8 Quantum phase transitions of bosons and fermions

8.1 Bose-Hubbard model

Hamiltonian:

$$\hat{H} = -\underbrace{w}_{\text{hopping parameter}} \sum_{\langle ij \rangle} \left(\hat{b}_i^\dagger \hat{b}_j + \hat{b}_j^\dagger \hat{b}_i \right) - \underbrace{\mu}_{\text{chemical potential}} \sum_i \hat{n}_i + \frac{1}{2} \underbrace{U}_{\text{on-site potential}} \sum_i \hat{n}_i (\hat{n}_i - 1)$$

with $\hat{n}_i = \hat{b}_i^\dagger \hat{b}_i$ "number operator" and $[\hat{b}_i, \hat{b}_j^\dagger] = \delta_{ij}$.

Low-temperature phases ($k_B T \ll w$):

(a) $U/w = 0$: Bose-Einstein condensate, all particles in single-particle ground state (for $d > 2$)

(b) $0 < U/w \ll 1$: Superfluid, $\langle \hat{b}_i \rangle \neq 0$

(c) $U/w \gg 1$: Mott insulator for integer filling $\langle \hat{n} \rangle := \frac{1}{M} \sum_i \langle \hat{n}_i \rangle \in \mathbb{N}$

Superfluid, $\langle \hat{b}_i \rangle \propto \delta n$, for noninteger filling $\langle \hat{n} \rangle \in \mathbb{N} + \delta n$

Experimental realization:

- Ultracold atoms on an optical lattice 

$\updownarrow V \sim \frac{1}{w}$
- Magnons at a field-driven QCP ($\mu \leftrightarrow B$)

8.2 Bose-Hubbard model: Mean-field theory

Order parameters :

$$\Psi_B = z w \langle \hat{b}_i \rangle \quad , \quad \hat{b}_i = \frac{1}{zw} \Psi_B + \delta\hat{b}_i$$

$\uparrow$ lattice coordination numbers

Mean-field decoupling (kinetic term):

$$\hat{H}_{MF} = \sum_i \left[-\mu \hat{n}_i + \frac{1}{2} U \hat{n}_i (\hat{n}_i - 1) - \Psi_B^* \hat{b}_i - \Psi_B \hat{b}_i^\dagger \right] \qquad \text{local}$$

Possible phases:

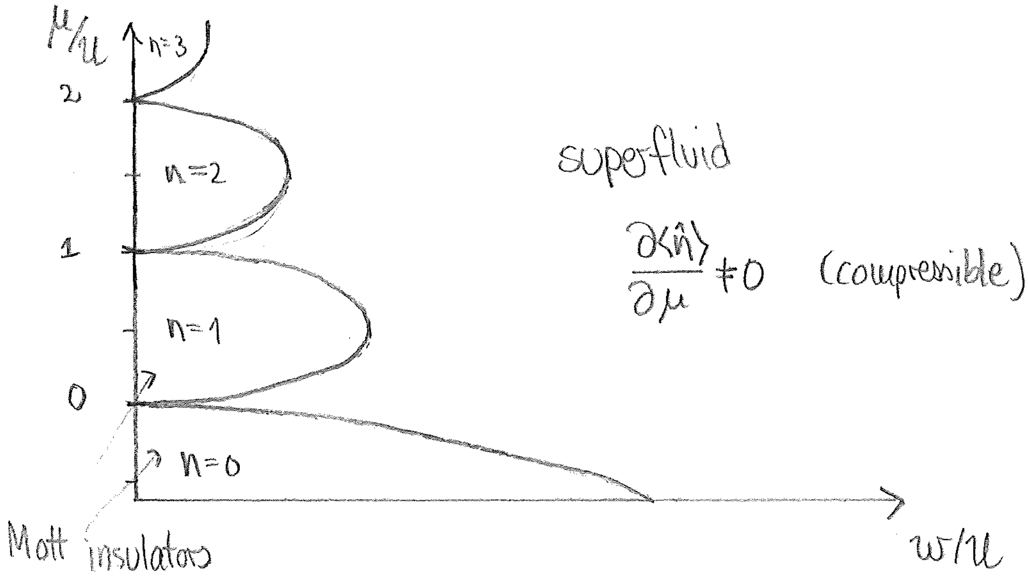
- $\Psi_B \neq 0$: superfluid , $U(1)$: $\Psi_B = |\Psi_B| e^{i\phi} \mapsto |\Psi_B| e^{i(\phi + \delta\phi)}$ spontaneously broken
- $\Psi_B = 0$: Mott insulator, bosons localized, no long-range order

Mean-field ground state for $w \to 0$:

$$\Psi_B = 0 \quad \text{with} \quad n = \langle \hat{n}_i \rangle = \begin{cases} 0 & \text{for } \mu/U < 0 \\ 1 & \text{for } 0 < \mu/U < 1 \\ 2 & \text{for } 1 < \mu/U < 2 \\ \vdots & \end{cases}$$

Remark: Ground state for finite w can be computed in standard QM perturbation theory (small w) or numerically

Mean-field phase diagram:



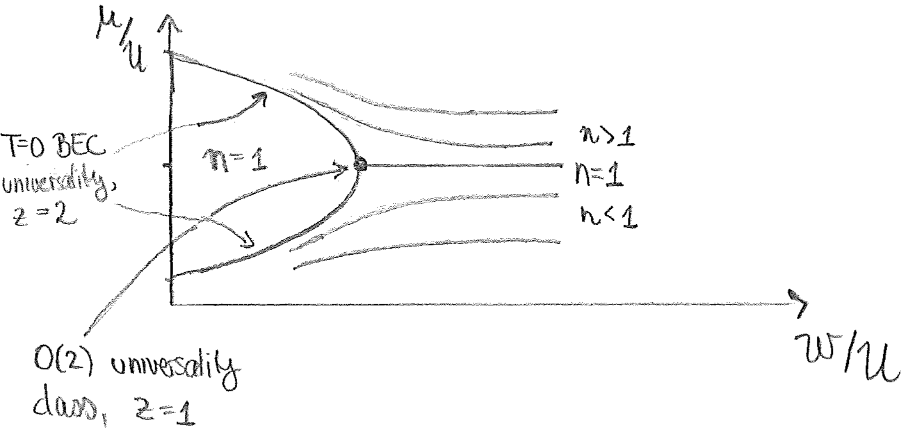
Superfluid: $\frac{\partial\langle\hat{n}\rangle}{\partial\mu} \neq 0$ (compressible)

Mott insulators: $\frac{\partial\langle\hat{n}\rangle}{\partial\mu} = 0$ (incompressible)

Remark: Phase diagram in qualitative agreement with quantum Monte Carlo simulations

8.3 Superfluid-insulator transition: Universality classes

Lines of constant density:



Coherent-state path integral:

$$Z_B = \int \mathcal{D}\Phi_i(\tau)\,\mathcal{D}\Phi_i^*(\tau)\; e^{-S_B[\Phi_i(\tau),\Phi_i^*(\tau)]}$$

with action:

$$S_B = \sum_i \int_0^{1/T} d\tau \left[\Phi_i^* \frac{\partial \Phi_i}{\partial \tau} - \mu \Phi_i^*\Phi_i + \frac{1}{2} U \Phi_i^*\Phi_i (\Phi_i^*\Phi_i - 1) \right]$$

$$- w \sum_{\langle ij \rangle} \int_0^{1/T} d\tau \left(\Phi_i^*\Phi_j + \Phi_j^*\Phi_i \right)$$

Hubbard-Stratonovich transformation:

$$Z_B = \int \mathcal{D}\Phi_i\,\mathcal{D}\Phi_i^*\,\mathcal{D}\Psi_{Bi}\,\mathcal{D}\Psi_{Bi}^*\; e^{-S_B'[\Phi_i,\Phi_i^*,\Psi_{Bi},\Psi_{Bi}^*]}$$

with action:

$$S_B' = \int_0^{1/T} d\tau \left[\sum_i \left(\Phi_i^* \frac{\partial \Phi_i}{\partial \tau} - \mu \Phi_i^*\Phi_i + \frac{1}{2} U \Phi_i^*\Phi_i (\Phi_i^*\Phi_i - 1) - \Psi_{Bi}\Phi_i^* - \Psi_{Bi}^*\Phi_i \right) \right.$$

$$\left. + \sum_{\langle ij \rangle} \Psi_{Bi}^*\, w_{ij}^{-1}\, \Psi_{Bj} \right]$$

and "hopping matrix":

$$w_{ij} = \begin{cases} w & \text{if } i,j \text{ are neighbors} \\ 0 & \text{otherwise} \end{cases}$$

Integration over Φ_i and Φ_i^*:

$$Z_B = \int \mathcal{D}\Psi_B \mathcal{D}\Psi_B^* \, e^{-S_B''[\Psi_B, \Psi_B^*]}$$

with "effective action" (continuum limit $\Psi_{Bi}(\tau) \mapsto \Psi_B(\tau, \vec{x})$):

$$S_B'' = \int d^d\vec{x} \int_0^{1/T} d\tau \left(K_1 \Psi_B^* \frac{\partial \Psi_B}{\partial \tau} + K_2 \left| \frac{\partial \Psi_B}{\partial \tau} \right|^2 + r |\Psi_B|^2 + K_3 |\vec{\nabla} \Psi_B|^2 + \frac{1}{2} U |\Psi_B|^4 + \ldots \right)$$

by symmetry.

U(1) gauge symmetry:

$$\Phi_i \longmapsto \Phi_i \, e^{i\varphi(\tau)}$$

$$\Psi_{Bi} \longmapsto \Psi_{Bi} \, e^{i\varphi(\tau)}$$

$$\mu \longmapsto \mu + i \frac{\partial \varphi}{\partial \tau}$$

with "gauge field" $\varphi(\tau)$.

Demanding gauge invariance of S_B'':

$$K_1 = -\frac{\partial r}{\partial \mu} \quad \Rightarrow \quad K_1 \text{ term present if transition can be tuned by changing } \mu$$

Quadratic vs. linear time derivative:

(a) Density $\langle \hat{n} \rangle$ fixed across transition:

- transition through tip of "Mott lobe", tunable by w only
- $K_1 = 0 \Rightarrow z = 1$
- $O(2)$ universality class in $d+1$ dimensions

(b) Density $\langle \hat{n} \rangle$ varies across transition:

- transition tunable by μ
- $K_1 \neq 0 \Rightarrow z = 2$
- $T=0$ BEC universality class with $\eta = 0$ and $\nu = \frac{1}{2}$ (quantum!)

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8.4 Dilute Bose gas

Hamiltonian:

$$\hat{H}_B = \sum_{\vec{k}} \frac{\vec{k}^2}{2m} \hat{b}_{\vec{k}}^\dagger \hat{b}_{\vec{k}} - \sum_i \mu \, \hat{n}_i + \frac{1}{2} \sum_i U \, \hat{n}_i (\hat{n}_i - 1)$$

Action:

$$S_B = \int d\tau \int d^d\vec{x} \left(\Phi^* \frac{\partial \Phi}{\partial \tau} + \frac{1}{2m} |\vec{\nabla} \Phi|^2 - \mu |\Phi|^2 + \frac{u}{2} |\Phi|^4 \right)$$

Phases at $T=0$:

(a) $\mu<0$: $\langle\Phi\rangle=0$ with density $\langle\Phi^*\Phi\rangle=0 \Rightarrow$ no particles

(b) $\mu>0$: $\langle\Phi\rangle\neq0$ superfluid with $\langle\Phi^*\Phi\rangle\neq0$

Remark: QCP at $\mu=0$ describes Mott-superfluid transition in Bose-Hubbard model (modulo integer background density)

RG flow (near $\mu=0$):

$$\frac{du}{d\ln b}=(4-d-z)u-\frac{u^2}{2} \qquad \text{with } u=\frac{S_d}{(2\pi)^d}\frac{2mU}{\Lambda^{2-d}}$$

$$\frac{d\tilde{\mu}}{d\ln b}=2\tilde{\mu} \qquad \text{with } \tilde{\mu}=\frac{\mu}{\Lambda^2}$$

with $\eta=0$ and $z=2$.

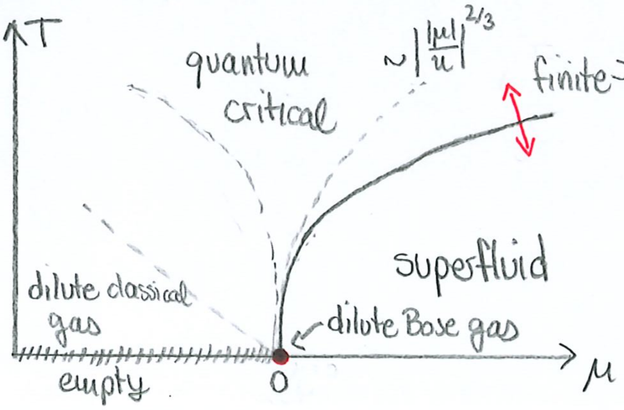
Critical behavior:

- $d\geq d_c^+=2$: u (dangerously) irrelevant, Gaussian criticality with $z=2$, $\eta=0$, and $\nu=\frac{1}{2}$,

$$\text{density } \langle\Phi^*\Phi\rangle=\begin{cases}0, & \mu<0\\ \frac{\mu}{u}+O(\mu^2), & \mu>0\end{cases}$$

- $d=1$: u relevant, non-Gaussian fixed point with $z=2$, still $\eta=0$ and $\nu=\frac{1}{2}$, equivalent to dilute 1D Fermi gas QCP

Phase diagram ($d=3$):



8.5 Dilute spinless Fermi gas

Hamiltonian (free fermions):

$$\hat{H}_F = \sum_{\vec{k}} \frac{\vec{k}^2}{2m} \hat{c}^+_{\vec{k}} \hat{c}_{\vec{k}} - \sum_i \mu \, \hat{c}^+_i \hat{c}_i \qquad \text{with } \{c_i, c_j^+\} = \delta_{ij}$$

Action:

$$S_F = \int d\tau \int d^d\vec{x} \left(\psi^* \frac{\partial \psi}{\partial \tau} + \frac{1}{2m} |\vec{\nabla}\psi|^2 - \mu |\psi|^2 \right)$$

where ψ and ψ^* are Grassmann variables, $\psi^2 = \psi^{*2} = 0$.

Remarks:

- On-site interaction impossible: $|\psi|^4 = 0$
- Non-local interactions such as $|\psi|^2 |\vec{\nabla}\psi|^2$ always irrelevant

Particle density:

$$\langle \psi^* \psi \rangle = \begin{cases} 0 & , \text{ for } \mu < 0 \\ \frac{S_d}{(2\pi)^d} \frac{(2m\mu)^{d/2}}{d} & , \text{ for } \mu > 0 \end{cases}$$

"Lifshitz transition"

with $S_d = \frac{2\pi^{d/2}}{\Gamma(d/2)}$ surface area of hypersphere.

Free energy density:

$$f_F = -T \int \frac{d^d\vec{k}}{(2\pi)^d} \ln\left[1 + e^{(\mu - \frac{\vec{k}^2}{2m})/T}\right] \quad \left[\begin{array}{l} \tilde{k} = \frac{k}{\sqrt{T}} \\ d^d\tilde{k} = T^{-d/2} d^d k \end{array}\right.$$

$$= T^{\frac{d+2}{2}} \tilde{\Phi}_f\left(\frac{\mu}{T}\right) = \mu^{\frac{d+2}{2}} \Phi_f\left(\frac{T}{\mu}\right)$$

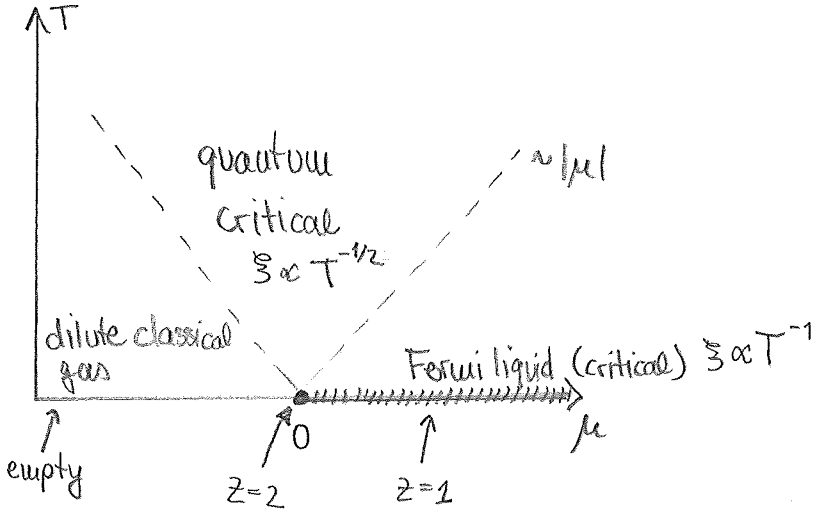
with universal scaling functions $\tilde{\Phi}_f$ and Φ_f.

Critical exponents:

$$f_F(\mu \to 0) \propto T^{\frac{d+z}{z}} \quad \Rightarrow z = 2$$

$$f_F(T \to 0) \propto |\mu|^{\nu(d+z)} \quad \Rightarrow \nu = \frac{1}{2}$$

Phase diagram:



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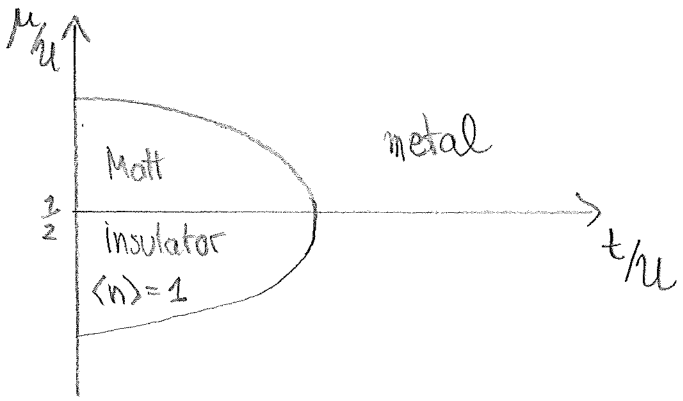
8.6 Fermi-Hubbard model on the square lattice
[8.4]

Hamiltonian:

$$\hat{H} = -t \sum_{\langle ij \rangle, \sigma} \left(\hat{c}_{i\sigma}^{\dagger} \hat{c}_{j\sigma} + \hat{c}_{j\sigma}^{\dagger} \hat{c}_{i\sigma} \right) - \mu \sum_{i,\sigma} \hat{n}_{i\sigma} + U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

Simplified phase diagram:



Antiferromagnetism in the Mott insulator:

(a) $t/U = 0$: • localized spins, 2^N-fold degenerate ground state

(b) $0 < t/U \ll 1$: • virtual hopping processes lead to energy gain of antiferromagnetic configurations

• effective model:

$$\hat{H} = J \sum \left(\hat{\vec{S}}_i \cdot \hat{\vec{S}}_j - \frac{1}{4} \right)$$

with $J = 4\frac{t^2}{U}$ and $\hat{\vec{S}}_i = \hat{c}_{i\sigma}^{\dagger} \vec{\tau}_{\sigma\sigma'} \hat{c}_{i\sigma'}$.

Pauli matrix

Remark: Phase diagram not fully understood, presumably rich:

- magnetic phases
- superconducting phases
- nematic phases
- spin liquids
- ⋮

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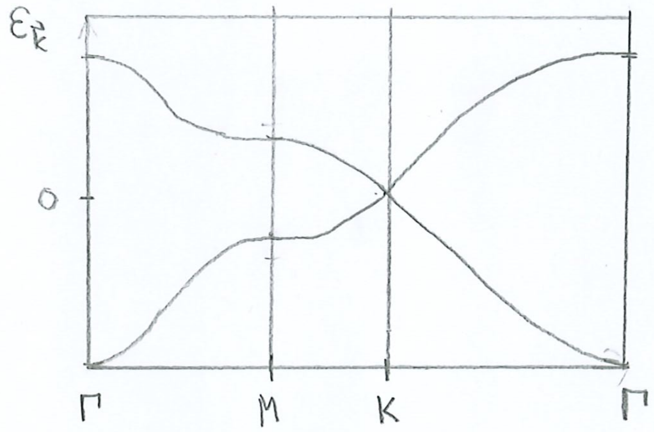
8.7 Fermi-Hubbard model on the honeycomb lattice

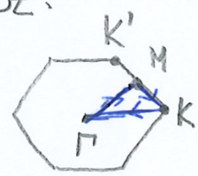
Spinless fermions with nearest-neighbor repulsion:

$$\hat{H} = -t \sum_{\langle ij \rangle} \left(\hat{a}_i^\dagger \hat{b}_j + \hat{b}_j^\dagger \hat{a}_i \right) + V \sum_{\langle ij \rangle} \hat{a}_i^\dagger \hat{a}_i \hat{b}_j^\dagger \hat{b}_j$$

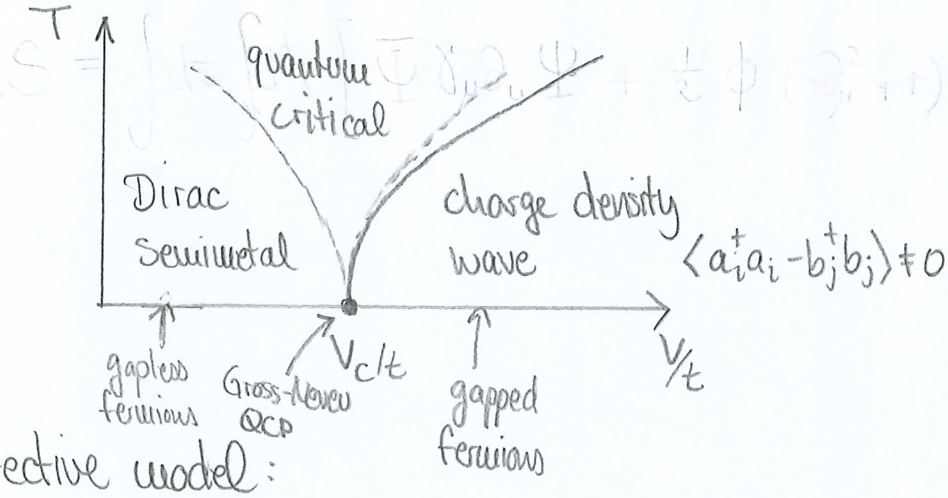
Energy dispersion ($V=0$):



BZ:



Phase diagram ($\mu=0$):



Effective model:

$$S = \int d\tau \int d^2\vec{x} \left[\bar{\Psi} \gamma_\mu \partial_\mu \Psi + g \phi \bar{\Psi} \Psi + \frac{1}{2} \phi (-\partial_\mu^2 + r) \phi + \lambda \phi^4 \right]$$

with

$$\Psi(\vec{q}, \omega) = \begin{pmatrix} a(\vec{K}+\vec{q}, \omega) \\ b(\vec{K}+\vec{q}, \omega) \\ a(-\vec{K}+\vec{q}, \omega) \\ b(-\vec{K}+\vec{q}, \omega) \end{pmatrix} \quad \text{and} \quad \bar{\Psi} \equiv \Psi^\dagger \gamma_0 \quad \text{with } \{\gamma_\mu, \gamma_\nu\} = 2 \delta_{\mu\nu} \mathbb{1}_4 ,$$

$\mu = 0, 1, 2$.

Critical behavior ($1/N$ expansion, ε expansion, QMC, conformal bootstrap):

$$\left.\begin{aligned} \eta_\phi &\simeq 0.51 \\ \eta_\psi &\simeq 0.087 \\ \nu &\simeq 0.91 \\ z &= 1 \end{aligned}\right\} \quad \text{2+1D Gross-Neveu universality class (quantum!)}$$

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