3. Bose-Hubbard Model

3.1. Hamiltonian and Mott-Insulator / Superfluid transition

Bose-Hubbard (BH) model in its simplest form:

$$\boxed{\hat{H} = -t\sum_{\langle ij\rangle}\left(b_i^{+}b_j + b_j^{+}b_i\right) - \mu\sum_i \hat{n}_i + \frac{U}{2}\sum_i \hat{n}_i(\hat{n}_i - 1)}$$

- b_i^{+}, b_i boson creation/annihilation operators on site i

  $\hat{n}_i := b_i^{+}b_i$ occupation-number operator

  boson commutator relations: $\left([\hat{A},\hat{B}] := \hat{A}\hat{B} - \hat{B}\hat{A} \right)$

  $$[b_i, b_j] = [b_i^{+}, b_j^{+}] = 0 \qquad [b_i, b_j^{+}] = \delta_{ij}$$

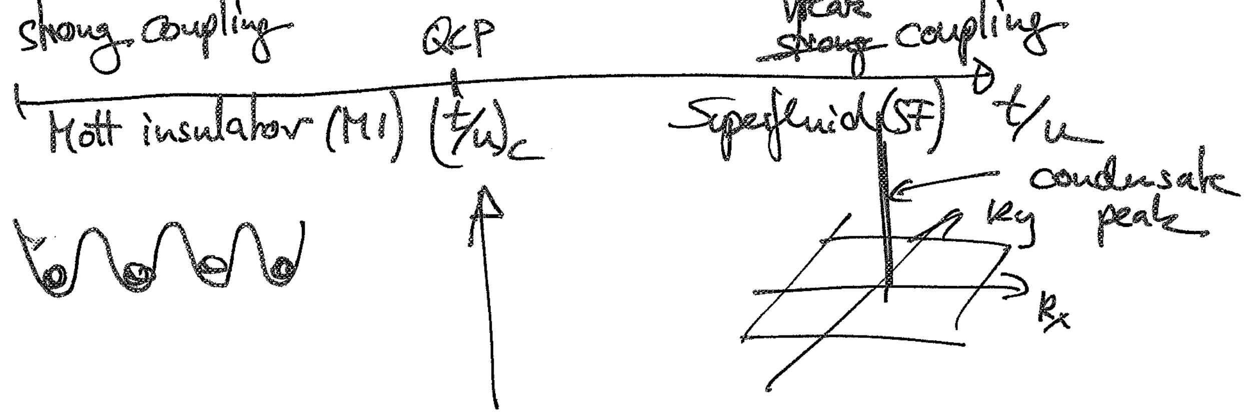
- t hopping amplitude between nearest-neighbor sites on a d-dim. hypercubic lattice

  ($\langle i,j\rangle$ denotes NN bonds)

  μ chemical potential (controls filling)

  U on-site repulsion between bosons

- Quantum-Phase Transition



location will depend on chemical potential μ

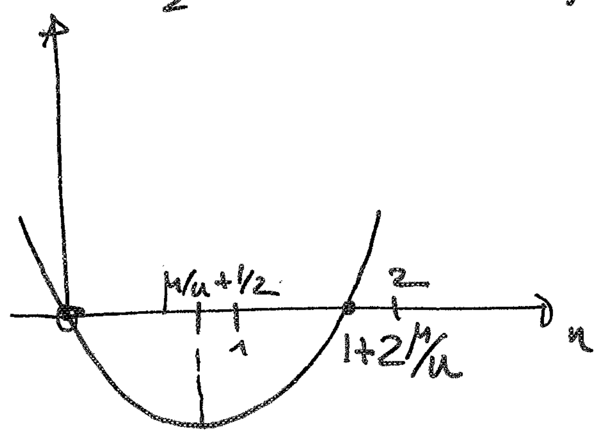
- atomic limit : $t/U \to 0$

$$\to \hat{H}_0 = -\mu \sum_i \hat{n}_i + \frac{U}{2} \sum_i \hat{n}_i(\hat{n}_i - 1)$$

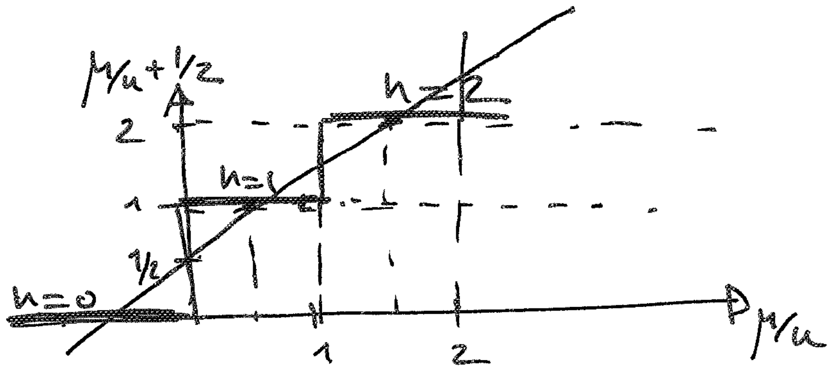
- diagonal in occupation-number basis
- no mixing of diffrent lattice sites

We obtain the ground state by minimizing
$\epsilon_0(n) = -\mu n + \frac{U}{2} n(n-1)$ with $n \in \{0, 1, \dots\}$
the number of bosons per site

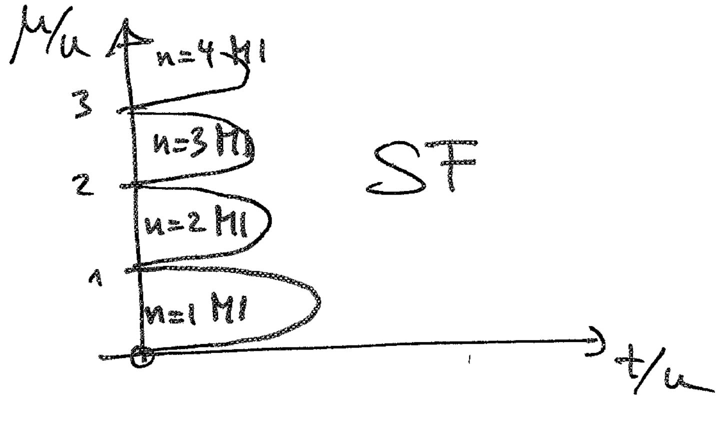
$$\epsilon_0(n) = \frac{U}{2} n(n - 1 - 2\mu/U)$$



$\epsilon_0(n)$ is minimized by the integer closest to $\mu/U + 1/2$



- We expect a phase diagram which looks like this



3.2. Coherent States for Bosons

- Our goal is to perform the quantum-to-classical mapping for the BH model

recipe: $$Z = \mathrm{Tr}\, e^{-\beta \hat{H}} = \sum\!\!\!\!\!\!\int_{\Phi} \langle \Phi | e^{-\beta \hat{H}} | \Phi \rangle$$

+ $|\Phi\rangle = \prod_i |\phi_i\rangle$: product state over quantum states on lattice sites
+ „$\sum$" for discrete, „$\int$" for continuous basis
+ In principle we can use any complete or overcomplete basis of the Hilbertspace

Trotter trick: $\beta/N = \Delta\tau$

$$Z = \sum\!\!\!\!\!\!\int_{\Phi} \langle \Phi | e^{-\Delta\tau \hat{H}} \; e^{-\Delta\tau \hat{H}} \; e^{-\Delta\tau \hat{H}} \cdots e^{-\Delta\tau \hat{H}} | \Phi \rangle$$

$$1 = \sum\!\!\!\!\!\!\int_{\Phi_1} |\Phi_1\rangle\langle\Phi_1| \qquad 1 = \sum\!\!\!\!\!\!\int_{\Phi_2} |\Phi_2\rangle\langle\Phi_2|$$

- What is the best basis for interacting bosons?
  → we want $\langle \Phi_j | e^{-\Delta\tau \hat{H}} | \Phi_{j+1} \rangle$ to be easy to evaluate
- We can always bring the Hamiltonian into a form where b^+'s are left of b's (normal ordering)

Hubbard interaction:

$$H_U = \frac{U}{2}\sum_i \hat{n}_i(\hat{n}_i - 1) = \frac{U}{2}\sum_i b_i^+ b_i (b_i^+ b_i - 1)$$

$$= \frac{U}{2}\sum_i b_i^+ b_i b_i^+ b_i - \frac{U}{2}\sum_i b_i^+ b_i$$

$$= \frac{U}{2}\sum_i b_i^+ b_i^+ b_i b_i$$

$$b_i b_i^+ = 1 + b_i^+ b_i$$

→ Bose-Hubbard Hamiltonian in normal ordering

$$\hat{H} = -t \sum_{\langle ij \rangle} (b_i^+ b_j + b_j^+ b_i) - \mu \sum_i b_i^+ b_i + \frac{U}{2} \sum_i b_i^+ b_i^+ b_i b_i$$

- Ideal solution: basis of eigenstates of annihilation operators

Why? $\langle \Phi_j | e^{-\Delta\tau \hat{H}} | \Phi_{j+1} \rangle$

$$\hat{=} \langle \Phi_j | 1 - \Delta\tau \hat{H} | \Phi_{j+1} \rangle$$

leads to matrix elements of the form

$$\langle \Phi_j | b^+ b^+ \cdots b b | \Phi_{j+1} \rangle$$

if $|\Phi\rangle$ is an eigenstate of b_i we can replace b by the eigenvalue

Same here, since

$$\langle \Phi_j | b^+ = (b | \Phi_j \rangle)^+$$

- We can indeed construct such a basis! This basis consisting of eigenstates of annihilation operators is known as <u>coherent state basis</u>

- Look at a single site first and drop lattice index i for the moment

$$\boxed{|\phi\rangle := e^{\phi b^+} |0\rangle}$$

$|0\rangle$ vacuum state (no boson)

ϕ complex number $\phi \in \mathbb{C}$

Claim 1: $|\phi\rangle$ is an eigenstate of b, $\boxed{b|\phi\rangle = \phi|\phi\rangle}$

Proof: $b|\phi\rangle = b e^{\phi b^+}|0\rangle$

$$= b\sum_{n=0}^{\infty} \frac{1}{n!}(\phi b^+)^n |0\rangle$$

$$= \sum_{n=0}^{\infty} \frac{\phi^n}{n!} b(b^+)^n|0\rangle$$

$$\underset{b|0\rangle=0}{=} \sum_{n=1}^{\infty} \frac{\phi^n}{n!} b(b^+)^n |0\rangle$$

$$= \sum_{n=1}^{\infty} \frac{\phi^n}{n!}\left(n(b^+)^{n-1} - (b^+)^n b\right)|0\rangle$$

$(*)$ $[b,(b^+)^n] = n(b^+)^{n-1}$

$$\underset{b|0\rangle=0}{=} \sum_{n=1}^{\infty} \frac{\phi^n}{(n-1)!}(b^+)^{n-1}|0\rangle$$

$$= \phi\sum_{n=0}^{\infty} \frac{\phi^n}{n!}(b^+)^n|0\rangle$$

$$= \phi|\phi\rangle$$

We can proof $(*)$ by complete induction over n:

$n=1$: $[b,b^+] = 1$ ✓

$n\to n+1$: Assume $(*)$ is true for n, show that it then also true for $n+1$!

$$[b,(b^+)^{n+1}] = [b,(b^+)^n b^+]$$

$$= (b^+)^n \underbrace{[b,b^+]}_{=1} + [b,(b^+)^n]\, b^+$$

$$\underset{(*)\text{for } n}{=} (b^+)^n + n(b^+)^{n-1} b^+$$

$$= (b^+)^n + n(b^+)^n$$

$$= (n+1)(b^+)^n$$ ✓

Claim 2: $\boxed{\langle\phi| b^\dagger = \langle\phi|\phi^*}$

Proof: $\langle\phi| b^\dagger = (b|\phi\rangle)^\dagger$

$= (\phi|\phi\rangle)^\dagger$

$= \langle\phi|\phi^*$

Claim 3: The overlap of two coherent states is given by

$$\boxed{\langle\phi|\phi'\rangle = e^{\phi^*\phi'}}$$

Proof: $\langle\phi|\phi'\rangle = \langle 0| e^{\phi^* b} e^{\phi' b^\dagger}|0\rangle$

$$= \sum_{n=0}^{\infty}\sum_{m=0}^{\infty} \frac{(\phi^*)^n}{n!}\frac{(\phi')^m}{m!} \underbrace{\langle 0| b^n (b^\dagger)^m |0\rangle}_{= \delta_{m,n}\langle 0|b^n (b^\dagger)^n|0\rangle}$$

$$= \sum_{n=0}^{\infty} \frac{(\phi^*\phi')^n}{(n!)^2} \langle 0| b^n (b^\dagger)^n |0\rangle$$

$$= \sum_{n=0}^{\infty} \frac{(\phi^*\phi')^n}{n!} \underbrace{\langle n|n\rangle}_{=1} = e^{\phi^*\phi'}$$

$(b^\dagger)^n|0\rangle = \sqrt{n!}\,|n\rangle$

$\langle 0|b^n = \sqrt{n!}\langle n|$

Note: ∘ For $\phi \neq \phi'$ the overlap is non-zero which means that the two coherent states are not orthogonal.
This however is not surprising, since the coherent state basis is an overcomplete basis

occupation number basis:
$\langle n|m\rangle = \delta_{mn}$
discrete, countable number of states

coherent states:
$\langle\phi|\phi'\rangle = e^{\phi^*\phi'}$
continuous, overcomplete

- We haven't normalized the coherent states,

$$\langle\phi|\phi\rangle = e^{|\phi|^2} \neq 1$$

We can easily normalize, but it is not important ($|\tilde{\phi}\rangle := e^{-\frac{1}{2}|\phi|^2}|\phi\rangle$)

Claim 4: The completeness relation is given by

$$\boxed{1 = \int \frac{d\phi^* d\phi}{2\pi i} e^{-\phi^*\phi} |\phi\rangle\langle\phi|} \qquad \phi^*\phi = |\phi|^2$$

Proof: $\phi = re^{i\theta}$, $\phi^* = re^{-i\theta}$

$$\int \frac{d\phi^* d\phi}{2\pi i} e^{-|\phi|^2}|\phi\rangle\langle\phi| = \frac{1}{\pi}\int_0^\infty r\,dr \int_0^{2\pi} d\theta\, e^{-r^2} |\phi\rangle\langle\phi|$$

$$= \frac{1}{\pi}\sum_{n,m=0}^{\infty} \frac{1}{\sqrt{n!}\sqrt{m!}} \int_0^\infty r\,dr \int_0^{2\pi} d\theta\, e^{-r^2} r^{n+m} e^{i(n-m)\theta} |n\rangle\langle m|$$

$$|\phi\rangle = e^{\phi b^+}|0\rangle = \sum_{n=0}^{\infty} \frac{1}{n!}\phi^n (b^+)^n|0\rangle = \sum_{n=0}^{\infty}\frac{1}{\sqrt{n!}}\phi^n|n\rangle = \sum_{n=0}^{\infty}\frac{r^n}{\sqrt{n!}}e^{in\theta}|n\rangle$$

$$= \sum_{n=0}^{\infty} \frac{1}{n!}\int_0^\infty dr\, 2r\, e^{-r^2} r^{2n} |n\rangle\langle n|$$

$$\underset{\substack{z=r^2 \\ dz = 2r\,dr}}{=} \sum_{n=0}^{\infty}\frac{1}{n!} \underbrace{\int_0^\infty dz\, e^{-z} z^n}_{=\Gamma(n+1) = n!} |n\rangle\langle n|$$

$$= \sum_{n=0}^{\infty} |n\rangle\langle n| = 1$$

- The results of this section can be easily generalized to the product states of coherent states on different lattice sites:

$$\boxed{|\Phi\rangle := |\phi_1, \phi_2, \dots\rangle = \prod_i |\phi_i\rangle_i}$$

$$|\Phi\rangle = e^{\sum_i \phi_i b_i^\dagger}|0\rangle, \qquad b_i|\Phi\rangle = \phi_i|\Phi\rangle,$$

$$\langle\Phi|\Phi'\rangle = e^{\Phi^*\Phi'} = e^{\sum_i \phi_i^*\phi_i'}$$

$$1 = \int \frac{d\Phi^* d\Phi}{2\pi i} e^{-\Phi^*\Phi}|\Phi\rangle\langle\Phi|$$

$$= \left(\prod_i \int \frac{d\phi_i^* d\phi_i}{2\pi i}\right) e^{-\sum_i \phi_i^*\phi_i}|\phi_1\phi_2\cdots\rangle\langle\phi_1,\phi_2\dots|$$

3.3. Coherent State Path Integral Representation of Partition Function

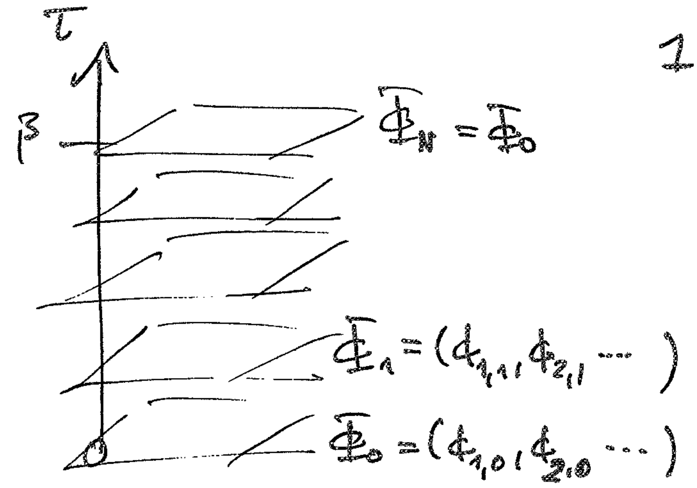
We use the coherent state basis $|\Phi\rangle$ to calculate the trace and resolve the identities in the trotter formula:

$$Z = \mathrm{Tr}\, e^{-\beta\hat{H}} = \int \frac{d\Phi^* d\Phi}{2\pi i}\langle\Phi|e^{-\beta\hat{H}}|\Phi\rangle$$

$$\underset{\Delta\tau=\beta/N}{=} \int \frac{d\Phi_0^* d\Phi_0}{2\pi i}\langle\Phi_0|e^{-\Delta\tau\hat{H}}\ e^{-\Delta\tau\hat{H}}\ e^{-\Delta\tau\hat{H}}\cdots e^{-\Delta\tau\hat{H}}|\Phi_0\rangle$$

$$1 = \int \frac{d\Phi_1^* d\Phi_1}{2\pi i} e^{-\Phi_1^*\Phi_1}|\Phi_1\rangle\langle\Phi_1|$$

$$1 = \int \frac{d\Phi_2^* d\Phi_2}{2\pi i} e^{-\Phi_2^*\Phi_2}|\Phi_2\rangle\langle\Phi_2|$$



$$Z = \left(\prod_\alpha \int \frac{d\Phi_\alpha^* d\Phi_\alpha}{2\pi i}\right)\left(\prod_\alpha \langle \Phi_\alpha | e^{-\Delta\tau \hat{H}} | \Phi_{\alpha+1}\rangle\right)\left(\prod_\alpha e^{-\Phi_\alpha^* \Phi_\alpha}\right)$$

Evaluation of matrix elements:

$$\langle \Phi_\alpha | e^{-\Delta\tau \hat{H}} | \Phi_{\alpha+1}\rangle \approx \langle \Phi_\alpha | 1 - \Delta\tau \hat{H} | \Phi_{\alpha+1}\rangle$$

$$\stackrel{(*)}{=} \left[1 - \Delta\tau\, H(\Phi_\alpha^*, \Phi_{\alpha+1})\right] \underbrace{\langle \Phi_\alpha | \Phi_{\alpha+1}\rangle}_{= e^{\Phi_\alpha^* \Phi_{\alpha+1}}}$$

$$\approx e^{-\Delta\tau H(\Phi_\alpha^*, \Phi_{\alpha+1}) + \Phi_\alpha^* \Phi_{\alpha+1}}$$

(*) $$\langle \Phi_\alpha | \hat{H} | \Phi_{\alpha+1}\rangle = \langle \Phi_\alpha | -t\sum_{\langle ij\rangle}(b_i^+ b_j + b_j^+ b_i) - \mu \sum_i b_i^+ b_i + \frac{U}{2}\sum_i b_i^+ b_i^+ b_i b_i | \Phi_{\alpha+1}\rangle$$

$$= \langle \Phi_\alpha | \Phi_{\alpha+1}\rangle \underbrace{\left(-t\sum_{\langle ij\rangle}(\phi_{i\alpha}^* \phi_{j,\alpha+1} + \phi_{j\alpha}^* \phi_{i,\alpha+1}) - \mu \sum_i \phi_{i\alpha}^* \phi_{i,\alpha+1} + \frac{U}{2}\sum_i (\phi_{i\alpha}^*)^2 \phi_{i,\alpha+1}^2\right)}_{H(\Phi_\alpha^*, \Phi_{\alpha+1})}$$

$$\rightarrow \quad Z = \left(\prod_\alpha \int \frac{d\Phi_\alpha^* d\Phi_\alpha}{2\pi i}\right) e^{\sum_\alpha \left\{ \Phi_\alpha^* (\Phi_{\alpha+1} - \Phi_\alpha) - \Delta\tau H(\Phi_\alpha^*, \Phi_{\alpha+1})\right\}}$$

Finally, we take the continuum limit in imaginary time direction:

$$\Phi_\alpha \rightarrow \Phi(\tau) \quad , \quad \sum_\alpha \Delta\tau \rightarrow \int_0^\beta d\tau$$

$$\frac{\Phi_{\alpha+1} - \Phi_\alpha}{\Delta\tau} \rightarrow \partial_\tau \Phi(\tau)$$

$$\rightarrow \quad Z = \int \mathcal{D}[\Phi^*, \Phi]\, e^{-S[\Phi^*, \Phi]}$$

$$S[\Phi^*, \Phi] = \int_0^\beta d\tau \left\{ -\Phi^*(\tau)\partial_\tau \Phi(\tau) + H(\Phi^*(\tau), \Phi(\tau))\right\}$$

$$\boxed{\begin{aligned} S = \sum_i \int_0^\beta d\tau \left\{ -\phi_i^*(\tau)\,\partial_\tau \phi_i(\tau) - \mu\, |\phi_i(\tau)|^2 + \frac{u}{2} |\phi_i(\tau)|^4 \right\} \\ - t \sum_{\langle ij \rangle} \int_0^\beta d\tau \left(\phi_i^*(\tau)\, \phi_j(\tau) + \phi_j^*(\tau)\phi_i(\tau) \right) \end{aligned}}$$

- Quantum field theory with complex fields $\phi_i(\tau) \in \mathbb{C}$
  → corresponds to $N=2$ real components
- We could also take the continuum limit in spatial directions. Hopping term will produce spatial gradient term $|\nabla \phi(\underline{r},\tau)|^2$

3.4. Hubbard – Stratonovich Transformation

- Mott - Insulator forms because of strong local repulsions U → strong coupling
- In the derived action $S[\phi^*,\phi]$, the interaction vertex ($|\phi|^4$ – term) is proportional to U and not expected to be small close to the MI - SF transition
- Goal: Find a <u>dual description</u> in which the „interaction vertex" $\sim |\psi|^4$ is small

  → Strong coupling expansion around the atomic limit ($t/u = 0$) in powers of t/u

- We decouple the off - diagonal (in the lattice - site index) hopping term by a <u>Hubbard - Stratonovich transformation</u>

<u>Step 1:</u> Introduce auxillary fields $\psi_i(\tau) \in \mathbb{C}$

$$Z = \int \mathcal{D}[\phi^*, \phi, \psi^*, \psi]\, e^{-(S_\phi^{(0)} + S_\psi^{(0)} + S_{\phi\psi})}$$

$$S_\phi^{(0)} = \int_0^\beta d\tau \sum_i \left\{ \phi_i^* \partial_\tau \phi_i - \mu |\phi_i|^2 + \frac{U}{2} |\phi_i|^4 \right\}$$

$$S_\psi^{(0)} = \int_0^\beta d\tau \sum_{ij} \psi_i^* (T^{-1})_{ij} \psi_j$$

$$S_{\phi\psi} = + \int_0^\beta d\tau \sum_i (\phi_i^* \psi_i + \phi_i \psi_i^*)$$

- T^{-1} denotes the inverse of the hopping matrix T ($T_{ij} = t$ for (i,j) NN and $T_{ij} = 0$ for all other bonds)
- We have simply rewritten the partition function Z. Integrating over the auxillary fields ψ^*, ψ, we obtain the original action $S[\phi^*, \phi] = S_\phi^{(0)} + \int_0^\beta d\tau \sum_{ij} \phi_i^* T_{ij} \phi_j$ (We only have to use the rules of Gaussian integration, completing the square etc...)

<u>Step 2:</u> We take the trace over (integrate over) the original bosonic fields ϕ^*, ϕ

$\rightarrow$ action $S[\psi^*, \psi]$ in terms of new fields only

$$Z = \int \mathcal{D}[\psi^*, \psi]\, e^{-S_\psi^{(0)}} \underbrace{\int \mathcal{D}[\phi^*, \phi]\, e^{-S_\phi^{(0)}}\, e^{-S_{\phi\psi}}}_{= Z_0 \langle e^{-S_{\phi\psi}} \rangle_0}$$

$$\left(Z_0 = \int \mathcal{D}[\phi^*, \phi]\, e^{-S_\phi^{(0)}} \right)$$

- $\langle e^{-S_{\phi\psi}} \rangle_0$ will depend only on ψ^*, ψ since we integrated over ϕ^*, ϕ

$$\rightarrow \quad Z = Z_0 \int \mathcal{D}[\psi^*,\psi] \, e^{-(S_\psi^{(0)} + S_\psi')}$$

$$S_\psi^{(0)} = \int_0^\beta d\tau \sum_i \psi_i^* (T^{-1})_{ij} \psi_j$$

$$\boxed{S_\psi'} = -\ln \langle e^{-S_{\phi\psi}} \rangle_0$$

$$\left(e^{-S_\psi'} \stackrel{!}{=} \langle e^{-S_{\phi\psi}} \rangle_0 \right) \quad = -\ln \left\langle \exp\left[-\int_0^\beta d\tau \sum_i \left(\phi_i^* \psi_i + \phi_i \psi_i^* \right) \right] \right\rangle_0$$

$$= -\ln \left\langle T_\tau \exp\left[-\int_0^\beta d\tau \sum_i \left(\psi_i(\tau) \, b_i^\dagger(\tau) + \psi_i^*(\tau) \, b(\tau) \right) \right] \right\rangle_0$$

- In the last step, we have re-expressed the average over bosonic fields $\phi_i(\tau)$ as an operator average, where

$$\boxed{b_i^\dagger(\tau) = e^{\hat{H}_0 \tau} \, b_i^\dagger \, e^{-\hat{H}_0 \tau}}$$

- T_τ is the time ordering operator, defined as

$$T_\tau \left(\hat{A}(\tau_1) \hat{B}(\tau_2) \right) = \begin{cases} \hat{A}(\tau_1) \hat{B}(\tau_2) & \text{if } \tau_1 \geq \tau_2 \\ \hat{B}(\tau_2) \hat{A}(\tau_1) & \text{if } \tau_1 < \tau_2 \end{cases}$$

- $\langle \dots \rangle_0$ denotes the average with respect to the local on-site Hamiltonian

$$\hat{H}_0 = \sum_i \left(\frac{U}{2} \hat{n}_i (\hat{n}_i - 1) - \mu \hat{n}_i \right) = \sum_i \hat{h}_i$$

$$\hat{h} = \frac{U}{2} \hat{n}(\hat{n} - 1) - \mu \hat{n}$$

Step 3: Expansion of S_ψ' up to the desired order in ψ

$$S_\psi' = -\ln\Big(1 + \frac{1}{2}\Big\langle T_\tau\Big[\int_0^\beta d\tau \sum_i \big(\psi_i(\tau) b_i^+(\tau) + h.c.\big)\Big]^2\Big\rangle_0 + \frac{1}{4!}\Big\langle T_\tau\Big[\int_0^\beta d\tau \sum_i \big(\psi_i(\tau) b_i^+(\tau) + h.c.\big)\Big]^4\Big\rangle_0 + \dots\Big)$$

$$= -\frac{1}{2}\Big\langle T_\tau\Big[\int_0^\beta d\tau \sum_i \big(\psi_i(\tau) b_i^+(\tau) + h.c\big)\Big]^2\Big\rangle_0$$

$$- \frac{1}{4!}\Big\langle T_\tau\Big[\int_0^\beta d\tau \sum_i \big(\psi_i(\tau) b_i^+(\tau) + h.c.\big)\Big]^4\Big\rangle_0$$

$$+ \frac{1}{8}\Big\langle T_\tau\Big[\int_0^\beta d\tau \sum_i \big(\psi_i(\tau) b_i^+(\tau) + h.c.\big)\Big]^2\Big\rangle_0^2 + \dots$$

$$= S_\psi'^{(2)} + S_\psi'^{(4)} + \dots$$

Evaluation of quadratic terms $S_\psi'^{(2)}$:

$$S_\psi'^{(2)} = -\int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \sum_{ij} \psi_i^*(\tau_1)\psi_j(\tau_2)\langle T_\tau b_i(\tau_1) b_j^+(\tau_2)\rangle_0$$

$$\underset{\substack{\tau=\tau_1 \\ \tau'=\tau_1-\tau_2}}{=} -\int d\tau \int_{-\beta}^{\beta} d\tau' \sum_{ij} \psi_i^*(\tau)\psi_j(\tau-\tau')\underbrace{\langle T_\tau b_i(\tau) b_i^+(\tau-\tau')\rangle_0}_{=\langle T_\tau b_i(\tau') b_i^+(0)\rangle_0}\delta_{ij}$$

$$\simeq -\int d\tau \int_{-\beta}^{\beta} d\tau' \sum_i \psi_i^*(\tau)\Big(\psi_i(\tau) - \partial_\tau\psi_i(\tau)\cdot\tau' + \frac{1}{2}\partial_\tau^2\psi_i(\tau)\tau'^2\Big)\langle T_\tau b_i(\tau') b_i^+(0)\rangle_0$$

$$\rightarrow \boxed{S_\psi'^{(2)} = \int_0^\beta d\tau \sum_i \left(K_1 \psi_i^* \partial_\tau \psi_i + K_2 |\partial_\tau \psi_i|^2 + g^{(0)} |\psi_i|^2 \right)}$$

$$g^{(0)} = - \int_{-\beta}^{\beta} d\tau \, \langle T_\tau \, b_i(\tau) b_i^+(0) \rangle_0$$

$$K_1 = + \int_{-\beta}^{\beta} d\tau \, \tau \, \langle T_\tau \, b_i(\tau) \, b_i^+(0) \rangle_0$$

$$K_2 = - \frac{1}{2} \int_{-\beta}^{\beta} d\tau \, \tau^2 \langle T_\tau \, b_i(\tau) b_i^+(0) \rangle_0$$

← Fourier transform of the single particle Green's function $G^{(0)}_{(\tau_1-\tau_2)} = - \langle T_\tau \, b_i(\tau_1) \, b_i^+(\tau_2) \rangle_0$ in the zero-frequency limit

This can easily be calculated since $\hat{H}_0$ is diagonal in the occupation number basis, $\hat{n}_i |n_i\rangle = n_i |n_i\rangle$. We can also drop the site index, since everything is diagonal in the site index.

$$\hat{h} = \frac{U}{2} \hat{n}(\hat{n}-1) - \mu \hat{n} \quad \longrightarrow \quad \text{eigenvalues} \quad \boxed{\epsilon(n) = \frac{U}{2} n(n-1) - \mu n}$$

Calculate single-particle Green's function

$$G^{(0)}(\tau_1-\tau_2) = - \langle T_\tau \, b(\tau_1) b^+(\tau_2) \rangle_0$$
$$= - \langle T_\tau \, b(\tau_1-\tau_2) \, b^+(0) \rangle_0$$

$\underline{\tau_1 \geq 2:}$

$$G^0(\tau_1-\tau_2) = - \langle b(\tau_1) b^+(\tau_2) \rangle_0$$
$$= - \frac{1}{Z_0} \sum_n e^{-\beta \epsilon(n)} \langle n | \, b(\tau_1) \, b^+(\tau_2) | n \rangle$$

$$= -\frac{1}{Z_0}\sum_n e^{-\beta\epsilon(n)} \langle n| e^{\hat H_0\tau_1} b\, e^{-\hat H_0 \tau_1} e^{\hat H_0\tau_2} b^+ e^{-\hat H_0\tau_2}|n\rangle$$

$$= -\frac{1}{Z_0}\sum_n e^{-\beta\epsilon(n)} e^{(\tau_1-\tau_2)\epsilon(n)} \langle n| b\, e^{-\hat H_0(\tau_1-\tau_2)} \underbrace{b^+|n\rangle}_{=\sqrt{n+1}\,|n+1\rangle}$$

$$= -\frac{1}{Z_0}\sum_n \sqrt{n+1}\, e^{-\beta\epsilon(n)} e^{-(\tau_1-\tau_2)(\epsilon(n+1)-\epsilon(n))} \quad \underbrace{\langle n|b|n+1\rangle}_{=\sqrt{n+1}}$$

$$= -\frac{1}{Z_0}\sum_n (n+1)\, e^{-\beta\epsilon(n)} e^{-(\tau_1-\tau_2)\epsilon_+(n)}$$

$$\boxed{\epsilon_+(n) := \epsilon(n+1) - \epsilon(n)}$$

$\tau_1 < \tau_2$: $\quad G^{(0)}(\tau_1-\tau_2) = -\langle b^+(\tau_2)\, b(\tau_1)$

$$= -\frac{1}{Z_0}\sum_n e^{-\beta\epsilon(n)} e^{-(\tau_1-\tau_2)\epsilon(n)} \langle n| b^+ e^{\hat H_0(\tau_1-\tau_2)} \underbrace{b\,|n\rangle}_{\sqrt{n}\,|n-1\rangle}$$

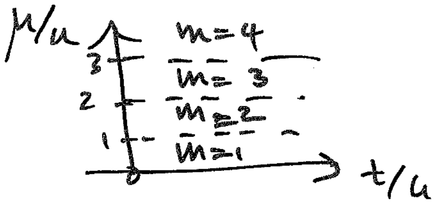
$$= -\frac{1}{Z_0}\sum_n \sqrt{n}\, e^{-\beta\epsilon(n)} e^{(\tau_1-\tau_2)(\epsilon(n-1)-\epsilon(n))} \quad \underbrace{\langle n|b^+|n-1\rangle}_{=\sqrt{n}}$$

$$= -\frac{1}{Z_0}\sum_n n\, e^{-\beta\epsilon(n)} e^{(\tau_1-\tau_2)\epsilon_-(n)}$$

$$\boxed{\epsilon_-(n) := \epsilon(n-1) - \epsilon(n)}$$

Low-temperature approximation:

For $T \ll U$ ($\beta U \gg 1$), the averages given by the above sums are dominated by the term $n = m$, with m the integer minimizing $\epsilon(n)$.



All the other terms will be exponentially small compared to the $n = m$ term.

$$\rightarrow \boxed{G^{0}(\tau=\tau_1-\tau_2) \simeq -\begin{cases}(m+1)\, e^{-\epsilon_+(m)\tau} & (\tau\geq 0)\\ m\; e^{\epsilon_-(m)\tau} & (\tau<0)\end{cases}}$$

We calculate the Fourier transform in the zero-frequency limit:

$$\boxed{\mathcal{G}^{(0)}} = \int_{-\beta}^{\beta} d\tau \; G^{0}(\tau)$$

$$= -m\int_{-\beta}^{0} d\tau\; e^{\epsilon_-(m)\tau} - (m+1)\int_{0}^{\beta} d\tau\; e^{-\epsilon_+(m)\tau}$$

$$= -\frac{m}{\epsilon_-(m)}\left(1-e^{-\beta\epsilon_-(m)}\right) + \frac{m+1}{\epsilon_+(m)}\left(e^{-\beta\epsilon_+(m)}-1\right)$$

$$\underset{\substack{\epsilon_\pm(m)>0\\ T\to 0}}{\simeq} \boxed{-\left(\frac{m}{\epsilon_-(m)}+\frac{m+1}{\epsilon_+(m)}\right)}$$

There is a simple trick to immediately obtain K_1, K_2.

Explicit form of $\epsilon_+(m), \epsilon_-(m)$:

$$\epsilon_\pm(m) = \epsilon(m\pm 1)-\epsilon(m) = \begin{cases} mU-\mu \\ (1-m)U+\mu\end{cases}$$

$$\rightarrow G^{(0)}(\tau) = -\begin{cases}(m+1)\, e^{-(mU-\mu)\tau} & (\tau\geq 0)\\ m\; e^{((1-m)U+\mu)\tau} & (\tau<0)\end{cases}$$

$$\rightarrow \tau G^{(0)}(\tau) = \frac{\partial G^{(0)}}{\partial\mu}, \quad \tau^2 G^{(0)}(\tau) = \frac{\partial^2 G^{(0)}}{\partial\mu^2}$$

$$\Rightarrow \boxed{K_1} = -\int_{-\beta}^{\beta} d\tau\; \tau\, G^{(0)}(\tau) = -\frac{\partial}{\partial\mu}\int_{-\beta}^{\beta} G^{(0)}(\tau) = \boxed{-\frac{\partial\mathcal{G}^{(0)}}{\partial\mu}}$$

$$\boxed{K_2} = \frac{1}{2}\int_{-\beta}^{\beta} d\tau\; \tau^2\, G^{(0)}(\tau) = \boxed{\frac{1}{2}\frac{\partial^2\mathcal{G}^{(0)}}{\partial\mu^2}}$$

- The evaluation of the quartic terms yields

$$\boxed{S_\psi'^{(4)} = H \int_0^\beta d\tau \sum_i |\psi_i|^4}$$

where the coefficient is related to the connected parts of the two-particle Green's function in the static limit. The calculation of

$$G^{\mathrm{II}}(\tau_1,\tau_2,\tau_3,\tau_4) = \langle T_\tau\, b(\tau_1)\, b(\tau_2)\, b^+(\tau_3)\, b^+(\tau_4)\rangle_0$$

is a bit tedious but straightforward.

→ for every possible time ordering, simply insert identities $1 = \sum_n |n\rangle\langle n|$ and evaluate the resulting products of matrix elements of bosonic creation and annihilation operators. [see K. Sengupta and N. Dupuis, Phys. Rev. A 71, 033629 (2005) for details]

Result:

$$\boxed{H = \left(\frac{m}{\epsilon_-(m)} + \frac{m+1}{\epsilon_+(m)}\right)\left(\frac{m}{\epsilon_-^2(m)} + \frac{m+1}{\epsilon_+^2(m)}\right) - \frac{m(m-1)}{\epsilon_-^2(m)\,\epsilon_{-2}(m)} - \frac{(m+1)(m+2)}{\epsilon_+^2(m)\,\epsilon_{+2}(m)}}$$

turns out that $H > 0$ for all μ, u and m

$$\left(\epsilon_{\pm 2} := \epsilon(m \pm 2) - \epsilon(m)\right)$$

We have derived the action $S[\psi^*,\psi]$ in the new complex fields ψ^*, ψ:

$$\boxed{\begin{aligned} S[\psi^*,\psi] &= S_\psi^{(0)} + S_\psi' \\ &= \int_0^\beta d\tau \sum_i \left\{ J^{(0)} |\psi_i|^2 + K_1 \psi_i^* \partial_\tau \psi + K_2 |\partial_\tau \psi_i|^2 + H |\psi_i|^4 \right\} \\ &\quad + \int_0^\beta d\tau \sum_{ij} (T^{-1})_{ij}\, \psi_i^* \psi_j \end{aligned}}$$

- Continuum limit and spatial gradient expansion
  $\to \psi = \psi(\underline{r}, \tau)$

The hopping matrix T with $T_{ij} = t$ for (i,j) NN, $T_{ij} = 0$ for all other (ij) is difficult to invert. However, we are only interested in the long-wavelength behavior

$$\int d\tau \sum_{ij} T_{ij} \phi_i^* \phi_j = t \int d\tau \sum_{\langle ij \rangle} (\phi_i^* \phi_j + c.c.)$$

$$= \int d\tau \int_k \left(2t \sum_{\alpha=1}^{d} \cos k_\alpha\right) \phi_k^* \phi_k$$

$$\underset{\text{small } k}{\simeq} \int d\tau \; t(z - k^2) \phi_k^* \phi_k$$

$\boxed{z = 2d}$ coordination number of hypercubic lattice

$\to$ dual action

$$S_\psi^{(0)} \simeq \int d\tau \int_k \frac{1}{t(z-k^2)} \psi_k^* \psi_k$$

$$\underset{\text{small } k}{\simeq} \int d\tau \int_k \Big(\underbrace{\frac{1}{zt}}_{|\psi|^2} + \underbrace{\frac{1}{z^2 t} k^2}_{|\nabla\psi|^2} \Big) \psi_k^* \psi_k$$

$\to$
$$\boxed{S[\psi^*, \psi] = \int d\tau \int d^d r \left\{ K_1 \psi^* \partial_\tau \psi + K_2 |\partial_\tau \psi|^2 + K_3 |\nabla \psi|^2 + R |\psi|^2 + H |\psi|^4 \right\}}$$

$$R = \frac{1}{zt} + \gamma^{(0)} = \frac{1}{zt} - \left(\frac{m+1}{\epsilon_+(m)} + \frac{m}{\epsilon_-(m)} \right)$$

$$K_1 = -\frac{\partial R}{\partial \mu}, \quad K_2 = \frac{1}{2} \frac{\partial^2 R}{\partial \mu^2}, \quad K_3 = \frac{1}{z^2 t}$$

H as given above

- $S[\psi^*, \psi]$ is the effective long-wavelength field theory for the Bose-Hubbard model in the strong-coupling regime $t \ll U$ (?)
- vertex H is of relative strength t/u
- What is the physical meaning of the fields ψ?

→ Look at the saddle point of $S[\phi^*, \phi, \psi^*, \psi]$:

$$0 = \frac{\delta S[\phi^*, \phi, \psi^*, \psi]}{\delta \psi_i^*} \quad \longrightarrow \quad \psi_i \sim \langle b_i \rangle$$

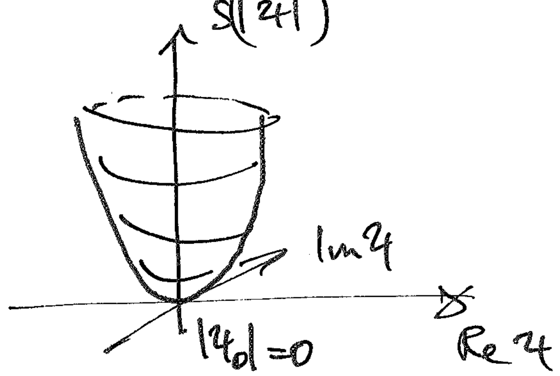
superfluid order parameter

3.5. Mean-Field Phase Diagram

We look for homogeneous configurations $\psi = \text{const}$ minimizing the action $S[\psi^*, \psi]$

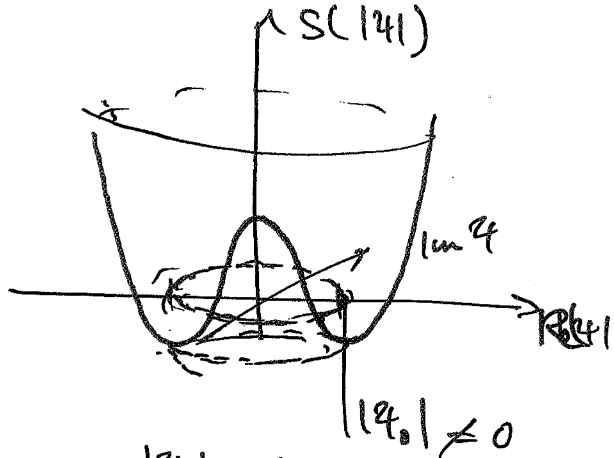
$$\rightarrow \quad S(|\psi|) = \beta V \left(R|\psi|^2 + H|\psi|^4 \right)$$

R > 0:



Mott insulator

R < 0:



$$|\psi_0| = \sqrt{-\frac{R}{2H}}$$

Superfluid

in SF, U(1) symmetry is spontaneously broken

- Superfluid order parameter vanishes as $|\psi_0| \sim (-R)^{1/2}$ as $R \to 0_-$

  → order-parameter exponent $\beta = 1/2$
  (This is characteristic of mean-field theory)

- In the Mott-insulator phase $(R>0)$, spectrum is gapped,

$$S[\psi^*,\psi] = \int d\tau \int d^d r \left\{ K_1 \psi^* \partial_\tau \psi + K_2 |\partial_\tau \psi|^2 + K_3 |\nabla\psi|^2 + R|\psi|^2 \right\}$$

$$= \int_{k\omega} \left(-iK_1\omega + K_2\omega^2 + K_3 k^2 + R\right) \psi^*_{(k\omega)} \psi(k,\omega)$$

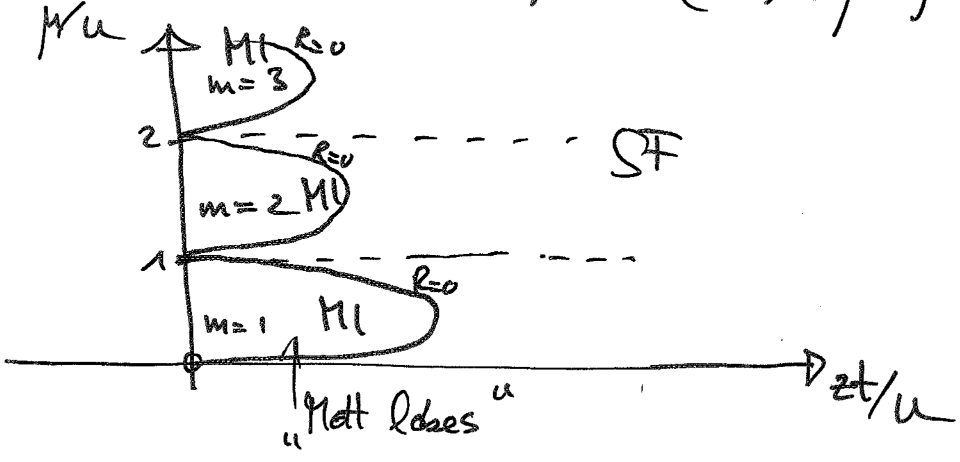
$$\psi(r,\tau) = \int_{k\omega} e^{-i(kr+\omega\tau)} \psi(k,\omega)$$

→ Correlations of superfluid order parameter decay exponentially at large distances

- We obtain the <u>mean-field phase boundary</u> from the condition $R=0$

$$R = R(t,\mu,U) = \frac{1}{zt} - \left(\frac{m+1}{\epsilon_+(m)} + \frac{m}{\epsilon_-(m)}\right)$$

$$= \frac{1}{zt} - \left(\frac{m+1}{mU-\mu} + \frac{m}{(1-m)U+\mu}\right)$$



- Mott insulator most stable for commensurate boson fillings (values of μ/u marking the tips of the Mott lobes)

$$\boxed{\left(\frac{\mu}{u}\right)_m = \sqrt{m(m+1)} - 1}$$

3.6. Dynamical Critical Exponent and Upper Critical Dimension

- In order to check the validity of the mean-field approximation, we have to determine the upper critical dimension D_u and compare with the effective dimension $D = d + z$

$D \geq D_u$: mean-field theory is valid and gives the right critical exponents

$\Leftrightarrow$ $d \geq D_u - z = d_u$

$\uparrow$ dimension of the quantum model

- What is the dynamical critical exponent z and the upper critical dimension d_u for the quantum-field theory describing the MI-SF transition?

$$S = \int d\tau \int d^d r \left\{ K_1 \psi^* \partial_\tau \psi + K_2 |\partial_\tau \psi|^2 + K_3 |\nabla \psi|^2 + R |\psi|^2 + H |\psi|^4 \right\}$$

quadratic action in the frequency / momentum domain

$$\left(\psi(\underline{r}, \tau) = \int_{\underline{k}\omega} \psi(\underline{k}, \omega)\, e^{-i(\underline{k}\underline{r} + \omega\tau)} \quad , \quad \int_{\underline{k}\omega} := \int \frac{d^d k}{(2\pi)^d} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \right)$$

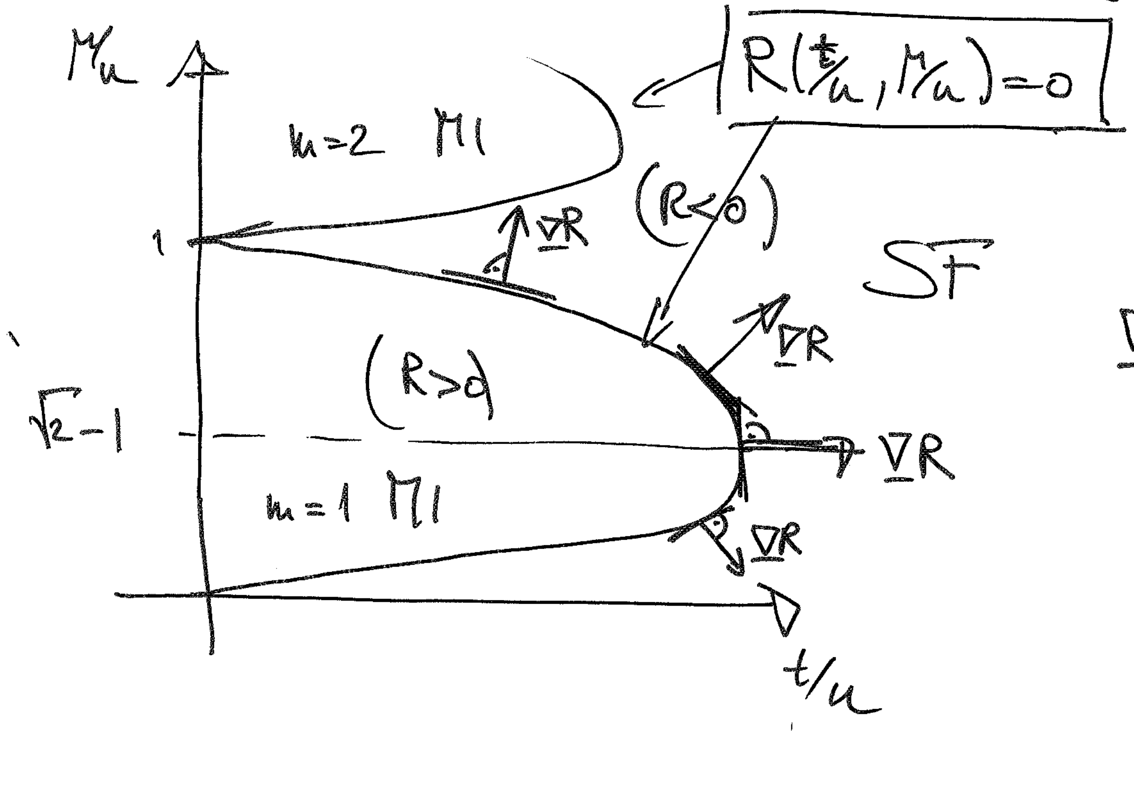
$$S_0 = \int_{\underline{k}\omega} \underbrace{\left(-i K_1 \omega + K_2 \omega^2 + K_3 k^2 + R \right)}_{\text{kernel } K(\underline{k}, \omega)} |\psi(\underline{k}, \omega)|^2$$

- We are interested in the long-wavelength behavior (small $\underline{k}$ and ω). Why have we kept the $\sim\omega^2$-term if there is an $\sim\omega$ term??

  → We have to make sure, that the prefactor K_1 is non-zero!

- Remember: $K_1 = -\frac{\partial R}{\partial \mu}$, $K_2 = \frac{1}{2} \frac{\partial^2 R}{\partial \mu^2}$

  K_1 and K_2 have a geometrical meaning. They are related to the slope and curvature of the mean-field phase boundary:



$$\underline{\nabla} R = \begin{pmatrix} \frac{\partial R}{\partial (t/u)} \\ \frac{\partial R}{\partial (\mu/u)} \end{pmatrix}$$

- We have to distinguish between <u>commensurate</u> and <u>incommensurate</u> fillings!

a) <u>Commensurate fillings</u> (tips of the Mott lobes)

$\underline{\nabla} R$ has no component in μ-direction

$$K_1 = \frac{\partial R}{\partial \mu} = 0$$

$\to$ Quantum Field Theory

$$\boxed{S_c = \int d\tau \int d^d r \left\{ K_2 |\partial_\tau \psi|^2 + K_3 |\nabla \psi|^2 + R|\psi|^2 + H |\psi|^4 \right\}}$$

<u>note:</u> K_2 ($\rightsquigarrow$ curvature) is always non-zero and has maximum at the tip

b) <u>incommensurate fillings</u>

$K_1 \neq 0$. In the small frequency limit we can neglect K_2. Dropping K_2 does not change the universality of the transition.

$$\boxed{S_{IC} = \int d\tau \int d^d r \left\{ K_1 \psi^* \partial_\tau \psi + K_3 |\nabla \psi|^2 + R|\psi|^2 + H |\psi|^4 \right\}}$$

- The dynamical critical exponent z can be obtained by setting the <u>kernel $\underline{K}(\underline{k}, \omega)$</u> for $R=0$ to zero. We expect $\boxed{\omega \sim k^z}$ as $k, \omega \to 0$

a) <u>commensurate fillings</u>

$$K_0(\underline{k}, \omega) = K_2 \omega^2 + K_3 k^2 = 0 \;\Rightarrow\; \omega \sim k$$

$$\Rightarrow \boxed{z = 1}$$

b) <u>incommensurate fillings</u>

$$K_0(\underline{k}, \omega) = -i K_1 \omega + K_3 k^2 \;\Rightarrow\; \omega \sim k^2 \;\Rightarrow\; \boxed{z = 2}$$

- To determine the upper critical dimension d_u, we rescale length and time by the correlation length ξ and the correlation time $\tau_c \sim \xi^z$ (only relevant length and time scales close to the transition)

$$\boxed{\tilde{r} = r/\xi} \qquad \boxed{\tilde{\tau} = \tau/\xi^z}$$

$$S_{IC} = \xi^{d+z} \int d\tilde{\tau} \int d^d\tilde{r} \left\{ \xi^{-z} K_1 \psi^* \partial_{\tilde{\tau}} \psi + \xi^{-2} K_3 |\tilde{\nabla}\psi|^2 + R|\psi|^2 + H|\psi|^4 \right\}$$

$$= \xi^{d+z-2} \int d\tilde{\tau} \int d^d\tilde{r} \left\{ \xi^{2-z} K_1 \psi^* \partial_{\tilde{\tau}} \psi + K_3 |\tilde{\nabla}\psi|^2 + R\xi^2 |\psi|^2 + H\xi^2 |\psi|^4 \right\}$$

$$= \int d\tilde{\tau} \int d^d\tilde{r} \left\{ \xi^{2-z} K_1 \tilde{\psi}^* \partial_{\tilde{\tau}} \tilde{\psi} + K_3 |\tilde{\nabla}\tilde{\psi}|^2 + R\xi^2 |\tilde{\psi}|^2 + H\xi^{4-(d+z)} |\tilde{\psi}|^4 \right\}$$

rescale fields to absorb prefactor

$$\boxed{\begin{aligned} \tilde{\psi} &= \psi/\xi^{-\lambda} \\ \lambda &= \frac{d+z-2}{2} \end{aligned}}$$

$$S_C = \int d\tilde{\tau} \int d^d\tilde{r} \left\{ \xi^{2-2z} K_2 |\partial_{\tilde{\tau}} \tilde{\psi}|^2 + K_3 |\tilde{\nabla}\tilde{\psi}|^2 + R\xi^2 |\tilde{\psi}|^2 + H\xi^{4-(d+z)} |\tilde{\psi}|^4 \right\}$$

- The form of the Kernel $K_0(\underline{k}, \omega)$ remains invariant if $z=2$ for incommensurate and $z=1$ for commensurate fillings

  (Consistent with previous result)

- After scale transformation, the interaction vertex is given by

$$\boxed{H' = H\,\xi^{4-(d+z)} = H\,\xi^{4-D}}$$

As we approach the transition, $\xi \to \infty$

$D > 4$: $H' \to 0$

vertex irrelevant at the transition, no influence on critical behavior, MF theory valid

$D < 4$: $H' \to \infty$

vertex is a relevant perturbation, MF theory gives wrong results

$\to D_u = 4 \iff \boxed{d_u = 4 - z = \begin{cases} 2 & \text{incommensurate} \\ 3 & \text{commensurate fillings} \end{cases}}$

E.g. in $d=3$ the mean-field theory adequately describes the MI-SF transition at incommensurate fillings but fails to describe the transition at the tips of the Mott lobes

- What is the physical reason why the universality of the transition is different at commensurate fillings?

$\to$ Suppression of density fluctuations. Phase fluctuations only, universality class of (3+1) dim. XY model