle = \exp\left[-\frac{k_{\mathbf{B}}Tr}{2J}\right]$$
$$\text{D=2} \qquad \frac{1}{(2\pi)^2}\frac{k_{\mathbf{B}}T}{J}\int \frac{1-\cos(\underline{q}\cdot\underline{r})}{q^2}d^2q \simeq \frac{k_{\mathbf{B}}T}{2\pi J}\ln\left(\frac{r}{a}\right) = \eta\ln\left(\frac{r}{a}\right) = \ln\left[\left(\frac{r}{a}\right)^{\eta}\right] \qquad \Rightarrow \qquad \langle\vec{S}(\underline{r})\cdot\vec{S}(\underline{0})\rangle = \left(\frac{r}{a}\right)^{-\eta}$$

with $\eta = k_{\mathbf{B}}T/(2\pi J)$.

Q3 Assuming the expression

$$\langle\vec{S}(\underline{r})\cdot\vec{S}(\underline{0})\rangle \sim \mathrm{e}^{-r/\xi} \qquad (3)$$

as definition of the correlation length ξ, **determine the dependence of** ξ on temperature in both the 1D and the 2D case.

A characteristic length scale of the spatial decay of pair-spin correlations, i.e. the correlation length, can be defined only for the 1D case and it is

$$\xi = \frac{2J}{k_{\mathbf{B}}T}$$

Note that this dependence is equal to the low-T expansion of the exact result.
For the 2D case, pair-spin correlations decay as a power law, namely it is scale free and a correlation length cannot be defined. As discussed during the correction in the class, this behavior represents the maximal degree of order that can be attained in the 2D classical XY model at low temperature. As the temperature exceeds a certain threshold, the decay of pair-spin correlations becomes exponential as in Eq.(3). In this high-T phase, the correlation length can then be defined and shows a very peculiar dependence on T*:*

$$\xi \sim \exp\left[\frac{\Delta}{(T-T_{\mathbf{KT}})^{1/2}}\right]$$

This correlation length diverges when the temperature $T_{\mathbf{KT}}$ *is approached from above. The temperature* $T_{\mathbf{KT}}$ *marks the transition from a power-law to an exponential decay of pair-spin correlations and is named after Kosterlitz and Thouless. Qualitatively, one can understand this change of regime as induced by the proliferation of vortices (or better the unbinding of vortex pairs). The next exercise focusses on a simple estimate of this temperature.*

Vortices in the 2D XY model

Besides the linear excitations described above, the Hamiltonian (1) is also compatible with vortex excitations. Vortices are topological excitations to some extent equivalent to domain walls in the 1D Ising model. In the two-dimensional case (D=2), it is convenient to parameterize the position of a certain spin on the XY plane through polar coordinates (r, ϕ). Then, the φ field is a function of this pair of coordinates, i.e., $\varphi(r, \phi)$.

In this description a vortex is represented, e.g., by a dependence of $\varphi(r, \phi) = \phi + \pi/2$ which yields the vector field $\vec{S}(r, \phi) = (\cos\varphi, \sin\varphi) = (-\sin\phi, \cos\phi)$.

Q1 Provide an estimate of the vortex energy $\mathcal{E}_{\text{vortex}}$ using this information, the Hamiltonian (1) and remembering that

$$\nabla\varphi = \left(\frac{\partial\varphi}{\partial r}, \frac{1}{r}\frac{\partial\varphi}{\partial\phi}\right).$$

For your convenience, set the extremes of integration $r_{\max} \simeq Na$ and $r_{\min} \simeq a$ (a lattice unit).

The Hamiltonian in equation (1) yields

$$\mathcal{E}_{\text{vortex}} = \frac{1}{2}J\int_{r_{\min}}^{r_{\max}} (\nabla\varphi)^2 d^2r = \frac{1}{2}J\int_{r_{\min}}^{r_{\max}} \left(0, \frac{1}{r}\right)^2 d^2r = \pi J\int_a^{Na} \frac{1}{r}dr = \pi J \ln N.$$

Q2 estimate of the entropy increase ΔS due to the creation of one vortex in an otherwise uniform ground state (with $\varphi(r,\phi) = \varphi_0$ =cst). This can be obtained by counting (roughly!) the number of lattice sites which can host the center of the vortex (vortex core).

For a system with $N \times N$ sites, a vortex core can be placed in N^2 sites. Hence,

$$\Delta S = k_B \ln\Omega = k_B \ln N^2 = 2k_B \ln N,$$

where Ω is the number of configurations.

Q3 Combining $\mathcal{E}_{\text{vortex}}$ and ΔS evaluate the free-energy variation associated with the creation of one vortex and draw your conclusions:

A rough estimate of the free-energy variation ΔF associated with the creation of a vortex at finite temperature T is given by

$$\Delta F = \mathcal{E}_{\text{vortex}} - T\Delta S = \pi J \ln N - 2Tk_B \ln N.$$

Q4 Is there a characteristic temperature T_c above which the formation of one vortex is favored?

To evaluate the Kosterlitz-Thouless temperature, we require that the free-energy variation estimated above be zero at $T_{\mathbf{KT}}$:

$$\Delta F\Big|_{T_{\mathbf{KT}}} = 0 \;\Leftrightarrow\; T_{\mathbf{KT}} = \frac{\pi J}{2k_B}.$$

Fit beta to data measured on Fe/W(111) films

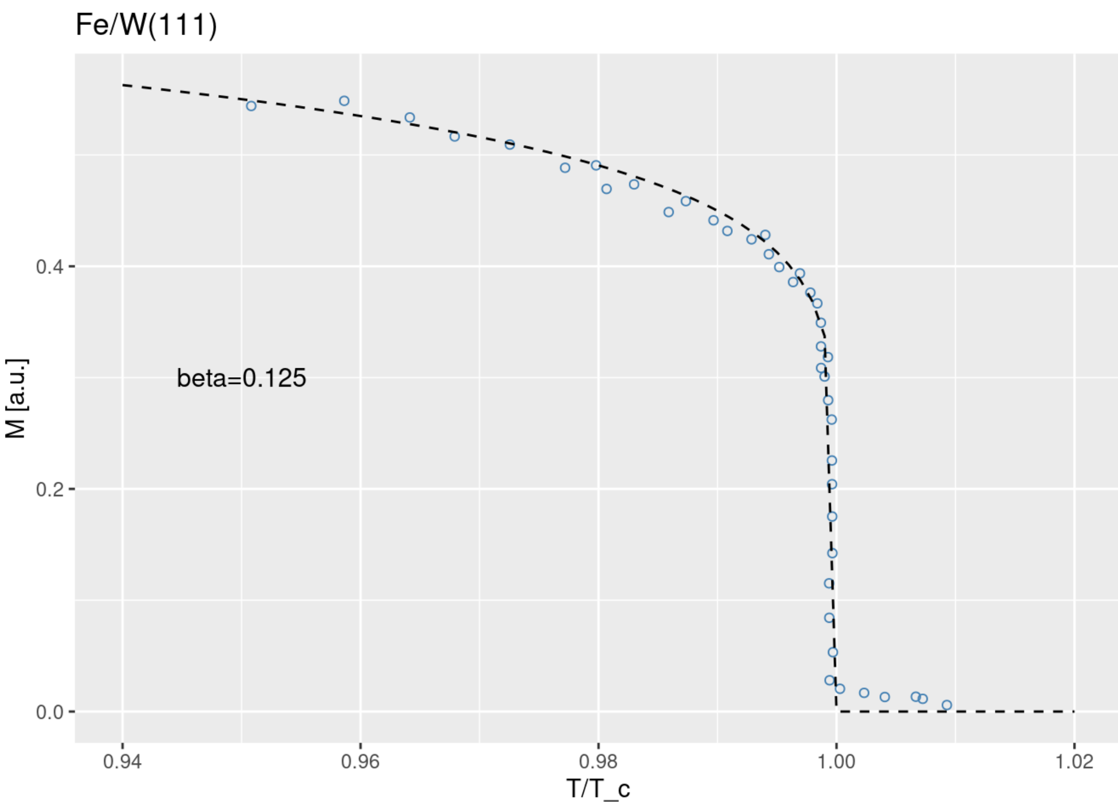
In the vicinity of T_c the spontaneous magnetization is expected to behave as

$$M(T) = \begin{cases} A\,(1-t)^\beta & \text{for} \quad t<1 \quad \text{i.e.} \quad T<T_c \\ 0 & \text{for} \quad t>1 \quad \text{i.e.} \quad T>T_c \end{cases}$$

with $t = T/T_c$. The script below loads data of the magnetization (in arbitrary units) versus t directly from the file "Data/beta_exponent.csv"

Q1 The mean-field prediction for the *critical exponent* defined above is $\beta = 1/2$. Fit the data by properly choosing the constant A and fixing β to the values: 1/2, 1/4 and 1/8.

To determine the parameters A and β you can change their values in the Rmd file and `knit` the document again.



Q2 Provide arguments that support your choice of β using the information that the data were collected on a film of Fe deposited on W(111) substrate, namely a 2D array of magnetic moments coupled ferromagnetically.

In the plot above we chose the parameters $A_0 = 0.8$ and $\beta_{\exp} = 1/8$. The later corresponds to the critical exponent of the 2D Ising model. The fact that the sample is a film is compatible with the dimensionality of the magnetic lattice (2D). The sample behaves as the Ising model (and not like the XY or Heisenberg model that would not sustain ferromagnetism at finite T) because an in-plane uniaxial anisotropy is present. We have not seen it in the course, but if the uniaxial anisotropy was out-of-plane, the dipolar interaction would have induced the formation of magnetic domains, leading to a vanishing global magnetization.

Q3 Explain with your own words why the prediction of the mean-field model is not accurate.

The mean-field model provides the correct critical exponents only for lattice dimensionality D $\geq$ 4; as the dimensionality of the magnetic lattice is reduced, the mean-field approximation becomes worse and worse.