Superfluid—Mott-insulator in lattice boson models: from RPA to functional renormalization group

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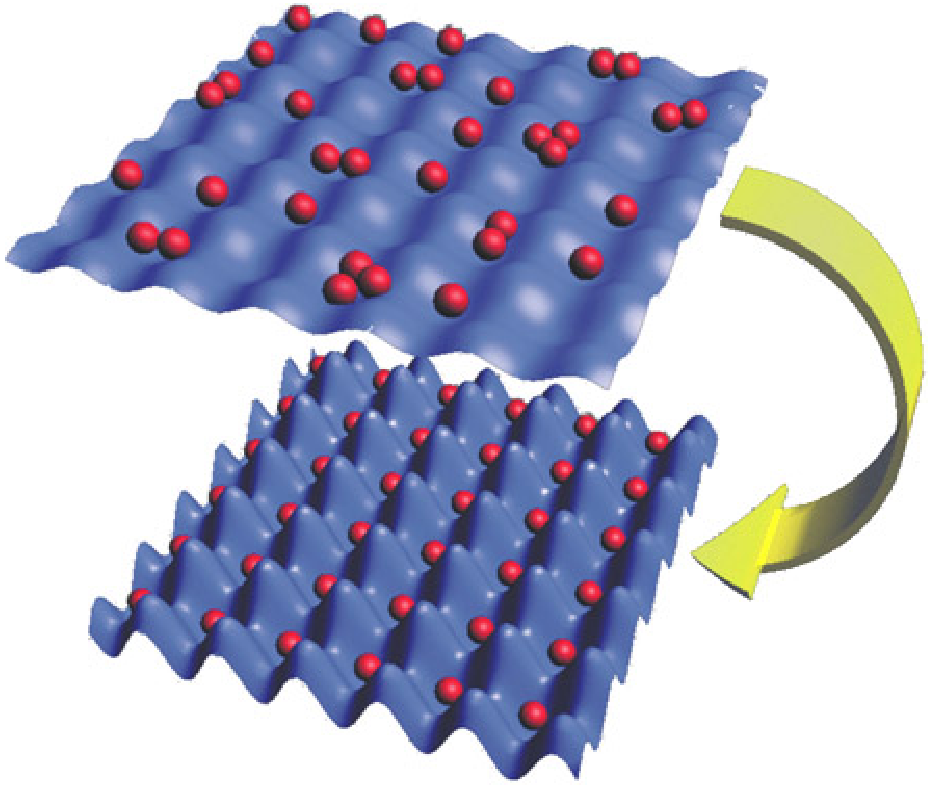
Bosons in an optical lattice



Superfluid to Mott insulator
quantum phase transition

M. Greiner, O. Mandel, T. Esslinger,
T.W. Hansch, and I. Bloch (Nature 2002)

[Picture: Quantum Optics Theory Group, Innsbruck university]

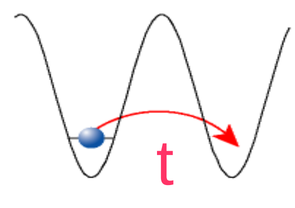
Outline

- Bose-Hubbard model
- Mean-field approximation and strong-coupling RPA
- Beyond RPA: functional renormalization group

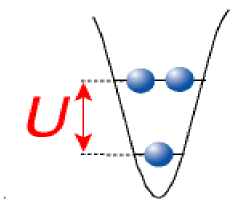
Bosons in an optical lattice: Bose-Hubbard model

$$\hat{H} = -t \sum_{\langle i,j \rangle} (\hat{\psi}_i^\dagger \hat{\psi}_j + \mathrm{h.c.}) - \mu \sum_i \hat{n}_i + \frac{U}{2} \sum_i \hat{n}_i(\hat{n}_i - 1), \qquad \hat{n}_i = \hat{\psi}_i^\dagger \hat{\psi}_i$$

Competition between tunneling



and on-site interaction

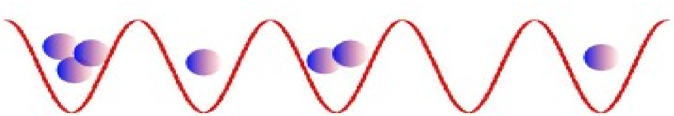


$t \gg U$

$t \ll U$ and integer filling (e.g. n=1)

Superfluid ground state

$$\Delta n_i \sim \langle n_i \rangle$$

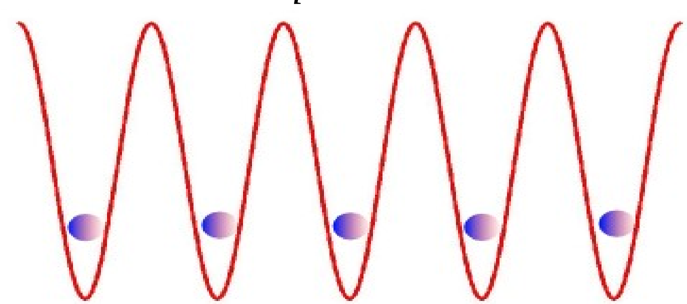


Macroscopic wave function $\Psi(\boldsymbol{r})$ with phase coherence

Mott insulator ground state

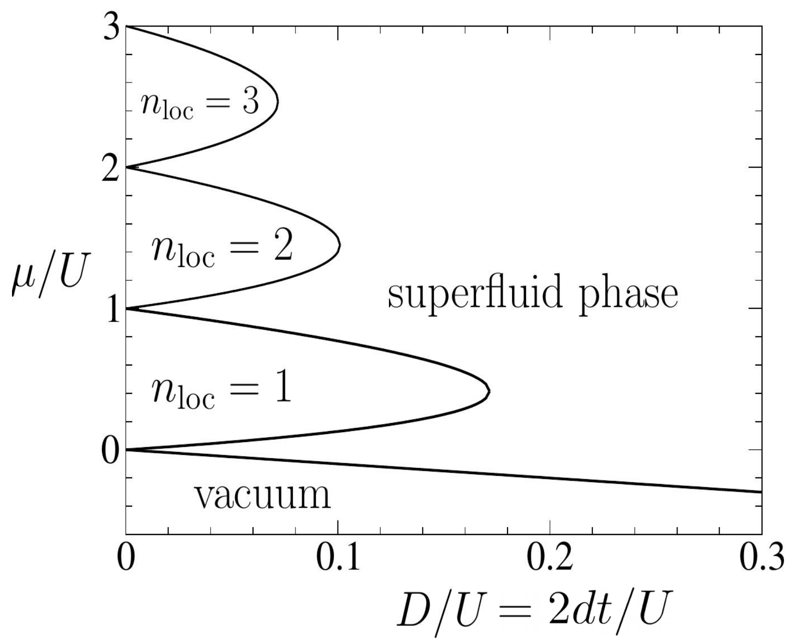
$$\langle n_i \rangle = 1$$

$$\Delta n_i \sim 0$$



Phase diagram of the Bose-Hubbard model

(hypercubic *d*-dimensional lattice)



Fisher et al., PRB '89

Mott insulator for integer fillings

Standard approach to superfluidity: Bogoliubov theory (mean-field theory plus Gaussian fluctuations: $\hat{\psi}_i = \langle \hat{\psi}_i \rangle + \delta \hat{\psi}_i$) always predicts the ground state to be superfluid.

Modified (strong-coupling) mean-field theory

(expansion about the local limit)

- Ising model

$$H = J \sum_{\langle i,j \rangle} \sigma_i \sigma_j - \sum_i h_i \sigma_i$$

$$H_{\mathrm{MF}} = J \sum_{\langle i,j \rangle} (\langle \sigma_i \rangle \sigma_j + \sigma_i \langle \sigma_j \rangle) - \sum_i h_i \sigma_i$$

single-site Hamiltonian

- Bose-Hubbard model

$$\hat{H} = -t \sum_{\langle i,j \rangle} (\hat{\psi}_i^\dagger \hat{\psi}_j + \mathrm{h.c.}) + \hat{H}_{\mathrm{loc}}$$

$$\hat{H}_{\mathrm{MF}} = -t \sum_{\langle i,j \rangle} (\langle \hat{\psi}_i^\dagger \rangle \hat{\psi}_j + \hat{\psi}_i^\dagger \langle \hat{\psi}_j \rangle + \mathrm{h.c.}) + \hat{H}_{\mathrm{loc}}$$

single-site Hamiltonian

$$E_0 = a_0 + a_2 |\langle \hat{\psi} \rangle|^2 + a_4 |\langle \hat{\psi} \rangle|^4$$

Ginzburg-Landau

Phase diagram qualitatively reproduced

Beyond (strong-coupling) mean-field: RPA

- Ising model

$$Z = \sum_{\{\sigma\}} e^{-\frac{1}{2}\sum_{i,j}\sigma_i K_{ij}\sigma_j}$$

$$= \sum_{\{\sigma\}} \int \prod_i d\varphi_i \; e^{-\frac{1}{2}\sum_{i,j}\varphi_i K^{-1}_{ij}\varphi_j + \sum_i \varphi_i \sigma_i}$$ Hubbard-Stratonovich

$$= \int \prod_i d\varphi_i \; e^{-\frac{1}{2}\sum_{i,j}\varphi_i K^{-1}_{ij}\varphi_j + \sum_i \ln 2\cosh\varphi_i}$$

$$\equiv \int \mathcal{D}[\varphi] \; e^{-\int d^d r \left\{\frac{1}{2}(\nabla\varphi)^2 + r_0\varphi^2 + u_0\varphi^4\right\}}$$

- Bose Hubbard model

$$Z = \int \mathcal{D}[\psi^*, \psi]\, e^{-\int_0^\beta d\tau \left\{\sum_i \psi_i^* \partial_\tau \psi_i + H[\psi^*,\psi]\right\}}$$

$$= \int \mathcal{D}[\psi^*, \psi]\, e^{\int_0^\beta d\tau \sum_{i,j} \psi_i^* t_{ij} \psi_j - S_{\rm loc}[\psi^*,\psi]}$$

$$= \int \mathcal{D}[\psi^*, \psi, \varphi^*, \varphi]\; e^{\int_0^\beta d\tau \left\{\sum_{i,j} \varphi_i^* t_{ij}^{-1} \varphi_j + \sum_i (\varphi_i^* \psi_i + \text{c.c.})\right\} - S_{\rm loc}[\psi^*,\psi]} \quad \text{(Hub.-Strat.)}$$

$$= Z_{\rm loc} \int \mathcal{D}[\varphi^*, \varphi]\;\, e^{\int_0^\beta d\tau \sum_{i,j} \varphi_i^* t_{ij}^{-1} \varphi_j} \left\langle e^{\int_0^\beta d\tau \sum_i (\varphi_i^* \psi_i + \text{c.c.})} \right\rangle_{\rm loc} \quad \text{(integrate out } \psi\text{)}$$

where $\langle \cdots \rangle_{\rm loc} = \dfrac{1}{Z_{\rm loc}} \displaystyle\int \mathcal{D}[\psi^*, \psi] \cdots e^{-S_{\rm loc}[\psi^*,\psi]}$

second-order cumulant expansion (t-expansion)

$$Z = \int \mathcal{D}[\varphi^*, \varphi]\; e^{-\sum_{\mathbf{q},\omega_n} \varphi^*(\mathbf{q},i\omega_n)[-t_{\mathbf{q}}^{-1} + G_{\rm loc}(i\omega_n)]\varphi(\mathbf{q},i\omega_n)}$$

Gaussian action

- Single-particle propagator

$$G(\mathbf{q}, i\omega_n) = -\langle\psi(\mathbf{q}, i\omega_n)\psi^*(\mathbf{q}, i\omega_n) = \frac{G_{\rm loc}(i\omega_n)}{1 - t_{\mathbf{q}} G_{\rm loc}(i\omega_n)}$$

RPA form
(cf. Hubbard I)

- Local propagator

$$G_{\rm loc}(i\omega_n) = \frac{n_{\rm loc}+1}{i\omega_n + \mu - U n_{\rm loc}} - \frac{n_{\rm loc}}{i\omega_n + \mu - U(n_{\rm loc}-1)}$$

Two-pole structure (particle and hole excitations of a single site): cannot be reproduced from perturbation theory (or Bogoliubov theory) but crucial to describe SF-MI transition.

- Instability of the Mott insulator $1 - t_{\mathbf{q}=0} G_{\rm loc}(i\omega_n = 0) = 0$

agrees with mean-field theory

Strong-coupling RPA

- exact in the local limit t=0
- describes qualitatively the phase diagram but not quantitatively
- mean-field-like treatment of hopping term: does not capture critical behavior of the SF-MI transition

Non-perturbative functional renormalization group (NPRG)

- NPRG: Wetterich'93... (reviews: Berges et al., Phys. Rep. '02, Delamotte arXiv '07)
- Lattice models: T. Machado & ND, Phys. Rev. E 82, 041128 (2010)
- Bose-Hubbard model: A. Rançon & ND

Family of models indexed by momentum scale *k*

$$\hat{H} + \Delta\hat{H}_\Lambda \quad \longrightarrow \quad \hat{H} + \Delta\hat{H}_k \quad \longrightarrow \quad \hat{H} + \Delta\hat{H}_{k=0} = \hat{H}$$

Reference system
=
local limit
(exact solution)

solve RG equation $\frac{d}{dk}(\cdots) = \cdots$

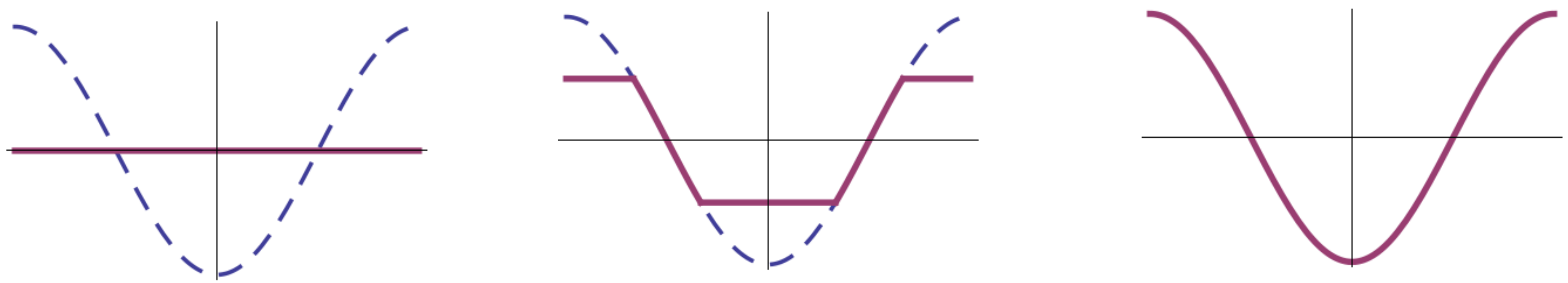
System of interest

Follow Wilson's RG idea: integrate short-distance degrees of freedom first

Practical implementation of the NPRG

$$\Delta \hat{H}_k = \sum_{\mathbf{q}} \hat{\psi}^\dagger(\mathbf{q}) R_k(\mathbf{q}) \hat{\psi}(\mathbf{q})$$

Effective hopping amplitude: $t_{\mathbf{q}} + R_k(\mathbf{q}) \equiv -2t\cos(q) + R_k(q) \quad \text{(1D)}$



$k = \Lambda = \sqrt{2d}$ $\qquad 0 < k < \Lambda$ $\qquad k = 0$

Local limit: decoupled sites

Solve RG equation

Which quantity do we calculate ?

- Effective action: (slightly modified) Legendre transform (Gibbs free energy)

$$Z_k[J^*, J] = \int \mathcal{D}[\psi^*, \psi]\; e^{-S[\psi^*,\psi]-\Delta S_k[\psi,\psi]+\int_0^\beta d\tau \sum_i (J_i^* \psi_i + \text{c.c.})}$$

$$\phi_i(\tau) = \langle \psi_i(\tau) \rangle$$

$$\Gamma_k[\phi^*, \phi] = -\ln Z_k[J^*, J] + \int_0^\beta d\tau \sum_i (J_i^* \phi_i + \text{c.c.}) - \Delta S_k[\phi^*, \phi]$$

- Initial condition of the RG flow

$$S + \Delta S_\Lambda = S_{\text{loc}}$$ local limit

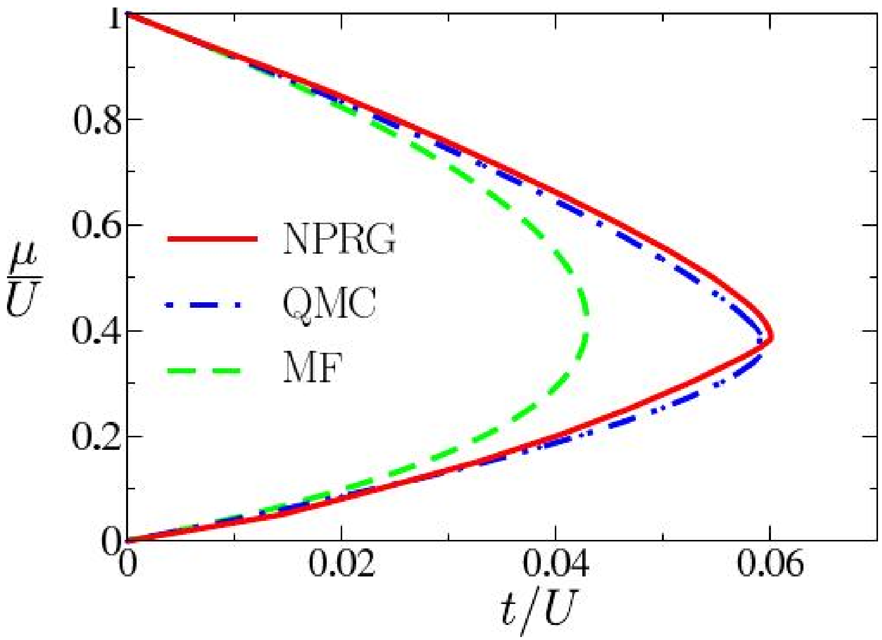
$$\Gamma_\Lambda = \Gamma_{\text{loc}} + \int_0^\beta d\tau \sum_{\mathbf{q}} \phi^*(\mathbf{q}) t_{\mathbf{q}} \phi(\mathbf{q})$$ RPA

- Exact RG equation (Wetterich'93)

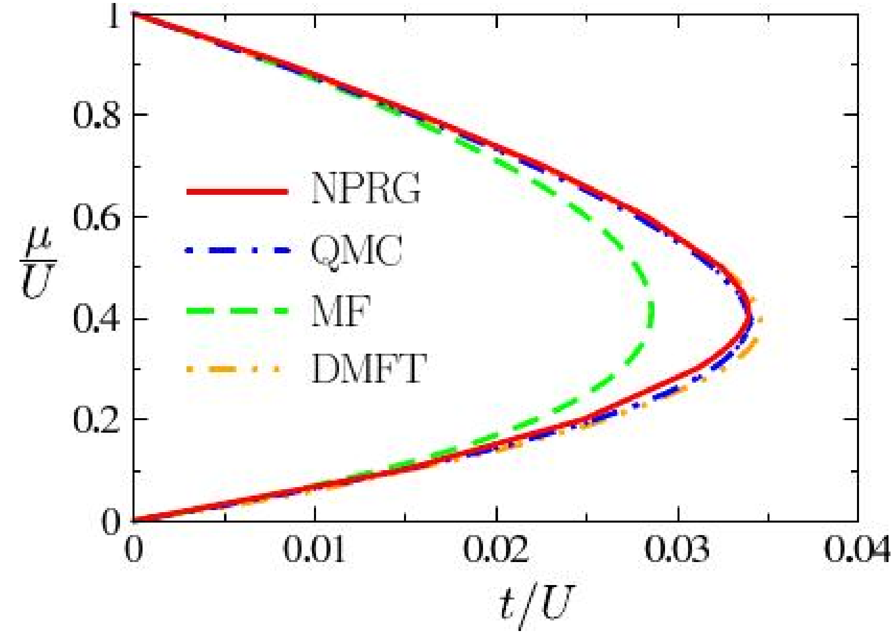
$$\partial_k \Gamma_k[\phi^*, \phi] = \frac{1}{2} \text{Tr} \left[\partial_k R_k \left(\Gamma_k^{(2)}[\phi^*, \phi] + R_k \right)^{-1} \right]$$ … can be solved approximately

Phase diagram

2D



3D



[QMC: B. Capogrosso-Sansone et al., DMFT: P. Anders et al.]

Critical behavior of the SF-MI transition at constant density (2D):

	NPRG	3D XY (MC)	RPA
$\nu =$	0.699	0.671	0.5
$\eta =$	0.049	0.038	0

Functional RG and quantum phase transitions

- Thermodynamics of a Bose gas near the SF-MI transition

  [A. Rançon & ND, PRA 2012]
- Universal equation of state of a dilute 2D Bose gas

  [A. Rançon & ND, PRA 2012]
- Thermodynamics in the vicinity of a relativistic quantum critical point in 2+1 dimensions

  [A. Rançon et al., PRE 2013]
- Higgs amplitude mode in the vicinity of a (2+1)-dimensional quantum critical point

  [A. Rançon & ND, PRB 2014, F. Rose et al., PRA 2015]
- Critical Casimir forces from the equation of state of quantum critical systems

  [A. Rançon et al., PRB 2016]
- Nonperturbative functional renormalization-group approach to transport in the vicinity of a (2+1)-dimensional O(N)-symmetric quantum critical point

  [F. Rose & ND, PRB 2017]

Thank you !