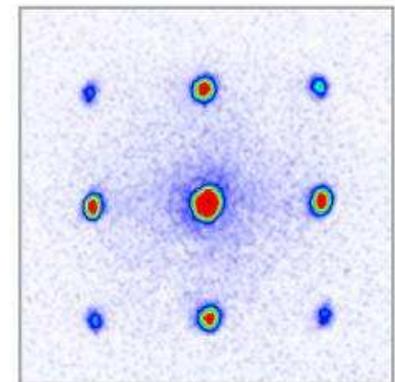


# Ultracold Atomic Gases in Optical Lattices



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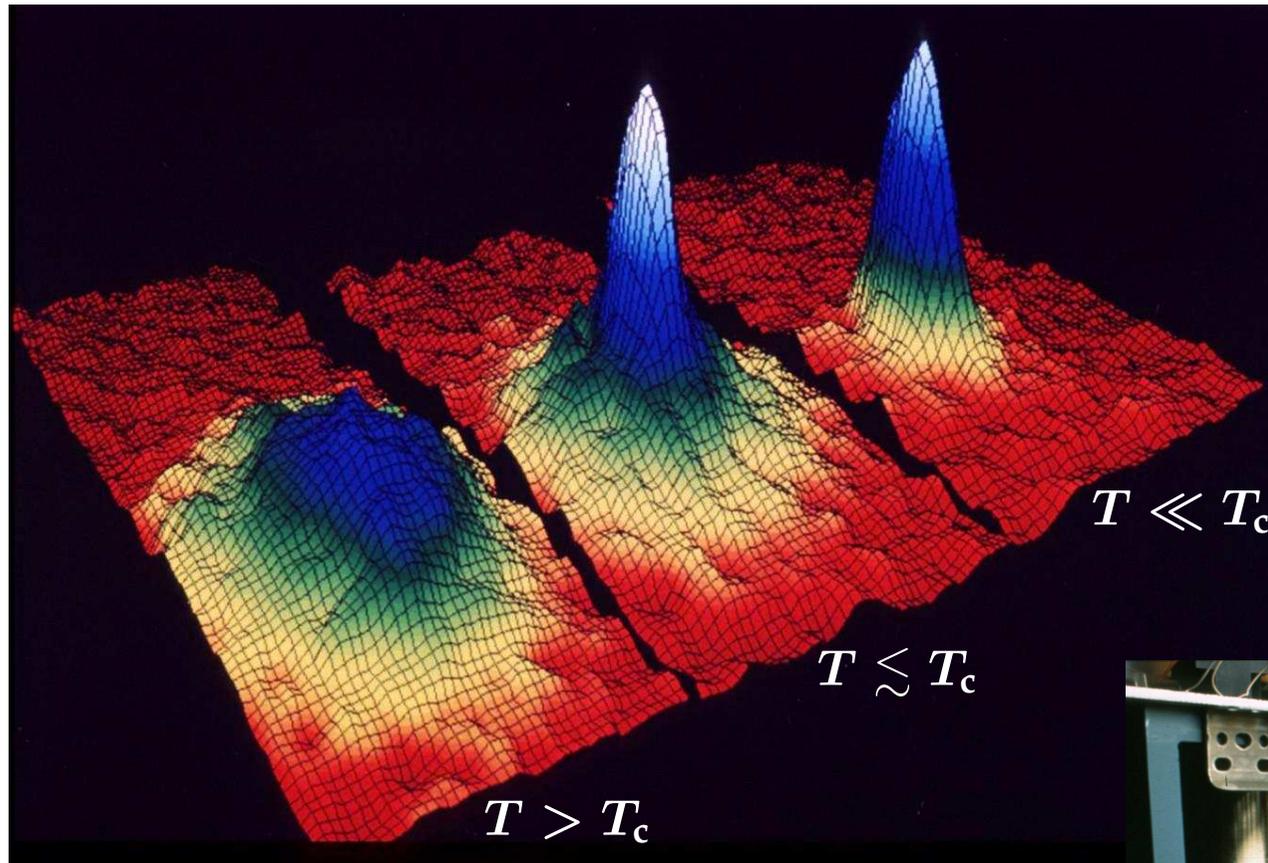


# Overview

- Ultracold Atomic Gases
- The Lattice Experiment
- Bose-Hubbard Model
- Condensation & Superfluidity
- Two-Color Superlattices
- Boson-Fermion Mixtures in Lattices

Boulder / Colorado — June 5th, 1995 — 10:54 am

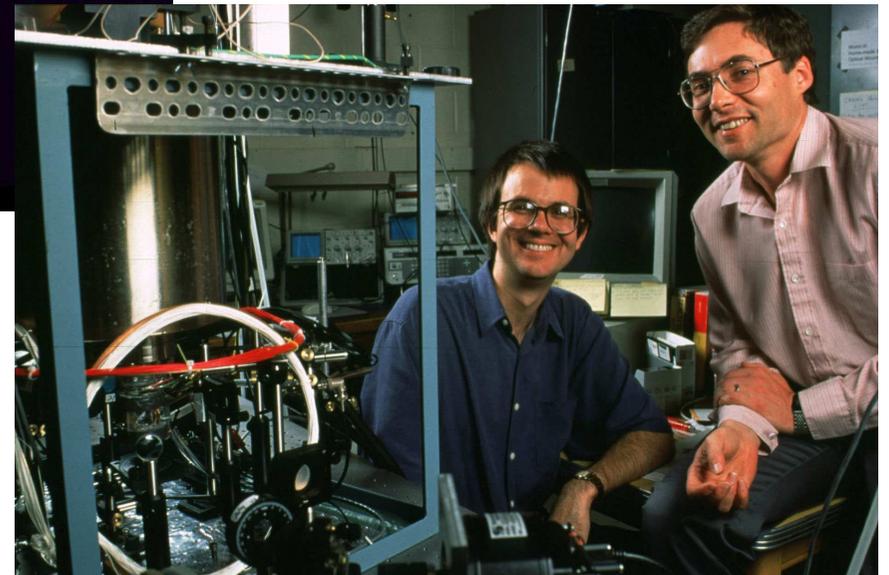
# BEC of Rubidium Atoms



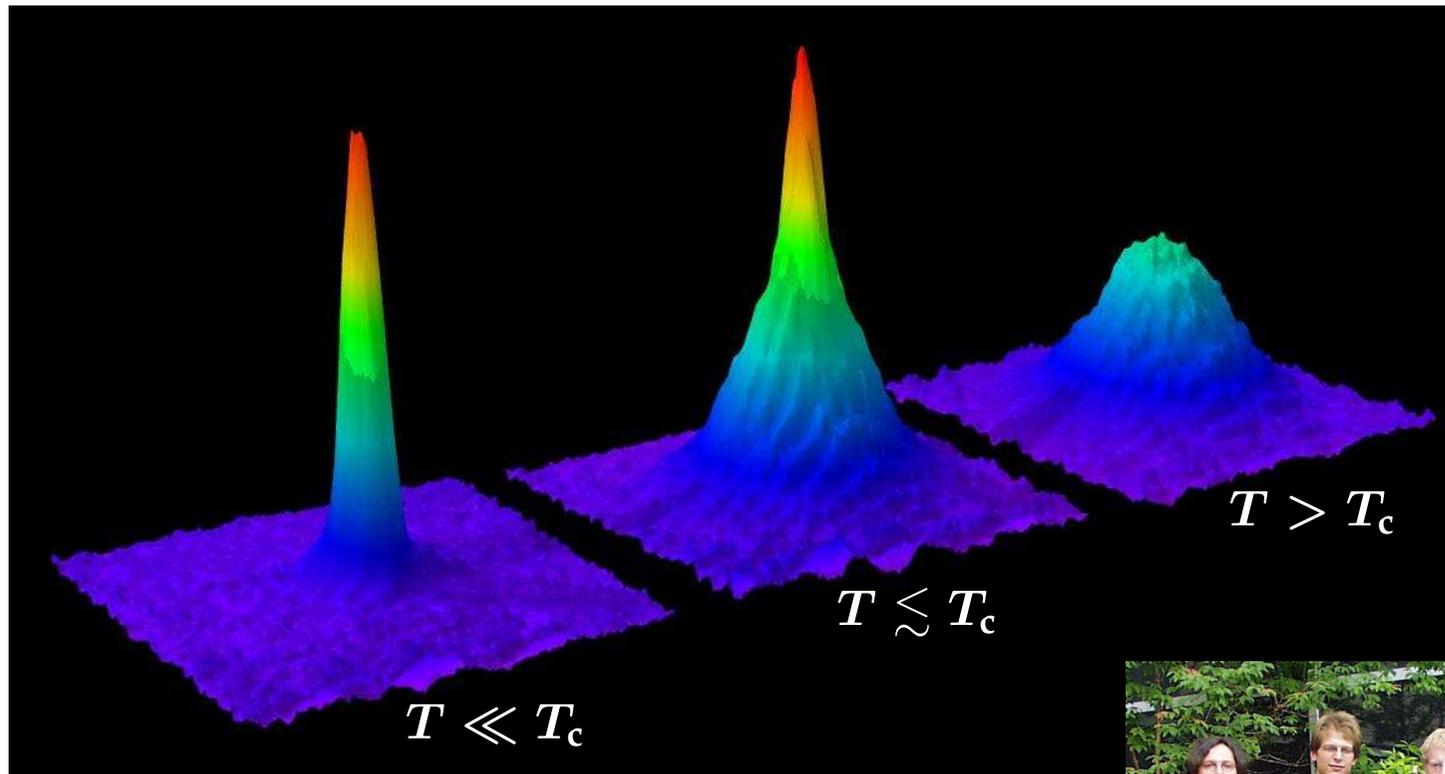
- $^{87}\text{Rb}$
- $N_{\text{initial}} \approx 10^6$
- $N_{\text{BEC}} \approx 2000$
- $T_c \approx 170\text{nK}$
- absorption image after 60 ms expansion

*E. Cornell, C. Wieman, et al.*  
(JILA, NIST, U of Colorado)

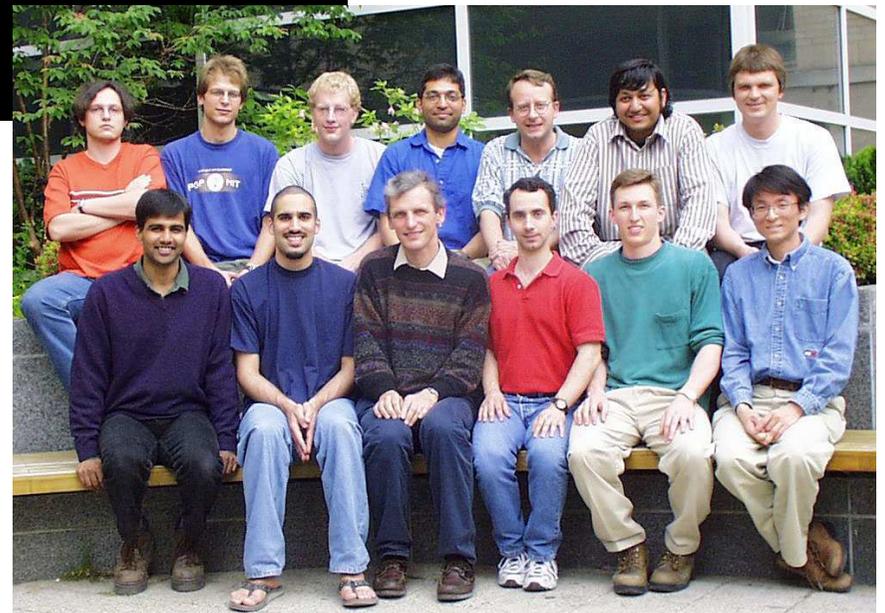
Nobel Prize in Physics 2001



Cambridge / Massachusetts — September 1995  
BEC with Sodium Atoms



- $^{23}\text{Na}$
- $N_{\text{initial}} \approx 10^9$
- $N_{\text{BEC}} \approx 5 \times 10^5$
- $T_c \approx 2 \mu\text{K}$
- absorption image after 60 ms expansion



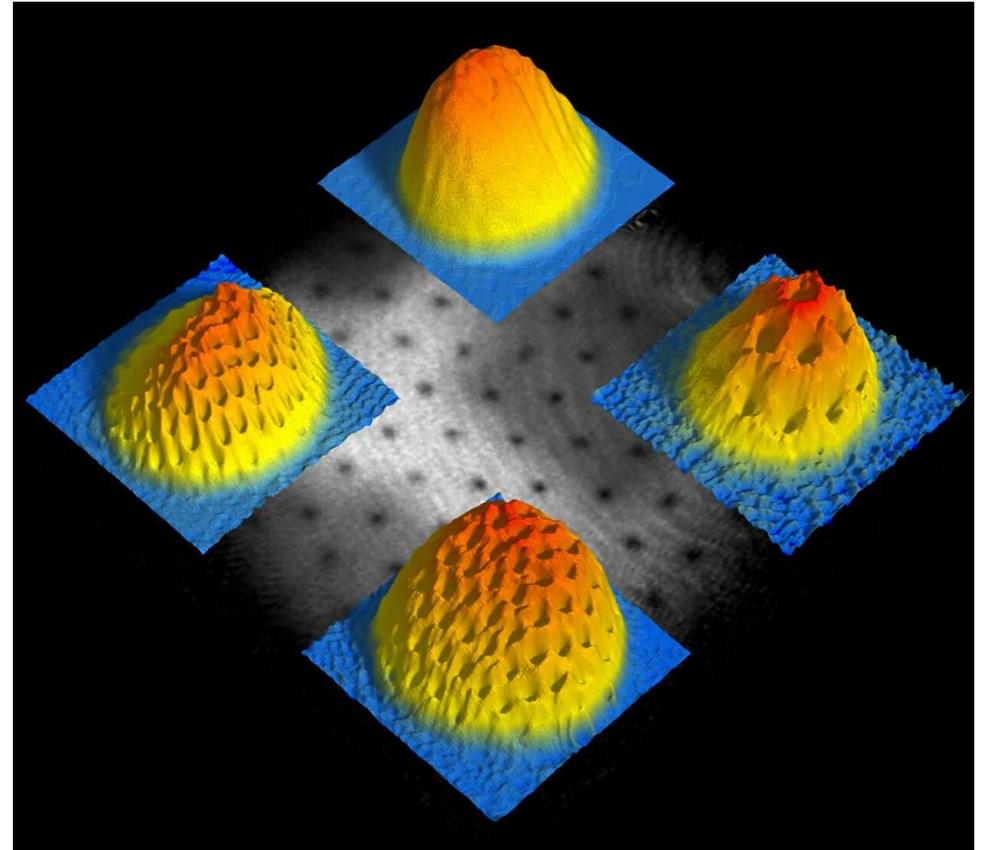
*W. Ketterle, et al.*  
(MIT)

Nobel Prize in Physics 2001

...over the Intervening Years

# Dynamics of Dilute Quantum Gases

- amazing experimental achievements
  - condensates of  $^1\text{H}$ ,  $^4\text{He}^*$ ,  $^7\text{Li}$ ,  $^{23}\text{Na}$ ,  $^{41}\text{K}$ ,  $^{85}\text{Rb}$ ,  $^{87}\text{Rb}$ ,  $^{133}\text{Cs}$ ,  $^{174}\text{Yb}$
  - vortices, vortex lattices and their dynamics
  - bright and dark solitons and soliton trains
  - collective excitations and collapse
  - boson-fermion mixtures and ultra-cold fermions

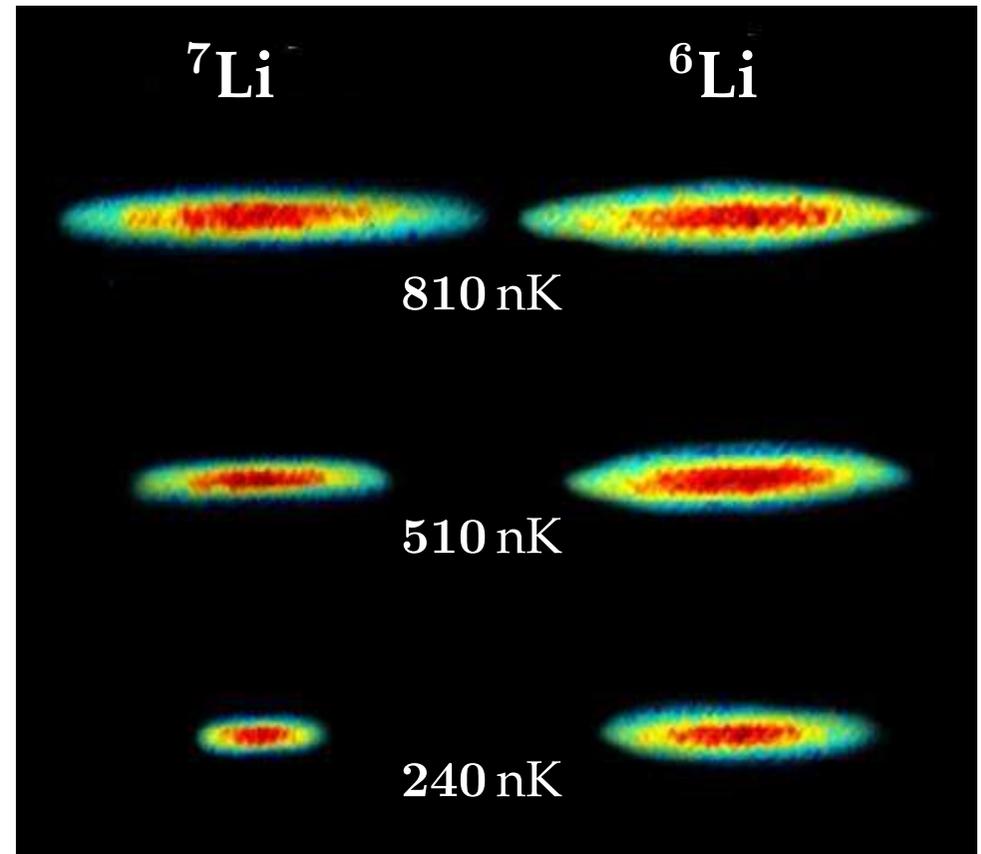


[W. Ketterle *et al.*; Science 292 (2001) 476]

...over the Intervening Years

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[R. Hulet *et al.*; Science 291 (2001) 2570]

everything well described within  
**mean-field theory** (Gross-Pitaevskii equation)

# The Advent of Correlations

**correlations** beyond  
mean-field begin to play a role

```
graph TD; A("correlations beyond mean-field begin to play a role") --> B("Feshbach Resonances"); A --> C("Optical Traps");
```

## Feshbach Resonances

- tuning of the scattering length over several orders of magnitude
- **coherent molecule formation:** molecular condensates, ultracold chemistry
- **BEC-BCS crossover:** generalized Cooper pairing, fermionic superfluidity

## Optical Traps

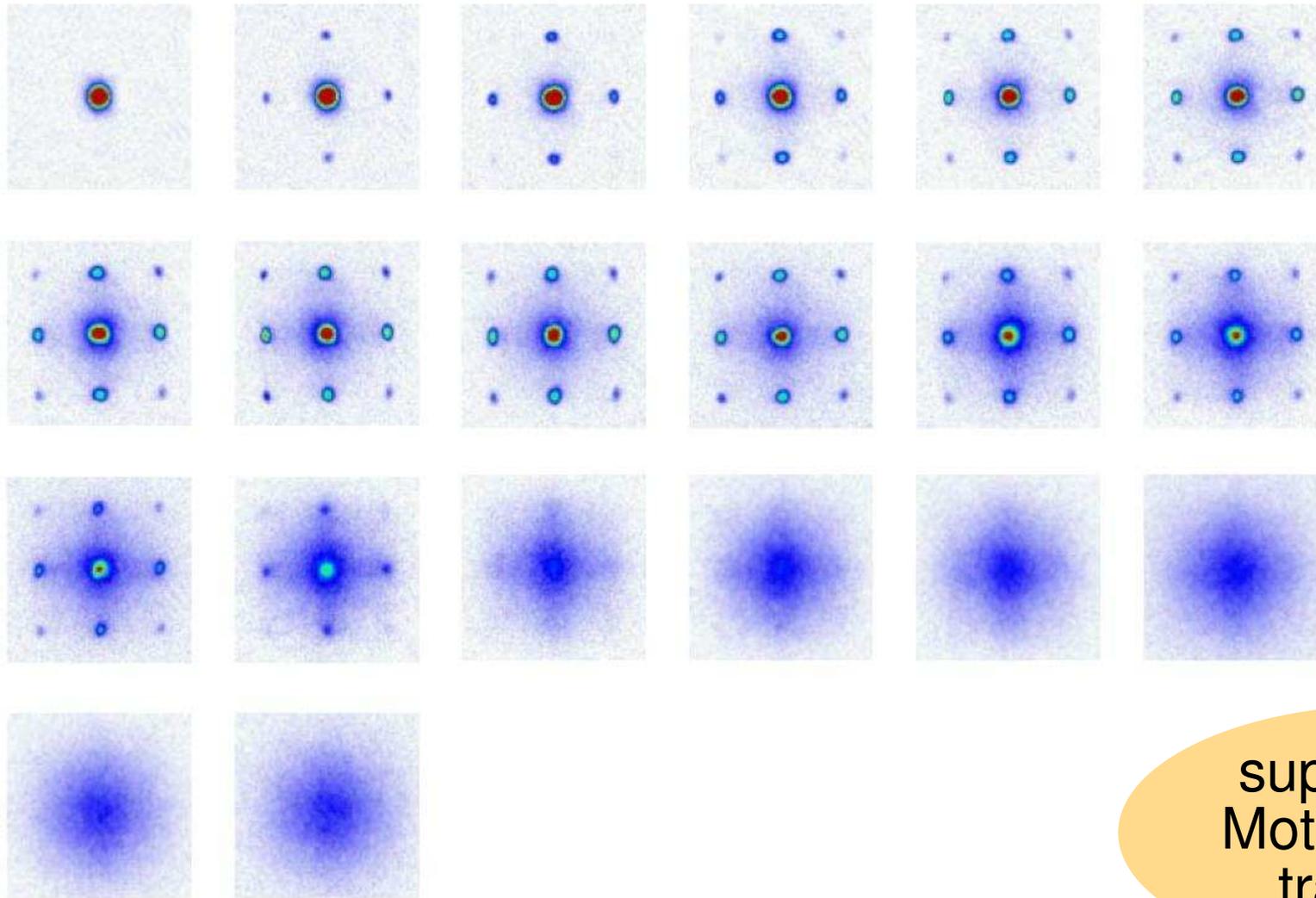
- tightly confining traps with a multitude of geometries
- **quasi 1D and 2D traps:** quantum gases in low dimensions
- **optical lattices in 1-3D:** band structure, quantum phase transitions, disorder, ...

# A Theoreticians' View of The Lattice Experiment

- produce a **Bose-Einstein condensate** of atoms in a magnetic trap
- load the condensate into an **optical standing-wave lattice** created by counter-propagating laser beams
- in a 3D lattice one ends up with **few atoms per lattice site** in a 1D lattice one can have thousands of atoms
- probe different physical regimes by varying **lattice depth** and **interaction strength**
- switch off the lattice, let the gas expand, and observe the **matter-wave interference pattern**

# Munich Experiment Interference Pattern

increasing lattice depth  $\longrightarrow$



characteristic  
interference pat-  
tern of array of  
coherent BECs

incoherent back-  
ground emerges  
and peaks van-  
ish

superfluid to  
Mott-insulator  
transition

[M. Greiner *et al.*; Nature 415 (2002) 39]

# Questions...

- How to describe ultracold bosons in a lattice?
- How to define **superfluid** and **condensate**?
- What is the **superfluid to Mott-insulator transition**?
- Are there **other quantum-phases** one can investigate?
- What happens if the lattice is **irregular**?
- What about **fermions**?

# Bose-Hubbard Model

# Bose-Hubbard Model

- one-dimensional lattice with  $N$  particles and  $I$  lattice sites at  $T = 0\text{K}$
- restrict Hilbert space to the **lowest energy band**
- localized Wannier wavefunctions  $w_i(x)$  with associated **occupation numbers**  $n_i$  for the individual sites  $i = 1 \dots I$
- represent  $N$ -boson state in complete basis of **Fock states**  $|\{n_1, \dots, n_I\}_\alpha\rangle$

$$|\Psi\rangle = \sum_{\alpha=1}^D C_\alpha |\{n_1, \dots, n_I\}_\alpha\rangle$$

- basis dimension  $D$  **grows dramatically** with  $I$  and  $N$

$I$	6	8	10	12	for $N/I = 1$
$D$	462	6435	92 378	1 352 078	

# Bose-Hubbard Hamiltonian

- second quantized Hamiltonian with respect to Wannier basis [Fisher *et al.* (1989); Jaksch *et al.* (1998)]

$$H_0 = -J \sum_{i=1}^I (a_{i+1}^\dagger a_i + \text{h.a.}) + \sum_{i=1}^I \epsilon_i n_i + \frac{V}{2} \sum_{i=1}^I n_i (n_i - 1)$$

tunneling between adjacent lattice sites      single-particle energy      on-site two-body interaction

- assumptions: (a) only lowest band, (b) constant nearest-neighbor hopping, (c) only short-range interactions

- ▶ describes **strongly correlated systems** as well as **pure condensates**
- ▶ **exact solution**: compute lowest eigenstates using Lanczos algorithms

# Simple Physical Quantities

- consider a regular lattice  $\rightarrow \epsilon_i = 0$
- solve eigenproblem for various  $V/J$

- **mean occupation numbers**

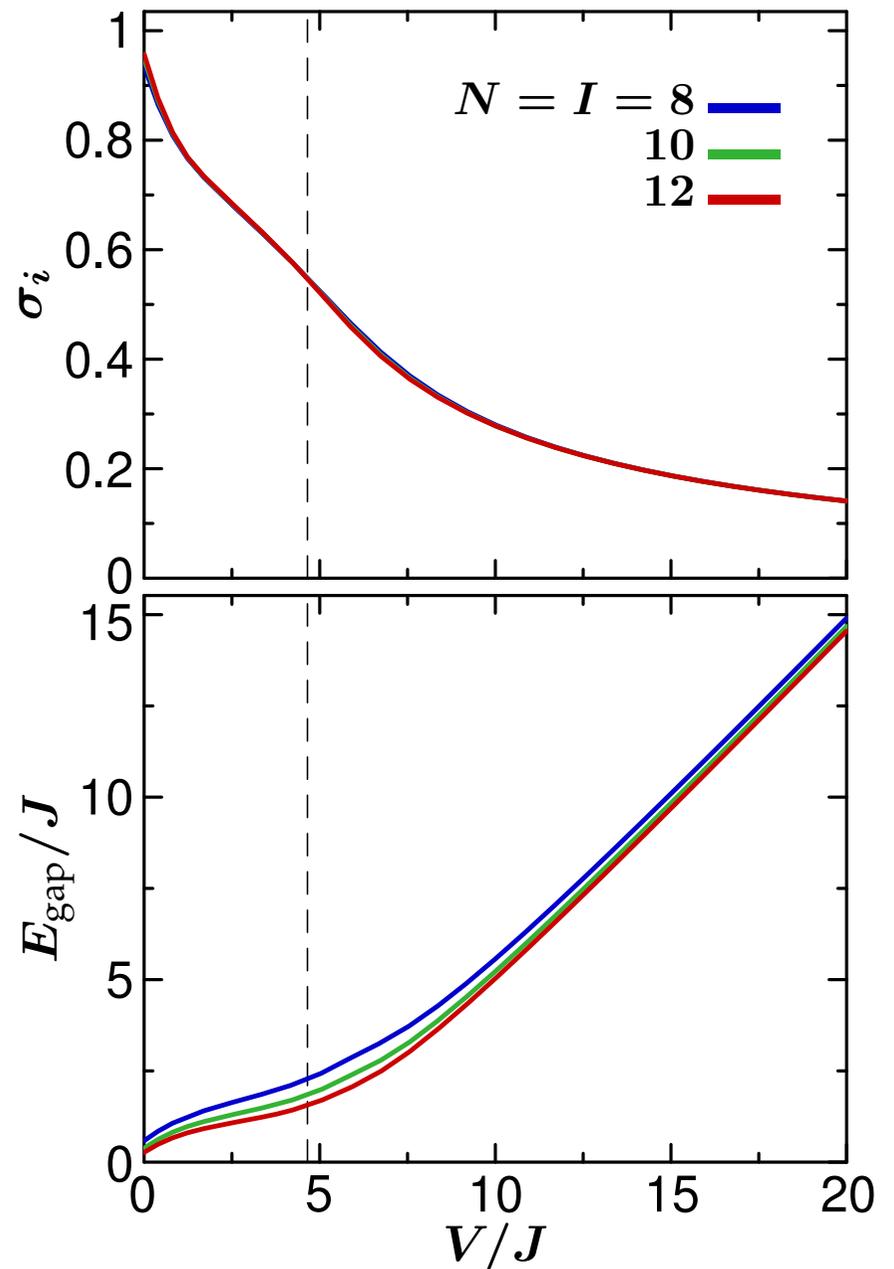
$$\bar{n}_i = \langle \Psi_0 | n_i | \Psi_0 \rangle$$

- **number fluctuations**

$$\sigma_i = \sqrt{\langle \Psi_0 | n_i^2 | \Psi_0 \rangle - \langle \Psi_0 | n_i | \Psi_0 \rangle^2}$$

- **energy gap**

$$E_{\text{gap}} = E_{\text{1st excited}} - E_0$$



# Condensate & Superfluidity

# Bose-Einstein Condensation

- eigensystem of the **one-body density matrix**

$$\rho_{ij}^{(1)} = \langle \Psi_0 | a_j^\dagger a_i | \Psi_0 \rangle$$

defines natural orbitals and the corresponding occupation numbers

- Onsager-Penrose criterion: **Bose-Einstein condensate** is present if one of the eigenvalues of  $\rho_{ij}^{(1)}$  is of order  $N$  (in the thermodynamic limit)

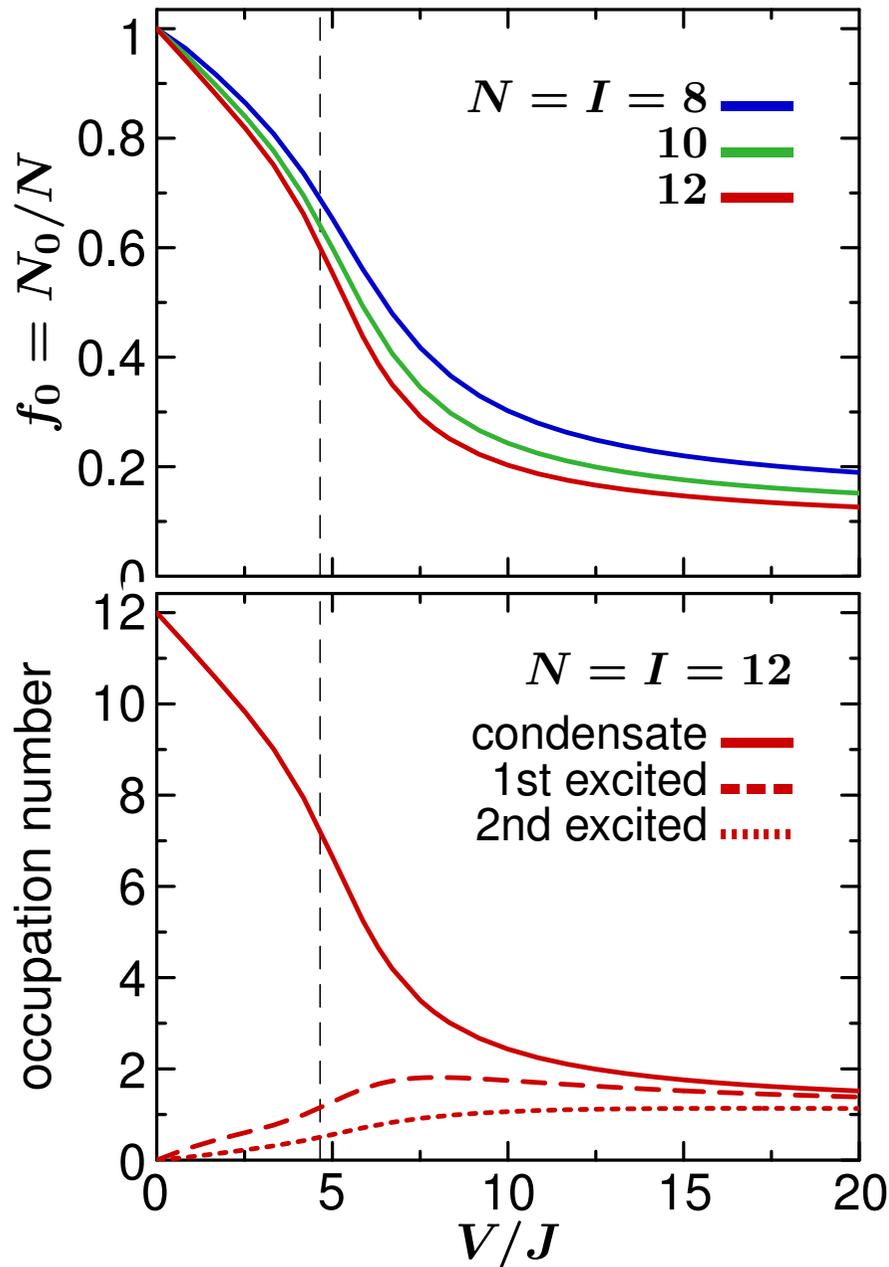
eigenvalue  $\rightarrow N_0$  : number of condensed particles  
eigenvector  $\rightarrow \phi_{0,i}$  : condensate wave function

- existence of a condensate implies **off-diagonal long range order**

$$\rho_{ij}^{(1)} \not\rightarrow 0 \quad \text{as} \quad |i - j| \rightarrow \infty$$

- in a regular lattice the natural orbitals are **quasimomentum eigenstates**

# Condensate & Quasimomentum Distribution



- pure condensate for  $V/J = 0$
- rapid depletion of the condensate with increasing  $V/J$
- finite size effect: condensate fraction in a finite lattice always  $\geq 1/I$
- states with larger quasimomentum are populated successively
- homogeneous occupation of the band in the limit of large  $V/J$

# What is Superfluidity?

- macroscopically the superfluid flow is **non-dissipative** and **irrotational**, i.e., it is described by the gradient of a scalar field

$$\vec{v}_{\text{SF}} \propto \vec{\nabla} \theta(\vec{x})$$

- **classical two-fluid picture**: only normal component responds to an imposed velocity field  $\vec{v}$  (moving walls), the superfluid stays at rest
- energy in the comoving frame differs from ground state energy in the rest frame by the **kinetic energy of the superflow**

$$E(\text{imposed } \vec{v}, \text{ comoving frame}) = E(\text{at rest}) + \frac{1}{2} M_{\text{SF}} \vec{v}^2$$

- ▶ these two ideas are basis for the **microscopic definition of superfluidity**

# Definition of Superfluidity

- the velocity field of the superfluid is defined by the **gradient of the phase** of the condensate wavefunction  $\phi_0(\vec{x})$

$$\vec{v}_{\text{SF}} = \frac{\hbar}{m} \vec{\nabla} \theta(\vec{x}) \quad \phi_0(\vec{x}) = e^{i\theta(\vec{x})} |\phi_0(\vec{x})|$$

- employ **twisted boundary conditions** to impose a linear phase variation

$$\Psi(\vec{x}_1, \dots, \vec{x}_i + L\vec{e}_1, \dots, \vec{x}_N) = e^{i\Theta} \Psi(\vec{x}_1, \dots, \vec{x}_i, \dots, \vec{x}_N) \quad \forall i$$

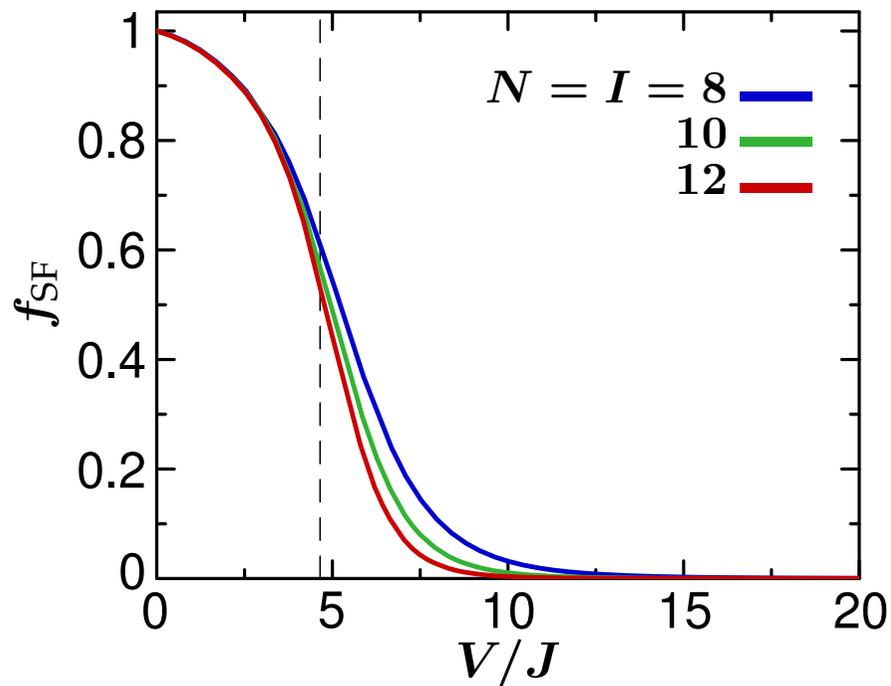
- the change in energy  $E_\Theta - E_0$  due to the phase twist is for small  $\Theta$  identified with the **kinetic energy of the superflow**

$$E_\Theta - E_0 = \frac{1}{2} M_{\text{SF}} v_{\text{SF}}^2 = \frac{1}{2} m N_{\text{SF}} v_{\text{SF}}^2$$

- superfluid fraction** = stiffness with respect to phase variations

$$F_{\text{SF}} = \frac{N_{\text{SF}}}{N} = \frac{2m L^2}{\hbar^2 N} \frac{E_\Theta - E_0}{\Theta^2} \quad \Theta \ll \pi$$

# Superfluid Fraction



- solve eigenvalue problem with & without imposed phase twist and directly compute  $E_{\Theta} - E_0$  and  $f_{\text{SF}}$
- $f_{\text{SF}}$  is the natural **order parameter** for the superfluid-insulator transition
- rapid decrease of  $f_{\text{SF}}$  in a narrow window in  $V/J$  already for small systems
- coupling to **excited states** is crucial for the vanishing of  $f_{\text{SF}}$  in the insulating phase

# Condensate -vs- Superfluid

## Condensate

- largest eigenvalue of the one-body density matrix
- involves only the ground state
- measure for off-diagonal long-range order / coherence

$$f_0 < f_{\text{SF}}$$

- non-condensed particles are dragged along with condensate
- liquid  $^4\text{He}$  at  $T = 0\text{K}$ :

$$f_0 \approx 0.1, \quad f_{\text{SF}} = 1$$

≠

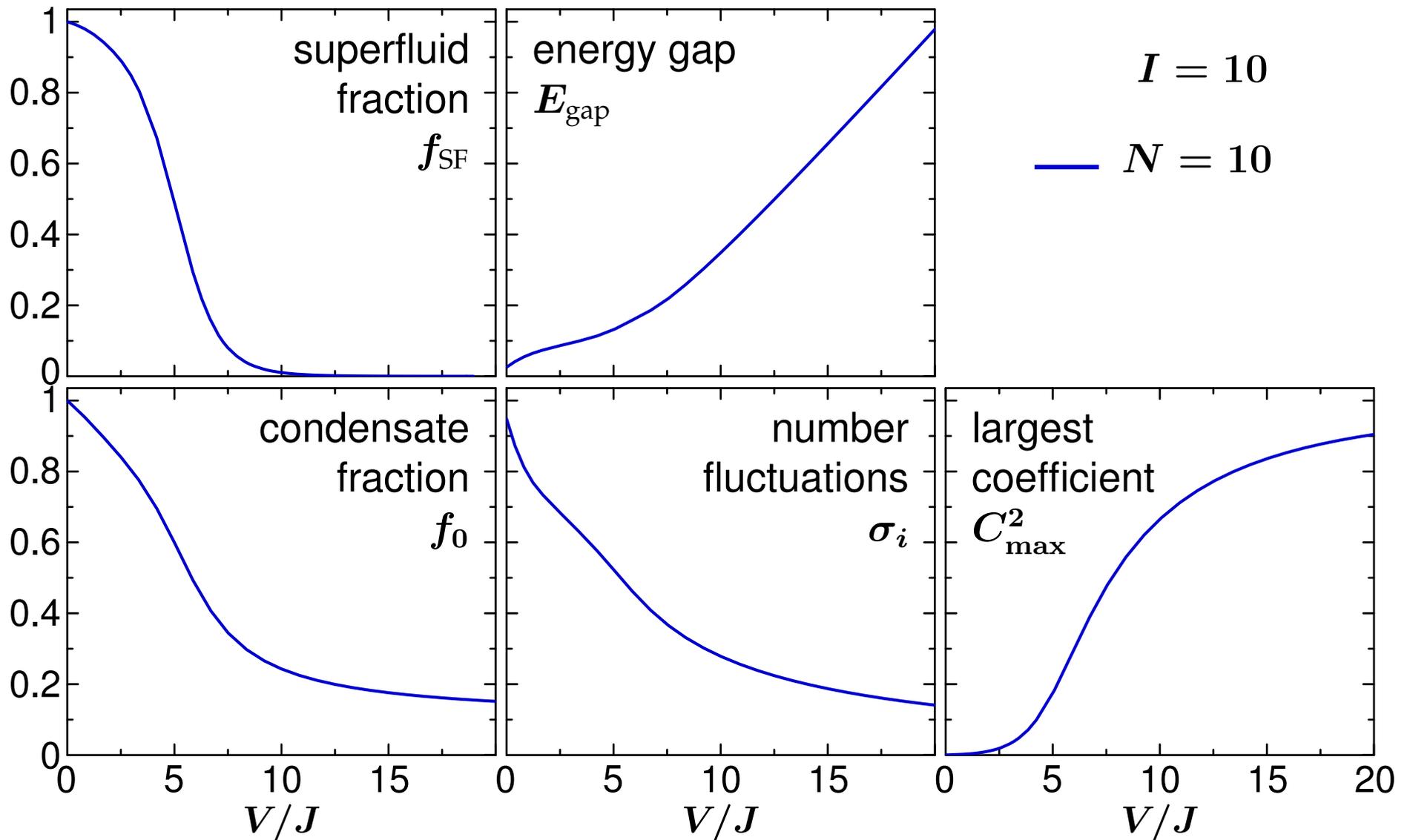
## Superfluid

- response of the system to an external perturbation
- depends crucially on the excited states of the system
- measures a flow property

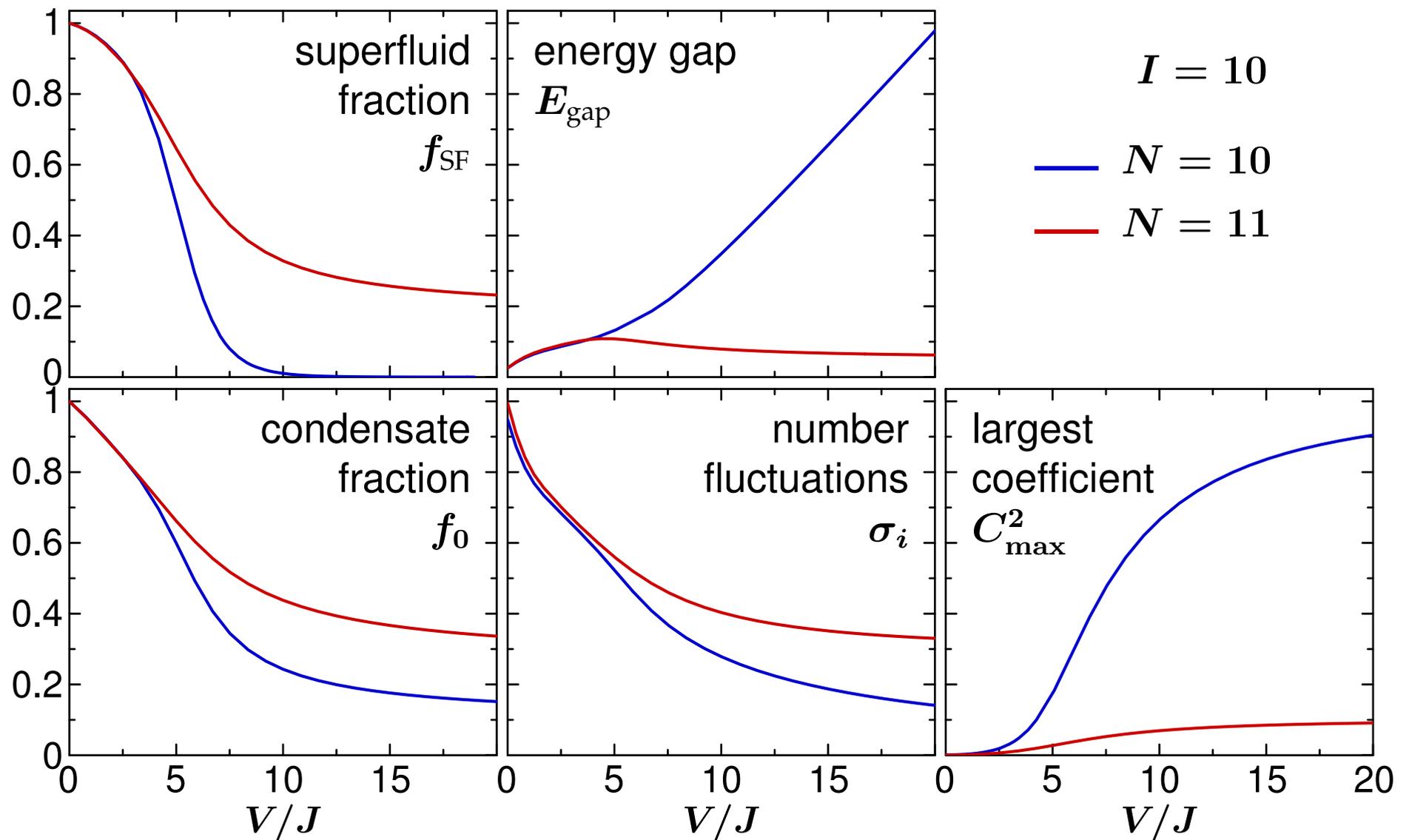
$$f_0 > f_{\text{SF}}$$

- part of the condensate has a reduced stiffness under phase variations
- seems to occur in systems with defects or disorder

# Superfluid to Mott-Insulator Transition

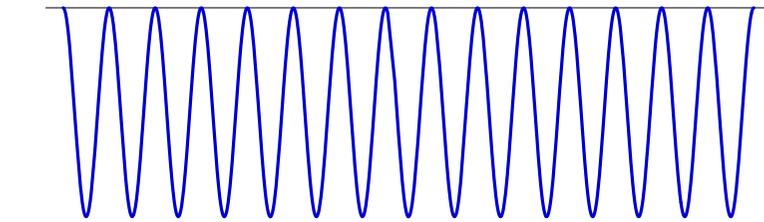


# Superfluid to Mott-Insulator Transition

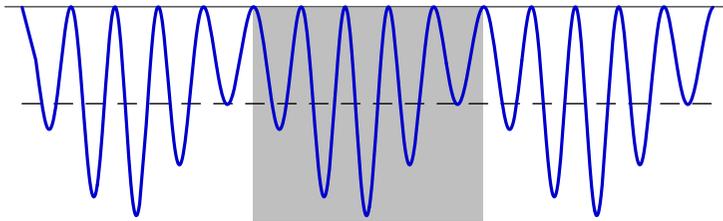


# Two-Color Superlattices

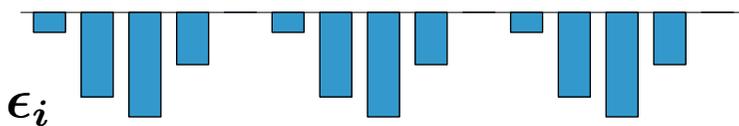
# Two-Color Superlattices



$U_1(x)$



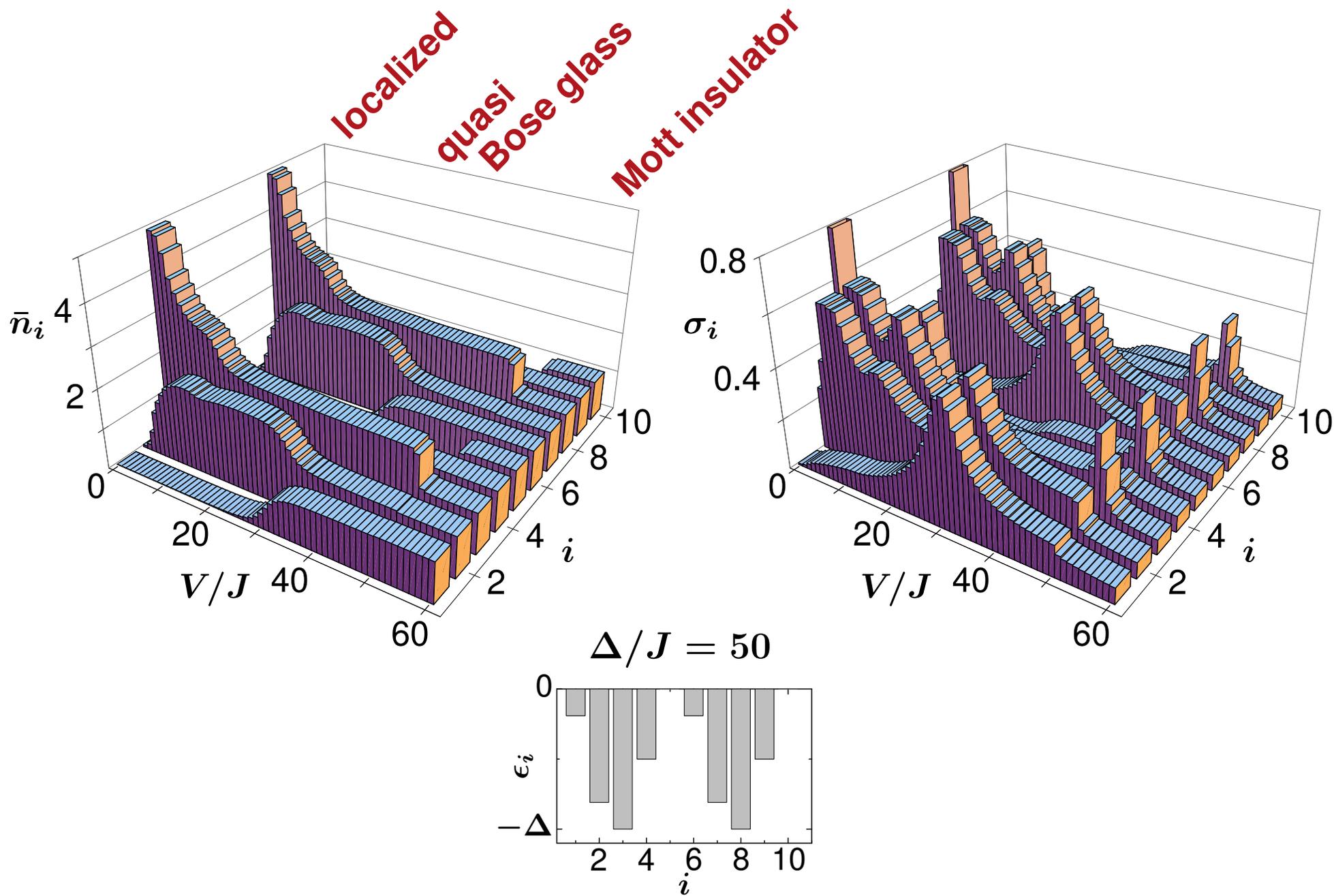
$U_{1+2}(x)$



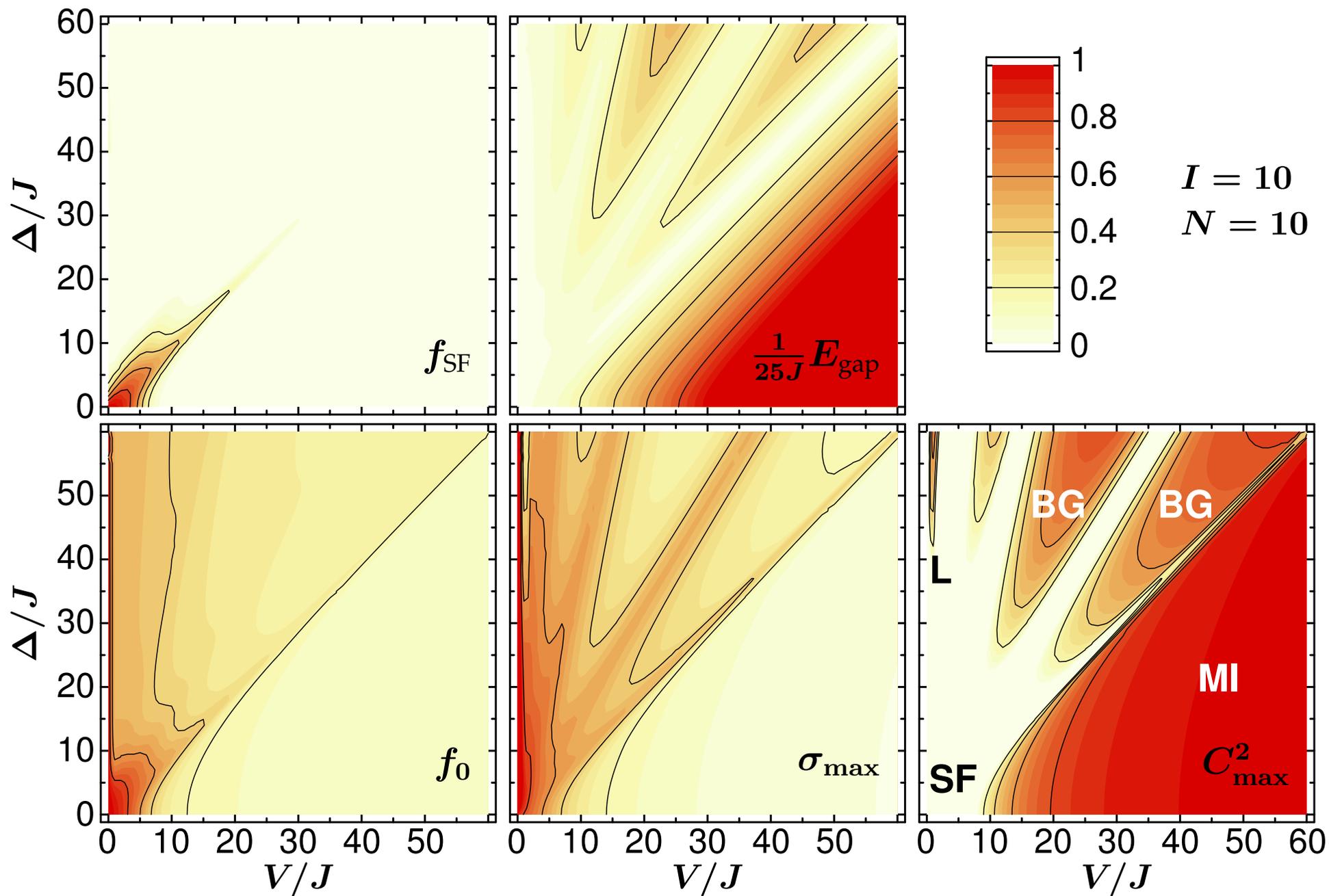
- start with a standing wave created by a laser with wavelength  $\lambda_1$
- add a second standing wave created by a laser with wavelength  $\lambda_2 = \frac{5}{7}\lambda_1$  and much smaller intensity (here 4%)
- potential exhibits a periodic modulation of the well-depth with a period of 5 sites
- Bose-Hubbard model: varying on-site energies  $\epsilon_i \in [0, -\Delta]$

► **controlled lattice irregularities** open novel possibilities to study “disorder” related effects; more complex topologies easily possible

# Interaction -vs- Lattice Irregularity



# $V$ - $\Delta$ Phase Diagrams



# Boson-Fermion Mixtures in Lattices

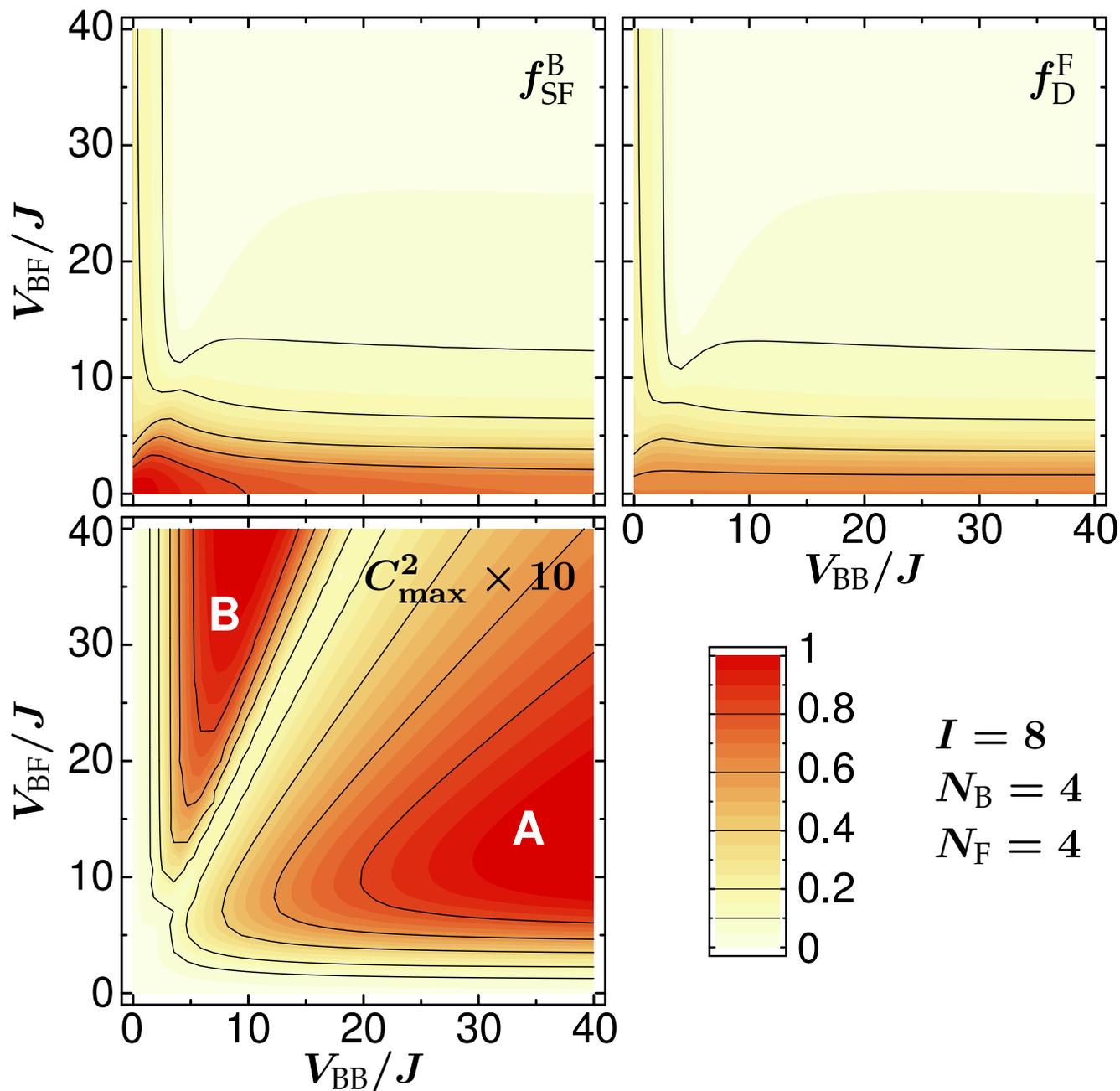
# Bose-Fermi-Hubbard Hamiltonian

- second quantized Hamiltonian containing boson (B) and fermion (F) operators [Albus et al. (2003)]

$$\begin{aligned} H_0 = & - J_B \sum_{i=1}^I (a_{i+1}^{B\dagger} a_i^B + \text{h.a.}) + \frac{V_{BB}}{2} \sum_{i=1}^I n_i^B (n_i^B - 1) \\ & - J_F \sum_{i=1}^I (a_{i+1}^{F\dagger} a_i^F + \text{h.a.}) + V_{BF} \sum_{i=1}^I n_i^B n_i^F \end{aligned}$$

- exact solution of eigenvalue problem in combined Fock-state representation
- in addition to ground state observables we employ two stiffnesses to characterize the various phases
  - **bosonic phase stiffness** → boson superfluid fraction
  - **fermionic phase stiffness** → Drude weight, fermionic conductivity

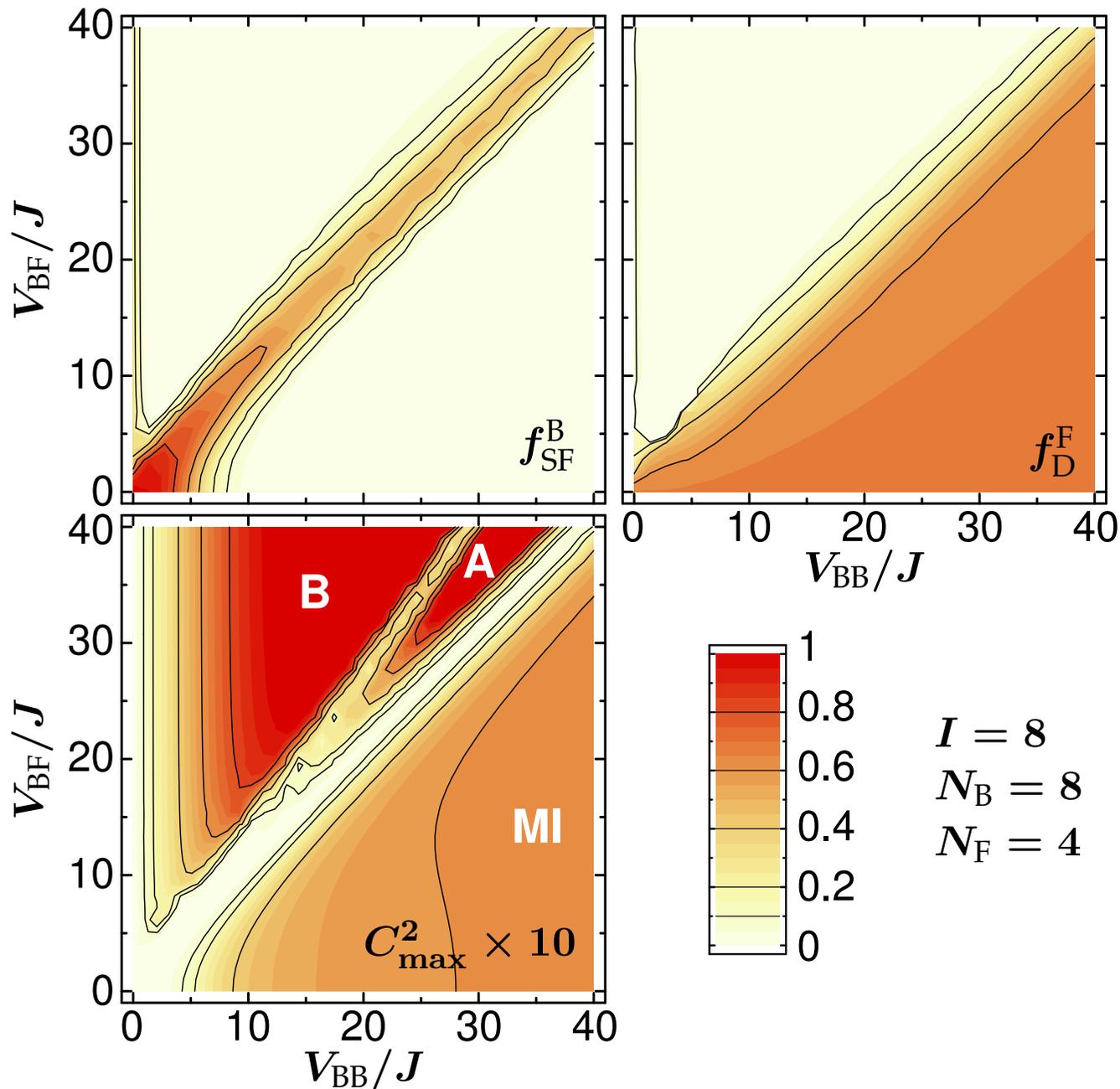
# $V_{\text{BB}}-V_{\text{BF}}$ Phase Diagrams



**A:** alternating boson-fermion occupation  
 → crystalline diagonal long-range order

**B:** continuous boson and fermion blocks  
 → component separation

# $V_{BB}$ - $V_{BF}$ Phase Diagrams



**A:** alternating boson-fermion occupation  
 → crystalline diagonal long-range order

**B:** continuous boson and fermion blocks  
 → component separation

**MI:** bosonic Mott insulator  
 → fermions not affected

# Summary

## ■ **superfluidity**

- stiffness under phase twists; depends crucially on the excitation spectrum

## ■ **condensate & coherence**

- property of the one-body density matrix of the ground state

## ■ **two-color superlattices**

- rich phase diagram with several insulating phases: localized, quasi Bose-glass, Mott-insulator

## ■ **boson-fermion mixtures in lattices**

- novel class of lattice systems with largely unexplored phase diagram

# Epilogue

- unique degree of **experimental control** makes ultracold atomic gases in optical lattices...
  - ideal model systems to study strong correlation effects (quantum phase transitions) and other solid-state questions
  - promising “hardware” for quantum information processing
- many **fascinating questions** still open...
  - fermions in lattices, attractive interactions & Cooper pairing
  - Bragg spectroscopy & dynamic structure factor
  - simulation of time-dependent optical lattices

# Epilogue

## ■ thanks to my collaborators

- M. Hild, F. Schmitt  
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- K. Burnett, J. Dunningham, K. Braun-Munzinger  
University of Oxford

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