4. Frustrated Quantum Antiferromagnets

4.1. Hamiltonian, Classical ground States and Linear Spin-Wave Theory

- The $J_1 - J_2$ Heisenberg model on a d-dim. hypercubic lattice

$$\hat{H} = J_1 \sum_{\langle ij \rangle} \hat{S}_i \hat{S}_j + J_2 \sum_{\langle\langle ij \rangle\rangle} \hat{S}_i \hat{S}_j$$

– $J_1, J_2 > 0$ (antiferromagnetic couplings)
– $\langle .,. \rangle$ Nearest-Neighbor (NN)
  $\langle\langle .,. \rangle\rangle$ Next-Nearest Neighbor (NNN) bonds

- $\hat{S}_i = (\hat{S}_i^x, \hat{S}_i^y, \hat{S}_i^z)$ spin operators, total spin $S = 1/2, 1, 3/2, \ldots$

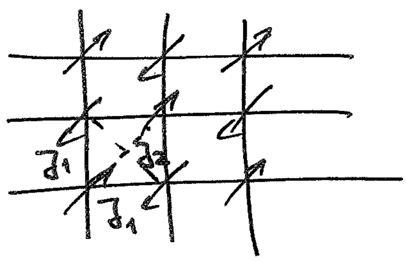
commutator relations: $[\hat{S}_i^\alpha, \hat{S}_j^\beta] = i\hbar \delta_{ij} \epsilon_{\alpha\beta\gamma} \hat{S}_i^\gamma$

$\epsilon_{\alpha\beta\gamma}$ antisymmetric tensor, $\epsilon_{xyz} = \epsilon_{zxy} = \epsilon_{yzx} = 1$

$\epsilon_{yxz} = \epsilon_{zyx} = \epsilon_{xzy} = -1$

all other elements are zero

- The system is frustrated, we cannot make NN and NNN bonds happy



ground state for small J_2

dimensionless parameter controlling the frustration:

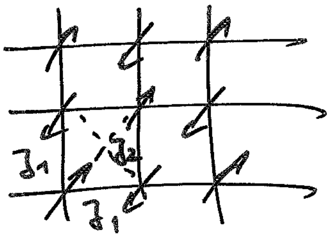
$$\boxed{\gamma = J_2 / J_1}$$

- Classical groundstates:

Look at limiting cases:

$\gamma = J_2/J_1 \ll 1$:

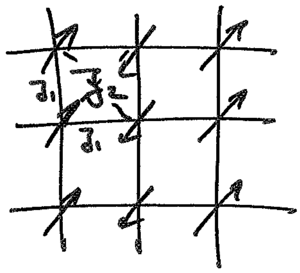
groundstate is the Neel antiferromagnet



NN bonds happy
NNN bonds unhappy

$\gamma = J_2/J_1 \gg 1$:

we should make the NNN bond happy



one NN bond is unhappy

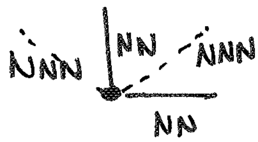
columnar antiferromagnet

ordering wave vector: $\vec{S}_i = S(0,0,e^{i\underline{Q}\,\underline{r}_i})$

$\underline{Q} = (\pi,\pi)$ $\qquad\qquad$ $\underline{Q} = (\pi, 0)$

- Comparison of energies of the two classical spin states

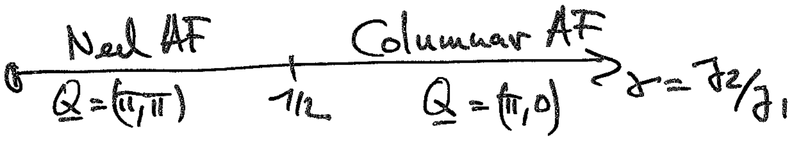
→ for every site, we have to count 2 NN and 2 NNN bonds



→ $E_{(\pi,\pi)} = -2J_1 + 2J_2$ $\qquad\qquad$ $E_{(\pi,0)} = -J_1 + J_1 - 2J_2 = -2J_2$

change of groundstate for $E_{(\pi,\pi)} = E_{(\pi,0)} \Leftrightarrow -2J_1 + 2J_2 = -2J_2$

$\Leftrightarrow \boxed{\gamma = J_2/J_1 = 1/2}$



- Quantum fluctuations are expected to induce paramagnetic state around $\gamma = 1/2$

- Classical limit corresponds to $S \to \infty$. Quantum fluctuations to lowest order in $1/S$ are captured in <u>linear spin-wave theory</u> (LSWT)

- classical ground state: $\vec{S}_i = S(0,0,\sigma_i)$, $\sigma_i = e^{i\underline{Q}\,\underline{r}_i} = \begin{cases} +1 & i \in A \\ -1 & i \in B \end{cases}$

  two sublattices A and $\underline{B}$:

$$\begin{array}{ccc} + & - & + \\ - & + & - \\ + & - & + \end{array} \qquad\qquad \begin{array}{ccc} + & - & + \\ + & - & + \\ + & - & + \end{array}$$

Neel AF $\qquad\qquad$ columnar AF

- Perform <u>spin rotation</u>:

$$\hat{S}_i^x = \hat{\tilde{S}}_i^x \,, \quad \hat{S}_i^y = \sigma_i \hat{\tilde{S}}_i^y \,, \quad \hat{S}_i^z = \sigma_i \hat{\tilde{S}}_i^z$$

- Transformation rotates all spins on sublattice B,
- Rotation preserves spin commutator relations
- In the rotated basis, the classical ground state is given by $\vec{\tilde{S}} = S(0,0,1)$

- Hamiltonian in the rotated spin basis

$$\begin{aligned} \hat{S}_i \hat{S}_j &= \hat{\tilde{S}}_i^x \hat{\tilde{S}}_j^x + \sigma_i \sigma_j \hat{\tilde{S}}_i^y \hat{\tilde{S}}_j^y + \sigma_i \sigma_j \hat{\tilde{S}}_i^z \hat{\tilde{S}}_j^z \\ &= \frac{1+\sigma_i\sigma_j}{4} \left(\hat{\tilde{S}}_i^+ \hat{\tilde{S}}_j^- + \hat{\tilde{S}}_i^- \hat{\tilde{S}}_j^+ \right) \\ &\quad + \frac{1-\sigma_i\sigma_j}{4} \left(\hat{\tilde{S}}_i^+ \hat{\tilde{S}}_j^+ + \hat{\tilde{S}}_i^- \hat{\tilde{S}}_j^- \right) \\ &\quad + \sigma_i \sigma_j \hat{\tilde{S}}_i^z \hat{\tilde{S}}_j^z \end{aligned}$$

where we have used that $\hat{\tilde{S}}_i^\pm = \hat{\tilde{S}}_i^x \pm i \hat{\tilde{S}}_i^y$

- Express the spin operators by Holstein - Primakoff (HP) bosons :

$$\boxed{\begin{aligned} \hat{\tilde{S}}_i^{+} &= \sqrt{2S - \hat{n}_i}\; b_i \\ \hat{\tilde{S}}_i^{-} &= b_i^{+} \sqrt{2S - \hat{n}_i} \\ \hat{\tilde{S}}_i^{z} &= S - \hat{n}_i \end{aligned}} \qquad \hat{n}_i = b_i^{+} b_i$$

Since $\hat{\tilde{S}}^z |S, m_S\rangle = m_S |S, m_S\rangle$ with $m_S = -S, -S+1, \dots, S-1, S$, we have to truncate ($\hbar = 1$) the bosonic Hilbertspace

- For large S, we can treat the HP bosons as conventional bosons and approximate the transformation by

$$\hat{\tilde{S}}_i^{+} = \sqrt{2S}\, b_i \qquad \hat{\tilde{S}}_i^{z} = S - b_i^{+} b_i$$
$$\hat{\tilde{S}}_i^{-} = \sqrt{2S}\, b_i^{+}$$

$$\rightarrow \hat{S}_i \hat{S}_j = S \frac{1+\sigma_i \sigma_j}{2} (b_i^{+} b_j + b_i b_j^{+}) + S \frac{1-\sigma_i\sigma_j}{2} (b_i^{+} b_j^{+} + b_i b_j)$$
$$+ \underbrace{\sigma_i \sigma_j S^2}_{\rightarrow \text{ classical energy}} - S \sigma_i \sigma_j (b_i^{+} b_i + b_j^{+} b_j) + \text{quartic term}$$

- The linear - spin wave Hamiltonian is given by the terms quadratic in the bosonic operators. For the Néel antiferromagnet :

$$\boxed{\frac{\hat{H}_{SW}^{(\pi,\pi)}}{S}} = J_1 \sum_{\langle ij \rangle} \left(b_i^{+} b_j^{+} + b_i b_j + b_i^{+} b_i + b_j^{+} b_j \right)$$
$$+ J_2 \sum_{\langle\langle ij \rangle\rangle} \left(b_i^{+} b_j + b_i b_j^{+} - b_i^{+} b_i - b_j^{+} b_j \right)$$

$$\underset{b_i^{+} = \int_q e^{i q r_i} b_q^{+}}{=} \boxed{\int_q \left\{ A_q^{(\pi,\pi)} (b_q^{+} b_q + b_{-q} b_{-q}^{+}) + B_q^{(\pi,\pi)} (b_q^{+} b_{-q}^{+} + b_{-q} b_q) \right\}}$$

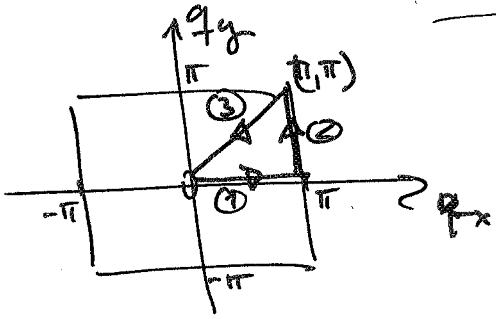
$$\boxed{\begin{aligned} A_q^{(\pi,\pi)} &= 2J_1 - 2J_2(1-\cos q_x \cos q_y) \\ B_q^{(\pi,\pi)} &= J_1(\cos q_x + \cos q_y) \end{aligned}}$$

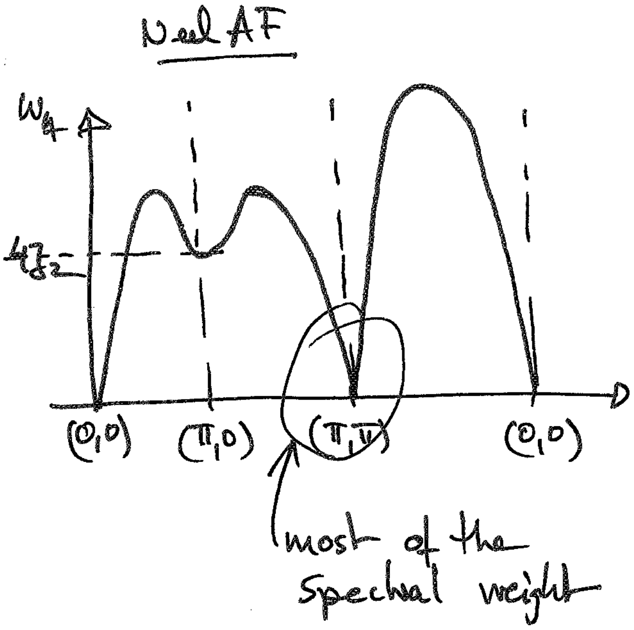
- For $\underline{Q}=(\pi,0)$ in the columnar antiferromagnet, the form factors are given by

$$\boxed{\begin{aligned} A_q^{(\pi,0)} &= J_1 \cos q_y + 2J_2 \\ B_q^{(\pi,0)} &= J_1 \cos q_x + 2J_2 \cos q_x \cos q_y \end{aligned}}$$

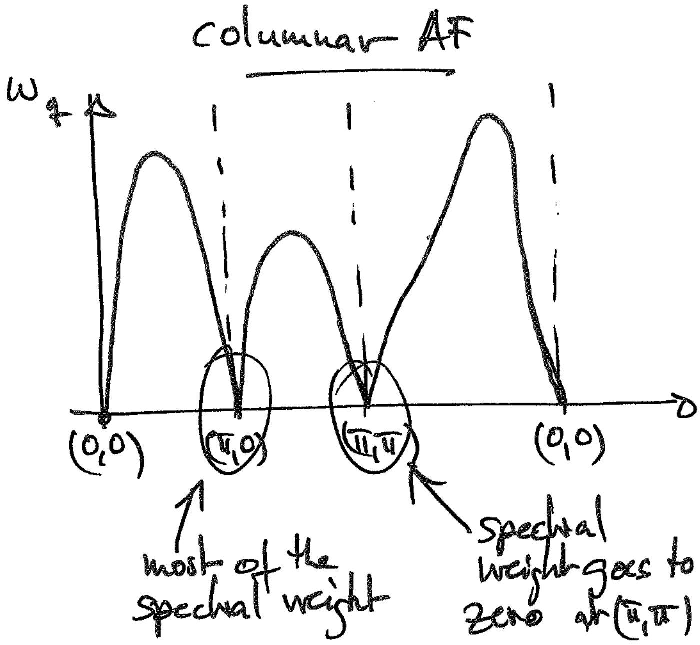
- We can diagonalize the spin-wave Hamiltonian by a Bogoliubov transformation

$$\to \quad H_{SW} = \int_q \omega_q \gamma_q^+ \gamma_q \quad \text{with} \quad \boxed{\omega_q = \sqrt{A_q^2 - B_q^2}}$$





Minimum at $(\pi,0)$ comes down as we increase $\gamma = J_2/J_1$



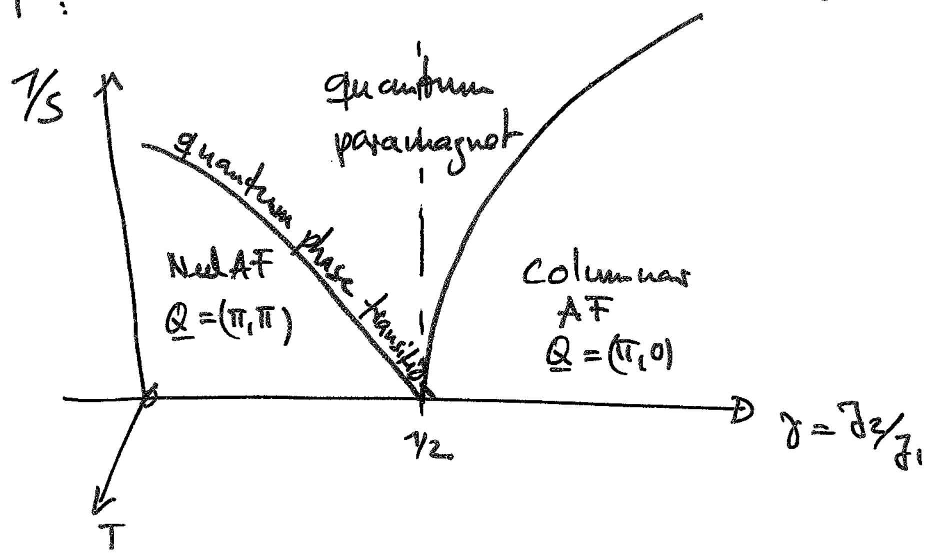
- How to estimate when quantum fluctuations destroy the different magnetic orders?
  - → For both phases calculate the staggered magnetization in the linear spin-wave approximation

$$m = \frac{1}{N}\sum_i \langle \hat{S}_i^z \rangle = S - \frac{1}{N}\sum_i \langle b_i^\dagger b_i \rangle = S - \int_{q \in BZ} \langle b_q^\dagger b_q \rangle$$

(Brilloin zone)

  - → Evaluate $\langle b_q^\dagger b_q \rangle$ by transforming to the new operator basis $\gamma_q^\dagger, \gamma_q$ in which H_{SW} is diagonal
  - → Calculate the resulting integral over $\underline{q} \in BZ$
  - → Phase transitions determined by the points where staggered magnetization vanishes

- Resulting zero-temperature phase diagram in LSWT:

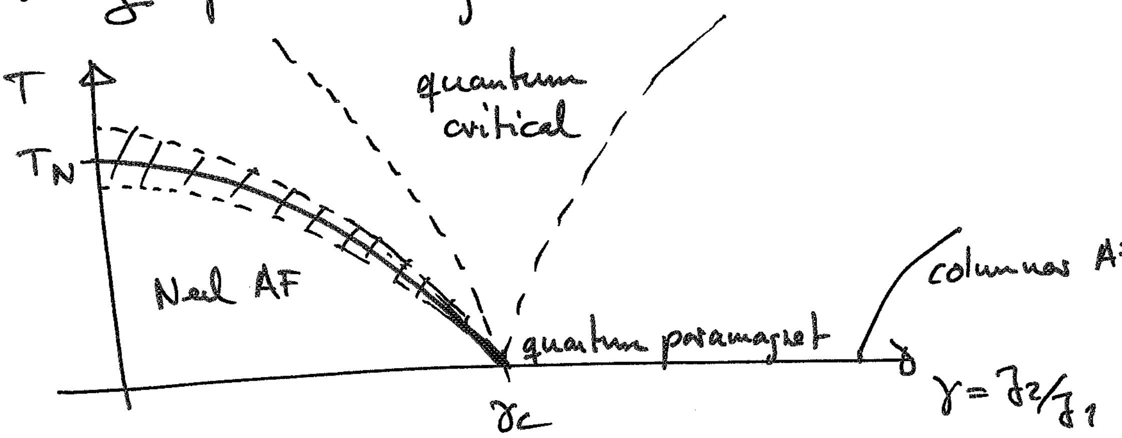


4.2. Classical Non-Linear Sigma Model

- We are interested in the nature of the transition from the Neel ordered phase to the quantum paramagnet
- Order parameter for the Neel ordered phase is the staggered magnetization $m = \langle \sigma_i \hat{S}_i^z \rangle = \langle \hat{S}_i^z \rangle$

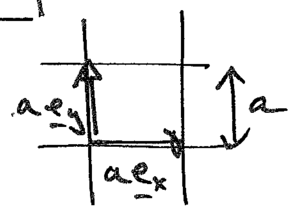
$$\langle \hat{\tilde{S}}^z(\underline{r})\, \hat{S}^z(0) \rangle \underset{|\underline{r}| \to \infty}{\sim} \begin{cases} m^2 & \text{Neel AF} \\ e^{-r/\xi} & \text{paramagnet} \end{cases}$$

- Long-range magnetic order can be destroyed by thermal or quantum fluctuations. We expect the following phase diagram



- In the introduction we have learned that sufficiently close to the thermal transition (shaded region) quantum fluctuations are irrelevant for the nature of the transition
- Therefore we first look at the <u>classical $J_1 - J_2$ model</u>
- Treat spins as <u>classical vectors</u>, introduce <u>staggered field</u>:

$$\boxed{\vec S_i = S \cdot \begin{cases} \vec n_i & i \in A \\ -\vec n_i & i \in B \end{cases}} \qquad \vec n_i \text{ unit vector } \boxed{\vec n_i^{\,2} = 1}$$



$$\mathcal{H} = -J_1 S^2 \sum_{\langle ij\rangle} \vec n_i \vec n_j + J_2 S^2 \sum_{\langle\langle ij\rangle\rangle} \vec n_i \vec n_j$$

$$= -\frac{J_1 S^2}{2} \sum_{\underline r} \vec n(\underline r) \Bigg[\sum_{\substack{\alpha = 1,\dots,d \\ \lambda = \pm 1}} \vec n(\underline r + \lambda a \underline e_\alpha) - \gamma \sum_{\substack{\alpha\beta \\ \lambda\lambda'}}^{(\alpha\neq\beta)} \vec n(\underline r + \lambda a \underline e_\alpha + \lambda' a \underline e_\beta) \Bigg]$$

$$= \frac{J_1 S^2}{4} \sum_{\underline r} \Bigg\{ \sum_{\alpha\lambda} \left[\vec n(\underline r) - \vec n(\underline r + \lambda a \underline e_\alpha)\right]^2 - \gamma \sum_{\substack{\alpha\beta \\ \lambda\lambda'}}^{(\alpha\neq\beta)} \left[\vec n(\underline r) - \vec n(\underline r + \lambda a \underline e_\alpha + \lambda' a \underline e_\beta)\right]^2 \Bigg\}$$

$$\xrightarrow{a\to 0} \frac{J_1 S^2}{4} a^{-d} \int d^d r \left\{ \sum_{\alpha\lambda} (\lambda a \partial_\alpha \vec{n})^2 - \gamma \sum_{\substack{\alpha\beta \\ \lambda\lambda'}}^{(\alpha\neq\beta)} (\lambda a \partial_\alpha \vec{n} + \lambda' a \partial_\beta \vec{n})^2 \right\}$$

$$= \frac{J_1 S^2}{4} a^{2-d} \int d^d r \left\{ 2(\nabla\vec{n})^2 - 2\gamma \underbrace{\sum_{\alpha\beta}^{(\alpha\neq\beta)} \left[(\partial_\alpha \vec{n})^2 + (\partial_\beta \vec{n})^2\right]}_{= 2(d-1)(\nabla\vec{n})^2} \right\}$$

$$= \underbrace{\frac{J_1 S^2}{2} a^{2-d} (1 - 2(d-1)\gamma)}_{=:\ \rho_s/2} \int d^d r \, (\nabla\vec{n})^2$$

ρ_s : spin stiffness

$$\boxed{Z = \int \mathcal{D}\vec{n} \; \delta(\vec{n}^2 - 1) \; e^{-\beta \rho_s/2 \int d^d r \, (\nabla\vec{n})^2}}$$

d-dim. non-linear sigma model (NLσM)

- We can generalize to an N-component vector field $\vec{n}(\underline{r})$ with $\vec{n}^2 = 1$.
- For J_1-J_2 Heisenberg model : $N = 3$
- Stiffness ρ_s can be tuned by $\gamma = J_2/J_1$ ($\rho_s \sim [1 - 2(d-1)\gamma]$)
- Action looks trivial (quadratic, just $(\nabla\vec{n})^2$ describing wave-like excitations)
- Non trivial problem because of constraint $\vec{n}^2(\underline{r}) = 1$
  $\rightarrow$ non linearity !

- The constraint allows us to express one component of the vector field $\vec{n}(\underline{r})$ by the other components

$$\boxed{\underbrace{\vec{n}(\underline{r})}_{N\text{-component vector}} = (\underbrace{\vec{\pi}(\underline{r})}_{(N-1)\text{-component vector}}, \sigma(\underline{r}))}$$

$\vec{n}^2(\underline{r}) = 1$

$$\Rightarrow \boxed{\vec{\pi}^2(\underline{r}) + \sigma^2(\underline{r}) = 1}$$

$$Z = \underbrace{\int \mathcal{D}\vec{n}}_{=\prod_{\underline{r}} \int d^N \vec{n}(r)} \underbrace{\delta(\vec{n}^2 - 1)}_{=\prod_{\underline{r}} \delta(\vec{n}^2(r) - 1)} e^{-\frac{1}{2t}\int d^d r\, (\nabla \vec{n})^2}$$

$\boxed{t := T/\rho_s}$ dimensionless temperature

$$= \int \mathcal{D}\vec{\pi} \int \mathcal{D}\sigma\, \delta(\sigma^2 + \vec{\pi}^2 - 1)\, e^{-\frac{1}{2t}\int d^d r \{(\nabla\vec{\pi})^2 + (\nabla\sigma)^2\}}$$

$$\overset{(*)}{=} \int \mathcal{D}\vec{\pi} \prod_{\underline{r}} \frac{1}{\sqrt{1-\vec{\pi}^2(\underline{r})}}\, e^{-\frac{1}{2t}\int d^d r \{(\nabla\vec{\pi})^2 + (\nabla\sqrt{1-\vec{\pi}^2})^2\}}$$

$$= \int \mathcal{D}\vec{\pi}\, e^{-\frac{1}{2t}\int d^d r \left\{ (\nabla\vec{\pi})^2 + \frac{(\vec{\pi}\nabla\vec{\pi})^2}{1-\vec{\pi}^2} + t \ln(1-\vec{\pi}^2) \right\}}$$

$$\left((*) \int dx\, \delta(x^2-a) f(x) = \int \frac{dz}{\sqrt{z}} \delta(z-a) f(\sqrt{z}) = f(\sqrt{a})/\sqrt{a} \right)$$

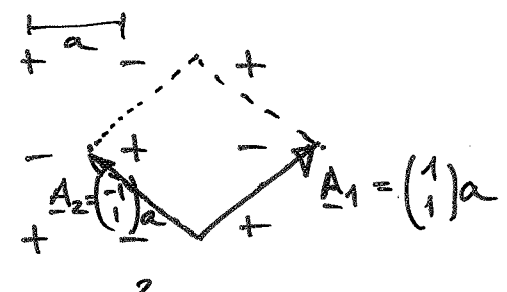
- Action $S[\vec{\pi}] = \frac{1}{2t}\int d^d r \left\{ (\nabla\vec{\pi})^2 + \frac{(\vec{\pi}\nabla\vec{\pi})^2}{1-\vec{\pi}^2} + t \ln(1-\vec{\pi}^2) \right\}$

contains <u>nontrivial vertex corrections</u>. They arrise from the constraint $\vec{n}^2 = 1$ in the non-linear sigma model.

- <u>Momentum cut-off Λ</u> :

- On the lattice, the volume of the unit cell is given by $V = 2a^d$ where the factor 2 comes from the fact that we have to include 2 spins (from sublattice A and B) in the unit cell

<u>e.g. in $d=2$</u>

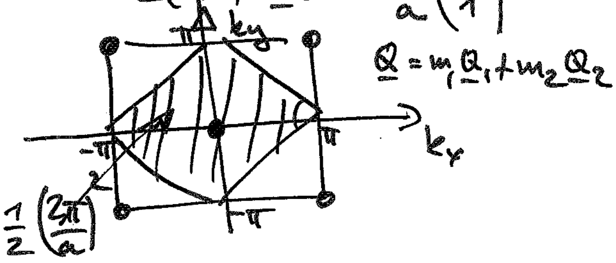


$V = \sqrt{2}^2 a^2 = 2a^2$

<u>in momentum space</u>

reciprocal lattice vectors defined by $\boxed{\underline{Q}_i \underline{A}_j = 2\pi \delta_{ij}}$

$\underline{Q}_1 = \frac{\pi}{a}\begin{pmatrix}1\\1\end{pmatrix}$, $\underline{Q}_2 = +\frac{\pi}{a}\begin{pmatrix}-1\\1\end{pmatrix}$

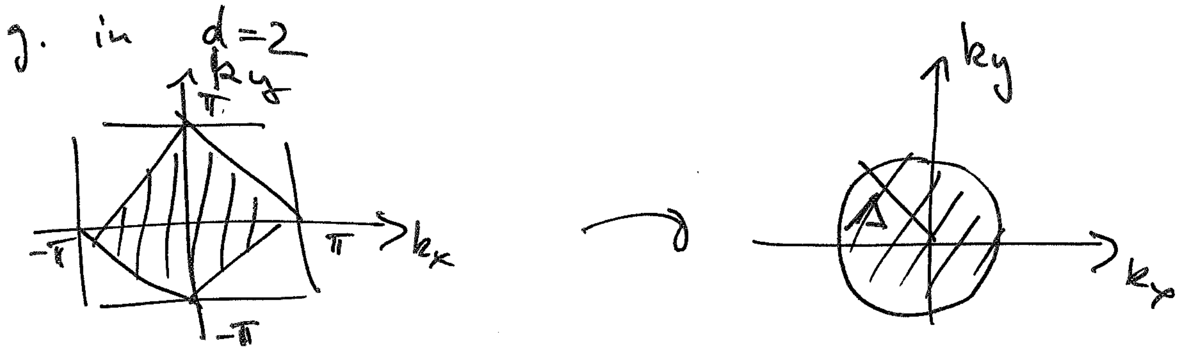


$\tilde{V} = \frac{1}{2}\left(\frac{2\pi}{a}\right)^2$

- In d dimensions, the volume of the magnetic Brillouin zone is $\boxed{\tilde{V} = \frac{1}{2}\left(\frac{2\pi}{a}\right)^d}$

- In the continuum theory, we should replace the hypercubic Brillouin zone by a sphere with radius Λ

e.g. in $d=2$



- Sometimes, Λ is determined by the condition that the volume of the Brillouin zone remains the same

$$\tilde{V} = \frac{1}{2}\left(\frac{2\pi}{a}\right)^d = K_d \Lambda^d \quad , \; K_d \text{ volume of } d\text{-dim. unit sphere}$$

$$\rightarrow \boxed{\Lambda = \frac{2}{\sqrt[d]{2K_d}} \frac{\pi}{a}}$$

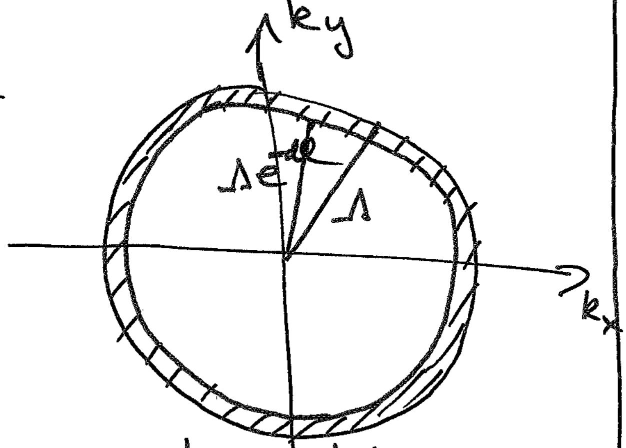
- Momentum cut-off corresponds to a small distance cut-off $\sim a \sim \frac{1}{\Lambda}$ in real space:

Coarse grained continuum theory is valid on scales larger than the lattice scale

4.3. Renormalization group of the classical model

General idea:

Eliminate an infinitesimal fraction of modes corresponding to the highest energies



momentum shell of thickness Λdl:
$\Lambda e^{-dl} \leq |\underline{k}| \leq \Lambda$

$\Downarrow$

Rescale momenta $\underline{k} \to \underline{k}\, e^{dl}$ that we end up with the original momentum cut-off Λ

$\Downarrow$

If the theory is renormalizable, the action S will have exactly the same functional form as before.

→ Identify renormalized coupling constants $g_1, \ldots, g_n$ (coefficients in the action)

$$\boxed{g_i(l+dl) = g_i(l) + dl \cdot F_i(g_1(l), \ldots, g_n(l))}$$

- We will obtain a set of coupled differential equations (RG flow equations) which describes the scale dependence of the coupling constants.
- In the following, we will explicitly derive the RG equations for the classical non-linear sigma model

$$Z = \int \mathcal{D}\vec{n}\; \delta(\vec{n}^2 - 1)\, e^{-S}$$

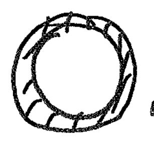
$$S = \frac{1}{2t} \int d^d r\; (\nabla \vec{n})^2$$

- One approach is based on the decomposition $\vec{n} = (\vec{\pi}, \sigma)$. The σ component is eliminated by using the constraint $\vec{\pi}^2 + \sigma^2 = 1$ leading to an action $S[\vec{\pi}]$ as discussed in the previous section
- As a next step, one decomposes the $\vec{\pi}$ field into a „slow" and a „fast" component:

$$\vec{\pi}(\underline{r}) = \int_{|\underline{k}| \le \Lambda} e^{i\underline{k}\underline{r}}\; \vec{\pi}(\underline{k})$$

$$= \int_{|\underline{k}| \le \Lambda e^{-dl}} e^{i\underline{k}\underline{r}}\; \vec{\pi}(\underline{k}) \;+\; \int_{\Lambda e^{-dl} \le |\underline{k}| \le \Lambda} e^{i\underline{k}\underline{r}}\; \vec{\pi}(\underline{k})$$


„slow"


„fast"

$$= \vec{\pi}_<(\underline{r}) \;+\; \vec{\pi}_>(\underline{r})$$

- We then take the trace over the fields $\vec{\pi}_>(\underline{r})$ which only depend on momenta from the outer momentum shell of thickness Λdl.

- This approach has been used to derive the RG equations

  a) for the classical NLσM:

  D. R. Nelson and R. A. Pelcovits, Phys. Rev. B16, 2191 (1977)

  b) for the quantum NLσM:

  S. Chakravarty, B. I. Halperin, and D. R. Nelson
  Phys. Rev. Lett. 60, 1057 (1988)
  Phys. Rev. B 39, 2344 (1989) !!! read this !!!

- Potential problems of this approach:

  1) We expand around a broken symmetry state $(\vec{\pi}, \sigma) = (0, 1)$, e.g. $\sigma = \sqrt{1-\vec{\pi}^2} \underset{\text{small } \vec{\pi}}{\simeq} 1 - \frac{1}{2}\vec{\pi}^2 + \ldots$

  But: We should not break the spin-rotational symmetry

  2) The potential $t \ln(1-\vec{\pi}^2) \simeq -t\vec{\pi}^2$ arrising from the Jacobian has a maximum at $\vec{\pi} = 0$ and therefore causes potential stability problems in the expansion around the $\vec{\pi} = 0$ state.

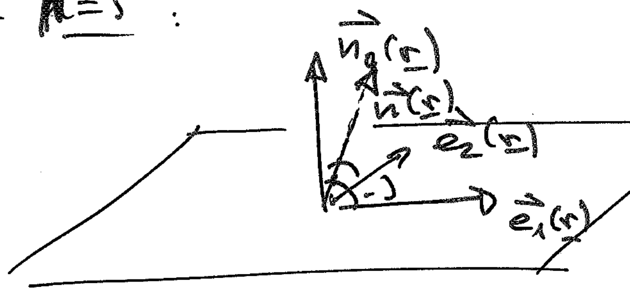
- In the following, we will use an alternative approach which does not break the spin-rotational symmetry [A.M. Polyakov, Phys. Lett. 59, 79 (1975)]

- After the elimination of fast modes with momenta from the outer shell $\Lambda e^{-dl} \leq |\underline{k}| \leq \Lambda$, we should obtain a new order parameter field $\vec{n}_0(\underline{r})$ which depends only on the "slow" modes $|\underline{k}| \leq \Lambda e^{-dl}$

- Since we eliminated only an infinitesimal fraction of modes, the differences between $\vec{n}_0(\underline{r})$ and $\vec{n}(\underline{r})$ should be very small

- We decompose $\vec{n}(\underline{r})$ into a component along $\vec{n}_0(\underline{r})$ and an orthonormal basis $\{\vec{e}_\alpha(\underline{r})\}$, $\alpha = 1, \dots, N-1$ spanning the orthogonal complement of $\vec{n}_0(\underline{r})$

e.g. in $N=3$:



$\left(\vec{n}_0(\underline{r}), \{\vec{e}_\alpha(\underline{r}) \,|\, \alpha = 1, \dots, N-1\}\right)$ orthonormal basis of $\mathbb{R}^N$

$$\vec{n}_0^{\,2}(\underline{r}) = 1 \qquad \forall \alpha = 1, \dots, N-1 : \ \vec{n}_0(\underline{r}) \cdot \vec{e}_\alpha(\underline{r}) = 0 , \quad \vec{e}_\alpha(\underline{r}) \cdot \vec{e}_\beta(\underline{r}) = \delta_{\alpha\beta}$$

Decomposition:

$$\boxed{\vec{n}(\underline{r}) = \sqrt{1-\phi^2(\underline{r})}\;\vec{n}_0(\underline{r}) + \sum_{\alpha=1}^{N-1} \phi_\alpha(\underline{r})\,\vec{e}_\alpha(\underline{r})}$$

$$\phi^2(\underline{r}) := \sum_{\alpha=1}^{N-1} \phi_\alpha^2(\underline{r})$$

- $\vec{n}_0(\underline{r}), \vec{e}_\alpha(\underline{r})$ orthonormal vector fields depending on „slow" modes
- $\phi_\alpha(\underline{r})$ are real-valued fields which depend on momenta from the shell $\Lambda e^{-dl} \le |\underline{k}| \le \Lambda$
- ϕ_α's should be small since $\vec{n}(\underline{r}) \approx \vec{n}_0(\underline{r})$ for an infinitesimally thin shell

- To decompose the action, we have to calculate

$$(\nabla\vec{n})^2 = \sum_{i=1}^{d} (\partial_i \vec{n})^2 \qquad \left(\partial_i = \frac{\partial}{\partial x_i}\right)$$

$$\partial_i \vec{n} = \frac{\sum_\alpha \phi_\alpha \partial_i \phi_\alpha}{\sqrt{1-\phi^2}}\,\vec{n}_0 + \sqrt{1-\phi^2}\,\partial_i \vec{n}_0 + \sum_\alpha \partial_i \phi_\alpha\,\vec{e}_\alpha + \sum_\alpha \phi_\alpha\,\partial_i \vec{e}_\alpha$$

We can use that $\partial_i \vec{n}_0 \perp \vec{n}_0$ $\quad \left(1 = \vec{n}_0^{\,2} \Rightarrow 0 = \partial_i \vec{n}_0^{\,2} = 2\vec{n}_0 \partial_i \vec{n}_0\right)$

$\rightarrow$ $\partial_i \vec{n}_0$ is a vector in the orthogonal complement of $\vec{n}_0$ and can be decomposed into its components along the basis vectors $\vec{e}_\alpha$

$$\boxed{\partial_i \vec{n}_0 = \sum_{\alpha=1}^{N-1} B_{i\alpha}\,\vec{e}_\alpha}$$

Likewise, we can decompose $\partial_i \vec{e}_\alpha$ as

$$\partial_i \vec{e}_\alpha = \sum_{\beta=1}^{N-1} A_{i\alpha\beta}\,\vec{e}_\beta + A_{i\alpha}\,\vec{n}_0$$

$$\boxed{A_{i\alpha\beta}} = \partial_i \vec{e}_\alpha \cdot \vec{e}_\beta = \partial_i (\underbrace{\vec{e}_\alpha \cdot \vec{e}_\beta}_{\delta_{\alpha\beta}}) - \vec{e}_\alpha \cdot \partial_i \vec{e}_\beta$$

$$= \boxed{-A_{i\beta\alpha}} \qquad \Rightarrow A_{i\alpha\alpha} = 0$$

which reflects that $\vec{e}_\alpha \perp \partial_i \vec{e}_\alpha$

$$\boxed{A_{i0}} = \vec{n}_0 \cdot \partial_i \vec{e}_\alpha = \partial_i (\underbrace{\vec{n}_0 \cdot \vec{e}_\alpha}_{=0}) - \vec{e}_\alpha \partial_i \vec{n}_0$$

$$= - \vec{e}_\alpha \cdot \sum_\beta B_{i\beta} \vec{e}_\beta = \boxed{-B_{i\alpha}}$$

$$\Rightarrow \boxed{\partial_i \vec{e}_\alpha = \sum_\beta A_{i\alpha\beta} \vec{e}_\beta - B_{i\alpha} \vec{n}_0}$$

- Putting things together:

$$\partial_i \vec{n} = \left(\sum_\alpha \frac{\phi_\alpha \partial_i \phi_\alpha}{\sqrt{1-\phi^2}} - \sum_\alpha B_{i\alpha} \phi_\alpha \right) \vec{n}_0$$

$$+ \sum_\alpha \left(\sqrt{1-\phi^2}\, B_{i\alpha} + \partial_i \phi_\alpha - \sum_\beta A_{i\alpha\beta} \phi_\beta \right) \vec{e}_\alpha$$

$$\Rightarrow (\partial_i \vec{n})^2 \underset{\substack{\text{up to} \\ \text{order } \phi^2}}{\simeq} \sum_{\alpha\beta} B_{i\alpha} B_{i\beta} \phi_\alpha \phi_\beta + \sum_\alpha \Big((1-\phi^2) B_{i\alpha}^2 + (\partial_i \phi_\alpha)^2 + 2 B_{i\alpha} \partial_i \phi_\alpha \Big)$$

We have dropped the terms containing $A_{i\alpha\beta}$. These fields are gauge degrees of freedom which can be transformed away by a change of basis in the orthogonal complement to $\vec{n}_0$.

[V. Cheropanov, I. Korenblit, A. Aharony, O. Entin-Wohlman, Eur. Phys. J. B 8, 511 (99)

$$(\nabla\vec{n})^2 = \sum_{i\alpha}\left\{ B_{i\alpha}^2 + (\partial_i\phi_\alpha)^2 + 2B_{i\alpha}\partial_i\phi_\alpha\right\}$$
$$+ \sum_{i\alpha\beta}\left\{ B_{i\alpha}B_{i\beta}\phi_\alpha\phi_\beta - B_{i\alpha}^2\phi_\beta^2\right\}$$

- The first term is simply $(\nabla\vec{u}_0)^2$:

$$\partial_i\vec{u}_0 = \sum_\alpha B_{i\alpha}\vec{e}_\alpha \Rightarrow (\nabla\vec{u}_0)^2 = \sum_i (\partial_i\vec{u}_0)^2 = \sum_{i\alpha\beta} B_{i\alpha}B_{i\beta}\underbrace{\vec{e}_\alpha\vec{e}_\beta}_{=\delta_{\alpha\beta}}$$
$$= \sum_{i\alpha}(B_{i\alpha})^2$$

$$\rightarrow \boxed{\begin{aligned} S &= \frac{1}{2t}\int d^dr\,(\nabla\vec{n})^2 \\ &= \overbrace{\frac{1}{2t}\int d^dr\,(\nabla\vec{u}_0)^2}^{=:\,S_0^<} + \overbrace{\frac{1}{2t}\int d^dr\sum_{i\alpha}(\partial_i\phi_\alpha)^2}^{=:\,S_0^>} \\ &\quad + \underbrace{\frac{1}{2t}\int d^dr\sum_{i\alpha}2B_{i\alpha}\partial_i\phi_\alpha}_{=:\,S_1} \\ &\quad + \underbrace{\frac{1}{2t}\int d^dr\sum_{i\alpha\beta}\left(B_{i\alpha}B_{i\beta}\phi_\alpha\phi_\beta - B_{i\alpha}^2\phi_\beta^2\right)}_{=:\,S_2}\end{aligned}}$$

- To implement the first step in the RG scheme, we have to integrate over the "fast" fields $\phi_\alpha(\underline{r})$ which only depend on momenta $\Lambda e^{-dl} \le |\underline{k}| \le \Lambda$ from the infinitesimal outer momentum shell.

$$Z = \int \mathcal{D}B \int \mathcal{D}\phi \; e^{-S[B,\phi]} = \int \mathcal{D}B \int \mathcal{D}\phi \; e^{-(S_0^<[B] + S_0^>[\phi] + S'[B,\phi])}$$

$$(S'[B,\phi] = S_1[B,\phi] + S_2[B,\phi])$$

$$= \int \mathcal{D}B \, e^{-S_0^<[B]} \int \mathcal{D}\phi \, e^{-S_0^>[\phi]} \, e^{-S'[B,\phi]}$$

$$= Z_0^> \int \mathcal{D}B \, e^{-S_0^<[B]} \langle e^{-S'[B,\phi]} \rangle_{0>}$$

$$= Z_0^> \int \mathcal{D}B \, e^{-S_0^<[B]} \left(1 - \langle S' \rangle_{0>} + \tfrac{1}{2} \langle S'^2 \rangle_{0>} + \dots \right)$$

$$= Z_0^> \int \mathcal{D}B \, e^{-(S_0^<[B] + \delta S^<[B])}$$

- The correction to the action $S_0^<[B] = \frac{1}{2t} \int d^d r \, (\nabla \vec{n}_0)^2$ is given by

$$\boxed{\delta S^<} = -\ln\left(1 - \langle S' \rangle_{0>} + \tfrac{1}{2} \langle S'^2 \rangle_{0>} + \dots\right)$$

$$\underset{\substack{\ln(1+\epsilon) \\ = \epsilon - \frac{1}{2}\epsilon^2}}{=} \langle S' \rangle_{0>} - \tfrac{1}{2} \langle S'^2 \rangle_{0>} + \tfrac{1}{2} \langle S' \rangle_{0>}^2 + \mathcal{O}(S'^4)$$

(where $S' = S_1 + S_2$)

S_1 linear in B and ϕ $\Rightarrow \langle S_1 \rangle_{0>} = 0$

S_2 – quadratic in both B and ϕ

$$\underset{\substack{\text{only} \\ \text{keep } \mathcal{O}(B^2)}}{=} \boxed{\langle S_2 \rangle_{0>} - \tfrac{1}{2} \langle S_1^2 \rangle_{0>}}$$

- We calculate the two contributions separately

$$\langle S_2 \rangle_{0>} = \frac{1}{2t}\int d^d r \sum_{i\alpha\beta}' \left\{ B_{i\alpha} B_{i\beta} \langle \phi_\alpha \phi_\beta \rangle_{0>} - B_{i\alpha}^2 \langle \phi_\beta^2 \rangle \right\}$$

$$-\frac{1}{2}\langle S_1^2 \rangle_{0>} = -\frac{1}{2t^2}\int d^d r \int d^d r' \sum_{\substack{ij\\ \alpha\beta}}' B_{i\alpha}(\underline{r}) B_{j\beta}(\underline{r}') \langle \partial_i \phi_\alpha(\underline{r}) \partial_j \phi_\beta(\underline{r}') \rangle_{0>}$$

- The averages $\langle \ldots \rangle_{0>}$ have to be taken over the shell with respect to the quadratic action

$$S_0^> = \frac{1}{2t}\int d^d r \sum_{i\alpha}' (\partial_i \phi_\alpha)^2 = \frac{1}{2t}\int d^d r \sum_{\alpha}' (\nabla \phi_\alpha)^2$$

$$= \frac{1}{2t}\int_k \sum_\alpha' k^2 \phi_\alpha(\underline{k}) \phi_\alpha(-\underline{k}) \qquad \text{(diagonal in } \underline{k} \text{ and } \alpha\text{)}$$

- As discussed before, we can read off the correlation function in k-space from the inverse of the kernel

$$\boxed{\langle \phi_\alpha(\underline{k}) \phi_\beta(\underline{k}') \rangle = \frac{t}{k^2} \delta_{\alpha\beta} \delta(\underline{k}+\underline{k}')}$$

- It follows that

$$\langle \phi_\alpha(\underline{r}) \phi_\beta(\underline{r}) \rangle_{0>} = \int_{\underline{k}\in \text{shell}} \int_{\underline{k}'\in\text{shell}} e^{i\underline{k}\underline{r}} e^{i\underline{k}'\underline{r}} \langle \phi_\alpha(\underline{k}) \phi_\beta(\underline{k}') \rangle$$

$$= t\delta_{\alpha\beta} \int_{\underline{k}\in\text{shell}} \frac{1}{k^2} = t\delta_{\alpha\beta} \int_{\Lambda e^{-dl} \le |\underline{k}| \le \Lambda} \frac{d^d k}{(2\pi)^d} \frac{1}{k^2}$$

$$= t\,\delta_{\alpha\beta} \frac{S_d}{(2\pi)^d} \int_{\Lambda e^{-dl}}^{\Lambda} dk\, k^{d-1} \frac{1}{k^2}$$

$$\boxed{\langle \phi_\alpha(r)\phi_\beta(r)\rangle_{0>} \simeq t\,\delta_{\alpha\beta}\frac{S_d}{(2\pi)^d}\Lambda^{d-3}(\Lambda-\Lambda e^{-dl}) = t\,\delta_{\alpha\beta}\frac{S_d}{(2\pi)^d}\Lambda^{d-2}\,dl}$$

- We use this result to calculate $\langle S_2\rangle_{0>}$:

$$\langle S_2\rangle_{0>} = \frac{1}{2t}\int d^d r \sum_{i\alpha\beta}\left\{ B_{i\alpha}B_{i\beta}\langle\phi_\alpha\phi_\beta\rangle_{0>} - B_{i\alpha}^2\langle\phi_\beta^2\rangle_{0>}\right\}$$

$$= \frac{1}{2}\int d^d r\sum_{i\alpha\beta}\frac{S_d}{(2\pi)^d}\Lambda^{d-2}dl\left(\delta_{\alpha\beta}B_{i\alpha}B_{i\beta} - B_{i\alpha}^2\right)$$

$$= \frac{1}{2}\frac{S_d}{(2\pi)^d}\Lambda^{d-2}\,dl\int d^d r\sum_{i\alpha} B_{i\alpha}^2 - \underbrace{(N-1)}_{\text{from summatio over }\beta}B_{i\alpha}^2$$

$$= -\frac{1}{2}\frac{S_d}{(2\pi)^d}\Lambda^{d-2}(N-2)\,dl\int d^d r\,(\nabla\vec{n}_0)^2$$

- It can be shown by a similar calculation that $\langle \partial_i\phi_\alpha(\underline{r})\,\partial_j\phi_\beta(\underline{r}')\rangle_{0>} = 0$ and hence $\langle S_1^2\rangle_{0>} = 0$

- After the elimination of „fast" modes (the fields ϕ_α), the action reads

$$S_0^< - \frac{1}{2}\frac{S_d}{(2\pi)^d}\Lambda^{d-2}(N-2)\,dl\int_{|\tilde{r}|\geq 1/\tilde{\Lambda}} d^d\tilde{r}\,(\tilde{\nabla}\vec{n}_0)^2 \qquad (\tilde{\Lambda} = \Lambda e^{-dl})$$

$$= \frac{1}{2t}\left[1 - t\frac{S_d}{(2\pi)^d}\Lambda^{d-2}(N-2)\,dl\right]\int_{|\tilde{r}|\geq 1/\tilde{\Lambda}} d^d\tilde{r}\,(\tilde{\nabla}\vec{n}_0)^2$$

- As a next step, we rescale the momenta, $\underline{k} \to e^{dl}\underline{k}$ that the momentum cut-off remains unchanged.

  Rescaling of momenta is equivalent to the rescaling of length

$$\underline{\tilde{r}} \to \underline{\tilde{r}}\, e^{-dl} = \underline{r}$$

$$\to \frac{1}{2t}\left[1 - \frac{S_d}{(2\pi)^d}\Lambda^{d-2}(N-2)t\, dl\right] \int_{|\tilde{r}| \geq 1/\tilde{\Lambda}} d^d\tilde{r}\, (\tilde{\nabla}\vec{n}_0)^2$$

$$= \frac{1}{2t}\left[1 - \frac{S_d}{(2\pi)^d}\Lambda^{d-2}(N-2)t\, dl\right] e^{(d-2)dl} \int_{|r| \geq 1/\Lambda} d^d r\, (\nabla\vec{n}_0)^2$$

- We can extract the renormalized coupling constant

$$\frac{1}{2t(l+dl)} = \frac{1}{2t(l)}\left[1 - \frac{S_d}{(2\pi)^d}\Lambda^{d-2}(N-2)\, t(l)\, dl\right]\left[1 + (d-2)dl\right]$$

$$\simeq \frac{1}{2t(l)}\left[1 + (d-2)dl - \frac{S_d}{(2\pi)^d}\Lambda^{d-2}(N-2)\, t(l)\, dl\right]$$

- <u>RG flow equation</u>

$$\underbrace{\frac{d}{dl}\frac{1}{t}}_{= -\frac{1}{t^2}\frac{dt}{dl}} = (d-2)\frac{1}{t} - \frac{S_d}{(2\pi)^d}\Lambda^{d-2}(N-2)$$

$$\to \boxed{\frac{dt}{dl} = (2-d)t + \frac{S_d}{(2\pi)^d}\Lambda^{d-2}(N-2)\, t^2}$$

- It is convenient to absorb prefactors by a simple rescaling,

$$\boxed{\tilde{t} := \frac{S_d}{(2\pi)^d} \Lambda^{d-2} \cdot t}$$

$$\rightarrow \boxed{\frac{d\tilde{t}}{dl} = (2-d)\tilde{t} + (N-2)\tilde{t}^2}$$

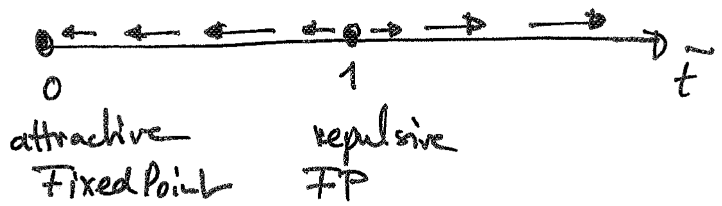
initial condition:

$$\tilde{t}(0) = \tilde{t}_0 = \frac{S_d}{(2\pi)^d} \Lambda^{d-2} \frac{T}{\rho_s}$$

- We discuss the RG equation in the case $N=3$ of the Heisenberg antiferromagnet ($\vec{n}$ is a three-component vector) in $d=3$ spatial dimension.

$$\boxed{\frac{d\tilde{t}}{dl} = -\tilde{t} + \tilde{t}^2} \quad , \quad \boxed{\tilde{t}_0 = \tilde{t}(0) = \frac{\Lambda}{2\pi^2} \frac{T}{\rho_s}} = \boxed{\frac{\Lambda a}{2\pi^2} \frac{T}{J_1 S^2 (1-4\gamma)}}$$

fixed points ($\frac{d\tilde{t}}{dl} = 0$) : $\tilde{t} = 0$ and $\tilde{t} = 1$



$\tilde{t} < 1$: RG flow is towards smaller values of $\tilde{t}$ since $\frac{d\tilde{t}}{dl} < 1$

$\tilde{t} > 1$: RG flow is towards larger values of $\tilde{t}$ since

$$\frac{d\tilde{t}}{dl} > 1$$

- What does this mean physically?

a) For $\tilde{t}(0) = \tilde{t}_0 < 1$ $\left(T < T_c = \frac{2\pi^2}{\Lambda a} J_1 S^2 (1-4\gamma)\right)$, the RG flow is towards the attractive fixed point $\tilde{t} = 0$ corresponding to $T = 0$ or $\rho_s = \infty$

→ going to larger scales, fluctuations of the order parameter are suppressed

→ system is ordered

b) for $\tilde{t}(0) = \tilde{t}_0 > 1$ $(T > T_c)$: $\tilde{t} \to \infty$

this corresponds to $T \to \infty$ or $\rho_s \to 0$

→ going to larger scales fluctuation become more severe

→ system is disordered

- We can solve the RG equation analytically:

$$\frac{d\tilde{t}}{dl} = -\tilde{t} + \tilde{t}^2 \quad , \quad \tilde{t}(0) = \tilde{t}_0$$

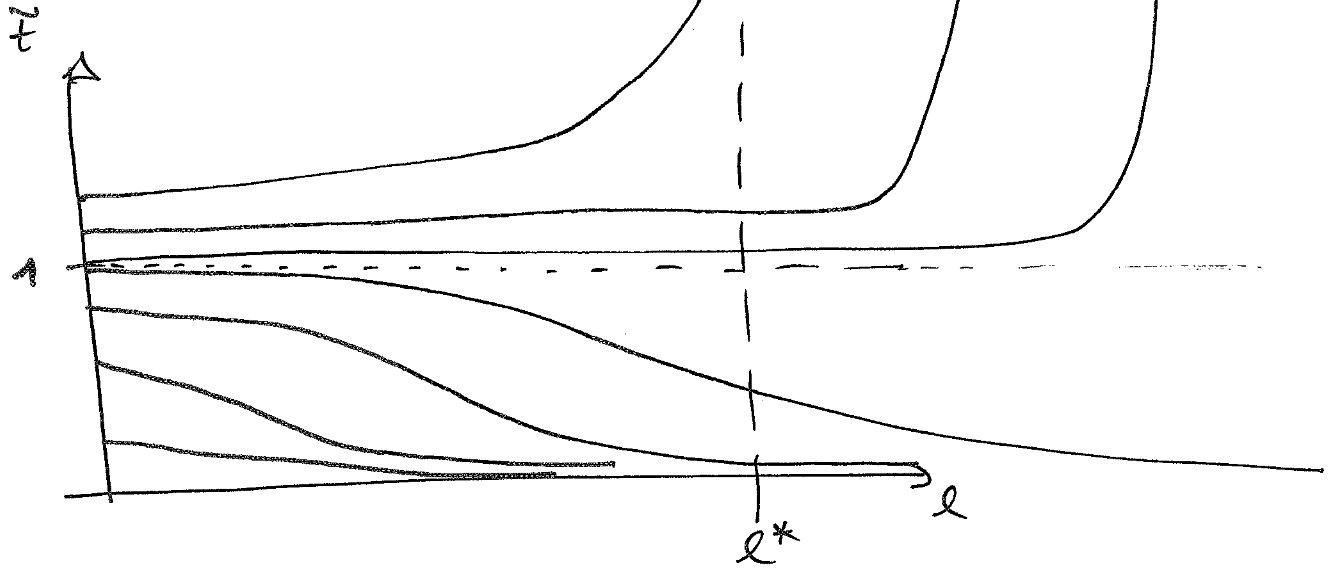
separation of variables:

$$\frac{d\tilde{t}}{\tilde{t}^2 - \tilde{t}} = dl \quad \rightarrow \quad \int_{\tilde{t}_0}^{\tilde{t}(l)} d\tilde{t} \, \underbrace{\frac{1}{\tilde{t}^2 - \tilde{t}}}_{\frac{1}{\tilde{t}-1} - \frac{1}{\tilde{t}}} = \int_0^l dl = l$$

$$\Leftrightarrow \quad l = \ln \frac{|\tilde{t}(l) - 1|}{\tilde{t}(l)} - \ln \frac{|\tilde{t}_0 - 1|}{\tilde{t}_0} = \ln \frac{\tilde{t}(l) - 1}{\tilde{t}_0 - 1} \frac{\tilde{t}_0}{\tilde{t}(l)}$$

$$\Rightarrow \quad \boxed{\tilde{t}(l) = \frac{\tilde{t}_0}{\tilde{t}_0 + (1 - \tilde{t}_0) e^l}}$$

$$\tilde{t}(l) = \frac{\tilde{t}_0}{\tilde{t}_0 + (1-\tilde{t}_0)e^l}$$



- For $\tilde{t}_0 > 1$ (disordered phase, $T > T_c$), $\tilde{t}$ diverges at a scale l^*,

$$\tilde{t}_0 = (\tilde{t}_0 - 1)e^{l^*} \Leftrightarrow e^{l^*} = \frac{\tilde{t}_0}{\tilde{t}_0 - 1} \Rightarrow l^* = \ln\frac{\tilde{t}_0}{\tilde{t}_0 - 1}$$

  → l^* shifts to larger and larger values as we approach the transition, $\tilde{t}_0 \to 1_+$ $(T \to T_c^+)$

  → divergence becomes sharper

- We can identify the correlation length as $\boxed{\xi = a \cdot e^{l^*}}$ with a the lattice constant

in our case:

$$\xi = a\frac{\tilde{t}_0}{\tilde{t}_0 - 1} = a\frac{T/T_c}{T/T_c - 1} = a\frac{T}{T - T_c}$$

⇒ The correlation length exponent is $\boxed{\nu = 1}$.

- Note that our result $\nu = 1$ is <u>not exact</u>:

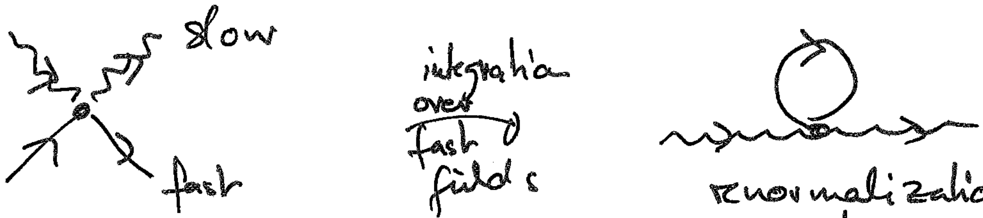
high resolution Monte-Carlo study of the classical Heisenberg model ($N=3$) in $d=3$ space dimension shows that

$$\boxed{\nu_{MC} = 0.7048 \pm 0.0030}$$

[K. Chen, A.M. Ferrenberg, D.P. Nelson, Phys. Rev. B 48, 3249 (1993)]

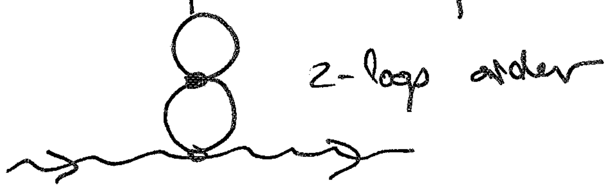
Why is our result not exact?

- We performed and RG calculation to "<u>1-loop order</u>"



renormalization of quadratic term $\sim (\nabla \vec{n}_0)^2$

- quadratic action is further renormalized by higher-order contributions from the expansion of the exponential function, e.g.



$$\to \quad \frac{d\tilde{t}}{dl} = -\tilde{t} + \tilde{t}^2 + c\,\tilde{t}^3 + \dots$$

→ shifted FP and different behavior in the vicinity of the FP (linearize around FP)

→ corrections to exponents

- Finally, let us look at the RG equation for $N=3$ and <u>$d=2$</u>:

$$\frac{d\tilde{t}}{dl} = \tilde{t}^2 \quad \Rightarrow \quad \tilde{t} \text{ diverges for any initial value } \tilde{t}_0 > 0 \,!$$

⇒ No long range order at finite temperature (→ Mermin Wagner theorem)

- Only for $d > 2$ a magnetically ordered phase is present at finite temperatures

$$\frac{d\tilde{t}}{dl} = \underbrace{(2-d)}_{<0}\tilde{t} + \tilde{t}^2 = \tilde{t}\left(\tilde{t} - (d-2)\right)$$

$$\tilde{t}_c = d-2 \quad \rightarrow \quad \boxed{d_c^- = 2} \text{ is the lower critical dimension}$$

4.4. Spin - Coherent states

- Goal is to derive the effective quantum field theory (Landau-Ginzburg action) for the frustrated $J_1 - J_2$ Heisenberg antiferromagnet
- We have to find the best set of quantum states (over complete basis of spin Hilbert space) to take the trace in the partition function and to resolve the identities in the Suzuki-Trotter formula
- Goal: Getting as close as possible to the classical order-parameter theory given by the classical NLσM

- In the following, we focus on a single quantum spin. For many spins on a lattice we can easily generalize the results by taking the product state of single-site quantum states

- <u>Conventional complete basis</u>:

Since $[\hat{S}^2, \hat{S}_z] = 0$, it is possible to find a simultaneous eigenbasis of $\hat{S}^2$ and $\hat{S}_z$

$|S, m\rangle$, $S = 1/2, 1, 3/2, 2, \ldots$

$m = -S, -S+1, \ldots, S-1, S$

(for a given S, there are $2S+1$ basis states with different m quantum numbers)

$$\hat{S}_z |S, m\rangle = \hbar m |S, m\rangle$$
$$\hat{S}^2 |S, m\rangle = \hbar^2 S(S+1) |S, m\rangle$$

<u>orthonormal basis</u> : $\langle S, m | S', m' \rangle = \delta_{SS'} \delta_{m,m'}$

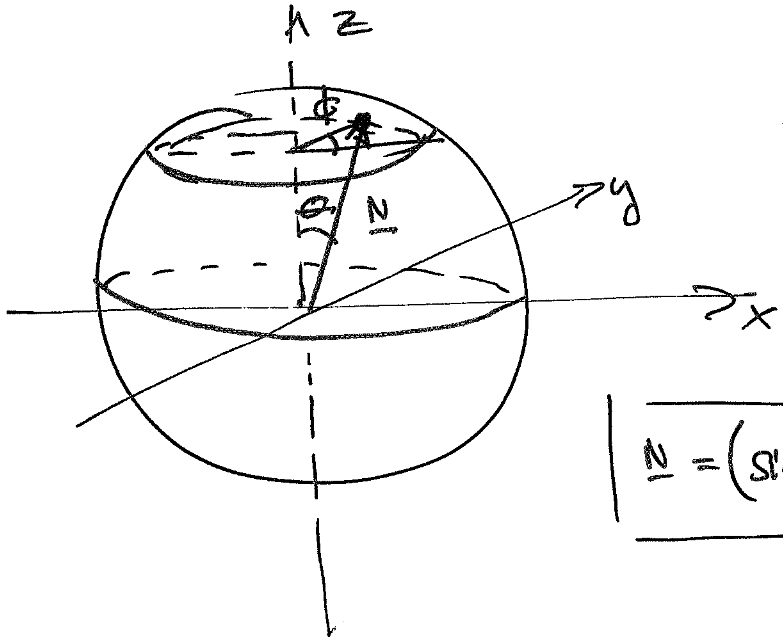
<u>completeness relation</u>: $1 = \sum_{S,m} |S, m\rangle\langle S, m|$

- <u>spin-coherent states</u>

To establish a connection to the classical order-parameter theory, we construct an overcomplete basis such that the eigenvalues of the spin operator $\hat{\underline{S}} = \begin{pmatrix} \hat{S}_x \\ \hat{S}_y \\ \hat{S}_z \end{pmatrix}$ are classical vectors

$$\hat{\underline{S}} |\underline{N}\rangle = S \underline{N} |\underline{N}\rangle \quad \left(\text{or } \langle \underline{N} | \hat{\underline{S}} | \underline{N} \rangle = S \underline{N} \right)$$

$\underline{N}$ an arbitrary unit vector , $\underline{N}^2 = 1$



spherical coordinates:

$$\boxed{\underline{N} = (\sin\theta\cos\phi\,,\ \sin\theta\sin\phi\,,\ \cos\theta)}$$

- The maximally polarized state $^{(m=s)}$ with $\hat{S}_z|s,s\rangle = (\hbar) s|s,s\rangle$ corresponds to $\underline{N} = \underline{N}_0 = (0,0,1)$ $(\hbar = 1)$

$$|\underline{N} = (0,0,1)\rangle = |s, m=s\rangle =: |\psi_0\rangle$$

- claim: The states $\boxed{|\underline{N}\rangle := \exp(z\hat{S}^+ - z^*\hat{S}^-)|\psi_0\rangle}$ with $\boxed{z = -\frac{\theta}{2}\exp(-i\phi)}$ have the desired property $\boxed{\langle\underline{N}|\hat{\underline{S}}|\underline{N}\rangle = s\underline{N}}$!

Proof: $\hat{\Omega} := z^*\hat{S}^- - z\hat{S}^+$, $|\underline{N}\rangle = \exp(-\hat{\Omega})|\psi_0\rangle$

$\hat{\Omega}$ is anti-hermitian, $\langle\underline{N}| = \langle\psi_0|\exp(\hat{\Omega})$

$\hat{\Omega}^+ = -\hat{\Omega}$

$$\langle\underline{N}|\hat{S}_z|\underline{N}\rangle = \langle\psi_0|e^{\hat{\Omega}}\hat{S}_z e^{-\hat{\Omega}}|\psi_0\rangle$$

$$\underset{\text{Baker-Hausdorff}}{=} \langle\psi_0|\hat{S}_z + [\hat{\Omega},\hat{S}_z] + \frac{1}{2}[\hat{\Omega},[\hat{\Omega},\hat{S}_z]] + \ldots|\psi_0\rangle$$

$$= \langle\psi_0|\sum_{k=0}^{\infty}\frac{1}{k!}\hat{A}_k|\psi_0\rangle$$

$$\hat{A}_0 = \hat{S}_z$$
$$\hat{A}_1 = [\hat{\Omega}, \hat{S}_z]$$
$$\hat{A}_2 = [\hat{\Omega}, [\hat{\Omega}, \hat{S}^z]]$$
$$\hat{A}_3 = [\hat{\Omega}, [\hat{\Omega}, [\hat{\Omega}, \hat{S}^z]]]$$
$$\vdots$$

$$\hat{A}_1 = [\hat{\Omega}, \hat{S}_z] = [z^* \hat{S}^- - z\hat{S}^+, \hat{S}_z] = z^* \hat{S}^- + z\hat{S}^+$$
$$[\hat{S}^\pm, \hat{S}_z] = \mp \hat{S}^\pm$$

$$\hat{A}_2 = [\hat{\Omega}, \hat{A}_1] = [z^* \hat{S}^- - z\hat{S}^+, z^* \hat{S}^- + z\hat{S}^+]$$
$$= 2z^* z [\hat{S}^-, \hat{S}^+] = -4z^* z \hat{S}_z$$

$$\hat{A}_3 = [\hat{\Omega}, \hat{A}_2] = -4z^* z [\hat{\Omega}, \hat{S}_z] = -4z^* z \hat{A}_1$$
$$\hat{A}_4 = [\hat{\Omega}, \hat{A}_3] = -4z^* z [\hat{\Omega}, \hat{A}_1] = (-4z^* z)^2 \hat{S}_z$$

$$\boxed{\hat{A}_k = \begin{cases} (-4z^* z)^{k/2} \hat{S}^z & \text{for } k = 0, 2, 4, \dots \\ (-4z^* z)^{(k-1)/2} (z^* \hat{S}^- + z\hat{S}^+) & \text{for } k = 1, 3, 5, \dots \end{cases}}$$

Since $\langle \psi_0 | \hat{S}^\pm | \psi_0 \rangle = 0$, only the $k = 0, 2, 4, \dots$ terms contribute

$$\rightarrow \langle \underline{N} | \hat{S}^z | \underline{N} \rangle = \langle \psi_0 | \sum_{k=0}^{\infty} \frac{1}{k!} \hat{A}_k | \psi_0 \rangle = \langle \psi_0 | \sum_{n=0}^{\infty} \frac{1}{(2n)!} \hat{A}_{2n} | \psi_0 \rangle$$

$$= \langle \psi_0 | \sum_{n=0}^{\infty} \frac{1}{(2n)!} (-4|z|^2)^n \underbrace{\hat{S}^z | \psi_0 \rangle}_{= S|\psi_0\rangle}$$

$$\underset{1 = \langle \psi_0 | \psi_0 \rangle}{=} S \sum_n \frac{(-1)^n}{(2n)!} (2|z|)^{2n} = S \cos(2|z|) \underset{z = -\frac{\theta}{2} \exp(-i\phi)}{=} S \cos\theta = S N_z$$

analogous: $\langle \underline{N} | \hat{S}^+ | \underline{N} \rangle = \ldots = -S \frac{z^*}{|z|} \sin(2|z|)$

$$= S \exp(-i\phi) \sin\theta$$

$$\langle \underline{N} | \hat{S}^- | \underline{N} \rangle = S \exp(i\phi) \sin\theta$$

$$\Rightarrow \begin{cases} \langle \underline{N} | \hat{S}_x | \underline{N} \rangle = \langle \underline{N} | \frac{\hat{S}^+ + \hat{S}^-}{2} | \underline{N} \rangle = S \cos\phi \sin\theta = S N_x \\ \langle \underline{N} | \hat{S}_y | \underline{N} \rangle = \langle \underline{N} | \frac{\hat{S}^+ - \hat{S}^-}{2i} | \underline{N} \rangle = S \sin\phi \sin\theta = S N_y \end{cases}$$

✓

other useful properties:

$$\boxed{\langle \underline{N} | \underline{N} \rangle = 1}$$ trivial

- completeness relation

$$\boxed{\frac{2S+1}{4\pi} \int d\mu(\underline{N}) \, |\underline{N}\rangle\langle\underline{N}| = 1}$$

measure: $\int d\mu(\underline{N}) := \int_{\mathbb{R}^3} d^3\underline{N} \, \delta(\underline{N}^2 - 1)$

4.5. Coherent State Path Integral for a single Quantum Spin

- $\hat{H}$ Hamiltonian of a single quantum spin $\hat{S}$, e.g. $\hat{H} = \underline{B} \cdot \hat{\underline{S}}$

- We calculate the partition function by taking the trace with respect to the coherent state basis

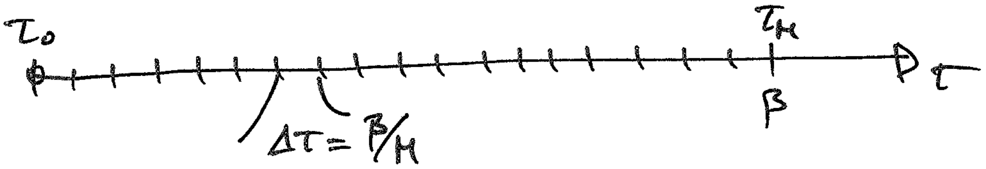
$$Z = \mathrm{Tr}\, e^{-\beta \hat{H}}$$

$$= \frac{2S+1}{4\pi} \int d\mu(\underline{N}) \; \langle \underline{N} | e^{-\beta \hat{H}} | \underline{N} \rangle$$

$$= \lim_{M\to\infty} \left(\prod_{i=1}^{M} \frac{2S+1}{4\pi} \int d\mu(\underline{N}(\tau_i)) \right) \langle \underline{N}(\tau_0 = 0) | e^{-\Delta\tau \hat{H}} | \underline{N}(\tau_1) \rangle$$

↑ Trotter formula

$$\cdot \langle \underline{N}(\tau_1) | e^{-\Delta\tau \hat{H}} | \underline{N}(\tau_2) \rangle \cdots \langle \underline{N}(\tau_{M-1}) | e^{-\Delta\tau \hat{H}} | \underline{N}(\tau_M = \tau_0) \rangle$$



Evaluation of the matrix elements of $e^{-\Delta\tau \hat{H}}$:

$$\langle \underline{N}(\tau_i) | e^{-\Delta\tau \hat{H}} | \underline{N}(\tau_i + \Delta\tau) \rangle$$

$$= \langle \underline{N}(\tau_i) | \underline{N}(\tau_i + \Delta\tau) \rangle - \Delta\tau \langle \underline{N}(\tau_i) | \hat{H} | \underline{N}(\tau_i) \rangle + \mathcal{O}(\Delta\tau^2)$$

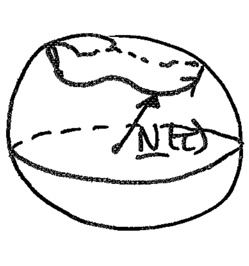
$$= 1 + \Delta\tau \langle \underline{N}(\tau_i) | \frac{d}{d\tau_i} | \underline{N}(\tau_i) \rangle - \Delta\tau \, H(S\underline{N}(\tau_i))$$

$$= e^{-\Delta\tau \left\{ H(S\underline{N}(\tau_i)) - \langle \underline{N}(\tau_i) | \frac{d}{d\tau_i} | \underline{N}(\tau_i) \rangle \right\}}$$

The partition function is given by

$$Z = \lim_{M\to\infty} \left(\prod_{i=1}^{M} \frac{2S+1}{4\pi} \int d\mu(\underline{N}(\tau_i)) \right) e^{-\sum_{i=1}^{M} \Delta\tau \left\{ H(S\underline{N}(\tau_i)) - \langle \underline{N}(\tau_i) | \frac{\partial}{\partial \tau_i} | \underline{N}(\tau_i) \rangle \right\}}$$

$$= \int_{\underline{N}(0) = \underline{N}(\beta)} \mathcal{D}\underline{N}(\tau) \, \delta(\underline{N}(\tau)^2 - 1) \, e^{-\int_0^\beta d\tau \left\{ H(S\underline{N}(\tau)) - \langle \underline{N}(\tau) | \frac{d}{d\tau} | \underline{N}(\tau) \rangle \right\}}$$



- First term is simply obtained by replacing the spin operator $\hat{S}$ by a classical vector $S \cdot \underline{N}$
- 2nd term results from overlap between coherent states (Berry phase)

$$S = S_H + S_B$$

$$= \int_0^\beta d\tau \, H(S\underline{N}(\tau)) \quad - \int_0^\beta d\tau \, \langle \underline{N}(\tau) | \frac{d}{d\tau} | \underline{N}(\tau) \rangle$$

- For the evaluation of the Berry phase term S_B, we have to evaluate the derivative

$$\frac{d}{d\tau} | \underline{N}(\tau) \rangle = \frac{d}{d\tau} \exp\left(z(\tau) \hat{S}_+ - z^*(\tau) \hat{S}_- \right) | \psi_0 \rangle$$

- We have to be very careful! In general, the operator $\hat{M}(\tau)$ does not commute with the operator $\frac{d}{d\tau} \hat{M}(\tau)$: $\quad [\hat{M}(\tau), \frac{d}{d\tau} \hat{M}(\tau)] \neq 0$
(This is also the case for the operator $\hat{\Omega}(\tau)$ in the exponent)

In this case $\quad \frac{d}{d\tau} \exp(\hat{M}(\tau)) \neq \frac{d\hat{M}}{d\tau} \exp(\hat{M})$!

The correct way of taking the derivative is given by the formula

$$\boxed{\frac{d}{d\tau} \exp(\hat{M}) = \int_0^1 du \; e^{\hat{M}(1-u)} \frac{d\hat{M}}{d\tau} e^{\hat{M}u}}$$

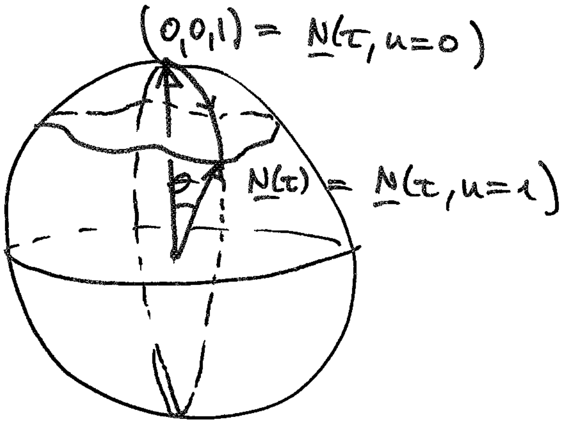
$$\rightarrow S_B = -\int_0^\beta d\tau \, \langle \underline{N}(\tau) | \frac{d}{d\tau} | \underline{N}(\tau) \rangle$$

$$= -\int_0^\beta d\tau \int_0^1 du \, \langle \underline{N}(\tau) | \, e^{(z\hat{S}^+ - z^*\hat{S}^-)(1-u)} \left(\frac{dz}{d\tau} \hat{S}^+ - \frac{dz^*}{d\tau} \hat{S}^- \right) \underbrace{e^{(z\hat{S}^+ - z^*\hat{S}^-)u} | \psi_0 \rangle}_{=: | \underline{N}(\tau, u) \rangle}$$

$$= -\int_0^\beta d\tau \int_0^1 du \, \langle \underline{N}(\tau, u) | \, \frac{dz}{d\tau} \hat{S}^+ - \frac{dz^*}{d\tau} \hat{S}^- \, | \underline{N}(\tau, u) \rangle$$

- What is the meaning of the states $|\underline{N}(\tau,u)\rangle = e^{(z\hat{S}^{+} - z^{*}\hat{S}^{-})u}\,|\psi_0\rangle$?

$$z = -\frac{\theta}{2}\,e^{-i\phi} \quad \Rightarrow \quad \text{Multiplication with } u\in[0,1] \text{ changes the } \theta \text{ angle}$$



- The Berry phase has a geometrical meaning:

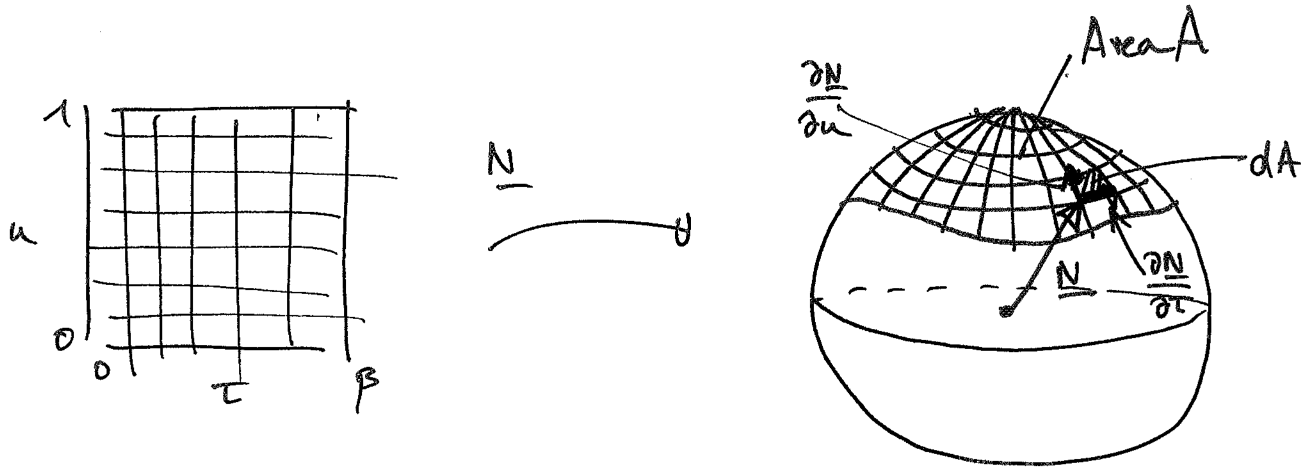
$$S_B = -\int_0^{\beta} d\tau \int_0^{1} du \;\langle \underline{N}(\tau,u)|\, \frac{dz}{d\tau}\hat{S}^{+} - \frac{dz^{*}}{d\tau}\hat{S}^{-}\,|\underline{N}(\tau,u)\rangle$$

$$= iS\int_0^{\beta} d\tau \int_0^{1} du \;\underbrace{\underline{N}\cdot\left(\frac{\partial \underline{N}}{\partial u} \times \frac{\partial \underline{N}}{\partial \tau}\right)}_{\text{surface area element } dA} = iSA$$

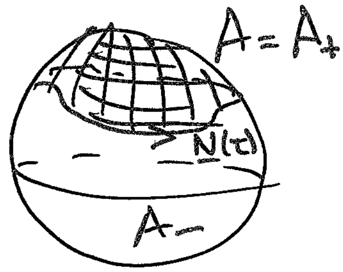
1) $\hat{S}^{\pm} = \hat{S}^{x} \pm i\hat{S}^{y}$

2) $\hat{S}^{\alpha}|\underline{N}(\tau,u)\rangle = S N_{\alpha}(\tau,u)\,|\underline{N}(\tau,u)\rangle$

3) definition of z



- The Berry phase is proportional to the area A on the surface of the unit sphere enclosed by the worldline $\underline{N}(\tau)$ ($\underline{N}(0) = \underline{N}(\beta) \Rightarrow$ closed line on unit sphere)



$$A_+ + A_- = S_3 = 4\pi$$

- It is called a phase because it is purely imaginary

4.6. Quantum NLσM and Berry Phases

- We continue to derive the effective field theory for the quantum antiferromagnet
- long-wavelength, large S description of dynamics of a d-dim. quantum AF in the vicinity of a ground state with collinear long-range Néel order
- coherent-state product state

$$|\underline{N}(\tau)\rangle = |\underline{N}(\underline{r}_1,\tau)\rangle \otimes |\underline{N}(\underline{r}_2,\tau)\rangle \otimes \dots$$

$$= \prod_i |\underline{N}(\underline{r}_i,\tau)\rangle$$

$\underline{r}_i$ are the sites of the d-dim. hypercubic lattice, i labels the sites

- After taking the trace and resolving the identities with respect to the product states $|\underline{N}(\tau)\rangle$ we obtain as a trivial generalization

$$Z = \int_{\substack{\underline{N}(\underline{r}_i,0) \\ = \underline{N}(\underline{r}_i,\beta)}} \mathcal{D}\underline{N}(\underline{r}_i,\tau)\ \delta(\underline{N}^2-1)\ e^{-S}$$

$$S = S_H + S_B$$

$$S_H = \int_0^\beta d\tau\ H(\{S\underline{N}(\underline{r}_i,\tau)\})$$

$$= -J_1 S^2 \int_0^\beta d\tau \left(\sum_{\langle ij\rangle} \underline{N}(\underline{r}_i,\tau)\,\underline{N}(\underline{r}_j,\tau) + \alpha \sum_{\langle\langle ij\rangle\rangle} \underline{N}(\underline{r}_i,\tau)\,\underline{N}(\underline{r}_j,\tau) \right)$$

$$S_B = iS \sum_i \int_0^\beta d\tau \int_0^1 du\ \underline{N}(\underline{r}_i,\tau,u) \cdot \left(\frac{\partial \underline{N}(\underline{r}_i,\tau,u)}{\partial u} \times \frac{\partial \underline{N}(\underline{r}_i,\tau,u)}{\partial \tau} \right)$$

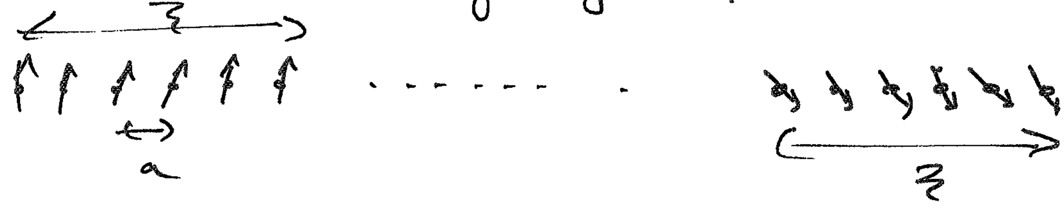
- Next step: To derive the effective continuum field theory for the Neel-order parameter we decompose the unit vector $\underline{N}(\underline{r}_i,\tau)$ as

$$\boxed{\underline{N}(\underline{r}_i,\tau) = \epsilon_i\ \underline{n}(\underline{r}_i,\tau)\sqrt{1-\underline{L}^2(\underline{r}_i,\tau)} + \underline{L}(\underline{r}_i,\tau)}$$

$$\underline{n}^2 = 1, \quad \underline{n}\cdot\underline{L} = 0, \quad \underline{L}^2 \ll 1$$

* $\epsilon_i = +1$ on sublattice A, $\epsilon_i = -1$ on sublattice B
* $\underline{n}(\underline{r}_i,\tau)$ describes the local orientation of the Neel ordering, varies slowly on the scale of the lattice spacing

* values of $\underline{n}$ can be considerably different on well separated points, leaving open the possibility of a quantum disordered phase with no long-range spin order



* $\underline{L}(\underline{r}_i,\tau)$ component of the spins which is perpendicular to the local orientation of the Néel order

• Insert the decomposition of $\underline{N}$ into $\mathcal{H}(\{S\underline{N}(\underline{r}_i,\tau)\})$ and expand the result in gradients and powers of $\underline{L}$. This yields in the continuum limit

$$\boxed{\mathcal{H} = \frac{1}{2}\int d^d\underline{r}\left(\rho_s(\underline{\nabla}\vec{n})^2 + \chi_\perp S^2 \underline{L}^2\right)}$$

$$\left(S_{\mathcal{H}} = \int_0^\beta d\tau\, \mathcal{H}[\vec{n},\vec{L}]\right)$$

Spin-wave stiffness:

$$\boxed{\rho_s = J_1[1 - 2(d-1)\gamma]\, S^2 a^{2-d}}$$

transverse susceptibility:

$$\boxed{\chi_\perp = 2d\, a^d J_1}$$

• Note: Theory becomes unstable at $\gamma = \frac{1}{2(d-1)}$ since $\rho_s = 0$. This is exactly the value $\gamma_c = J_2/J_1$ of the classical transition

- Calculation of the Berry-phase term in terms of $\underline{n}$ and $\underline{L}$: $\quad \underline{N} = \epsilon_i \underline{n}\sqrt{1-\underline{L}^2} + \underline{L}$, $\underline{L} \perp \underline{n}$

$$S_B = iS \sum_i \int_0^\beta d\tau \int_0^1 du \; \underline{N}(\underline{r}_i, \tau, u) \cdot \left(\frac{\partial \underline{N}(\underline{r}_i,\tau,u)}{\partial u} \times \frac{\partial \underline{N}(\underline{r}_i,\tau,u)}{\partial \tau} \right)$$

$$= \underbrace{iS \sum_i \epsilon_i \int_0^\beta d\tau \int_0^1 du \; \underline{n}_i \cdot \left(\frac{\partial \underline{n}_i}{\partial u} \times \frac{\partial \underline{n}_i}{\partial \tau} \right)}_{= S_B'}$$

$$- iS \int d^d \underline{r} \int_0^\beta d\tau \; \underline{L}(\underline{r},\tau) \left(\underline{n}(\underline{r},\tau) \times \frac{\partial \underline{n}(\underline{r},\tau)}{\partial \tau} \right) + \mathcal{O}(L^3)$$

* The first term S_B' looks like the original Berry phase term but now for the order parameter field $\underline{n}_i$
* It alternates between the two sublattices → no continuum limit possible
* In the second term, we took the continuum limit and integrated over the dummy variable u
* We have decomposed S_B into a smooth part and a residual Berry phase term S_B'

- In the order-parameter field $\underline{n}$ and the perpendicular field $\underline{L}$, the quantum-field theory for the quantum antiferromagnet is given by

$$\boxed{\begin{aligned} Z &= \int \mathcal{D}\underline{n}\, \delta(\underline{n}^2-1) \int \mathcal{D}\underline{L}\; e^{-\left(S[\underline{n},\underline{L}] + S_B'\right)} \\ S[\underline{n},\underline{L}] &= \frac{1}{2}\int_0^\beta d\tau \int d^d\underline{r} \left\{ \rho_s (\nabla \underline{n})^2 + \chi_\perp s^2 \underline{L}^2 - 2iS\underline{L}\cdot\left(\underline{n}\times\frac{\partial \underline{n}}{\partial \tau}\right)\right\} \end{aligned}}$$

- The modes associated with the field $\underline{L}$ are massive (and dispersionless)

  → they should not be important in the effective long wavelength theory

- We can integrate over the field $\underline{L}$. The functional integral over $\underline{L}$ is easy to calculate since it is a gaussian integral.

completing the square:

$$\chi_\perp S^2 \underline{L}^2 - 2iS\underline{L}\left(\underline{n}\times\frac{\partial \underline{n}}{\partial\tau}\right)$$

$$= \chi_\perp S^2\left[\underline{L}^2 - \frac{2i}{\chi_\perp S}\left(\underline{n}\times\frac{\partial\underline{n}}{\partial\tau}\right)\underline{L}\right]$$

$$= \chi_\perp S^2\left[\left(\underline{L} - \frac{i}{\chi_\perp S}\left(\underline{n}\times\frac{\partial\underline{n}}{\partial\tau}\right)\right)^2 + \frac{1}{\chi_\perp^2 S^2}\left(\underline{n}\times\frac{\partial\underline{n}}{\partial\tau}\right)^2\right]$$

$$= \chi_\perp S^2\left(\underline{L} - \frac{i}{\chi_\perp S}\left(\underline{n}\times\frac{\partial\underline{n}}{\partial\tau}\right)\right)^2 + \frac{1}{\chi_\perp}\left(\underline{n}\times\frac{\partial\underline{n}}{\partial\tau}\right)^2$$

$$\underline{n}^2 = 1 \Rightarrow \underline{n} \perp \frac{\partial\underline{n}}{\partial\tau}$$

$$\Rightarrow \left(\underline{n}\times\frac{\partial\underline{n}}{\partial\tau}\right)^2 = \underbrace{|\underline{n}|^2}_{=1}\left(\frac{\partial\underline{n}}{\partial\tau}\right)^2 \underbrace{\sin^2\phi}_{=1} = \left(\frac{\partial\underline{n}}{\partial\tau}\right)^2$$

- Therefore the effective field theory is given by the <u>(d+1)-dim. non-linear sigma model</u> <u>augmented by the residual Berry phase term</u>:

$$\boxed{\begin{aligned} Z &= \int \mathcal{D}\underline{n}\,\delta(\underline{n}^2-1)\, e^{-(S[\underline{n}] + S_B')} \\ S[\underline{n}] &= \frac{\rho_s}{2}\int_0^\beta d\tau \int d^d r \left\{ (\nabla_r \underline{n})^2 + \frac{1}{\chi_\perp \rho_s}\left(\frac{\partial\underline{n}}{\partial\tau}\right)^2 \right\} \end{aligned}}$$

- Quantum-field theory with dynamical exponent $\underline{z=1}$. In momentum space and frequency domain: $(T=0)$

$$S = \frac{\rho_s}{2} \int_{\underline{k}\omega} \left(k^2 + \frac{1}{\chi_\perp \rho_s} \omega^2 \right) \underline{n}^*(\underline{k}\omega)\, \underline{n}(\underline{k}\omega)$$

look at pole of the kernel: $\omega = \sqrt{\chi_\perp \rho_s}\, |\underline{k}|$

$\Rightarrow z=1$

- This is to be expected since spin-waves have a linear dispersion at low energies. We have found that the spin-wave velocity is given by

$$\underline{c} = \sqrt{\chi_\perp \rho_s} = \boxed{\sqrt{2d}\, a J_1 S \sqrt{1-2(d-1)\gamma}}$$

Note that this is exactly the same result as obtained in linear spin-wave theory by expanding $\omega(q) = \sqrt{A_q^2 - B_q^2}$ around $q=0$ (or $\underline{q}=(\pi,\pi)$)