Mott-insulator and superfluid phases of correlated bosons – the bosonic dynamical mean-field approach with the strong coupling impurity solver

Anna Kauch

Center for Electronic Correlations and Magnetism
Institute of Physics, University of Augsburg

EKM

Universität Augsburg University

TRR 80

Collaboration: Krzysztof Byczuk, Dieter Vollhardt

Prague, 7^{th} December, 2010

Outline

- Non-interactiong bosons and the Bose-Einstein condensation
- Bose-Hubbard model and the static mean-field solution

- Bosons in optical lattices

- Bosonic dynamical mean-field theory (B-DMFT)
- Strong-coupling solution of the B-DMFT equations
- Results for the phase diagram and spectral functions

- Summary and outlook

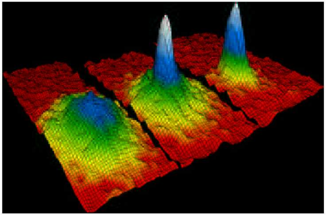
Non-interacting bosons

The number of particles is given by Bose-Einstein distribution

$$N = \sum_{\mathbf{k}} \frac{1}{e^{\frac{\epsilon_{\mathbf{k}} - \mu}{k_B T}} - 1} = \int_0^\infty \frac{N_0(\epsilon) \mathrm{d}\epsilon}{e^{\frac{\epsilon - \mu}{k_B T}} - 1}$$

- For $N > N_c(T)$ or $T < T_c(N)$ the lowest energy state becomes macroscopically occupied and has to be treated separately

$$N = N^{BEC} + \int_0^\infty \frac{N_0(\epsilon) \mathrm{d}\epsilon}{e^{\frac{\epsilon - \mu}{k_B T}} - 1}$$



M.H. Anderson et al, *Nature* (1995)

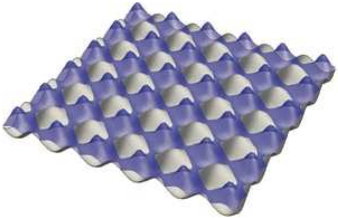
Non-interacting bosons on a lattice ($N_L = \#$ lattice sites)

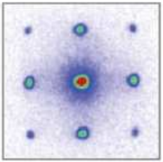
- Kinetic energy

$$H_{kin} = \sum_{ij} t_{ij} b_i^\dagger b_j$$

$$\langle H_{kin} \rangle = \sum_{ij} t_{ij} \langle b_i^\dagger b_j \rangle \qquad \langle b_i^\dagger b_j \rangle = \underbrace{\frac{N^{BEC}}{N_L}}_{\text{condensed bosons}} + \underbrace{\frac{1}{N_L} \sum_{\mathbf{k} \neq 0} n_{\mathbf{k}} e^{-i\mathbf{k}(\mathbf{R}_i - \mathbf{R}_j)}}_{\text{normal bosons}}$$

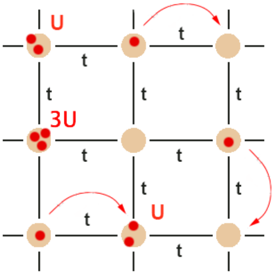
Bose-Einstein condensate on an optical lattice





Bose-Hubbard model

$$H = \sum_{ij} t_{ij} b_i^\dagger b_j + \frac{1}{2} U \sum_i n_i (n_i - 1)$$

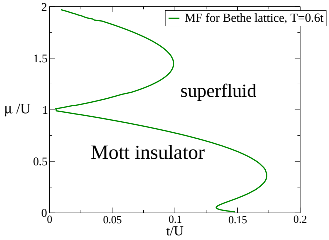


Standard approximations to the Bose-Hubbard model

- Bogoliubov approximation (dilute Bose gas): $b_i = \langle b_i \rangle + \tilde{b}_i$, where $\langle b_i \rangle$ is a complex number (classical variable) (Bogoliubov, 1947)
- Weak coupling expansion – valid for small U
- Gutzwiller (static) mean field (Fisher, 1989)

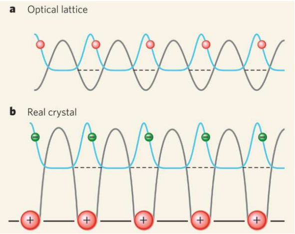
$$H_{MF} = \frac{1}{2} Un(n-1) - \mu n + zt\phi b^\dagger + zt\phi^* b \qquad \phi = \langle b \rangle_{MF}$$

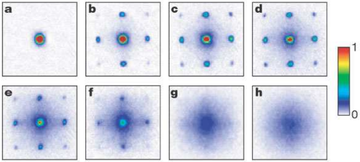
The mean-field phase diagram

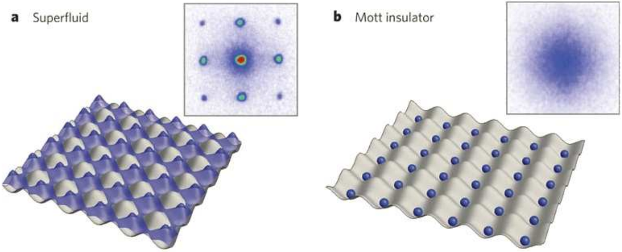


- Strong-coupling expansion in t around the atomic limit – valid for small t

Bose-Hubbard model in optical lattices







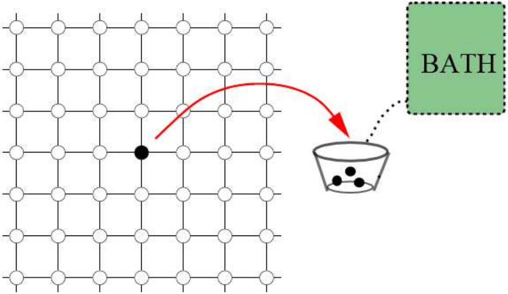
Greiner et al *Nature* (2002, 2009)

Bosonic dynamical mean-field theory

The bosonic Hubbard model

$$H = \sum_{ij} t_{ij} b_i^\dagger b_j + \frac{1}{2} U \sum_i n_i (n_i - 1)$$

Effective single-site problem

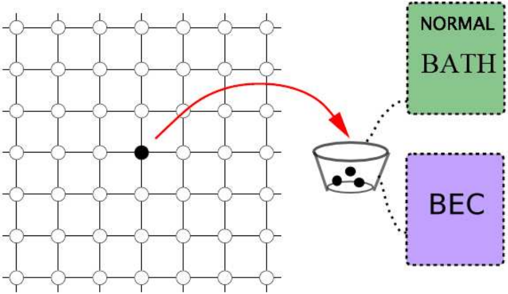


Bosonic dynamical mean-field theory

The bosonic Hubbard model

$$H = \sum_{ij} t_{ij} b_i^\dagger b_j + \frac{1}{2} U \sum_i n_i (n_i - 1)$$

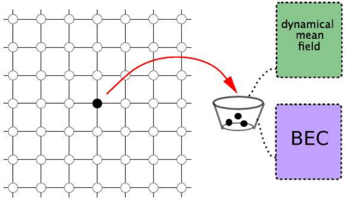
Effective single-site problem



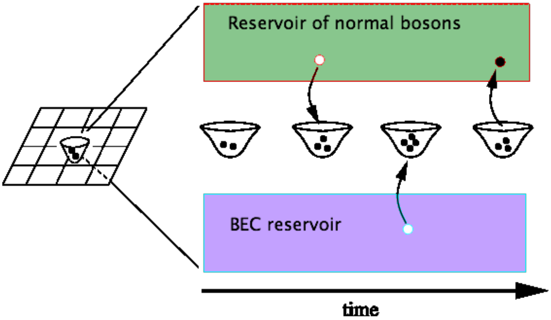
K. Byczuk and D. Vollhardt *Phys. Rev. B* **77**, 235106 (2008)

Bosonic dynamical mean-field theory

Spatial correlations are treated on mean-field level



Local correlations in time are captured exactly



The bosonic dynamical mean-field theory (B-DMFT)

- comprehensive (valid for all values of U, t, n and T), thermodynamicaly consistent and conserving approximation
- treats normal and condensed bosons on equal footing
- exact in the limit of $d \to \infty$ or $Z \to \infty$

When taking the limit $d \to \infty$, the hopping amplitudes t_{ij} have to be rescaled for the kinetic energy to remain finite.

Scalling of hopping amplitudes for lattice bosons

$$\text{Normal bosons}: \quad \langle H_{kin} \rangle = -\underbrace{t}_{\frac{1}{\sqrt{Z}}} \sum_i \underbrace{\sum_{j(NN\ i)}}_{Z} \underbrace{\langle b_i^\dagger b_j \rangle}_{\frac{1}{\sqrt{Z}}} \neq \infty, 0 \quad \Rightarrow \quad \text{rescaling} \quad t = \frac{t^*}{\sqrt{Z}}$$

$$\text{BEC bosons}: \quad \langle H_{kin} \rangle = -\underbrace{t}_{\frac{1}{Z}} \sum_i \underbrace{\sum_{j(NN\ i)}}_{Z} \underbrace{\langle b_i^\dagger \rangle \langle b_j \rangle}_{Z-\text{independent}} \neq \infty, 0 \quad \Rightarrow \quad \text{rescaling} \quad t = \frac{t^*}{Z}$$

The action for the bosonic Hubbard model

$$S = \int_0^\beta d\tau \left[\sum_i b_i^*(\tau)(\frac{\partial}{\partial \tau} - \mu) b_i(\tau) + \sum_{ij} t_{ij} b_i^*(\tau) b_j(\tau) + \frac{1}{2} \sum_i U n_i(\tau)(n_i(\tau) - 1) \right]$$

$$\Downarrow$$

B-DMFT:
$d \to \infty$
(with hoppings rescaled <u>differently</u> for normal bosons and BEC)

$$S_{local} = \int_0^\beta d\tau b^*(\tau)(\frac{\partial}{\partial \tau} - \mu) b(\tau) + \frac{1}{2} \int_0^\beta d\tau U n(\tau)(n(\tau) - 1) + \kappa \int_0^\beta d\tau \mathbf{\Phi}^\dagger(\tau) \mathbf{b}(\tau) +$$
$$+ \int_0^\beta d\tau \int_0^\beta d\tau' \; \mathbf{b}^\dagger(\tau) \mathbf{\Delta}(\tau - \tau') \mathbf{b}(\tau')$$

- Both the dynamical mean-field (hybridization) $\mathbf{\Delta}(\tau - \tau')$ and the BEC order parameter $\mathbf{\Phi}(\tau)$ are obtained self-consistently.
- κ is a lattice dependent parameter $\kappa = \sum_{i \neq 0} t_{i0}$

K. Byczuk and D. Vollhardt *Phys. Rev. B* **77**, 235106 (2008)

The B-DMFT equations

- The local Green function is given by

$$\mathbf{G}(\tau-\tau') = \begin{pmatrix} G_{11}(\tau-\tau') & G_{12}(\tau-\tau') \\ G_{21}(\tau-\tau') & G_{22}(\tau-\tau') \end{pmatrix} = -\langle T_\tau \mathbf{b}(\tau)\mathbf{b}^\dagger(\tau')\rangle_{\mathbf{S_{local}}}$$

  Note the Nambu notation: $\mathbf{b}^\dagger = (b^\dagger, b)$

- The BEC order parameter ϕ is given by

$$\phi = \langle b(\tau)\rangle_{S_{\boldsymbol{local}}}$$

- $\mathbf{\Delta}(\tau-\tau')$ can be calculated using $\mathbf{G}(\tau-\tau')$ with the help of lattice Hilbert transform

$$\mathbf{G}(\omega_n) = \int N_0(\epsilon)\left[\begin{pmatrix} i\omega_n+\mu-\epsilon & 0 \\ 0 & -i\omega_n+\mu-\epsilon \end{pmatrix} - \mathbf{\Sigma}(i\omega_n)\right]^{-1}$$

  and Dyson equation

$$\mathbf{\Sigma}(i\omega_n) = \begin{pmatrix} i\omega_n+\mu & 0 \\ 0 & -i\omega_n+\mu \end{pmatrix} - \mathbf{\Delta}(i\omega_n) - [\mathbf{G}(i\omega_n)]^{-1}$$

- For Bethe lattice $\mathbf{\Delta}(\tau-\tau') = t^2\mathbf{G}(\tau-\tau')$ and $\mathbf{\Phi} = (\phi, \phi^*)$

Existing solutions

- Exact diagonalization:
  - A. Hubener, M. Snoek, and W. Hofstetter *Phys. Rev. B* **80**, 245109 (2009)
  - Wen-Jun Hu and Ning-Hua Tong *Phys. Rev. B* **80**, 245110 (2009)
- Continuous time quantum Monte Carlo
  - P. Anders, E. Gull, L. Pollet, M. Troyer, and P. Werner *Phys. Rev. Lett.* **105**, 096402 (2010)
- Strong-coupling expansion in hybridization (presented here)

Bosonic DMFT vs. fermionic

- Two hybridization functions $\Delta_{11}(\tau)$, $\Delta_{12}(\tau)$ instead of one to be obtained self-consistently
- Order parameter Φ
- Infinitely large Hilbert space – ED more CPU time consuming
- No analogue of particle-hole symmetry
- No "30 years of Kondo physics" behind – no ready-to-use solvers

Linked-cluster expansion (LCE) in hybridization

The B-DMFT local action S_{loc} we split into two parts:

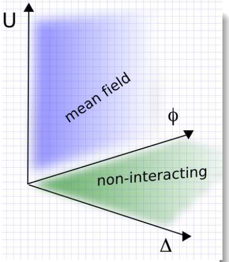
$$S_{loc} = \underbrace{\int_0^\beta d\tau b^*(\tau)(\frac{\partial}{\partial\tau} - \mu)b(\tau) + \frac{1}{2}\int_0^\beta d\tau U n(\tau)(n(\tau)-1) + \kappa\int_0^\beta d\tau \mathbf{\Phi}^\dagger(\tau)\mathbf{b}(\tau)}_{S_0\text{ -- treated exactly}} +$$

$$+ \underbrace{\int_0^\beta d\tau \int_0^\beta d\tau'\ \mathbf{b}^\dagger(\tau)\mathbf{\Delta}(\tau,\tau')\mathbf{b}(\tau')}_{\text{LCE with respect to hybridization } \mathbf{\Delta}}$$

Benchmarks

- Exact in the atomic limit ($t = 0$)
- For $\Delta = 0$ reduces to the mean-field theory
- The results obey Hugenholtz-Pines theorem

$$\Sigma_{11}(k=0,\omega=0) - \Sigma_{12}(k=0,\omega=0) = \mu$$



Hybridization expansion in more detail

We split the B-DMFT local action into S_0 and S'

$$S_{loc} = S_0 + S' = S_0 + \int_0^\beta d\tau \int_0^\beta d\tau' \ \mathbf{b}^\dagger(\tau)\Delta(\tau,\tau')\mathbf{b}(\tau')$$

The partition function

$$Z = \int Db^* Db e^{-S} = Z_0 \langle e^{-S'} \rangle_0$$

The ensemble average $\langle \cdots \rangle_0$ and Z_0 are given by

$$\langle \cdots \rangle_0 \equiv \frac{1}{Z_0} \int Db^* Db e^{-S_0} \cdots \qquad Z_0 = \int Db^* Db e^{-S_0}$$

Next we perform the linked-cluster expansion with respect to S'

$$\langle e^{-S'} \rangle_0 = 1 - \int_0^\beta d\tau \int_0^\beta d\tau' \ \langle T_\tau \mathbf{b}^\dagger(\tau)\Delta(\tau,\tau')\mathbf{b}(\tau') \rangle_0 +$$

$$+\frac{1}{2!} \int_0^\beta d\tau_1 \int_0^\beta d\tau_1' \int_0^\beta d\tau_2 \int_0^\beta d\tau_2' \ \langle T_\tau \mathbf{b}^\dagger(\tau_1)\Delta(\tau_1,\tau_1')\mathbf{b}(\tau_1') \ \mathbf{b}^\dagger(\tau_2)\Delta(\tau_2,\tau_2')\mathbf{b}(\tau_2') \rangle_0 + \dots$$

With the use of linked-cluster theorem we put connected averages back into the exponent

$$\langle e^{-S'}\rangle_0 = \exp\Big\{-\int_0^\beta d\tau \int_0^\beta d\tau' \ \langle T_\tau \mathbf{b}^\dagger(\tau)\Delta(\tau,\tau')\mathbf{b}(\tau')\rangle_0^{connected} +$$

$$+\frac{1}{2!}\int_0^\beta\int_0^\beta\int_0^\beta\int_0^\beta \langle T_\tau \mathbf{b}^\dagger(\tau_1)\Delta(\tau_1,\tau_1')\mathbf{b}(\tau_1') \ \mathbf{b}^\dagger(\tau_2)\Delta(\tau_2,\tau_2')\mathbf{b}(\tau_2')\rangle_0^{connected} + \dots\Big\}$$

We can obtain now the Green functions

$$G_{11}(\tau-\tau') = -\langle T_\tau b(\tau)b^*(\tau')\rangle_0 + \int_0^\beta d\tau_1 \int_0^\beta d\tau_1' \ \langle T_\tau b(\tau)\mathbf{b}^\dagger(\tau_1)\Delta(\tau_1,\tau_1')\mathbf{b}(\tau_1')b^*(\tau')\rangle_0^{cn}$$

$$G_{12}(\tau-\tau') = -\langle T_\tau b(\tau)b(\tau')\rangle_0 + \int_0^\beta d\tau_1 \int_0^\beta d\tau_1' \ \langle T_\tau b(\tau)\mathbf{b}^\dagger(\tau_1)\Delta(\tau_1,\tau_1')\mathbf{b}(\tau_1')b(\tau')\rangle_0^{cn}$$

The order parameter of the BEC

$$\phi = \langle b(\tau)\rangle_0 + \int_0^\beta d\tau_1 \int_0^\beta d\tau_1' \ \langle T_\tau b(\tau)\mathbf{b}^\dagger(\tau_1)\Delta(\tau_1,\tau_1')\mathbf{b}(\tau_1')\rangle_0^{cn}$$

Having obtained $\mathbf{G}(\tau, \tau')$ and the BEC order parameter ϕ

- Using B-DMFT equations, we can obtain new $\Delta(\tau, \tau')$ from $\mathbf{G}(\tau, \tau')$
- Then the new $\Delta(\tau, \tau')$ and ϕ are used to obtain a new $\mathbf{G}(\tau, \tau')$ until the self-consistent solution is reached

Remarks

- The averages $\langle \cdots \rangle_0$ are calculated with the use of the Hamiltonian representation

$$\langle \cdots \rangle_0 = \frac{1}{Z_0} Tr(e^{-\beta H_0} \cdots)$$

$$\text{where} \quad H_0 = \frac{1}{2} Un(n-1) - \mu n + \kappa \phi b^\dagger + \kappa \phi^* b$$

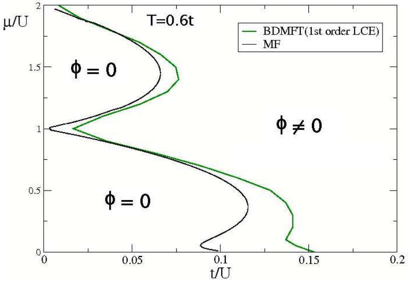
  has to be diagonalized numerically

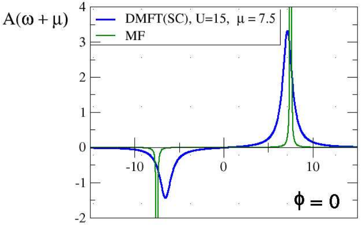
- The number of bosons on one site has to be cut off – otherwise the Hilbert space is infinitely large

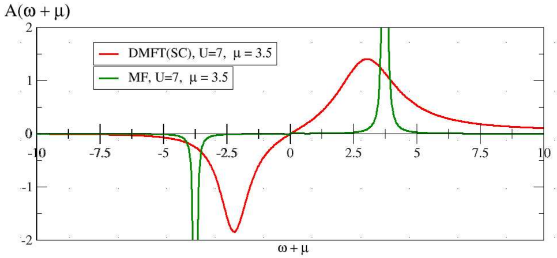
- There is a trivial hysteresis – if we start from a solution with $\phi = 0$ we never reach the solution with $\phi \neq 0$

Comparison with MF results

Phase diagram and spectral functions in the B-DMFT (first order LCE in Δ) and MF approximations



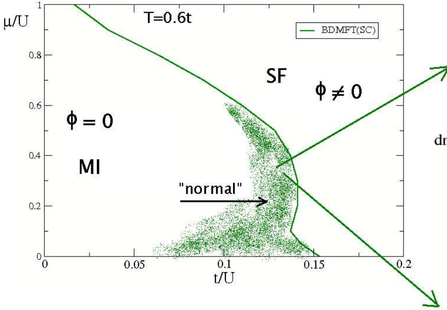


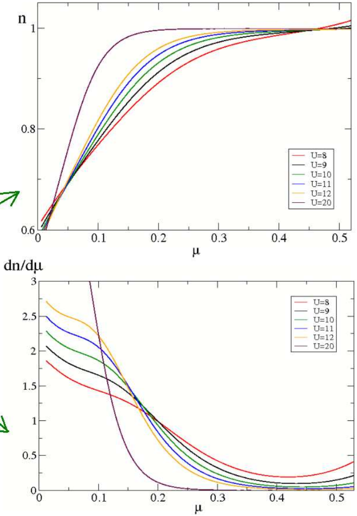


Phase diagram obtained with first order LCE in Δ in B-DMFT

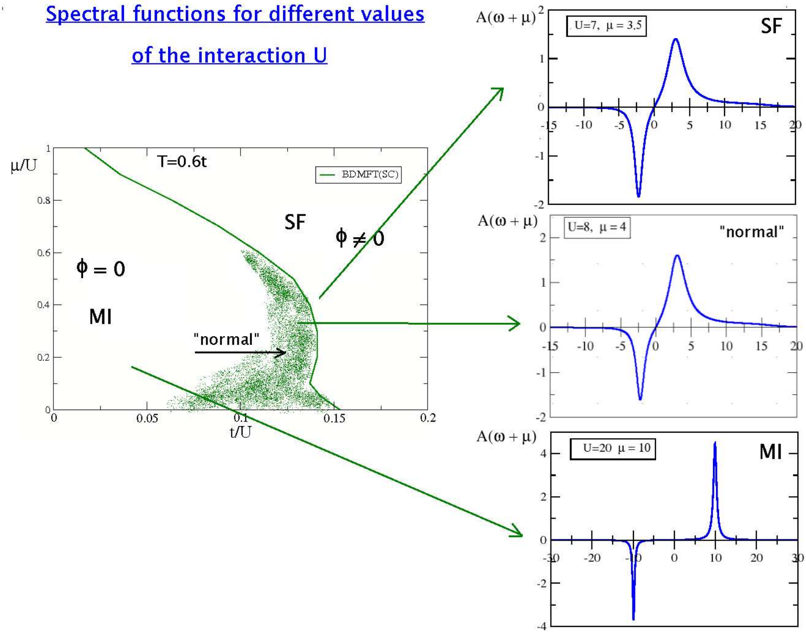
Compressibility for different values of the interaction U

A "normal" (compressible) phase is present:





$A(\omega + \mu)$ for the Bethe lattice (Padé)



Conclusions and outlook

The strong coupling expansion solution of the BDMFT

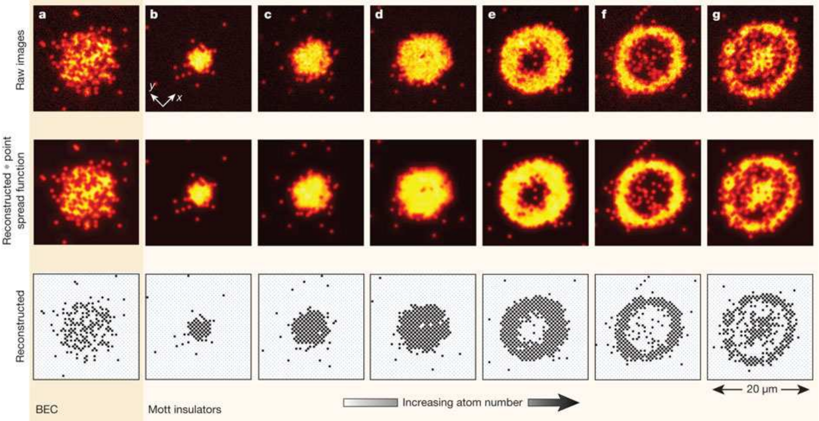
- Describes normal and condensed bosons on equal footing
- Gives access to spectral functions in Mott-insulating, normal and BEC phases
- Reproduces Hugenholtz-Pines theorem

- The validity of the first order LCE expansion is limited to the vicinity of the Mott phase

Outlook

- Multi-species bosons – simulators of magnetic systems
- Disorder? Non-equilibrium?
- LDA + B-DMFT, real-space B-DMFT
- Bose-Fermi mixtures

Real space images of bosons in optical lattice



Bloch et al *Nature* (2010)