

# 8 Quantum phase transitions of bosons and fermions

## 8.1 Bose-Hubbard model

Hamiltonian:

$$\hat{H} = -w \sum_{\langle ij \rangle} (\hat{b}_i^\dagger \hat{b}_j + \hat{b}_j^\dagger \hat{b}_i) - \mu \sum_i \hat{n}_i + \frac{1}{2} U \sum_i \hat{n}_i (\hat{n}_i - 1)$$

hopping parameter                      chemical potential                      on-site potential

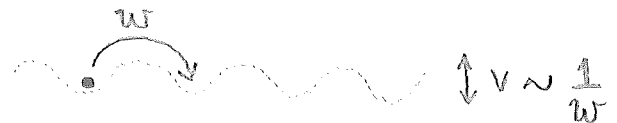
with  $\hat{n}_i = \hat{b}_i^\dagger \hat{b}_i$  "number operator" and  $[\hat{b}_i, \hat{b}_j^\dagger] = \delta_{ij}$ .

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

Experimental realization:

- Ultracold atoms on an optical lattice



- Magnons at a field-driven QCP ( $\mu \leftrightarrow B$ )

## 8.2 Bose-Hubbard model: Mean-field theory

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Order parameters:

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

↑  
lattice coordination number

Mean-field decoupling (kinetic term):

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

Possible phases:

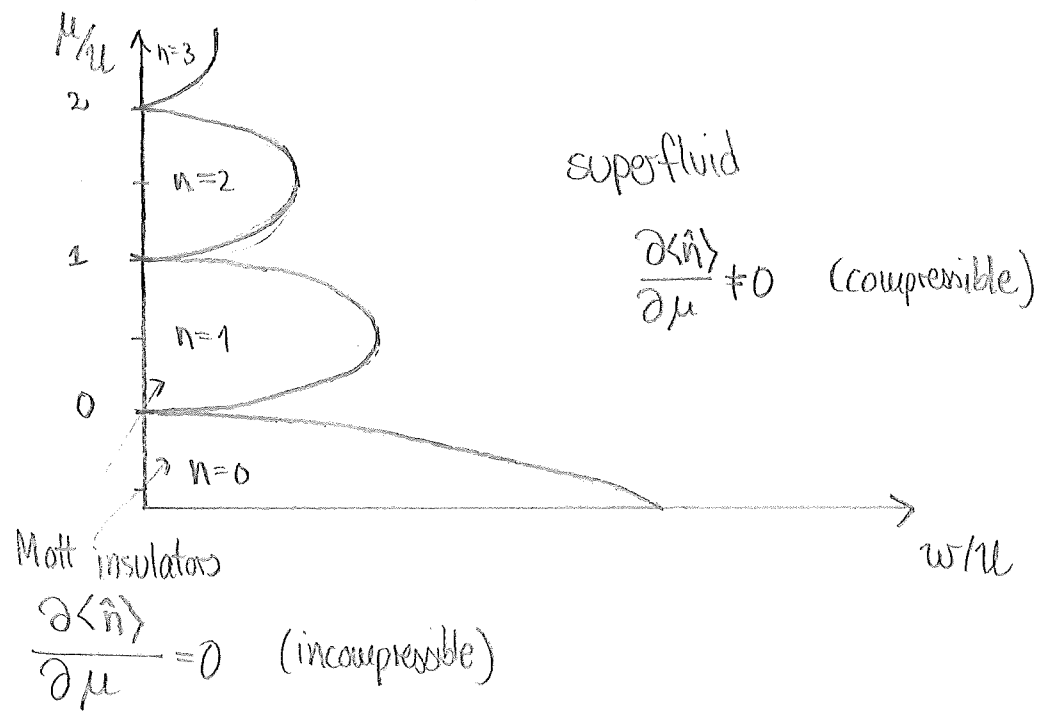
- $\Psi_B \neq 0$ : superfluid,  $U(1)$ :  $\Psi_B = |\Psi_B| e^{i\phi} \mapsto |\Psi_B| e^{i(\phi + \delta\phi)}$  spontaneously broken
- $\Psi_B = 0$ : Mott insulator, bosons localized, no long-range order

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

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

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

# Mean-field phase diagram:

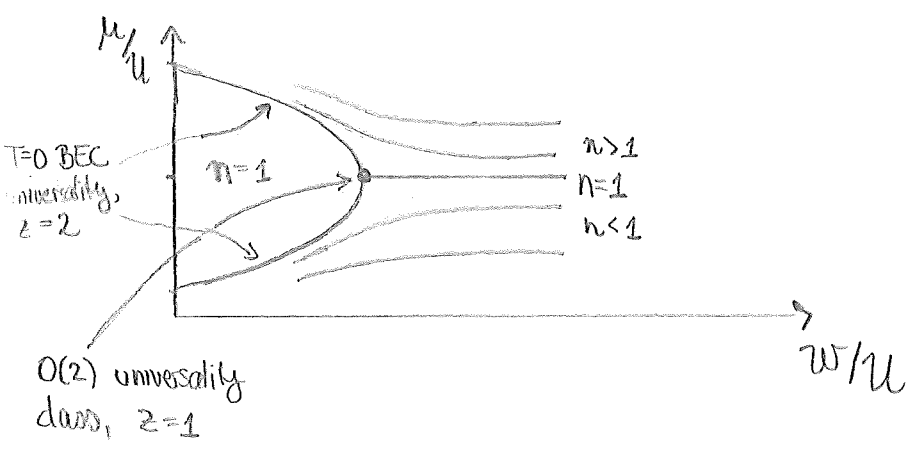


Remark: Phase diagram in qualitative agreement with quantum Monte Carlo simulations

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## 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:

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

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:

$$S'_B = \int_0^{1/\tau} d\tau \left[ \sum_i \left( \Phi_i^* \frac{\partial \Phi_i}{\partial \tau} - \mu \Phi_i^* \Phi_i + \frac{1}{2} U \Phi_i^* \Phi_i (\Phi_i^* \Phi_i - 1) - \Psi_{Bi}^* \Phi_i - \Psi_{Bi} \Phi_i^* \right) + \sum_{\langle ij \rangle} \Psi_{Bi}^* w_{ij}^{-1} \Psi_{Bj} \right]$$

and "hopping matrix":

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

Integration over  $\Phi_i$  and  $\Phi_i^*$ :

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

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

$$S_B'' = \int d^d \vec{x} \int_0^{1\hbar} d\tau \left( K_1 \Phi_B^* \frac{\partial \Phi_B}{\partial \tau} + K_2 \left| \frac{\partial \Phi_B}{\partial \tau} \right|^2 + \tau |\Phi_B|^2 + K_3 |\vec{\nabla} \Phi_B|^2 + \frac{1}{2} U |\Phi_B|^4 + \dots \right)$$

by symmetry.

U(1) gauge symmetry:

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

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

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

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

Demanding gauge invariance of  $S_B''$ :

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

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

## 8.4 Dilute Bose gas

Hamiltonian:

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

Action:

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

Phases at  $T=0$ :

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

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

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

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

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

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

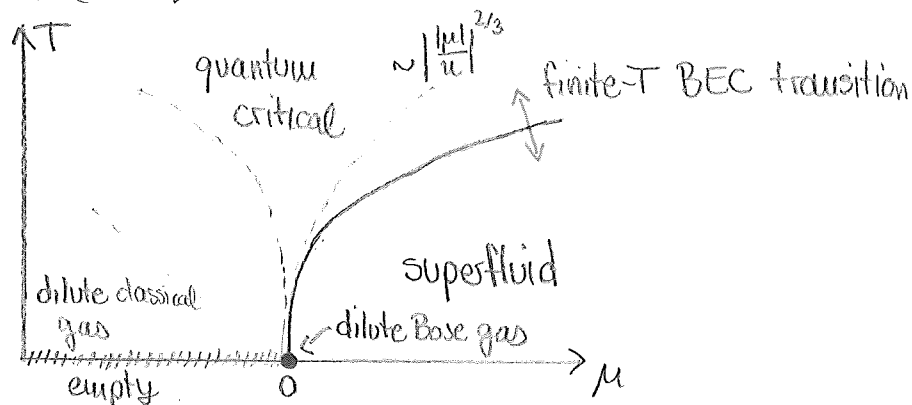
with  $\eta=0$  and  $z=2$ .

Critical behavior:

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

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Hamiltonian (free fermions):

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

Action:

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

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

Remarks:

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

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

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

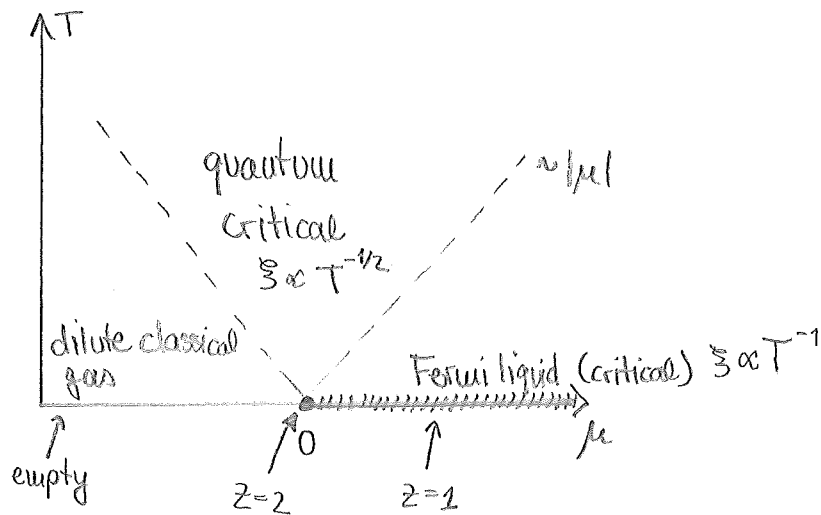
with universal scaling functions  $\tilde{\Phi}_f$  and  $\bar{\Phi}_f$ .

Critical exponents:

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

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

Phase diagram:

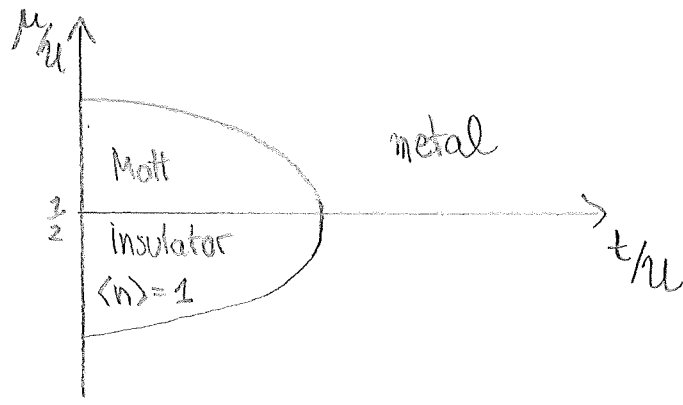


# 8.6 Fermi-Hubbard model on the square lattice

Hamiltonian:

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

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:

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

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

↑ Pauli matrix

Remark: Phase diagram not fully understood, presumably rich:

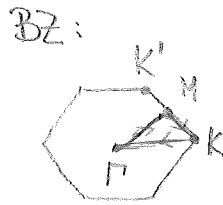
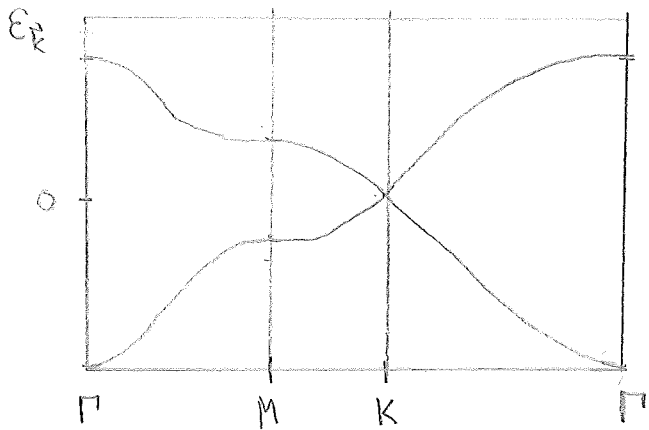
- magnetic phases
- superconducting phases
- nematic phases
- spin liquids
- ...

# 8.7 Fermi-Hubbard model on the honeycomb lattice

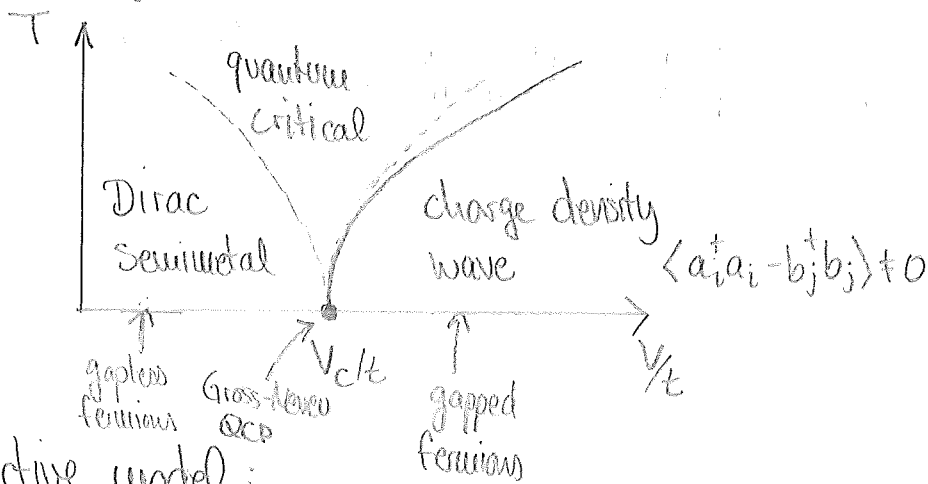
Spinless fermions with nearest-neighbor repulsion:

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

Energy dispersion ( $V=0$ ):



Phase diagram ( $\mu=0$ ):



Effective model:

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

with

$$\Psi_{\vec{q}, \omega} = \begin{pmatrix} a(\vec{K} + \vec{q}, \omega) \\ b(\vec{K} + \vec{q}, \omega) \\ a(-\vec{K} + \vec{q}, \omega) \\ b(-\vec{K} + \vec{q}, \omega) \end{pmatrix} \quad \text{and} \quad \bar{\Psi} \equiv \Psi^\dagger \gamma_0 \quad \text{with} \quad \{\gamma_\mu, \gamma_\nu\} = 2\delta_{\mu\nu} \mathbb{1}_4, \quad \mu = 0, 1, 2, 3$$

Critical behavior ( $\epsilon_N$  expansion,  $\epsilon$  expansion,  $\mathcal{O}(\text{MC})$ , conformal bootstrap):

(98)

$$\eta_\phi \simeq 0.51$$

$$\eta_\psi \simeq 0.087$$

$$\nu \simeq 0.91$$

$$z = 1$$

} 2+1D Gross-Neveu universality class (quantum!)

[JHEP02(2023)036]

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