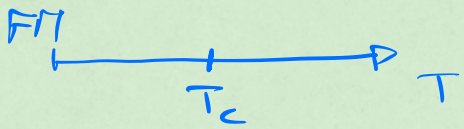
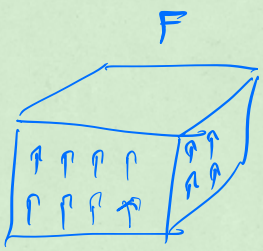
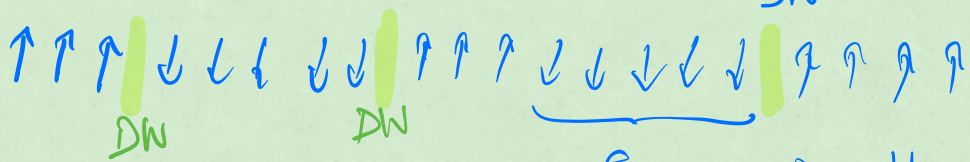
Lecture 28.11.2022





~ ∘ ~

1D Ising $T \neq 0$ Landau's argum.



ξ corr. length

$\xi \sim e^{2J/k_BT}$ $\quad E_{DW} = 2J$

$\chi \sim \frac{\xi}{T}$ magnetic susceptibility spin chains

2D Ising — ∘ — Peierls Argument.

$\Delta F = F_{path} - F_{uniform} = 2J\ell - k_B T \ln \Gamma_\ell$

$\Gamma_\ell = p^\ell \qquad p \leq 3$ (self avoiding path)

$\Delta F = 2J\ell - k_B T \ln(p^\ell) = 2J\ell - kT\,\ell \ln(p)$

$= \ell [2J - k_B T \ln p]$

$\Delta F > 0 \qquad k_B T < \frac{2J}{\ln p}$ stay in g.s. SPONTANEOUS MAG.

$\Delta F < 0 \qquad k_B T > \frac{2J}{\ln p}$ split into domains

NO SPONT. MAGN.

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2D lattice

An argument similar to the Landau's one, holding for the 1D Ising model, can be developed for the 2D system as well. In this case we should refer to the possibility of reversing a cluster of spins enclosed in a perimeter of l lattice sites and embedded in a region of spins all pointing in the same direction, as sketched in Fig. 6.3. For simplicity we consider a square lattice and sharp domain walls, meaning that all the spins are assumed to point either along $S^z = +1$ (outward) or along $S^z = -1$ (inward). The total cost in terms of exchange energy is of the order $\sim 2Jl$. To estimate the entropy variation due to the creation of a reversed cluster in an otherwise uniform spin configuration, we can think of a self-avoiding random walk. Suppose that a walker can move with one step from the center of a square in Fig. 6.3 to the center of a neighboring square. At each step the walker has at most

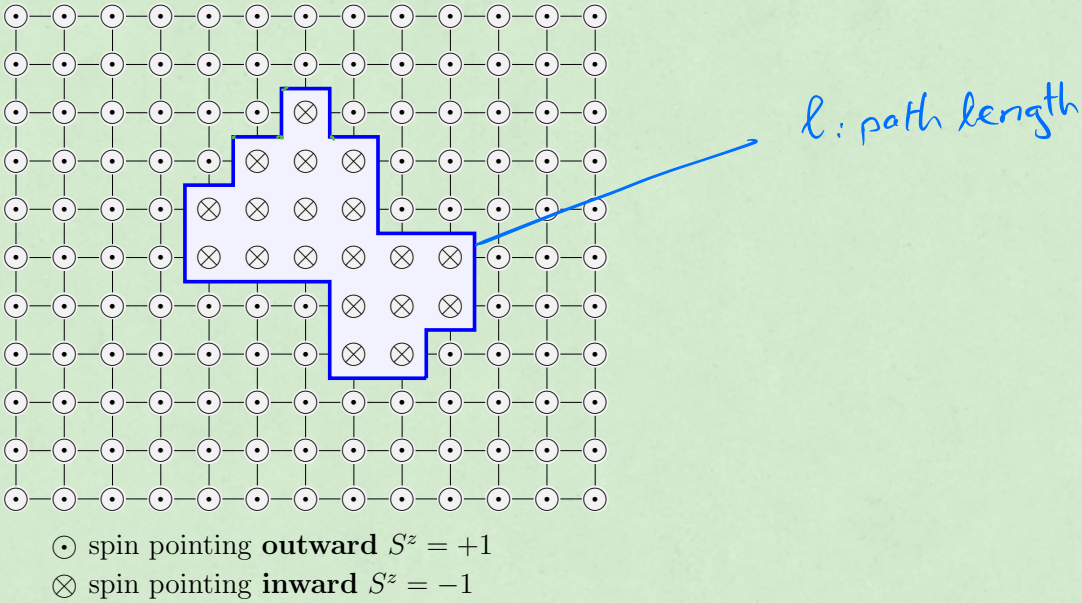


Figure 6.3: Schematic representation of a cluster of spins pointing along $S^z = -1$ (inward) in a 2D Ising lattice in which all the other spins point along $S^z = +1$ (outward). The perimeter of the cluster l is highlighted with a blue thick line.

1. Compute $Z = \operatorname{Tr}_{\{S^z(\underline{n})\}} e^{-\beta \mathcal{H}(\{S_i^z(\underline{n})\})}$

2^N terms $\qquad S^z(\underline{n}) = \pm 1$ Ising.

2. $F = -KT \ln[Z(B,T)]$

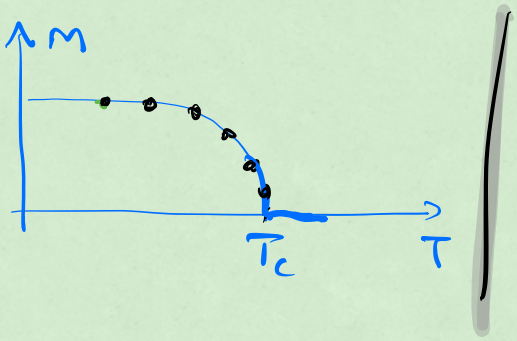
$m = -\frac{1}{N}\frac{\partial F}{\partial B}$ th. average of atomic magnetic moment

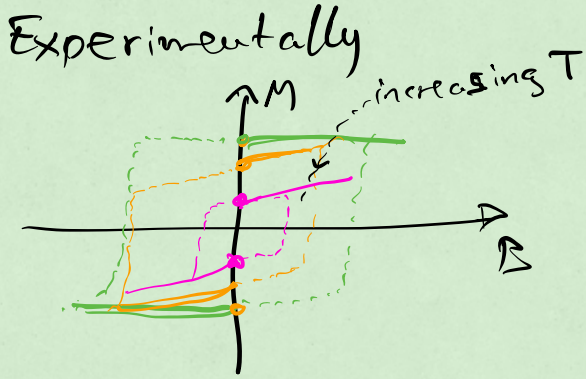
3. SPONTANEOUS MAGNET.

$m(T,0) = \lim_{B \to 0^+} m(B,T)$ $\begin{cases} \neq 0 & \text{FM} \\ = 0 & \text{NO FM} \end{cases}$

4. if 3. yields FM

$m(T,0) \sim (T_c - T)^{\beta}$ β critical exponent





m is continuous @ T_c

$\chi = \frac{\partial m}{\partial B}$ is discontinuous @ T_c $\Rightarrow$ 2nd order phase Transition

three choices of which way to go, since it has to avoid itself (the walker cannot take a step back in the direction where it came from). A possible random walk is highlighted with a thick line in the figure. Based on these simple considerations, we expect the number of closed loops corresponding to the perimeter l to be of the order p^l, with $p < 3$. As a result, the free-energy variation associated with the flip of a cluster delimited by a perimeter l is roughly $\Delta F = 2J\,l - k_{\rm B}T\,l\ln p$. Therefore, for $T < 2J/(k_{\rm B}\ln p)$ the ordered phase – with all the spin aligned along $S^z = +1$ – should be stable against the formation of large domains with reversed spins. This argument for the existence of an ordered low-temperature phase in this 2D Ising model and, thus, of a finite Curie temperature $T_{\rm c}$ was first put forward by Peierls – in more precise terms.

Rigorous results

The Ising model represents a particularly lucky case in which the heuristic arguments given above can be checked by solving the problem analytically. Even if we will not derive these results, it is useful to recall which steps should be followed to prove rigorously whether a model is consistent with a phase with **spontaneous** magnetization (finite magnetization in zero external field) for $T \neq 0$ or not. To this end, one has to compute:

1. the partition function

$$\mathcal{Z} = \mathcal{T}r\left\{e^{-\beta\mathcal{H}[\{S^z(\underline{n})\}]}\right\} \tag{6.20}$$

   where $\beta = 1/(k_{\rm B}T)$ and the trace is obtained by letting each discrete variable take the two possible values $S^z(\underline{n}) = \pm 1$ ($\mathcal{Z}$ is a sum with 2^N terms!)

2. the thermal average of the magnetic moment

$$m(T,B) = -\frac{1}{N}\frac{\partial F}{\partial B} = \frac{1}{N}\frac{1}{\beta}\frac{\partial \ln \mathcal{Z}}{\partial B} \tag{6.21}$$

3. the limit

$$m(T,0) = \lim_{B\to 0^+} m(T,B) \tag{6.22}$$

   and evaluate if there exists a temperature $T_{\rm c}$ below which the limit (6.22) takes a value different from zero.

This procedure can be carried out analytically for the Ising model in 1D and 2D producing different results:

2D Ising model

$\beta = 1/8$

$k_B T_c = \dfrac{2J}{\ln(1+\sqrt{2})}$

$\simeq 2.27\, J$

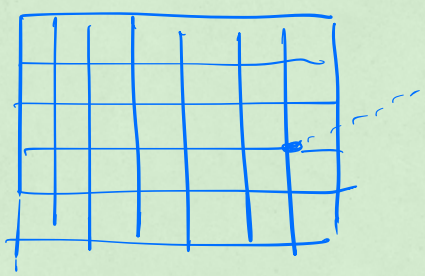
(Onsager 1944)

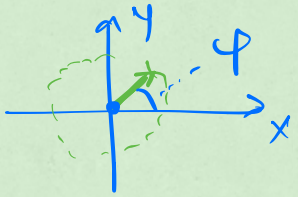
Mean field App.

$\beta = 1/2$

$k_B T_c = z J$

$= 4 J$ (2d lattice)





XY MODEL

$$\mathcal{H} = -\frac{J}{2} \sum_{(\vec{n},\vec{n}')}^{N.N.} \vec{S}(\vec{n}) \cdot \vec{S}(\vec{n}') = -\frac{J}{2} \sum_{\vec{n}\vec{n}'} \cos\left(\varphi(\vec{n}) - \varphi(\vec{n}')\right)$$

$$\cos(\Delta\varphi) \simeq 1 - \frac{1}{2}(\Delta\varphi)^2 + \dots$$ linearization

- For 1D, no spontaneous magnetization is possible at any finite temperature.

- For 2D, a spontaneous magnetization appears for $T < T_c$. The transition temperature is given by

$$\sinh\left(\frac{2J}{k_B T_c}\right) = 1 \quad \Rightarrow \quad T_c = \frac{2}{\ln(1+\sqrt{2})}\frac{J}{k_B} \simeq 2.27\frac{J}{k_B}\,. \tag{6.23}$$

  The comparison with the MF theory shows that the latter typically overestimates the transition temperature: The critical temperature of the 2D Ising model reported in Eq. (6.23) has to be compared with $T_c^{MF} = 4J/k_B$ ($z_n = 4$ for a square lattice). Expanding the spontaneous magnetization close to T_c yields

$$m(T,0) \sim (T_c - T)^{\frac{1}{8}}\,. \tag{6.24}$$

  Thus, for the 2D Ising model the exact value of the critical exponent is $\beta = 1/8$, at odds with the MF value $\beta^{MF} = 1/2$.

Indeed both these exact results obtained for the 1D and 2D Ising model show that the MFA overlooks some important features of the transition from the paramagnetic to the ferromagnetic phase, possibly occurring upon lowering the temperature.

Chapter 7

Spin models with continuous symmetry

Lecture: 28.11.2022

7.1 The XY model

When consistent with the symmetry of the problem, the quantum mechanical operators representing the effective spin of a magnetic atom can be replaced by a two-component classical vector $\vec{S} = (\cos\varphi, \sin\varphi)$, living – say – on the XY plane. An *ensemble* of such spins, disposed on a lattice and coupled via the exchange interaction, defines the classical XY model, whose Hamiltonian can be expressed in terms of the angle φ formed by each spin with some lattice direction:

$$\mathcal{H} = -\frac{1}{2}J \sum_{|\underline{n}-\underline{n}'|=1} \vec{S}(\underline{n}) \cdot \vec{S}(\underline{n}') = -\frac{1}{2}J \sum_{|\underline{n}-\underline{n}'|=1} \cos(\varphi(\underline{n}) - \varphi(\underline{n}')) \,. \tag{7.1}$$

Concretely, it can be energetically convenient for the magnetic moments of a solid to lie in a planar configuration when an easy-plane single-ion anisotropy is present. Alternatively, a planar configuration can be stabilized by the dipole-dipole interaction, of magnetostatic origin.

In this session we will derive a necessary condition for the two main classical-spin models with continuous symmetry – the XY and the Heisenberg model – to be compatible with a phase with spontaneous magnetization. This argument relies on

- a linearization of the pair-spin interaction

- the use of the equipartition theorem.

Since we will consider Hamitlonians in which the d.o.f. of spins sitting at different lattice sites are coupled, after the linearization we will obtain a quadratic Hamiltonian whose d.o.f. are still coupled with each other. Due to this fact, the results obtained in Chapter 5 for the ideal gas – in which quadratic d.o.f. are not coupled with each other – cannot be applied at this stage. Instead, some judicious transformation of coordinates will be needed in order to decouple the d.o.f. of the linearized spin Hamiltonian. This transformation is the same as the one used to decouple the d.o.f. of a chain of harmonic oscillators and, subsequently, apply the equipartition theorem. Therefore, we find it convenient to reproduce this calculation for the chain of harmonic oscillators before moving to the systems of our interest.

Chain of harmonic oscillators

We consider an array of harmonic oscillators on a 1D lattice. The d.o.f. of this problem are the diplacements u_k of individual atoms from their minimal energy position. The Hamiltonian for these *elastic excitations* reads

$$\mathcal{H} = \sum_{k=1}^{N} \frac{m}{2} \dot{u}_k^2 + \frac{1}{2} \sum_{k=1}^{N} K_e \left(u_{k+1} - u_k \right)^2 \tag{7.2}$$

The first summation on the r.h.s. represents the kinetic energy and can be handled similarly to the case of the ideal gas[1]. The second summation represents the potential energy of coupled harmonic oscillators. Clearly, the eqauipartition theorem cannot be applied to this portion of the Hamiltonian straightforwardly, though the variables u_k still contribute as a quadratic form.

[1]The only difference is that now atoms are disposed on a lattice and, therefore, there is no $N!$ term in the partition function to account for the correct Boltzmann counting.

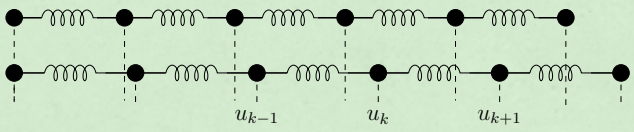


Figure 7.1: Schematic representation of the displacement field u_k in the 1D chain of harmonic oscillators described in the main text.

By means of the discrete Fourier transformation

$$u_k = \frac{1}{\sqrt{N}} \sum_q \tilde{u}_q e^{iqk}$$

the Hamiltonian (7.2) can be rewritten as

$$\mathcal{H} = \sum_q \left[K_e \left(1 - \cos q\right) |\tilde{u}_q|^2 + \frac{1}{2} m \, |\dot{\tilde{u}}_q|^2 \right] ,$$

namely in a form in which the new d.o.f. $\tilde{u}_q$ are not coupled with each other anymore. Note that the prefactor of $|\tilde{u}_q|^2$ is not constant but depends on q. At this point we can treat $\tilde{u}_q$ and $\dot{\tilde{u}}_q$ on the same footing as we did for p_x in the ideal gas calculation and obtain

$$\begin{aligned} K_e \left(1 - \cos q\right) \langle |\tilde{u}_q|^2 \rangle &= \frac{1}{2} k_B T \\ \frac{1}{2} m \langle |\dot{\tilde{u}}_q|^2 \rangle &= \frac{1}{2} k_B T \, . \end{aligned}$$

The first equation provides the thermal average of the Fourier amplitudes of the displacement field u_k. Knowing these quantities it is possible to determine the behavior of the averaged squared displacements of atoms in real space by inverting the Fourier transformation:

$$\langle u_k^2 \rangle = \frac{1}{N} \sum_q \langle |\tilde{u}_q|^2 \rangle = \frac{1}{N} \sum_q \frac{k_B T}{2 K_e \left(1 - \cos q\right)}$$

where in the last passage we have used the equipartition theorem. The summation on the wave-numbers q is usually evaluated taking the continuum limit

$$\frac{1}{N} \sum_q \to \frac{1}{2\pi} \int dq$$

and expanding $(1 - \cos q)$ at the denominator for small values of q:

$$\langle u_k^2 \rangle = \frac{1}{2\pi} \frac{k_B T}{K_e} \int_{q_{min}}^{q_{max}} \frac{dq}{q^2}$$

where the extremes of integration can be assumed $q_{min} = \pi/N$ (N being the number of atoms in the chain) and $q_{max} \to \infty$. Obviously, the integral above diverges for any $T \neq 0$ in the thermodynamic limit $N \to \infty$, meaning that the thermal average of square displacements diverges as well. The same calculations could be repeated for D=2 and D=3: only in the last case the

integral does not diverge. This argument is used to state that crystals cannot exist both in 1D and in 2D, because they are unstable w.r.t. thermal fluctuations. Later on we will adapt this calculation to rule out ferromagnetism at finite temperature for classical spin models with continuous symmetry, i.e., the XY and the Heisenberg model.

From the knowledge of $\langle|\tilde{u}_q|^2\rangle$ also the averaged correlation between the displacements of atoms sitting at different sites in real space can be computed:

$$\begin{aligned}\langle(u_{k+r}-u_k)^2\rangle &= \frac{2}{N}\sum_q \left[1-\cos(qr)\right]\langle|\tilde{u}_q|^2\rangle \\ &= \frac{2}{N}\sum_q \left[1-\cos(qr)\right]\frac{k_BT}{2K_e\,(1-\cos q)}\,.\end{aligned} \tag{7.3}$$

For spin models, this quantity is directly related to the behavior of the pair-spin correlation function.

Linear excitations of the XY model

Now we are ready to apply the formalism introduced in the previous section to discuss the properties of the XY model at finite temperature. One important aspect is that the Hamiltonian (7.1) is not quadratic in the d.o.f. $\varphi(\underline{n})$. However, if we limit ourselves to considering small variations of the $\varphi(\underline{n})$ angle between neighboring sites, the Hamiltonian takes the form

$$\mathcal{H} = -\frac{1}{4}J\sum_{|\underline{n}-\underline{n}'|=1}\left(\varphi(\underline{n})-\varphi(\underline{n}')\right)^2 + \text{const.} \tag{7.4}$$

Each pairs of nearest neighbors yields a contribution that can be expressed as the derivative of a continuous variable. For instance, for the coupling between two neighboring spins of a spin chain one has

$$(\varphi_{k+1}-\varphi_k)^2 \to (\partial_x\varphi)^2\ .$$

For lattices with higher dimensionality (with sites disposed along Cartesian axes) the coupling of one spin with its neighbors along different directions produces terms containing the derivatives $\partial_y\varphi$ and $\partial_z\varphi$. Therefore, the XY Hamiltonian is generally written in the continuum formalism as

$$\mathcal{H} = \frac{1}{2}J\int(\nabla\varphi)^2\,d^{\mathrm{D}}r\,. \tag{7.5}$$

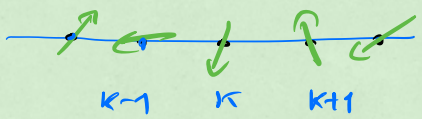
Note that in the continuum limit the factor one-half that was introduced in the Hamiltonian (7.1) to avoid double counting of interactions is not needed.

XY model : linear excitations

$$H = \frac{1}{2} J \frac{1}{2} \sum_{\substack{\underline{n}\,\underline{n}' \\ (NN)}} (\varphi(\underline{n}) - \varphi(\underline{n}'))^2 + \dots$$ LINEARIZED

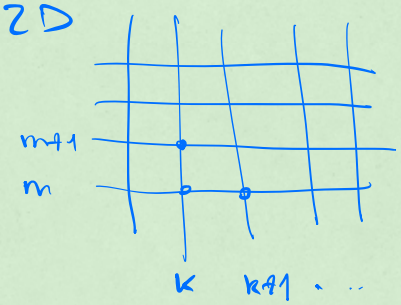
CONTINUUM LIMIT

1D



$$(\varphi_{k+1} - \varphi_k)^2 \sim (\partial_x \varphi)^2 \quad \text{where } \varphi(x)$$

2D



$$(\varphi(\underline{n}) - \varphi(\underline{n}'))^2 \sim (\nabla\varphi)^2$$

with $(\underline{n}\,\underline{n}')$ N.N. where $\varphi(x,y)$

$$\mathcal{H} = \frac{J}{2} \int (\nabla\varphi)^2 \, d^D\underline{r} + \dots$$ with $\varphi(\underline{r})$

F.T. ↓

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

$$\left\langle \frac{J}{2} q^2 |\tilde{\varphi}(q)|^2 \frac{d^D q}{(2\pi)^D} \right\rangle = \frac{k_B T}{2}$$

$$\frac{J}{2} q^2 \langle |\tilde{\varphi}(q)|^2 \rangle = \frac{k_B T}{2}$$

$$\boxed{\langle |\tilde{\varphi}(q)|^2 \rangle = \frac{kT}{J q^2}}$$

↓ Assignment: 10-week

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

xy 1D $\quad C(r) \simeq e^{-r/\xi}$

with $\xi \simeq \frac{J}{2kT}$ ⇐ linear excitations destroy FM

VS

Ising 1D $\quad C(r) \simeq e^{-r/\xi}$

with $\xi \sim \exp\left(\frac{2J}{kT}\right)$ ⇐ Domain Walls destroy FM

Fourier space

Equipartition thm

$$\frac{J}{2}\frac{1}{(2\pi)^d}\int q^2\,|\tilde{\varphi}(q)|^2\,d^dq \Rightarrow q^2\frac{J}{2}\langle|\tilde{\varphi}(q)|^2\rangle = \frac{kT}{2}$$

$\mathbb{R}$ space

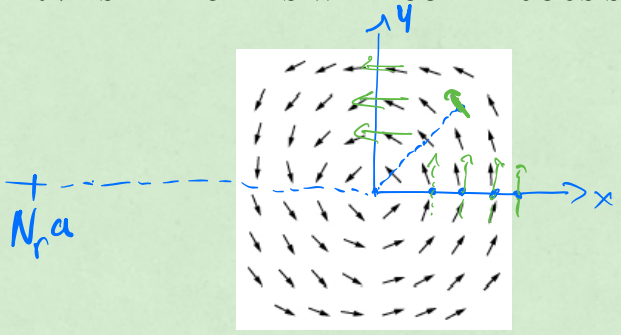
$$\frac{J}{2}\int (\nabla\varphi)^2\,d^Dr$$

$$\langle[\varphi(\underline{r})-\varphi(0)]^2\rangle_{th}$$

$$\langle\varphi^2(0)\rangle$$

$\Rightarrow$ Mermin Wagner theorem.

- applies to xy & Heisenberg model
- chain of harmonic oscillators.



spatial
$(x,y) \to (r,\phi)$
coord.

$\varphi(r,\phi) = \phi + \frac{\pi}{2}$

Figure 7.2: Sketch of a vortex excitation in the 2D XY model.

Similarly to what done for the 1D chain of harmonic oscillators, the Hamiltonian (7.5) can be decoupled passing to the Fourier space

$$\mathcal{H} = \frac{1}{2} J \frac{1}{(2\pi)^{\mathrm{D}}} \int q^2 |\tilde{\varphi}(q)|^2 \, d^{\mathrm{D}} q \tag{7.6}$$

in such a way that the *equipartition theorem* can be applied to evaluate the thermal averages of the Fourier amplitudes $\langle |\tilde{\varphi}(q)|^2 \rangle$. In the assignment, you will see that from the knowledge of this quantity the low-temperature behavior of pair-spin correlations

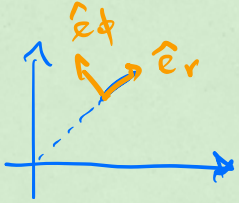
$$\langle \vec{S}(\underline{r}) \cdot \vec{S}(\underline{0}) \rangle \tag{7.7}$$

can be determined, the result being remarkably different for the 1D and the 2D case.

Vortices in the 2D XY model

Besides the linear excitations described above, the Hamiltonian (7.5) 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 $\vec{S}(r, \phi) = (\cos\varphi, \sin\varphi) = (-\sin\phi, \cos\phi)$.

$\varphi = \phi + \frac{\pi}{2} \Rightarrow H \approx \frac{J}{2} \int (\nabla\phi)^2 \, d^2 r$



Classroom activity: free energy of one vortex excitation

Q1 Provide an estimate of the vortex energy $\mathcal{E}_{\text{vortex}}$ using this information, the Hamiltonian (7.5) and remembering that

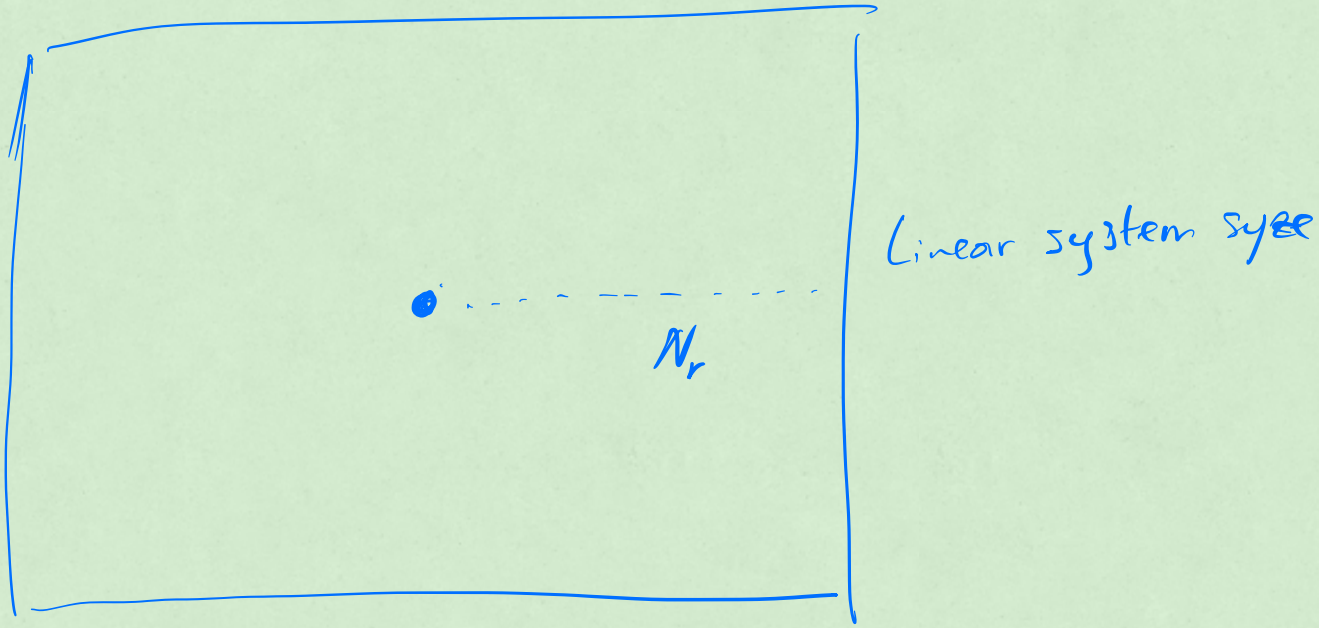
$$\nabla\varphi = \left(\frac{\partial\varphi}{\partial r}, \frac{1}{r}\frac{\partial\varphi}{\partial\phi}\right) = \left(0, \frac{1}{r}\right)$$

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

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

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

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



$$\nabla\phi = \left(0 ; \frac{1}{r}\right)$$

$$\mathcal{H} = \frac{J}{2}\int (\nabla\varphi)^2 \, d^2r = \frac{J}{2}\int_{r_{min}}^{r_{max}} \frac{1}{r^2}\, dr \int_0^{2\pi} d\phi$$

$$= \frac{J}{2}\, 2\pi \int_{r_{min}}^{r_{max}} \frac{dr}{r} = \pi J \ln\left(\frac{r_{max}}{r_{min}}\right)$$

$$\Delta E = E_{vortex} - E_{unif} = \pi J \ln\left(\frac{N_r a}{a}\right)$$

$$\simeq \pi J \ln(N_r)$$

$$S_{vortex} \sim k_B \ln(N_r^2)$$

$$\Delta F = \Delta E - S_{vortex} = \pi J \ln(N_r) - 2k_B T \ln(N_r)$$

$$= \left(\pi J - 2 k_B T\right) \ln(N_r)$$

$\Delta F > 0$ $\quad k_B T < \frac{\pi J}{2}$ $\quad$ Vortices do NOT form

$\Delta F < 0$ $\quad k_B T > \frac{\pi J}{2}$ $\quad$ Vortices form spontaneously

The formation of vortices in reality interplays with linear excitations, which for 2D case suffice to turn FM order into an algebraic decay of $C(r)$