

§2. Symmetry breaking and phase transitions

* Goldstone mode

- O(2) quantum rotor model

$$\hat{H} = \sum_j \frac{\hat{L}_j^2}{2C} - J \sum_{\langle ij \rangle} \cos(\hat{\theta}_i - \hat{\theta}_j) \quad J > 0 \\ C > 0$$

$$[\hat{\theta}_j, \hat{L}_l] = i \delta_{jl} \quad (\hbar = 1)$$

$$|\hat{\theta}| \theta\rangle = |\theta| \theta\rangle, \theta \in [0, 2\pi)$$

$\Rightarrow -J \sum_{\langle ij \rangle} \cos(\hat{\theta}_i - \hat{\theta}_j)$ favors ordered state

$|\theta_1, \theta_2, \dots\rangle$ with $\theta_1 = \theta_2 = \dots$

$$\hat{L}|m\rangle = m|m\rangle, m=0, \pm 1, \dots$$

$\Rightarrow \sum_j \frac{\hat{L}_j^2}{2C}$ favors disordered state

$|m_1=0, m_2=0, \dots\rangle$

Note that $|m=0\rangle = \int_0^{2\pi} d\theta |\theta\rangle \langle \theta | m=0 \rangle = \frac{1}{\sqrt{2\pi}} \int_0^{2\pi} d\theta |\theta\rangle$

Physics of the O(2) quantum rotor model:

- 1) competition between two terms
- 2) thermal fluctuations

Path integral formulation:

$$Z = \int D\theta(\tau) e^{-\int_0^\beta d\tau \left[\sum_j \frac{c}{2} \dot{\theta}_j^2 - J \sum_{\langle ij \rangle} \cos(\theta_i - \theta_j) \right]}$$

Starting point: perfectly ordered state

$$\theta_j(\tau) = \langle \theta \rangle \quad \text{"classical path"}$$

$$\theta_j = \langle \theta \rangle + \delta\theta_j \quad \text{"fluctuations around the classical path"}$$

$$\Rightarrow Z = \int D\delta\theta e^{-\int_0^\beta d\tau \left[\sum_j \frac{c}{2} \delta\dot{\theta}_j^2 - J \sum_{\langle ij \rangle} \cos(\delta\theta_i - \delta\theta_j) \right]}$$

assume $\delta\theta_i - \delta\theta_j$ small

$$\cos(\delta\theta_i - \delta\theta_j) \approx 1 - (\delta\theta_i - \delta\theta_j)^2 + \dots$$

(needs justification!)

$$\approx \int D\delta\theta e^{-\int_0^\beta d\tau \left[\sum_j \frac{c}{2} \delta\dot{\theta}_j^2 + \frac{J}{2} \sum_{\langle ij \rangle} (\delta\theta_i - \delta\theta_j)^2 \right]}$$

$\underbrace{\qquad\qquad\qquad}_{S_0}$

Fourier transformation:

$$\delta\theta_j(\tau) = \frac{1}{\sqrt{\beta N}} \sum_{\vec{k}, i\omega_n} e^{i\vec{k} \cdot \vec{R}_j - i\omega_n \tau} \Theta(\vec{k}, i\omega_n)$$

Bosonic Matsubara frequency

$$\omega_n = \frac{2\pi n}{\beta}, \quad n = 0, \pm 1, \dots$$

$$\Theta(\vec{k}, i\omega_n) = \Theta^*(-\vec{k}, -i\omega_n),$$

since $\delta\theta_j(\tau)$ is real

\vec{k} point in the first Brillouin zone (FBZ)

$$k_l \in (-\frac{\pi}{a}, \frac{\pi}{a}]$$

$$l = 1, 2, \dots, d \quad a: \text{lattice spacing}$$

Two terms in the action.

$$\int_0^\beta d\tau \sum_j \frac{c}{2} \delta \dot{\theta}_j(\tau)^2 = \int_0^\beta d\tau \sum_j \frac{c}{2} \frac{1}{\beta N} \sum_{\vec{k}, i w_n} \sum_{\vec{k}', i w_n'} e^{i(\vec{k} + \vec{k}') \cdot \vec{R}_j}$$

$$\times e^{-i(w_n + w_n')\tau} (-i w_n) (-i w_n') \Theta(\vec{k}, i w_n) \Theta(\vec{k}', i w_n)$$

$$= \sum_{\vec{k}, i w_n} \frac{c}{2} w_n^2 \Theta(\vec{k}, i w_n) \Theta(-\vec{k}, -i w_n)$$

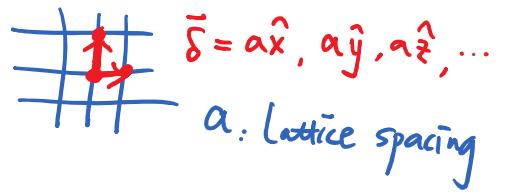
$$\left\{ \begin{array}{l} \frac{1}{\beta} \int_0^\beta d\tau e^{i(w_n - w_m)\tau} = \delta_{w_n, w_m} \\ \frac{1}{N} \sum_j e^{i(\vec{k} - \vec{k}') \cdot \vec{R}_j} = \delta_{\vec{k}, \vec{k}'} \end{array} \right.$$

$$\int_0^\beta d\tau \frac{J}{2} \sum_{\langle i,j \rangle} (\delta \theta_i - \delta \theta_j)^2 = \int_0^\beta d\tau \frac{J}{2} \sum_{\langle i,j \rangle} (\delta \theta_i^2 + \delta \theta_j^2 - 2 \delta \theta_i \delta \theta_j)$$

$$= \int_0^\beta d\tau \left[J d \sum_j \delta \theta_j^2 - J \sum_j \sum_{\vec{s}} \delta \theta_j \delta \theta_{j+\vec{s}} \right]$$

spatial dimensions

count neighbors:



$$= \int_0^\beta d\tau \left[J d \sum_j \frac{1}{\beta N} \sum_{\substack{\vec{k}, i w_n \\ \vec{k}', i w_n'}} e^{i(\vec{k} + \vec{k}') \cdot \vec{R}_j - i(w_n + w_n')\tau} \Theta(\vec{k}, i w_n) \Theta(\vec{k}', i w_n') \right]$$

$$- J \sum_j \sum_{\vec{s}} \frac{1}{\beta N} \sum_{\substack{\vec{k}, i w_n \\ \vec{k}', i w_n'}} e^{i(\vec{k} + \vec{k}') \cdot \vec{R}_j - i(w_n + w_n')\tau + i \vec{k} \cdot \vec{s}} \Theta(\vec{k}, i w_n) \Theta(\vec{k}', i w_n')$$

$$= \sum_{\vec{k}, i w_n} \left(J d - J \sum_{\vec{s}} e^{i \vec{k} \cdot \vec{s}} \right) \Theta(\vec{k}, i w_n) \Theta(-\vec{k}, -i w_n)$$

$$\sum_{\ell=1}^d \cos(k_\ell a) \quad (\text{use the symmetry of } \vec{k} \leftrightarrow -\vec{k})$$

$$= \sum_{\vec{k}, i w_n} J \sum_{\ell=1}^d \left[1 - \cos(k_\ell a) \right] \Theta(\vec{k}, i w_n) \Theta(-\vec{k}, -i w_n)$$

The partition function becomes

$$Z = \int \prod_{\vec{k}, i\omega_n} d\Omega(\vec{k}, i\omega_n) e^{-S_0}$$

$$S_0 = \sum_{\vec{k}, i\omega_n} \left\{ \frac{C}{2} \omega_n^2 + J \sum_{\ell=1}^d [1 - \cos(k_\ell a)] \right\} \Omega(\vec{k}, i\omega_n) \Omega(-\vec{k}, -i\omega_n)$$

This describes a set of harmonic oscillators !

$$\begin{aligned} Z &= \int D\chi(t) e^{-\int_0^t dt' \left[\frac{1}{2} m \dot{\chi}(t')^2 + \frac{1}{2} m \omega^2 \chi(t')^2 \right]} \\ &\quad \downarrow \chi(t) = \frac{1}{\sqrt{N}} \sum_{i\omega_n} e^{-i\omega_n t} \chi(i\omega_n) \\ &= \int \prod_{i\omega_n} \chi(i\omega_n) e^{-\sum_{i\omega_n} \frac{1}{2} m (\omega_n^2 + \omega^2) \chi(i\omega_n) \chi(-i\omega_n)} \\ &\quad \downarrow \text{frequency} \end{aligned}$$

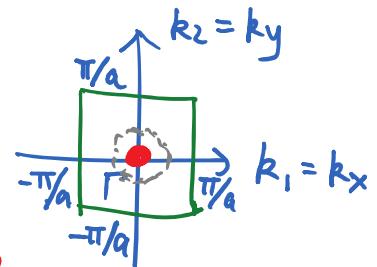
Hamiltonian formulation: $\hat{H} = \hbar \omega \hat{a}^\dagger \hat{a}$

For our problem, each \vec{k} point has an associated harmonic oscillator with frequency

$$\omega_{\vec{k}}^2 = \frac{2J}{C} \sum_{\ell=1}^d [1 - \cos(k_\ell a)]$$

Consider small \vec{k} (close to P point):

$$\omega_{\vec{k}}^2 \simeq \frac{J}{C} \sum_{\ell=1}^d (k_\ell a)^2 = \frac{Ja^2}{C} |\vec{k}|^2 \rightarrow 0 \quad \text{for } |\vec{k}| \rightarrow 0$$

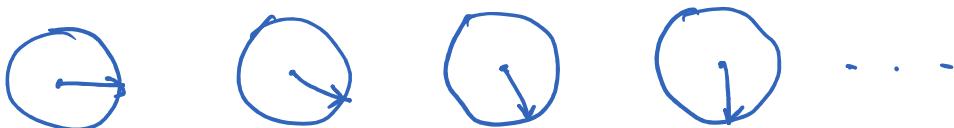


Gapless bosonic excitations !

Acoustic mode with linear dispersion:

$$\omega_{\vec{k}} = v_s |\vec{k}|$$

velocity $v_s = \sqrt{\frac{Ja^2}{c}}$



Small $\theta_i - \theta_j$ costs small energies $\sim O(1/L)$

\uparrow
System size

This is due to the infinite number of degenerate ground states, which are connected to each other by $O(2)$ rotations.

symmetry of the Hamiltonian

Goldstone mode tries to "restore" the broken symmetry!

\hookrightarrow doesn't show up if there are only discrete symmetries.
(e.g. Z_2 in Ising models)

Goldstone theorem:

broken of continuous symmetry \Rightarrow gapless Goldstone bosons

Examples: translation symmetry \Rightarrow acoustic phonon
spin-rotational symmetry \Rightarrow magnon

Refined version:

For "relativistic theories" (linear dispersion $\omega_{\vec{k}} \sim v_s |\vec{k}|$)

↑ ↑
Lorentz symmetry "speed of light"

Symmetry of the Hamiltonian: G

Symmetry of the ground state: H

Number (#) of Goldstone bosons

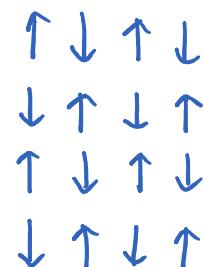
= # of generators of G

- # of generators of H

Example: Magnons in quantum antiferromagnets

$$G = SU(2)$$

$$H = U(1)$$



$$\# \text{ of magnons} = 3 - 1 = 2$$

$$\hat{S}_x, \hat{S}_y, \hat{S}_z$$

Note that this doesn't work for $SU(2)$ spin-1 ferromagnets which have a single branch of magnon with quadratic dispersion $\omega_{\vec{k}} \propto |\vec{k}|^2$, since it is "nonrelativistic".

* Mermin-Wagner theorem

Thermal fluctuations ($T > 0$)

Quantum fluctuations ($T = 0$)

zero-point motion of Goldstone bosons

Q: Does the long-range order survive?

In other word: Is the symmetry really broken?

How to quantify?

order parameter & correlation functions

Path integral formulation:

$$\langle \cos \hat{\theta}_j \rangle = \frac{1}{Z} \text{Tr}(e^{-\beta \hat{H}} \cos \hat{\theta}_j)$$

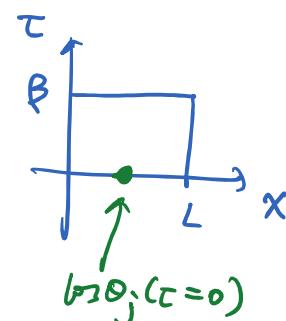
$$= \frac{1}{Z} \int \prod_{k=0}^{N-1} d\theta_k \langle \theta_0 | e^{-\beta \hat{H}} | \theta_{N-1} \rangle \cdots \langle \theta_1 | e^{-\beta \hat{H}} \underbrace{\cos \hat{\theta}_j}_{\parallel} | \theta_0 \rangle$$

$$= \frac{1}{Z} \int D\theta(\tau) \underbrace{\cos \theta_j(\tau=0)}_{-\tilde{S}[\theta]} e^{-\tilde{S}[\theta]}$$

$$\cos \theta_{k=0,j} | \theta_0 \rangle$$

In fact, $\tau=0$ can be replaced

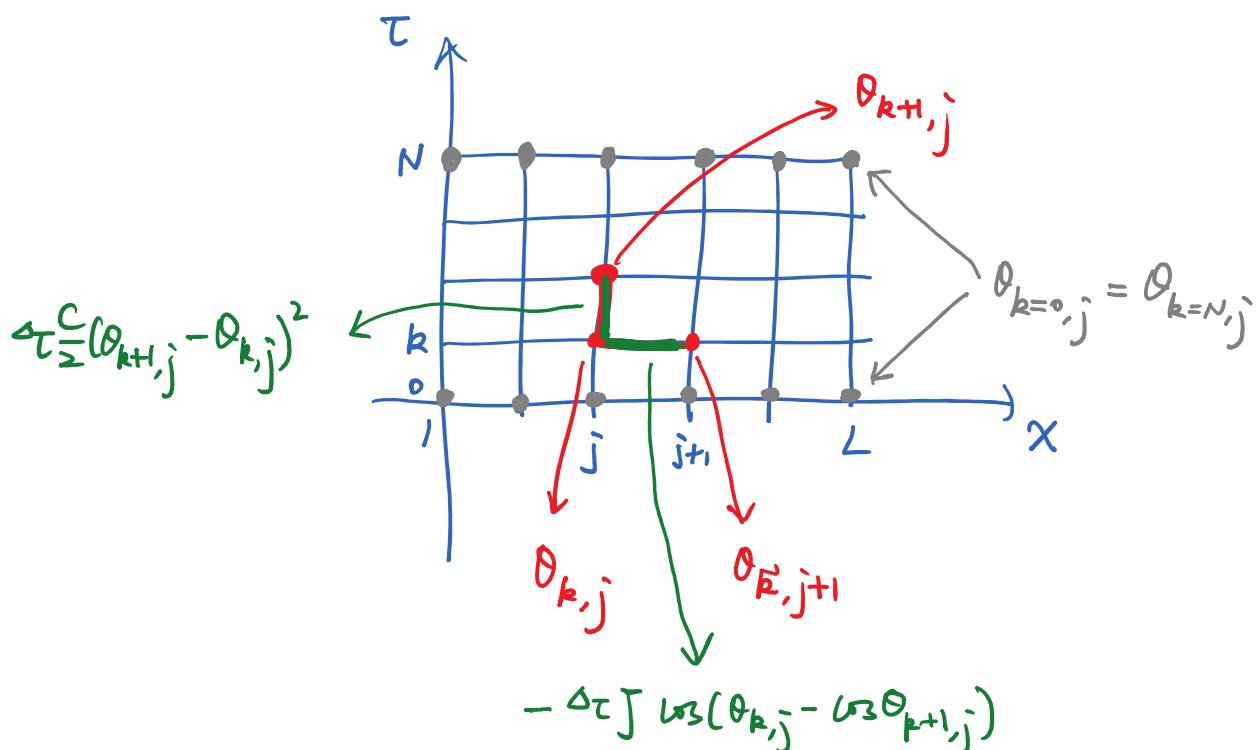
by other τ due to translation invariance
in imaginary-time direction.



Side remark: World-line Monte Carlo simulation

Example: $d=1$ $O(2)$ quantum rotor model

$$\begin{aligned} Z &= \int D\theta(\tau) e^{-\int_0^{\beta} d\tau \left[\frac{C}{2} \sum_j \dot{\theta}_j^2(\tau) - J \sum_{\langle i,j \rangle} \cos(\theta_i - \theta_j) \right]} \\ &= \lim_{\substack{\Delta\tau \rightarrow 0 \\ (N \rightarrow \infty)}} \int \prod_{k=0}^{N-1} \prod_{j=1}^L d\theta_{k,j} \xrightarrow{\text{label for the imaginary time}} \\ &\times e^{-\Delta\tau \left[\frac{C}{2} \sum_{k=0}^{N-1} \sum_{j=1}^L (\theta_{k+1,j} - \theta_{k,j})^2 - J \sum_{k=0}^{N-1} \sum_{\langle i,j \rangle} \cos(\theta_{k,i} - \theta_{k,j}) \right]} \\ &\quad \xrightarrow{\text{coupling along}} \quad \xrightarrow{\text{coupling along}} \\ &\quad \text{imaginary-time direction} \quad \text{spatial direction} \end{aligned}$$



\Rightarrow (1+1)-dimensional classical partition function
with positive Boltzmann weight $e^{-\tilde{H}(\{\theta\})}$!

$$Z = \int \prod_{k,j} d\theta_{k,j} e^{-\tilde{H}(\{\theta\})}$$

$$\langle \cos \theta_j \rangle = \frac{\int \prod_{k,j} d\theta_{k,j} \cos \theta_{k=0,j} e^{-\tilde{H}(\{\theta\})}}{\int \prod_{k,j} d\theta_{k,j} e^{-\tilde{H}(\{\theta\})}}$$

↑

perfect form for Monte-Carlo samplings!

(No "sign problem" in this case)