Ultracold Bose Gases in Optical Lattices:

Superfluidity, Interference, Disorder

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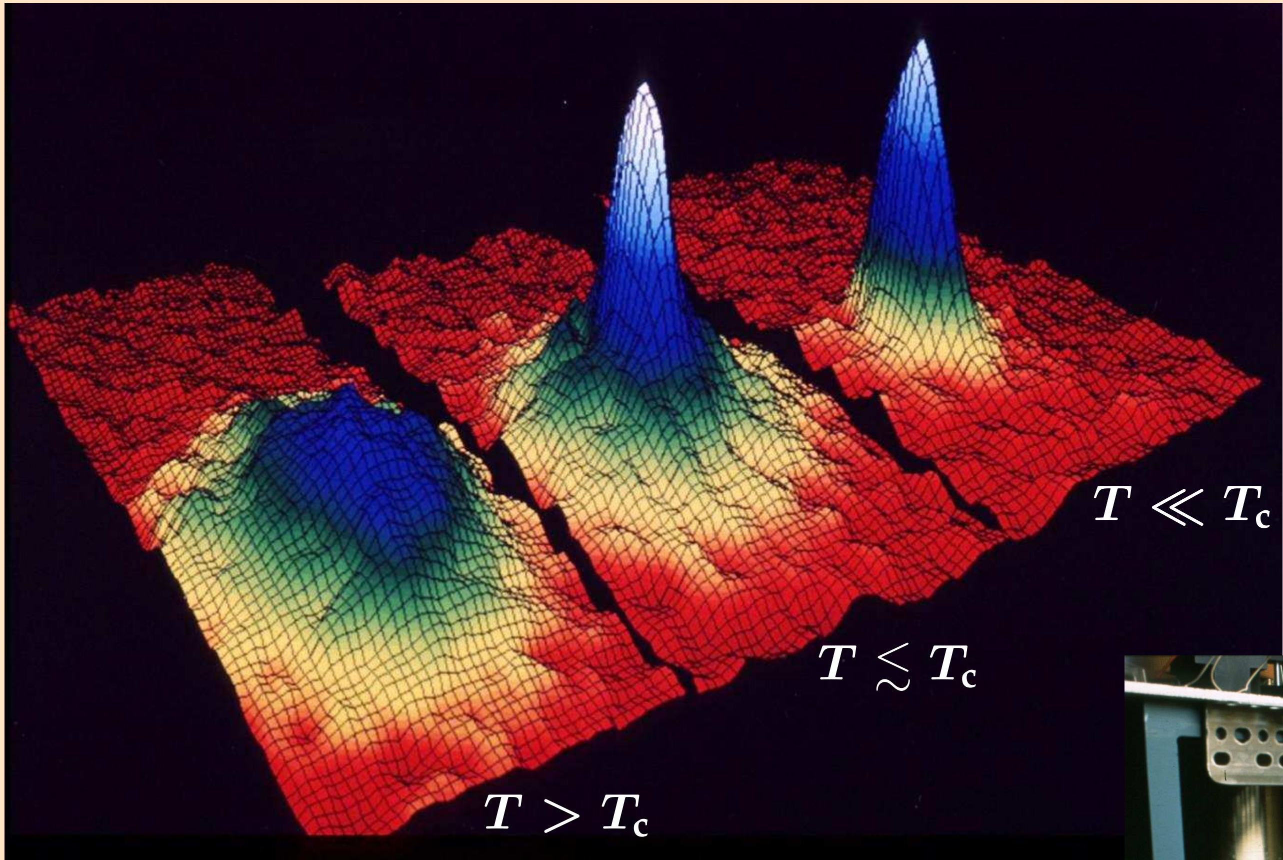
Overview

- Introduction
- Bose-Hubbard Model
- Condensate & Superfluidity
- Matter-Wave Interference Pattern
- Superfluid to Mott-Insulator Transition
- Two-Colour Lattices

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

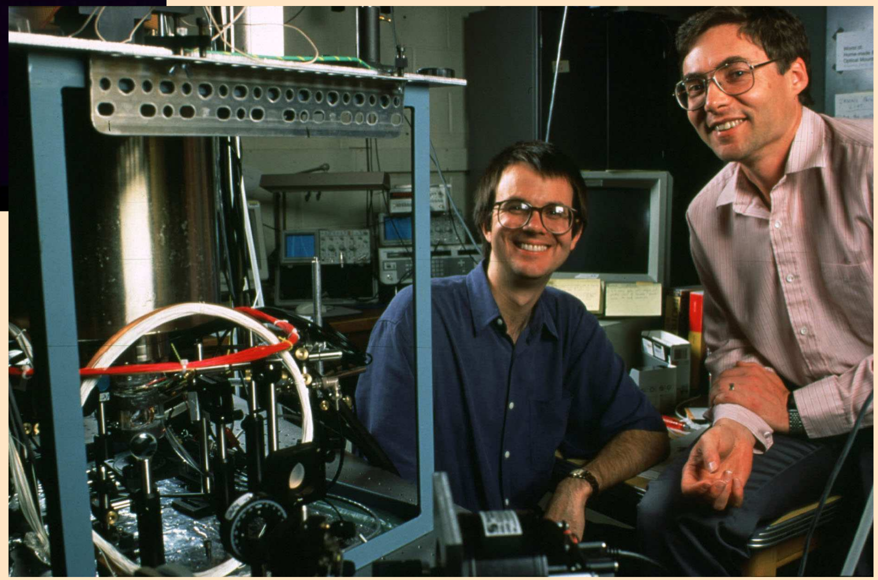
BEC of Rubidium Atoms



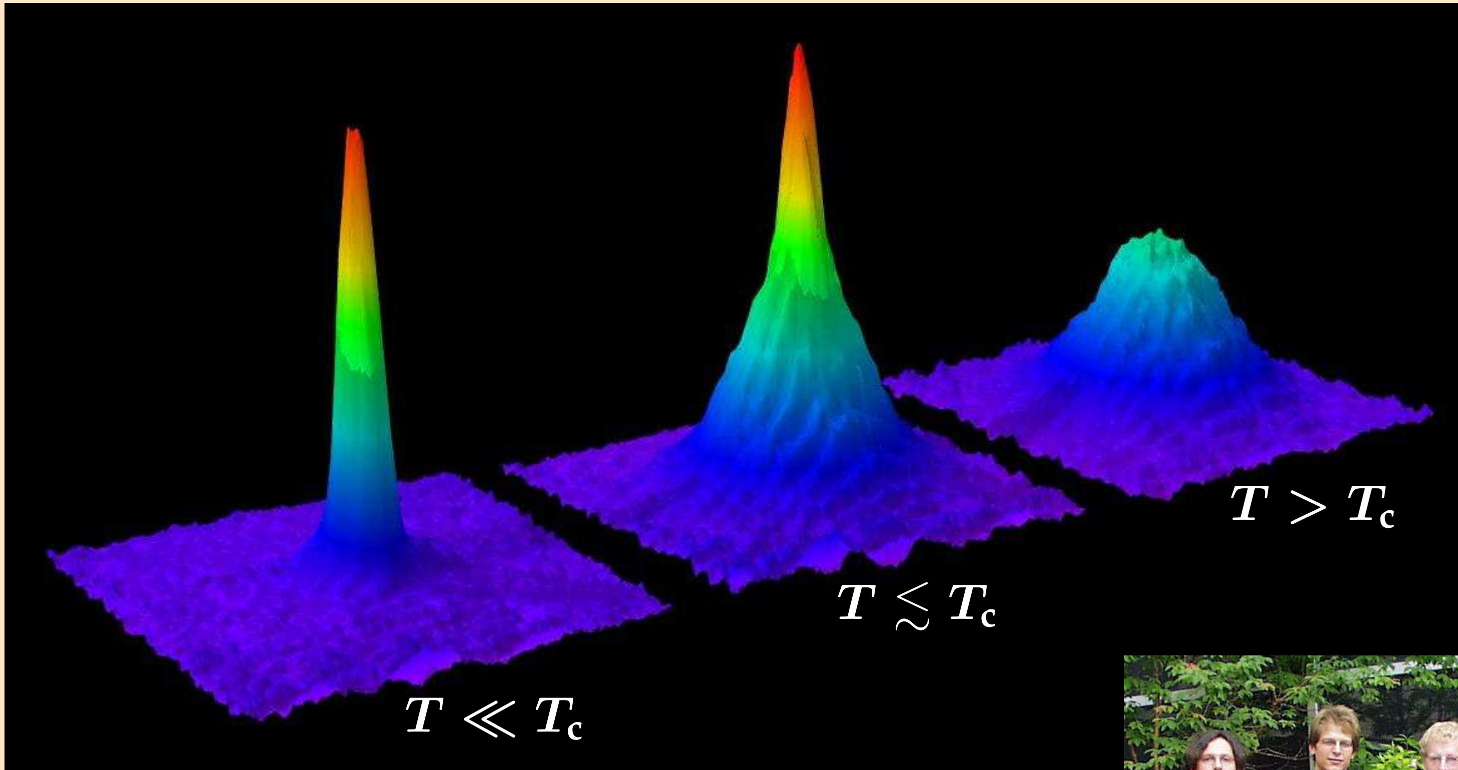
- ^{87}Rb $(F = 2, m_F = 2)$
- $N_{\text{initial}} \approx 10^6$
- $N_{\text{BEC}} \approx 2000$
- $T_c \approx 170$nK
- absorption image after $60\,$ms expansion
- 0.2mm $\times$ 0.27mm

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

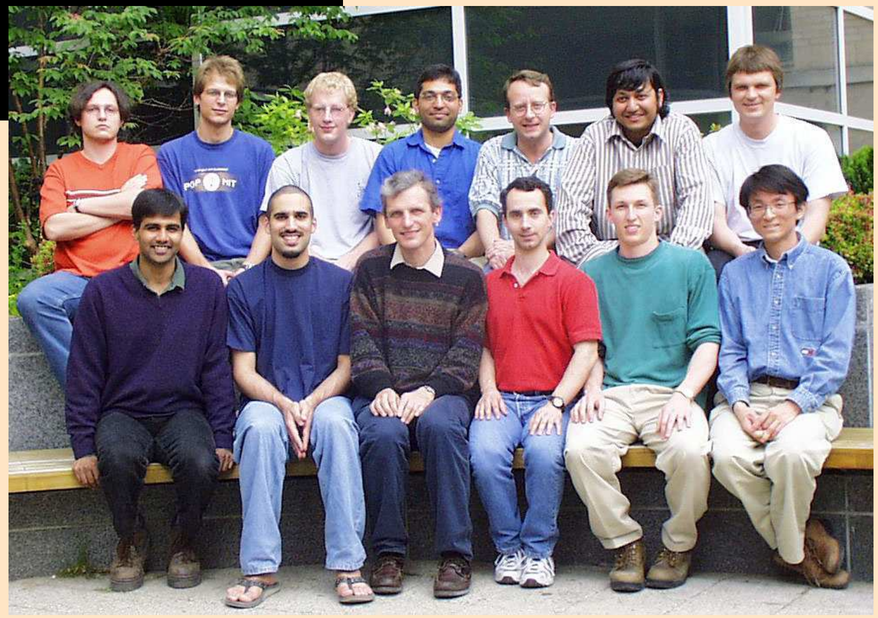
Nobel Prize in Physics 2001



BEC with Sodium Atoms



- ^{23}Na $(F=1, m_F=-1)$
- $N_{\text{initial}} \approx 10^9$
- $N_{\text{BEC}} \approx 5 \times 10^5$
- $T_c \approx 2\,\mu$K
- absorption image after $60\,$ms expansion
- 1mm $\times$ 1mm

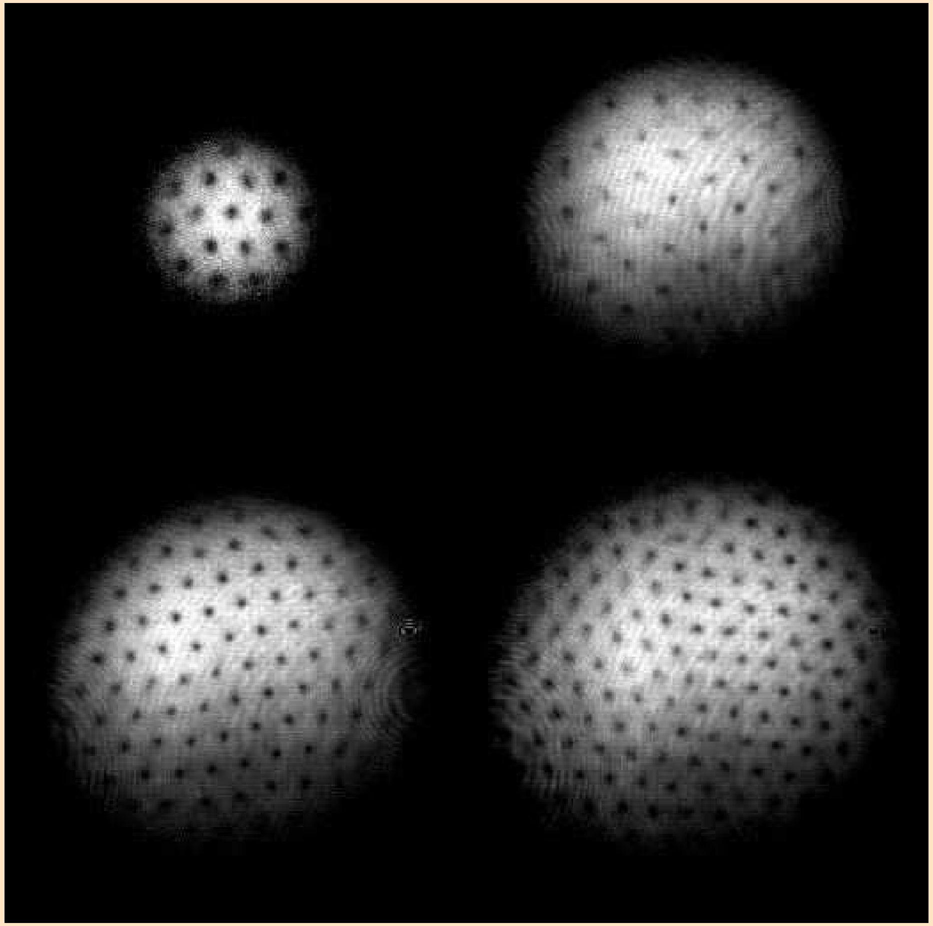


W. Ketterle, et al.
(MIT)

Nobel Prize in Physics 2001

Dynamics of Dilute Quantum Gases

- amazing experimental achievements
  - condensates of $^{1}\mathrm{H}$, $^{4}\mathrm{He}^{\star}$, $^{7}\mathrm{Li}$, $^{23}\mathrm{Na}$, $^{41}\mathrm{K}$, $^{85}\mathrm{Rb}$, $^{87}\mathrm{Rb}$, $^{133}\mathrm{Cs}$
  - vortices, vortex lattices and their dynamics
  - bright and dark solitons and soliton trains
  - collective modes: monopole, dipole, quadrupole, scissors,...
  - atom laser



Ketterle group, Science 292, 476-479 (2001)

- ► all these phenomena are well described in the framework of a **mean-field theory**, i.e., the Gross-Pitaevskii equation
- ► **correlations** (effects beyond mean-field) do not play a significant role...

The Advent of Correlations

correlations beyond the realm of a mean-field description begin to play a role in present day experiments

Feshbach Resonances

- allow to tune the scattering length (effective interaction strength) over several orders of magnitude and to switch the sign
- **strong interaction regime**, collapse of the Bose gas due to attractive interactions
- **coherent molecule formation** by sweeping through a Feshbach resonance

Optical Traps

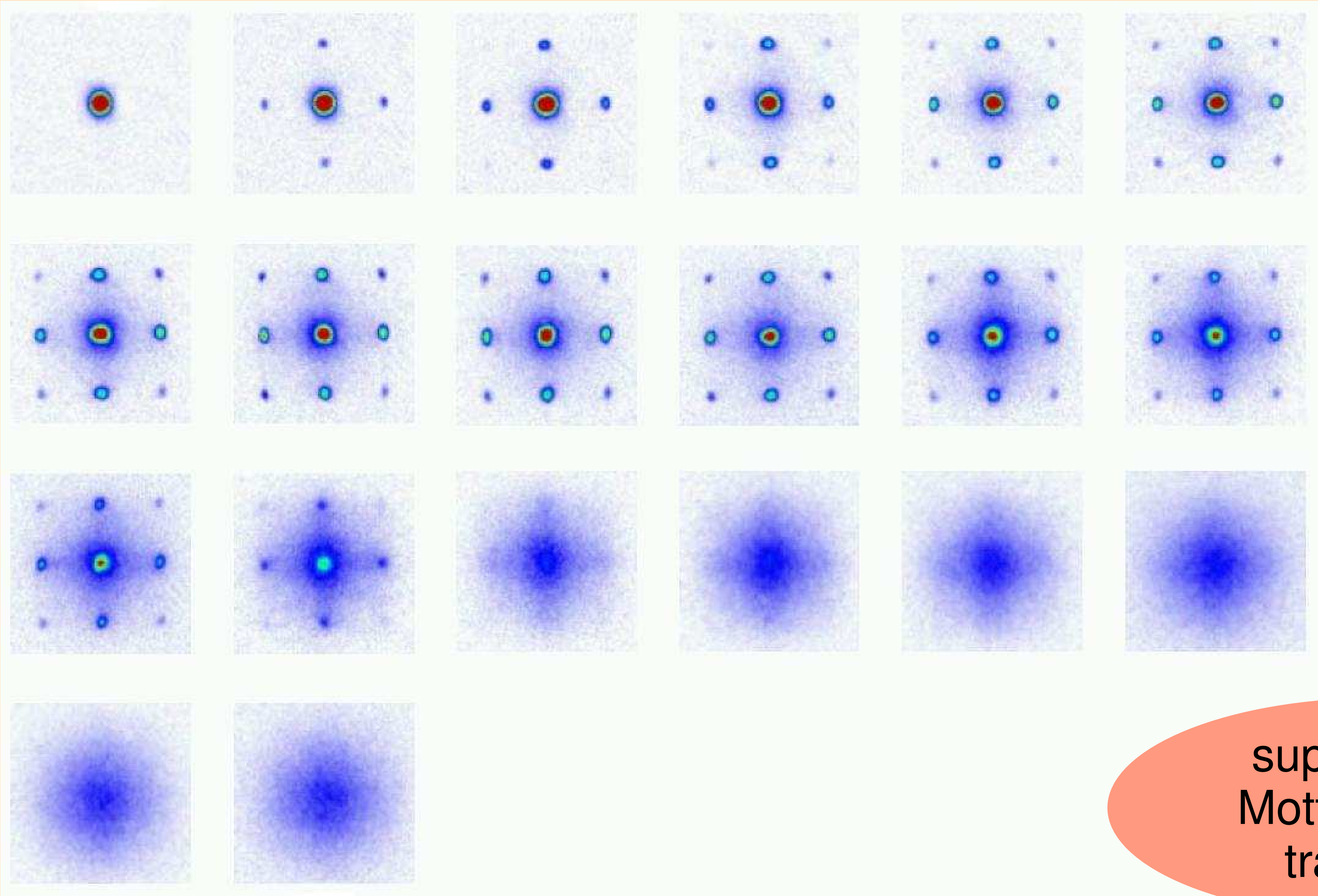
- allow to build very tightly confining traps with a multitude of geometries (using AC Stark shift)
- **quasi 1D and 2D traps**: quantum gases in low dimensions (Tonks gas, boson-fermion mapping, ...)
- **optical lattices in 1D, 2D and 3D**: quantum phase transitions, Mott-insulator, disorder, ...

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 by slowly increasing the laser intensity
- in a 3D lattice one ends up with **few atoms per lattice site** (favourable to study quantum phase transitions) in a 1D lattice one can have thousands of atoms
- by varying the **lattice depth** and the **interaction strength** one can probe different physical regimes
- switch off the lattice and let the gas expand for some time and observe the **matter-wave interference pattern**

Interference Pattern

increasing lattice depth ⟶



characteristic interference pattern of an array of coherent BECs emerges

incoherent background appears and peaks vanish slowly

superfluid to Mott-insulator transition

M. Greiner, *et al.*, Nature 415 (2002) 39

http://www.mpq.mpg.de/˜haensch/bec/experiments/mott.html

Many Questions

- How to describe ultracold bosons in a lattice?
- What is the **superfluid to Mott-insulator transition**?
- How to define **superfluidity**?
- What is the relation between **condensate** and superfluidity?
- What does the **interference pattern** tell about superfluidity?
- Are there **other quantum-phase transitions** one can investigate?
- What happens if the lattice potential is **irregular**?

Bose-Hubbard Model

Bose-Hubbard Model

- one-dimensional lattice with N particles and I lattice sites
- restricted Hilbert space: describe interacting many-body system in a basis of localised single-particle wave functions at the individual lattice sites
- solid-state language: consider only the **lowest band** and use the localised **Wannier functions** $w_i(x)$ as a basis
- represent many-boson state in a basis of **Fock states** $|n_1, ..., n_I\rangle$ with occupation numbers for the different localised Wannier states
- creation and annihilation operators for a boson localised at site i

$$\hat{a}_i^\dagger |n_1, ..., n_i, ..., n_I\rangle = \sqrt{n_i + 1}\, |n_1, ..., n_i + 1, ..., n_I\rangle$$
$$\hat{a}_i |n_1, ..., n_i, ..., n_I\rangle = \sqrt{n_i}\, |n_1, ..., n_i - 1, ..., n_I\rangle$$

$$\hat{n}_i = \hat{a}_i^\dagger \hat{a}_i$$

Bose-Hubbard Hamiltonian

- second quantised many-body Hamiltonian in restricted Hilbert space

$$\hat{\mathbf{H}}_0 = \underbrace{-J \sum_{i=1}^{I} (\hat{\mathbf{a}}_{i+1}^\dagger \hat{\mathbf{a}}_i + \mathrm{h.a.})}_{\text{tunnelling between adjacent lattice sites}} + \underbrace{\sum_{i=1}^{I} \epsilon_i \, \hat{\mathbf{n}}_i}_{\text{single-particle energy}} + \underbrace{\frac{V}{2} \sum_{i=1}^{I} \hat{\mathbf{n}}_i (\hat{\mathbf{n}}_i - 1)}_{\text{on-site two-body interaction}}$$

- the parameters J, ϵ_i, and V are given by matrix elements of the different terms of the continuous Hamiltonian in the Wannier basis

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

▶ Bose-Hubbard model is able to describe **strongly correlated systems** as well as **pure condensates**

Exact Numerical Solution

- solve matrix eigenvalue problem for the Bose-Hubbard Hamiltonian in a complete basis of Fock states $|n_1^{(\alpha)}, ..., n_I^{(\alpha)}\rangle$ with $\alpha = 1, ..., D$ for given N

$$|\Psi\rangle = \sum_{\alpha=1}^{D} C_\alpha |n_1^{(\alpha)}, ..., n_I^{(\alpha)}\rangle$$

- problem: the number D of basis states **grows dramatically**

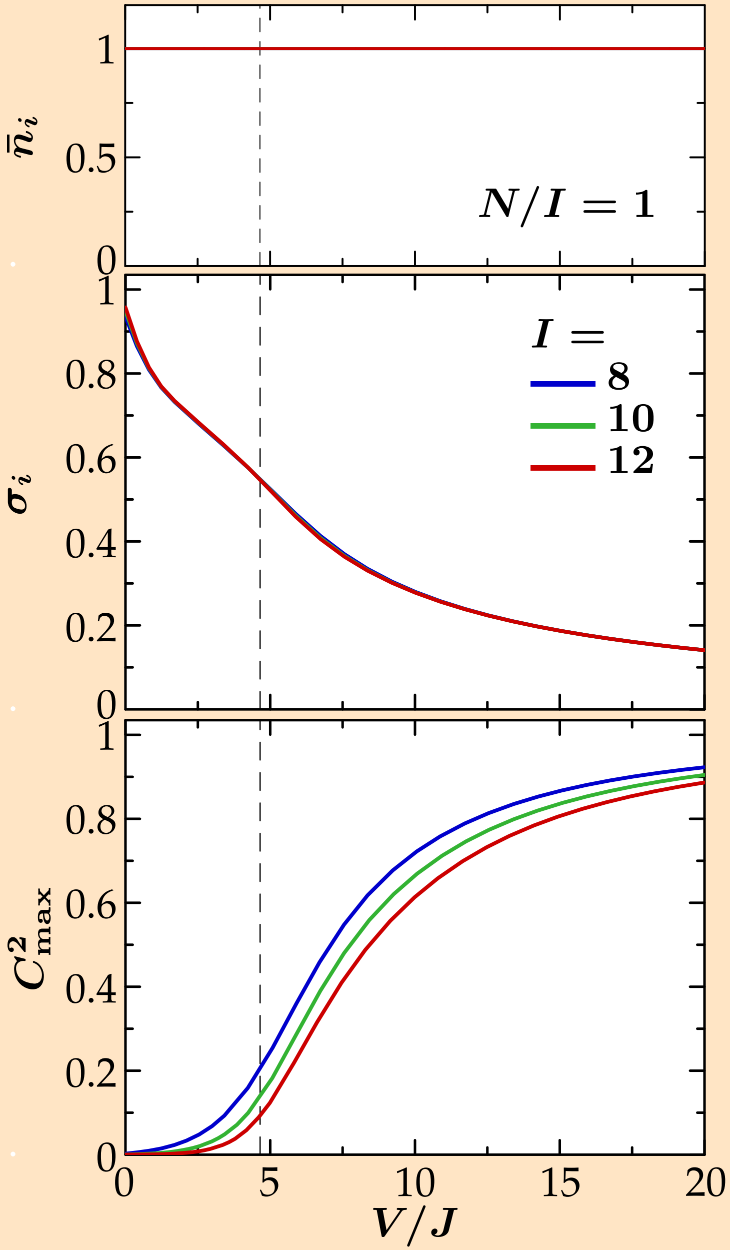
I	6	8	10	12
D	462	6435	92378	1352078

for $N/I = 1$

- use efficient iterative Lanczos algorithm to compute the lowest eigenvalues and eigenvectors of the sparse Hamilton matrix

- ▶ larger systems can be described by computationally very involved Monte Carlo methods (typically up to $I \sim 1000$)
- ▶ there are several approximation schemes, each applicable in very restricted parameter regimes only; none can describe the phase transition correctly

Simple Quantities



- calculate ground state $|\Psi_0\rangle$ for a sequence of values for V/J
- **mean occupation number**
$$\bar{n}_i = \langle\Psi_0|\,\hat{n}_i\,|\Psi_0\rangle$$
- **number fluctuations**
$$\sigma_i = \Big[\langle\Psi_0|\,\hat{n}_i^2\,|\Psi_0\rangle - \langle\Psi_0|\,\hat{n}_i\,|\Psi_0\rangle^2\Big]^{1/2}$$
- **largest coefficient**
$$C^2_{\max} = \max(C^2_\alpha)$$

▶ small V/J: hopping dominates; superpositions of many number states are favoured

▶ large V/J: interaction dominates; number states with smallest occupation numbers are preferred

Condensate & Superfluidity

General Definition of the
Bose-Einstein Condensate

- What does BE condensation mean in a strongly correlated many-body system?

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

$$\rho_{ij}^{(1)} = \langle \Psi_0 | \, \hat{a}_i^\dagger \hat{a}_j \, | \Psi_0 \rangle$$

  define the natural orbitals and the eigenvalues the corresp. occupation numbers

- Onsager-Penrose criterion: if one of the eigenvalues of $\rho_{ij}^{(1)}$ is of order N, such that N_0/N remains finite in the *thermodynamic limit*, then a **Bose-Einstein condensate** is present

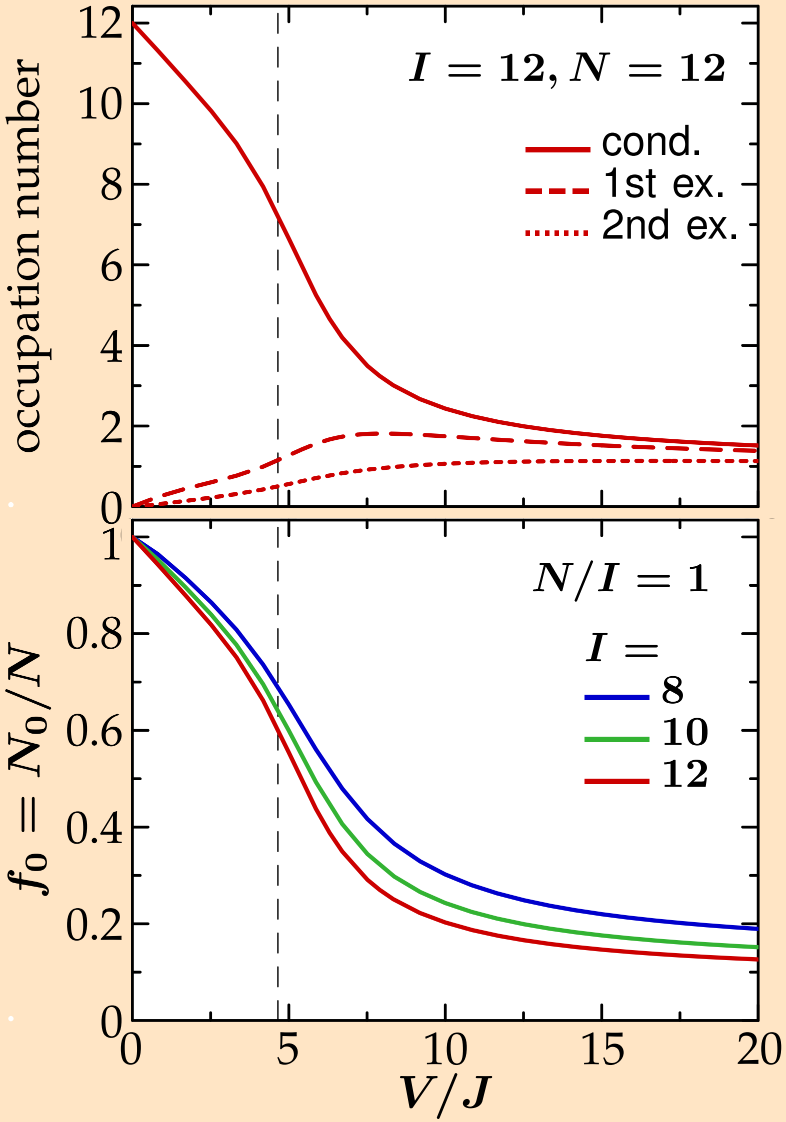
$$\begin{array}{rcccl} \text{eigenvalue} & \longrightarrow & N_0 & : & \text{number of condensed particles} \\ \text{eigenvector} & \longrightarrow & \phi_{0,i} & : & \text{condensate wave function} \end{array}$$

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

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

- in a regular lattice the natural orbitals are **quasi-momentum eigenstates**

Condensate Fraction



- noninteracting system: only the condensate state is populated
- with increasing V/J condensate is depleted and higher orbitals (larger q) are successively populated
- uniform population of the orbitals (band) in the strong interaction limit
- significant finite size effects: condensate fraction in a finite lattice always $\geq 1/I$
- one cannot judge about the absence of a condensate in the Penrose-Onsager sense in a finite size system

What is Superfluidity?

There is no "one-size-fits-all" definition of superfluidity!

Elliott H. Lieb, et al., cond-mat/0205570

What is Superfluidity?

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

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

- classical two-fluid picture: if a velocity field $\vec{v}$ is imposed (moving walls), then only the normal component responds, the superfluid component stays at rest
- the energy in the comoving frame differs from the ground state energy E_0 in the rest frame by the **kinetic energy of the superflow**

$$E(\text{imposed } \vec{v},\ \text{comoving frame}) = E_0 + \tfrac{1}{2} M_{\mathrm{SF}}\, \vec{v}^2$$

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

▶ NB: this is not the Landau picture of superfluidity and we do not consider the stability of the superflow (critical velocity)

Definition of Superfluidity

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

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

- to probe superfluidity (formally) we impose a linear phase variation onto the system, e.g., by **twisted boundary conditions** for the many-body wave function

$$\Psi(\vec{x}_1, ..., \vec{x}_i + L\vec{e}_1, ..., \vec{x}_N) = \mathrm{e}^{\mathrm{i}\Theta}\;\Psi(\vec{x}_1, ..., \vec{x}_i, ..., \vec{x}_N) \qquad \forall i$$

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

$$E_\Theta - E_0 = \tfrac{1}{2}M_{\mathrm{SF}}\;v_{\mathrm{SF}}^2 = \tfrac{1}{2}mN_{\mathrm{SF}}\;v_{\mathrm{SF}}^2$$

- **superfluid fraction** is proportional to the energy change due to the phase twist

$$\boxed{f_{\mathrm{SF}} = \frac{N_{\mathrm{SF}}}{N} = \frac{2m\,L^2}{\hbar^2 N}\,\frac{E_\Theta - E_0}{\Theta^2} \qquad\qquad (\Theta \to 0)}$$

Superfluidity on the Lattice

- **superfluid fraction** for a one-dimensional lattice with I sites and N particles

$$f_{\mathrm{SF}} = \frac{I^2}{JN}\,\frac{E_\Theta - E_0}{\Theta^2}$$

- twisted boundary conditions not feasible for a discrete system: use a unitary transformation to map the phase twist onto the Hamilton operator

- **twisted Hamiltonian** has a modified hopping term which contains the so called Peierls phase factors

$$\hat{\mathrm{H}}_\Theta \;=\; -J\sum_{i=1}^{I}(\mathrm{e}^{-\mathrm{i}\Theta/I}\,\hat{\mathrm{a}}^\dagger_{i+1}\hat{\mathrm{a}}_i + \mathrm{h.a.}) \;+\; \cdots$$

▶ procedure: solve the eigenvalue problem for the original and the twisted Bose-Hubbard Hamiltonian (with periodic BCs) to obtain E_0 and E_Θ

▶ phase factors can be engineered in experiment by accelerating the lattice or adding a linear potential → basis for schemes to **probe superfluidity directly**

Superfluid Fraction

- calculate the energy difference $E_\Theta - E_0$ induced by a small phase twist Θ in second order perturbation theory

$$\hat{\mathrm{H}}_\Theta \simeq \hat{\mathrm{H}}_0 + \frac{\Theta}{I}\hat{\mathrm{J}} - \frac{\Theta^2}{2I^2}\hat{\mathrm{T}} = \hat{\mathrm{H}}_0 + \hat{\mathrm{H}}_{\mathrm{pert}}$$

$$\hat{\mathrm{T}} = -J\sum_i(\hat{\mathrm{a}}_{i+1}^\dagger\hat{\mathrm{a}}_i + \mathrm{h.a.})$$
$$\hat{\mathrm{J}} = \mathrm{i}J\sum_i(\hat{\mathrm{a}}_{i+1}^\dagger\hat{\mathrm{a}}_i - \mathrm{h.a.})$$

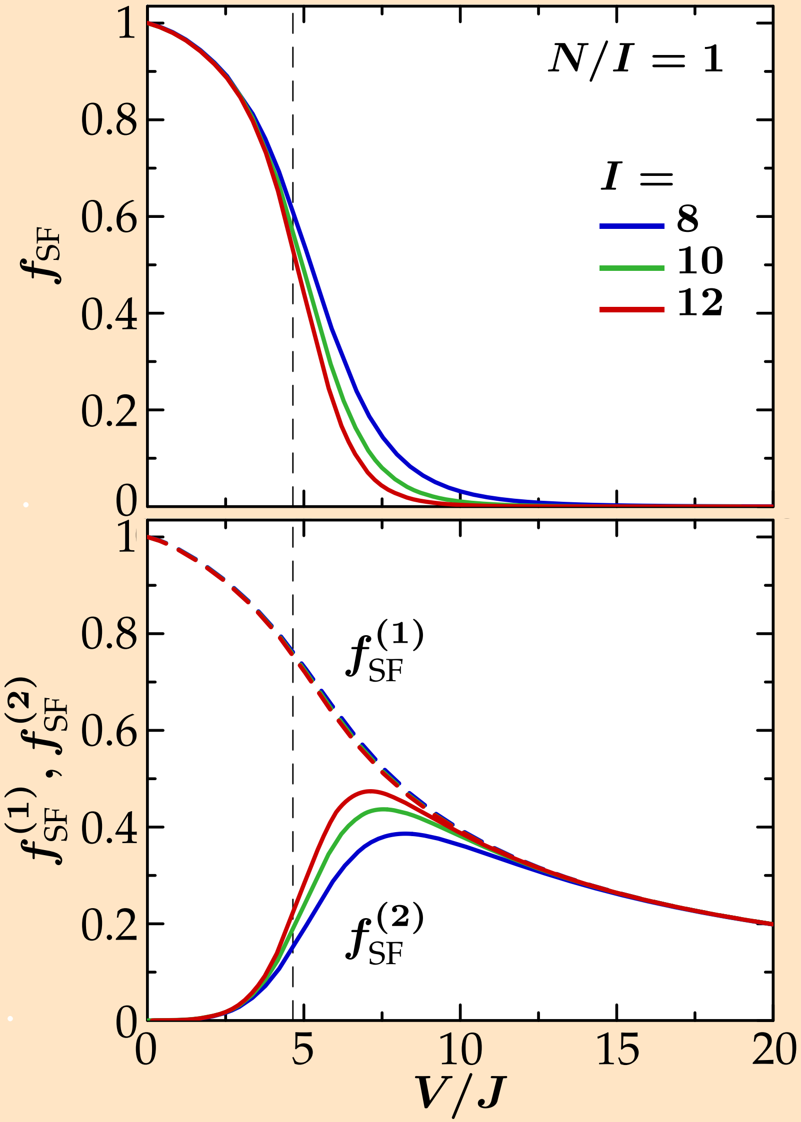
- including all contributions to the energy difference up to order Θ^2 gives for the superfluid fraction

$$f_{\mathrm{SF}} = f_{\mathrm{SF}}^{(1)} - f_{\mathrm{SF}}^{(2)}$$

$$f_{\mathrm{SF}}^{(1)} = -\frac{1}{2NJ}\langle\Psi_0|\,\hat{\mathrm{T}}\,|\Psi_0\rangle \qquad f_{\mathrm{SF}}^{(2)} = \frac{1}{NJ}\sum_{\nu\neq 0}\frac{|\langle\Psi_\nu|\,\hat{\mathrm{J}}\,|\Psi_0\rangle|^2}{E_\nu - E_0}$$

- **1st order term**: depends only on the ground state expectation value of $\hat{\mathrm{T}}$
- **2nd order term**: couples to the **whole excitation spectrum of $\hat{\mathrm{H}}_0$**
- the superfluid fraction measures the **response** of the system to an external perturbation (phase twist)

Superfluid Fraction



- superfluid fraction is the natural **order parameter** for the superfluid-insulator transition
- rapid decrease of f_{SF} in a narrow window in V/J already for small systems
- transition region in good agreement with Monte Carlo calculations for $(V/J)_{crit}$

- $f_{SF}^{(1)}$ decreases only very slowly
- vanishing of f_{SF} in the insulating phase is due to a cancellation between $f_{SF}^{(1)}$ and $f_{SF}^{(2)}$
- coupling to **excited states** is crucial for the vanishing of f_{SF} in the insulating phase

Condensate -vs- Superfluidity

condensate $\neq$ superfluid

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

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

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

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

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

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

- part of the condensate is not superfluid, i.e., it has a reduced rigidity against phase variations
- seems to occur in systems with defects or disorder

Matter-Wave Interference Pattern

Interference Pattern

- switch off the lattice and let the gas expand for some time τ
- free expansion described by the spreading of a Gaussian wave packet $G_i(\vec{y},t)$
- intensity $\mathcal{I}(\vec{y})$ observed at a point $\vec{y}$ after expansion time τ

$$\mathcal{I}(\vec{y}) = \left\langle \Psi_0 \right| \hat{\mathrm{A}}^\dagger(\vec{y}) \hat{\mathrm{A}}(\vec{y}) \left| \Psi_0 \right\rangle \qquad \hat{\mathrm{A}}(\vec{y}) = \sum_{i=1}^{I} G_i(\vec{y},\tau)\, \hat{\mathrm{a}}_i$$

- discard all information about the intensity envelope and take into account only the phase terms in the far-field

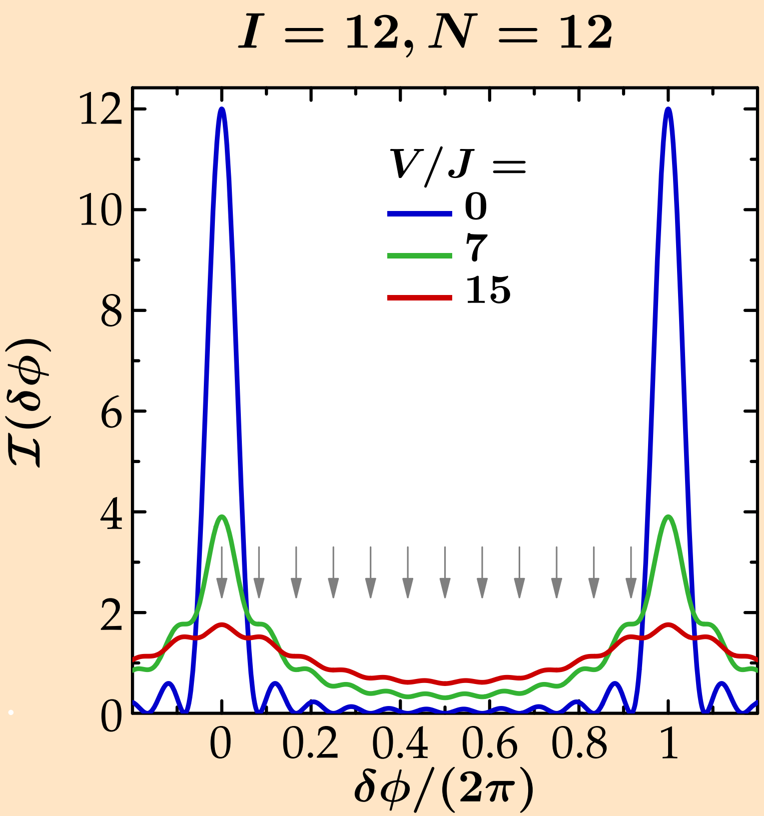
$$G_i(\vec{y},\tau) \;\longrightarrow\; \mathrm{e}^{\mathrm{i}\,\phi_i(\vec{y},\tau)} \;\longrightarrow\; \mathrm{e}^{\mathrm{i}\,\delta\phi(\vec{y},\tau)\,i}$$

- intensity as function of phase difference $\delta\phi$

$$\mathcal{I}(\delta\phi) = \frac{1}{I} \sum_{i,j=1}^{I} \mathrm{e}^{\mathrm{i}\;\delta\phi\;(j-i)} \underbrace{\left\langle \Psi_0 \right| \hat{\mathrm{a}}_i^\dagger \hat{\mathrm{a}}_j \left| \Psi_0 \right\rangle}_{\rho_{ij}^{(1)}}$$

▸ interference pattern gives information on the one-body density matrix of the ground state, e.g. the **quasi-momentum distribution**

Interference Pattern



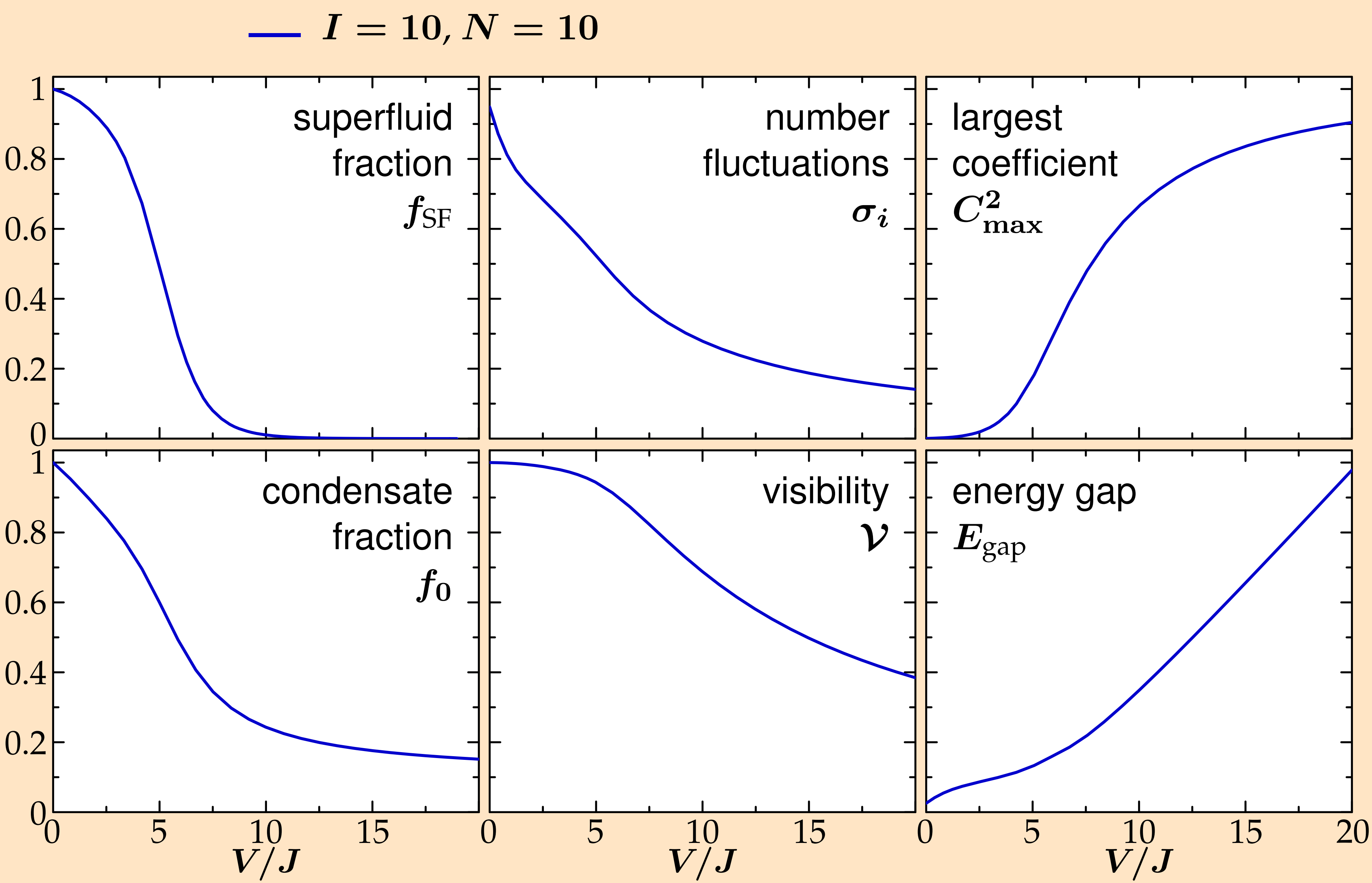
- peaks at $\delta\phi = 0, \pm 2\pi, \ldots$ correspond to the principal interference peaks seen in experiment
- with increasing V/J principal peaks are depleted and broadened; background emerges
- equivalently: with increasing V/J the condensate is depleted and the band is filled successively

▶ pronounced fringes still visible in the insulating phase

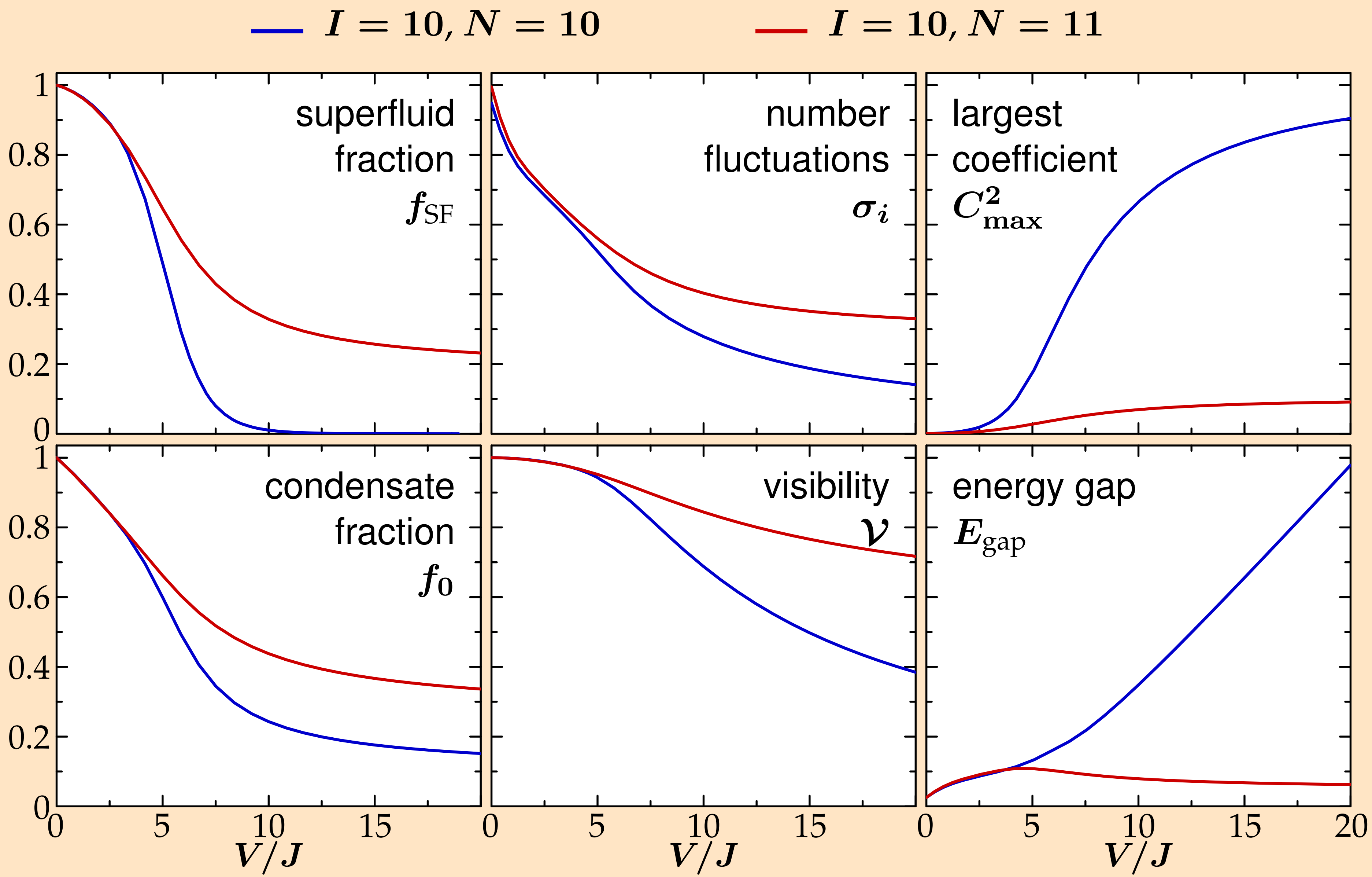
▶ fringes are a measure for **coherence properties** not for superfluidity

Superfluid to Mott-Insulator Transition

Relevant Quantities



Relevant Quantities



Superfluid to Mott-Insulator Transition

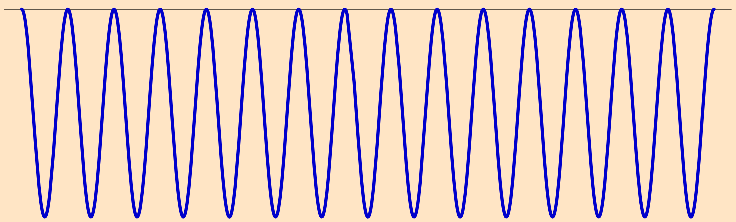
- **quantum phase transition** for commensurate fillings governed by the competition between kinetic energy (large fluctuations) and repulsive interactions (small occupation numbers)

	superfluid regime	Mott-insulator regime
ground state	superpos. of many FS	almost pure FS
number fluctuations	large	small
superfluid fraction	finite	zero
energy gap	small	increasing
interference fringes	present	slowly vanishing

- **order parameter** of the transition is the superfluid fraction f_{SF}, which depends crucially on the excited states
- ground state quantities (like interference pattern, fluctuations, etc.) cannot give direct information on superfluidity or the phase transition
- one has to devise specialised experimental schemes to probe superfluidity directly

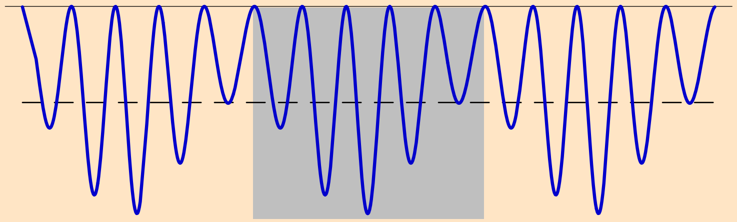
Two-Colour Superlattices

Two-Colour Superlattices



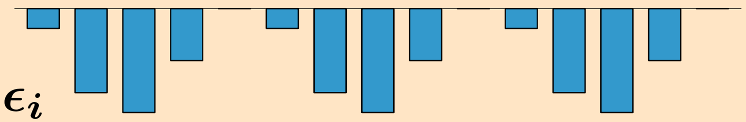
$U_1(x)$

- start with the conventional standing wave created by a laser with wavelength λ_1



$U_{1+2}(x)$

- 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

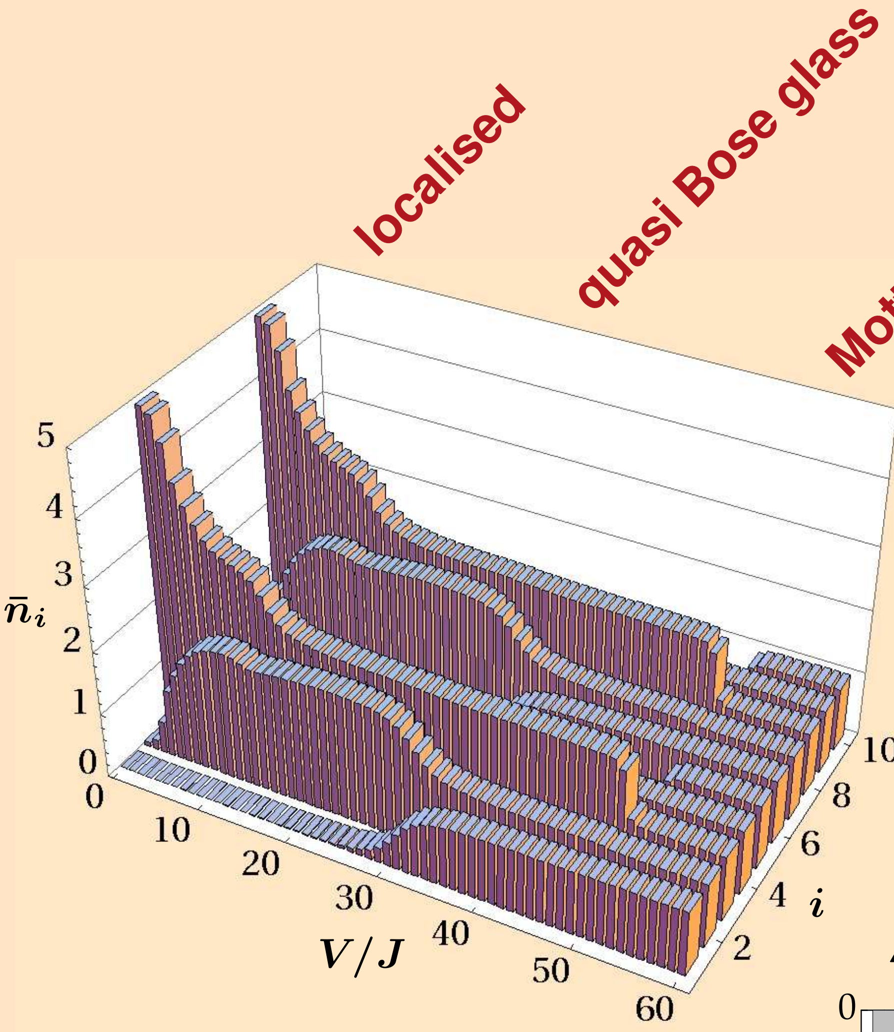


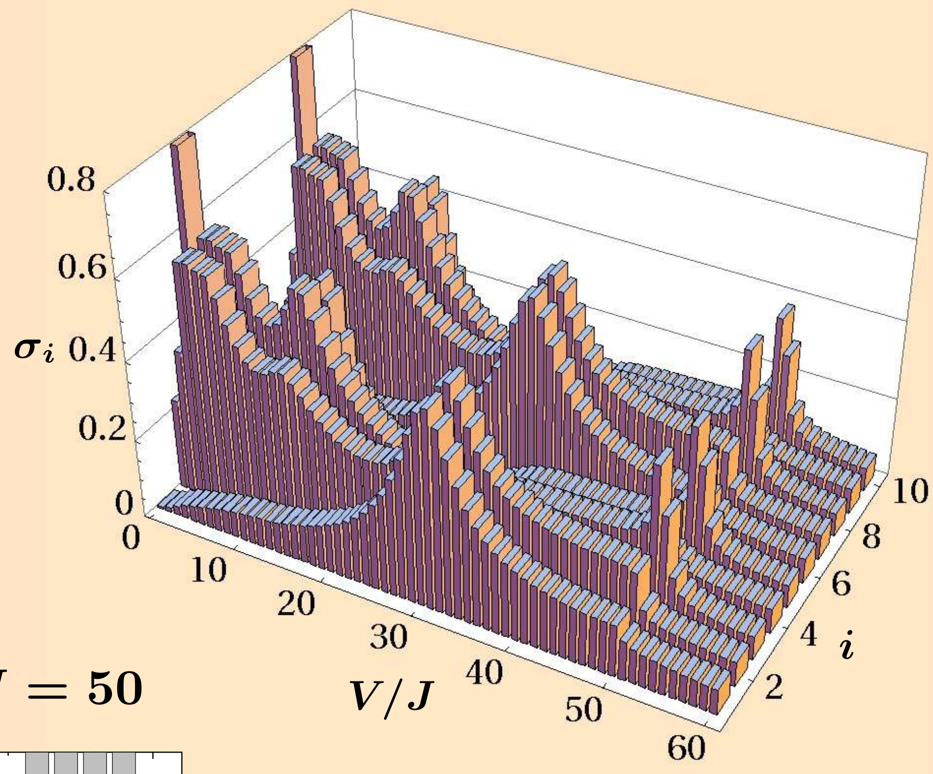
ϵ_i

- in the language of the Bose-Hubbard model this means varying on-site energies ϵ_i
- amplitude Δ of the modulation is controlled by the intensity of the second laser

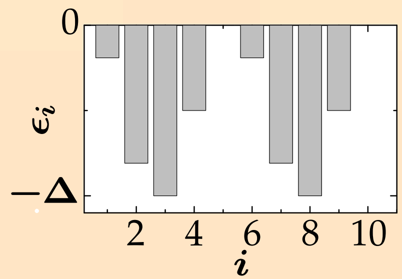
▶ these completely controlled lattice irregularities open novel possibilities to study fundamental **“disorder” effects**; more complex topologies easily possible

Interaction -vs- Lattice Irregularity

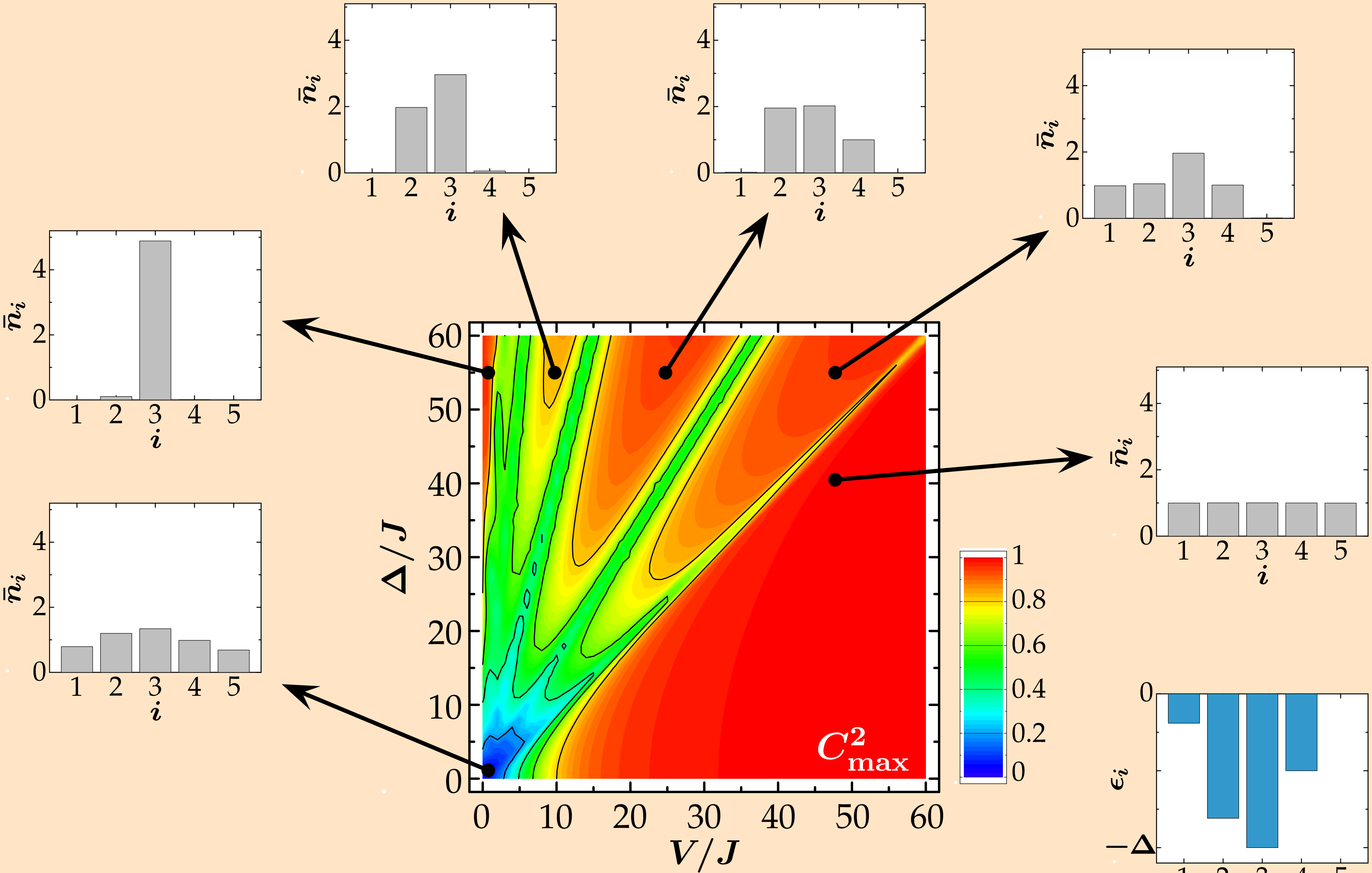




$\Delta/J = 50$

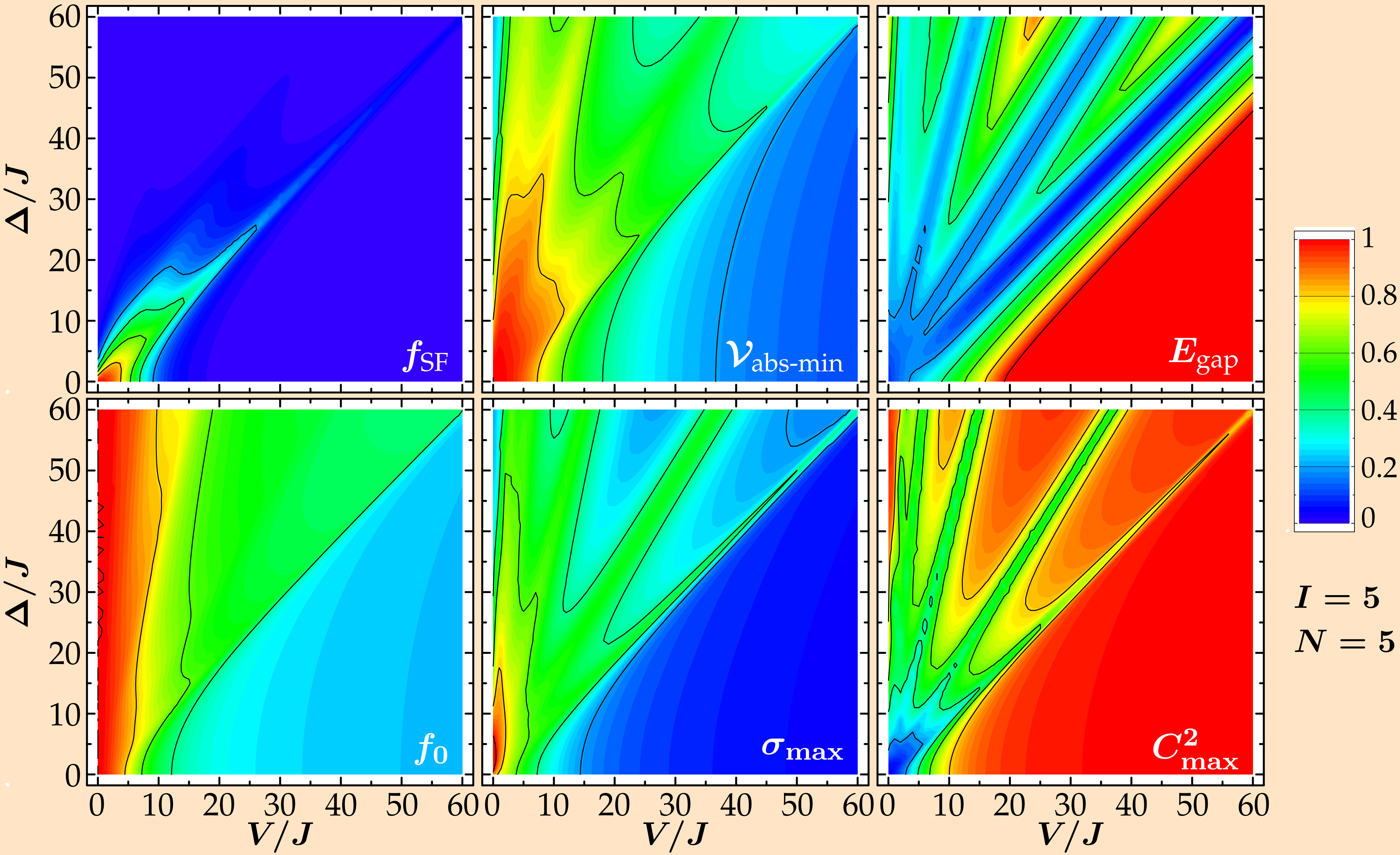


V-Δ Phase Diagram



$I = 5, N = 5$

More Phase Diagrams



Two-Colour Superlattices

- three competing terms in the Bose-Hubbard Hamiltonian generate a rich phase diagram with various quantum phase transitions
  - **hopping**: prefers wide distribution of occupation number
  - **interaction**: favours small occupation numbers
  - **lattice irregularity**: prefers large occupation numbers at deep wells
- several distinct insulating phases
  - **localised phase**: all particles localised at the deepest wells of each unit cell; large fluctuations
  - **quasi Bose glass**: integer non-uniform occupation with small fluctuations; rearrangements between different configurations
  - **Mott insulator**: whenever $V \gtrsim \Delta$ the uniform Mott-insulator phase appears for commensurate fillings

The Bottom Line

- optical lattices open a new chapter in the book of degenerate quantum gases

- ideal laboratory to study the **physics of lattice systems**
  - full control over all relevant parameters: interaction strength, tunnelling coefficient, lattice topology
  - powerful detection methods: momentum distribution, Bragg diffraction
  - different statistics: bosons, fermions, boson-fermion mixtures

- fascinating applications in **quantum information processing** and in **few-body physics**

Supplements

Condensate and Quasi-Momentum Distribution

- Bose-Hubbard model uses Wannier functions $w(x-\xi_i)$ as natural representation of the state; Bloch functions $\psi_q(x)$ are obtained through

$$\psi_q(x) = \frac{1}{\sqrt{I}} \sum_{i=1}^{I} \mathrm{e}^{-\mathrm{i}q\xi_i}\, w(x-\xi_i)$$

- define creation $\hat{\mathrm{c}}_q^\dagger$ and annihilation operators $\hat{\mathrm{c}}_q$ for bosons in Bloch states $\psi_q(x)$ with quasi-momentum q

$$\hat{\mathrm{c}}_q^\dagger = \frac{1}{\sqrt{I}} \sum_{i=1}^{I} \mathrm{e}^{-\mathrm{i}q\xi_i}\, \hat{\mathrm{a}}_i^\dagger \qquad \text{with} \qquad q = \frac{2\pi}{aI} \times \text{integer}$$

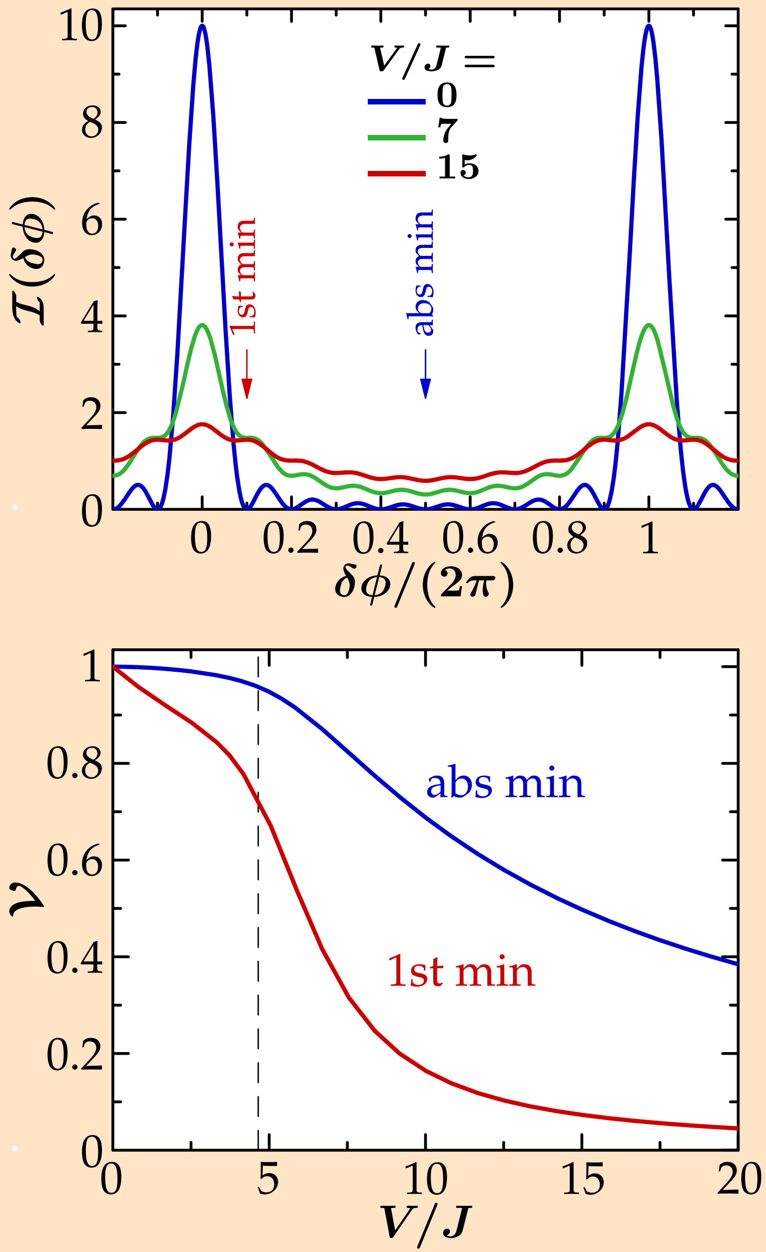
- occupation numbers for the Bloch states, i.e., **quasi-momentum distribution**

$$\tilde{n}_q = \langle \Psi_0 | \hat{\mathrm{c}}_q^\dagger \hat{\mathrm{c}}_q | \Psi_0 \rangle = \frac{1}{I} \sum_{i,j=1}^{I} \mathrm{e}^{\mathrm{i}q(\xi_j-\xi_i)} \langle \Psi_0 | \hat{\mathrm{a}}_i^\dagger \hat{\mathrm{a}}_j | \Psi_0 \rangle$$

- quasi-momentum $q=0$ Bloch state corresponds to the **condensate state**

$$N_0 = \tilde{n}_{q=0}$$

Interference Pattern & Visibility



- wanted: simple measure for the presence or absence of fringes
- standard definition of fringe visibility

$$\mathcal{V} = \frac{\mathcal{I}_{\mathrm{max}} - \mathcal{I}_{\mathrm{min}}}{\mathcal{I}_{\mathrm{max}} + \mathcal{I}_{\mathrm{min}}}$$

■ $\mathcal{I}_{\mathrm{min}}$ = absolute minimum

- measures non-uniformity of quasi-momentum distribution
- very insensitive

■ $\mathcal{I}_{\mathrm{min}}$ = first minimum

- measures occupation difference between condensate and 1st excited Bloch state
- better sensitivity but problematic experimentally