Quantum Phases of Bosonic Atoms in Optical Lattices

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Overview

- The Experiment
- Bose-Hubbard Model
- Condensate & Superfluid
- Matter-Wave Interference Pattern
- Superfluid to Mott-Insulator Transition
- Two-Colour Superlattices

A Theoreticians' View of

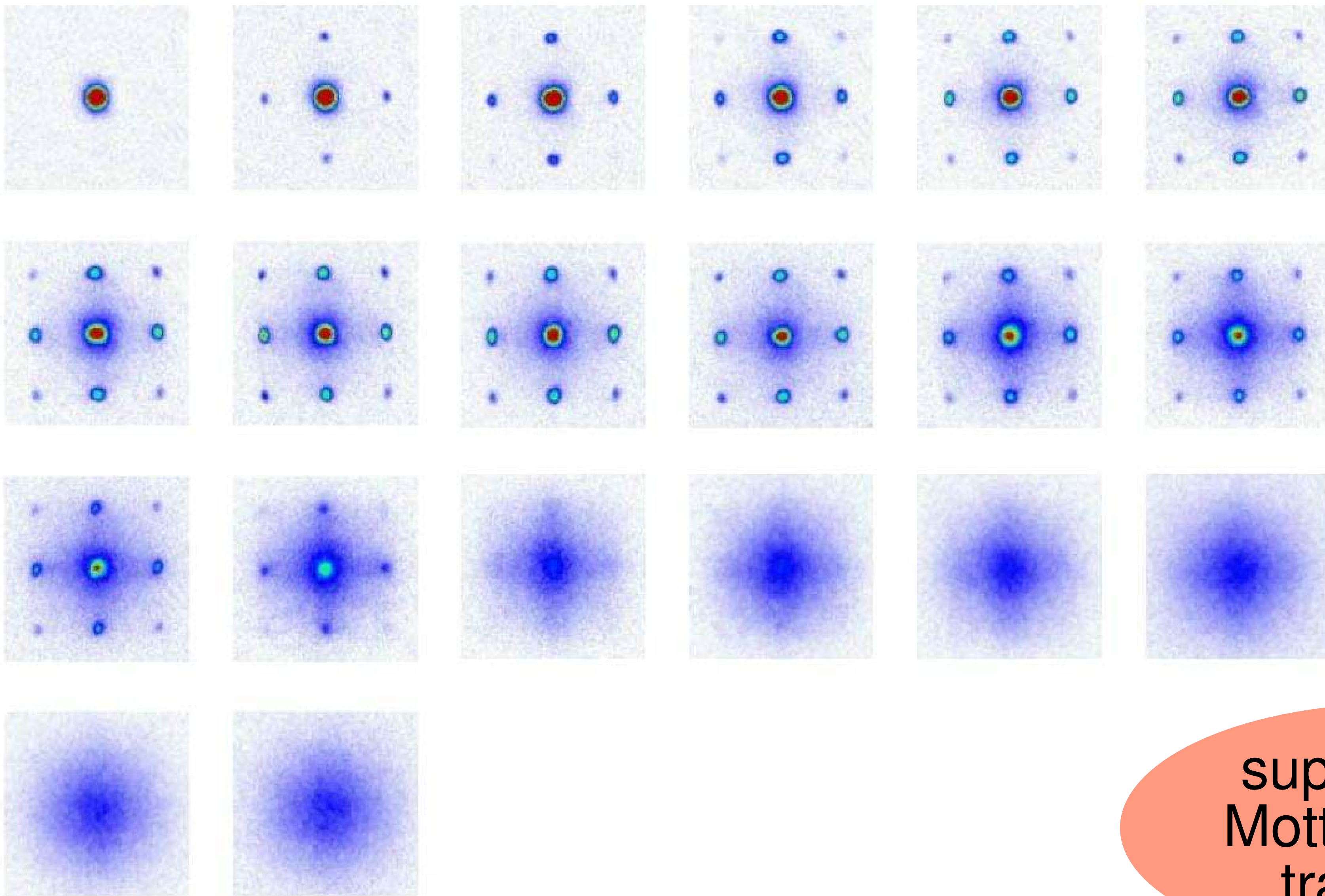
The Lattice Experiment

- 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 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**

Munich Experiment

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]

Questions...

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

Bose-Hubbard Model

Bose-Hubbard Model

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

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

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

I	6	8	10	12
D	462	6435	92 378	1 352 078

for $N/I = 1$

Bose-Hubbard Hamiltonian

- second quantised Hamiltonian in terms of the associated creation, annihilation, and number operators [Fisher et al. (1989); Jaksch et al. (1998)]

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

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

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

▶ **exact solution**: compute the lowest eigenstates of $\hat{\mathrm{H}}_0$ using iterative Lanczos algorithms

Simple Physical Quantities

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

- **mean occupation numbers**

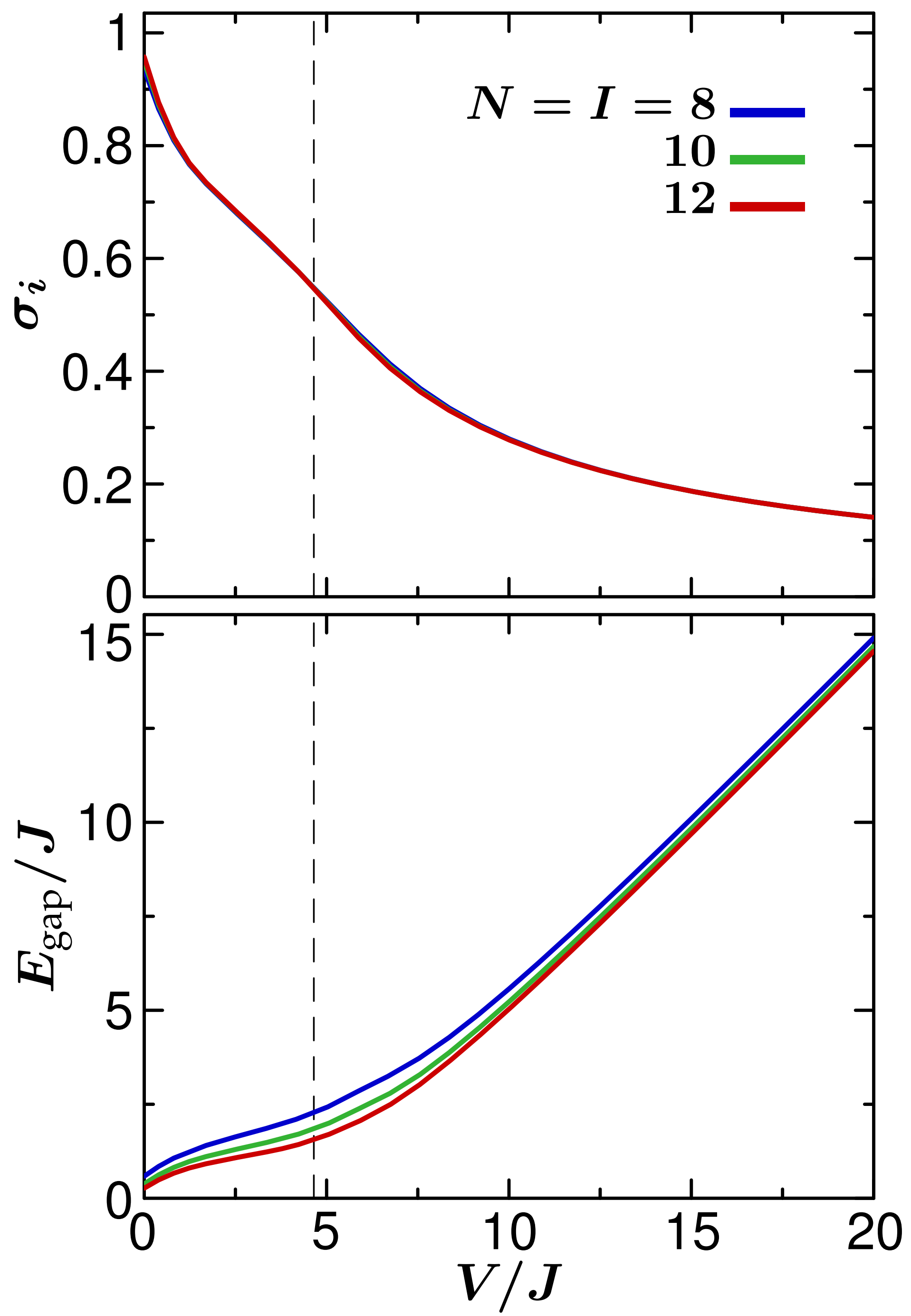
$$\bar{n}_i = \langle \Psi_0 | \,\hat{n}_i\, | \Psi_0 \rangle$$

- **number fluctuations**

$$\sigma_i = \sqrt{\langle \Psi_0 | \,\hat{n}_i^2\, | \Psi_0 \rangle - \langle \Psi_0 | \,\hat{n}_i\, | \Psi_0 \rangle^2}$$

- **energy gap**

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



Condensate & Superfluidity

General Definition of the
Bose-Einstein Condensate

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

$$\rho^{(1)}_{ij} = \left\langle \Psi_0 \right| \hat{a}^\dagger_i \hat{a}_j \left| \Psi_0 \right\rangle$$

  defines natural orbitals and the corresponding occupation numbers

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

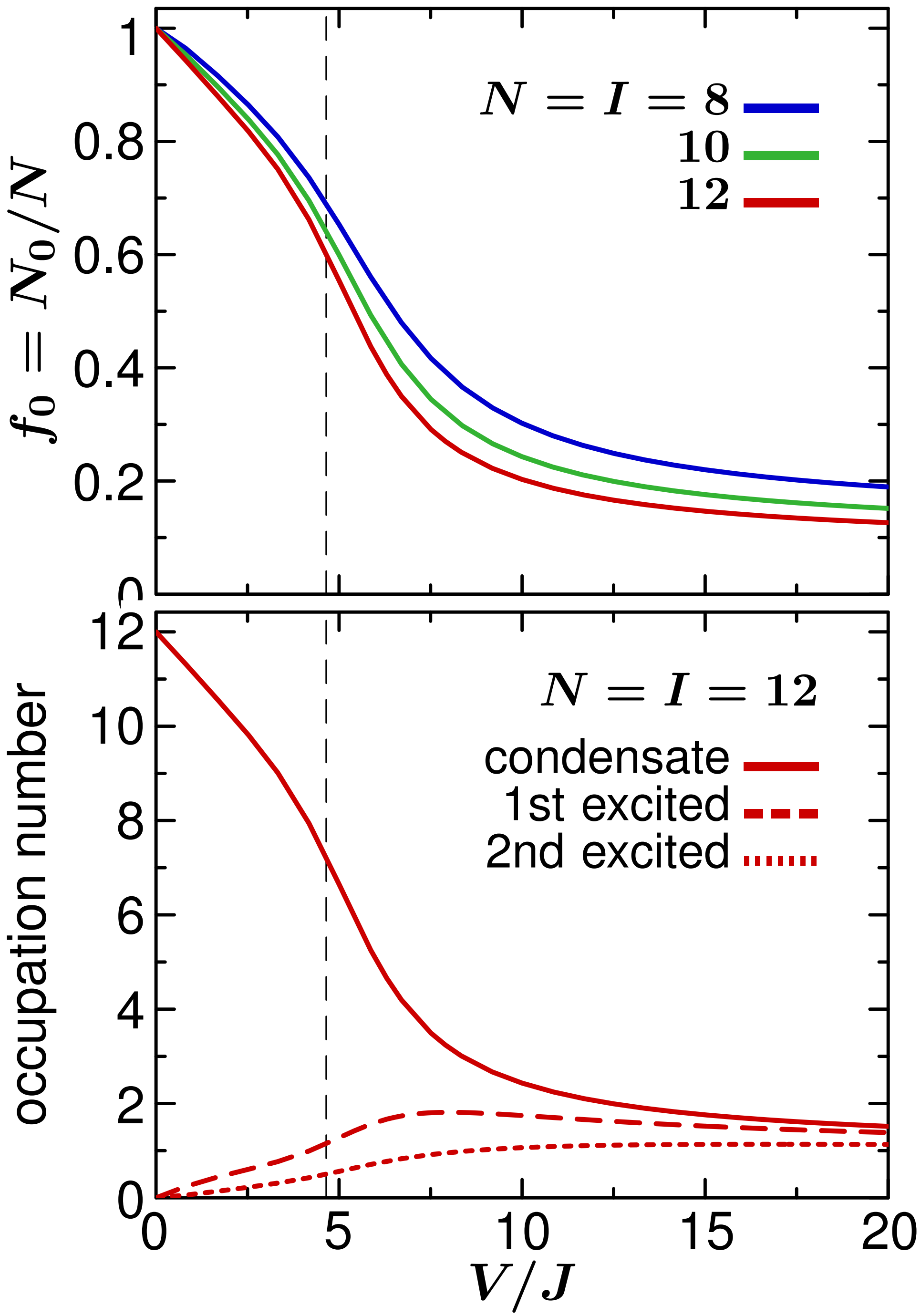
eigenvalue	$\longrightarrow$	N_0	:	number of condensed particles
eigenvector	$\longrightarrow$	$\phi_{0,i}$	:	condensate wave function

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

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

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

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

- 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**

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

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

Microscopic

Definition of Superfluidity

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

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

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

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

- 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**

$$E_\Theta - E_0 = \tfrac{1}{2} M_{\mathrm{SF}} \, v_{\mathrm{SF}}^2 = \tfrac{1}{2} m N_{\mathrm{SF}} \, v_{\mathrm{SF}}^2$$

- **superfluid fraction** $=$ rigidity with respect to phase variations

$$\boxed{F_{\mathrm{SF}} = \frac{N_{\mathrm{SF}}}{N} = \frac{2m\,L^2}{\hbar^2 N} \, \frac{E_\Theta - E_0}{\Theta^2}} \qquad \Theta \ll \pi$$

Superfluidity on the Lattice

- express F_{SF} in terms of the parameters of the Bose-Hubbard model

$$F_{\text{SF}} = \frac{m}{m^\star}\, f_{\text{SF}} \qquad\qquad \boxed{f_{\text{SF}} = \frac{I^2}{JN}\,\frac{E_\Theta - E_0}{\Theta^2}}$$

$$I = L/a \qquad J = \hbar^2/(2m^\star a^2)$$

  - $\frac{m}{m^\star}$: reduction of flow by the lattice itself
  - f_{SF} : interaction-induced depletion relevant for quantum phase transitions

- map phase twist onto Hamiltonian ➔ **twisted Hamiltonian** containing additional phase factors

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

- solve the eigenvalue problem of $\hat{\mathrm{H}}_\Theta$ and $\hat{\mathrm{H}}_0$ (with periodic BCs) and directly compute $E_\Theta - E_0$ and f_{SF}

Perturbative Calculation of the

Superfluid Fraction

- calculate $\boldsymbol{E_\Theta - E_0}$ in a perturbative expansion for small $\boldsymbol{\Theta}$ around the untwisted Hamiltonian $\hat{\mathrm{H}}_0$
- exact expression for $\boldsymbol{f_{\text{SF}}}$ in the limit $\boldsymbol{\Theta \to 0}$

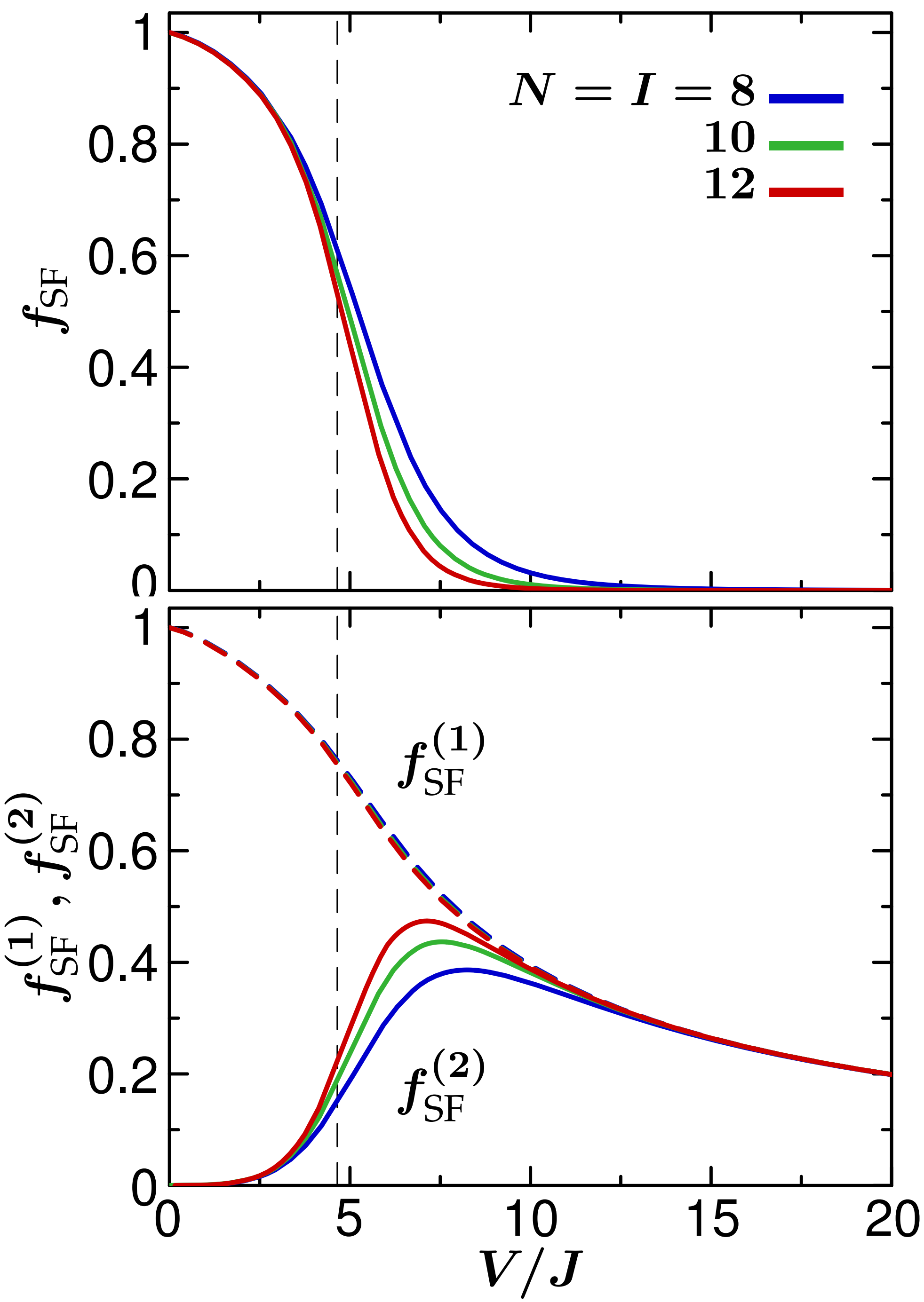
$$f_{\text{SF}} = f_{\text{SF}}^{(1)} - f_{\text{SF}}^{(2)}$$

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

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

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

$\neq$

Superfluid

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

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

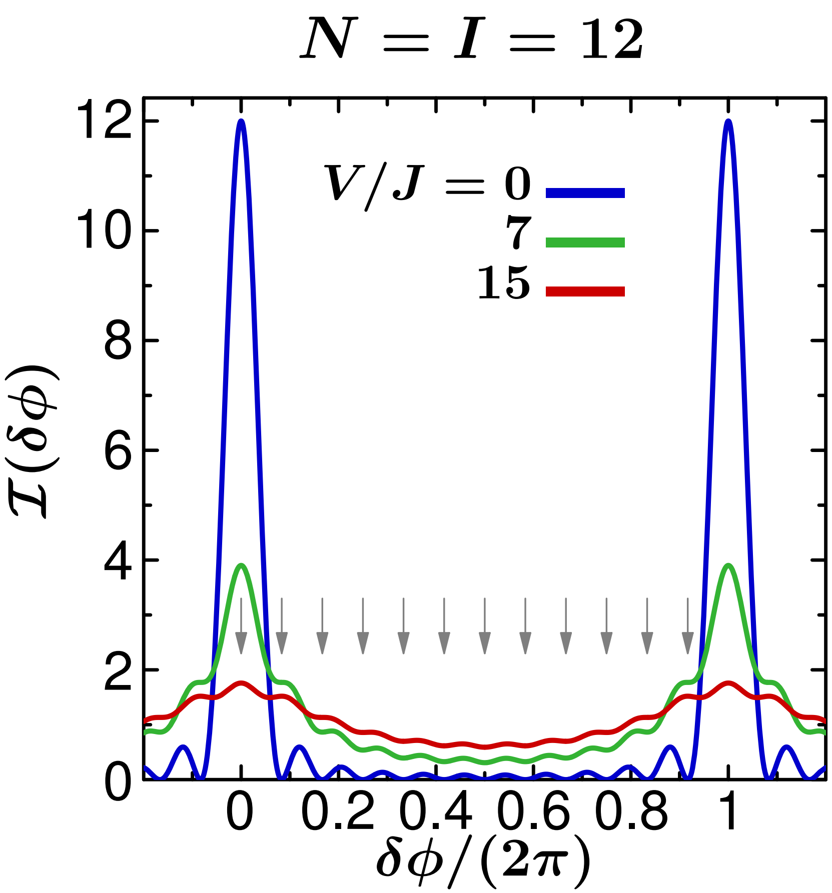
- non-condensed particles are dragged along with condensate
- liquid ^{4}He at $T = 0$K:

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

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

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

What about the Interference Pattern?



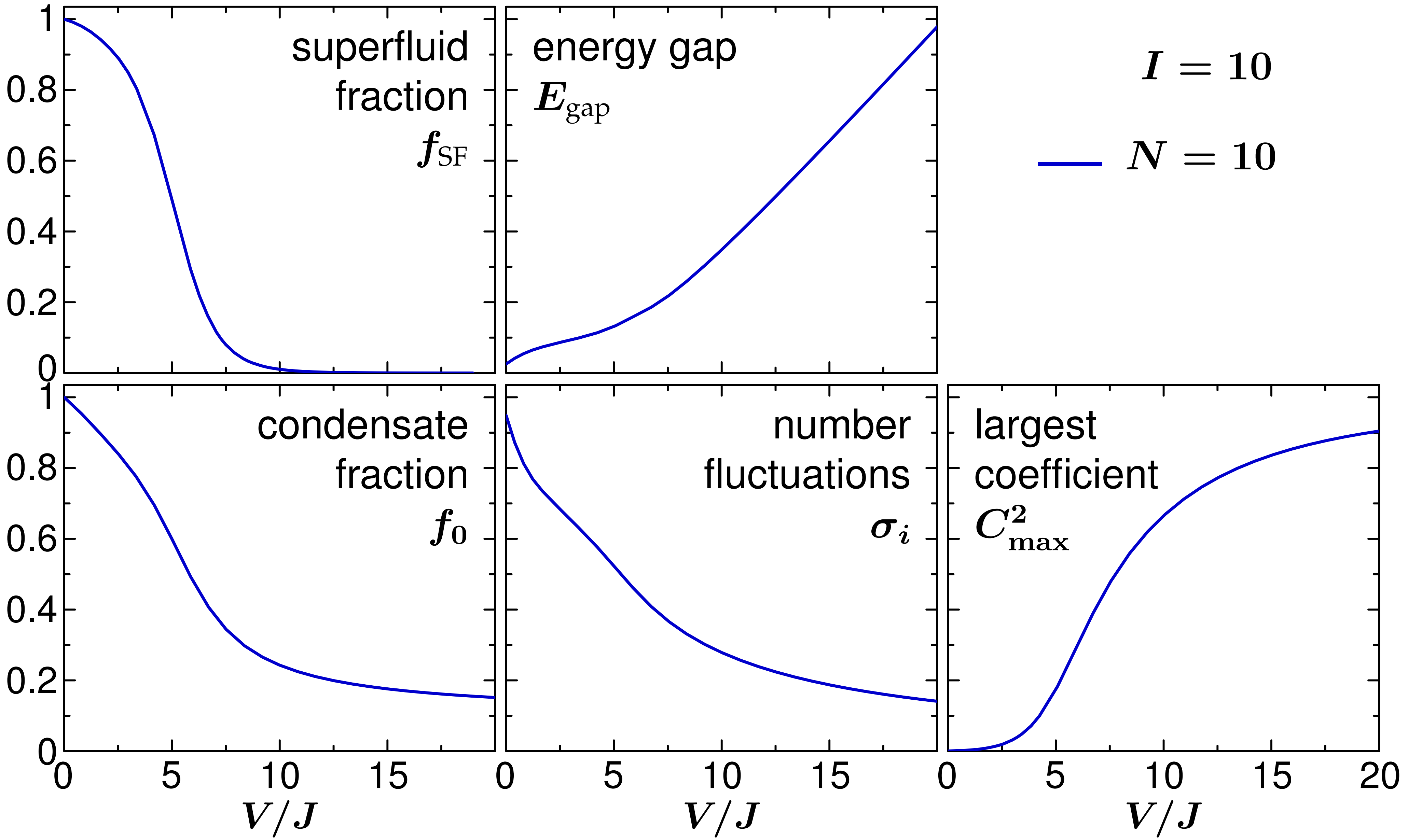
- interference fringes are a measure for the coherence properties
- intensity in the far-field as function of phase difference $\delta\phi$

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

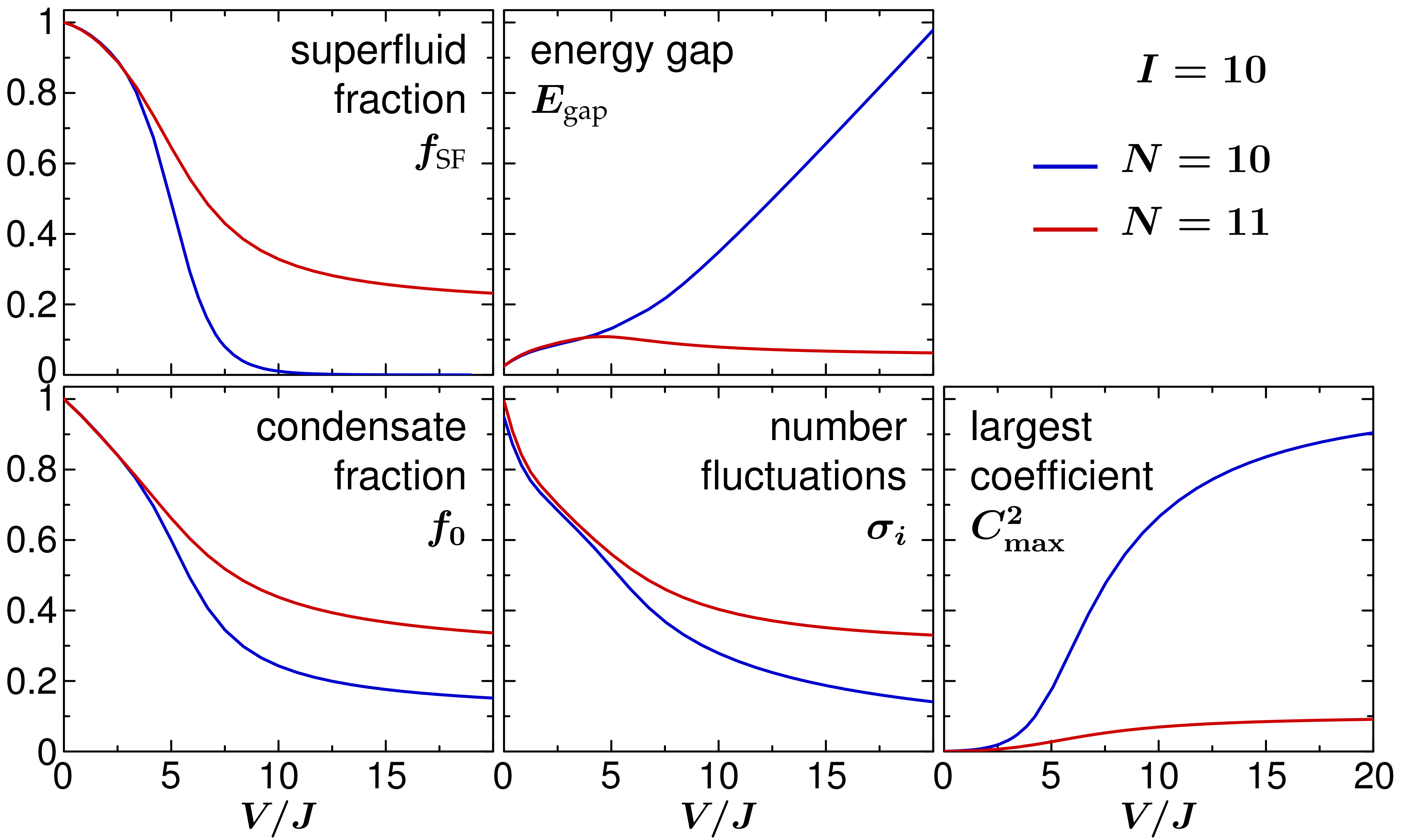
- determined entirely by the one-body density matrix of the ground state

► fringes tell something about **conden-sate** and quasimomentum distribution but **not about superfluidity**

Superfluid to Mott-Insulator Transition

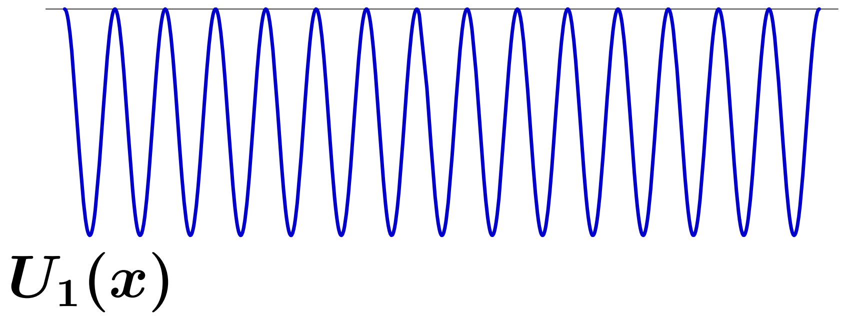


Superfluid to Mott-Insulator Transition

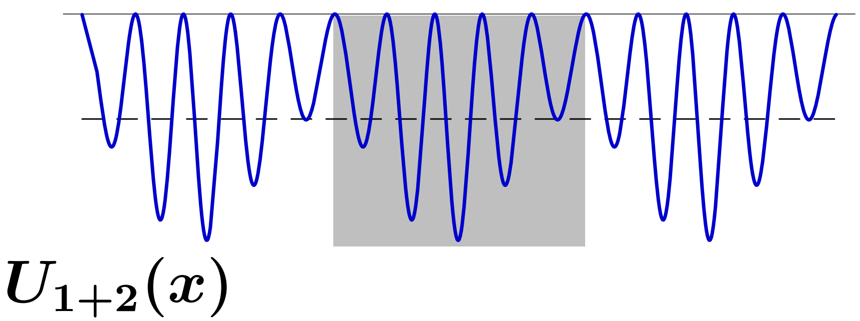


Two-Colour Superlattices

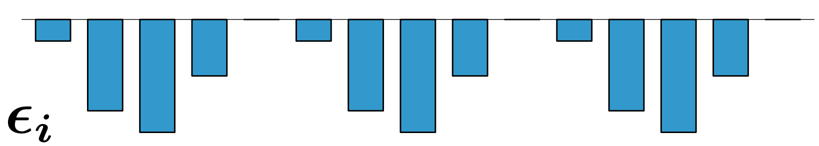
Two-Colour Superlattices



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



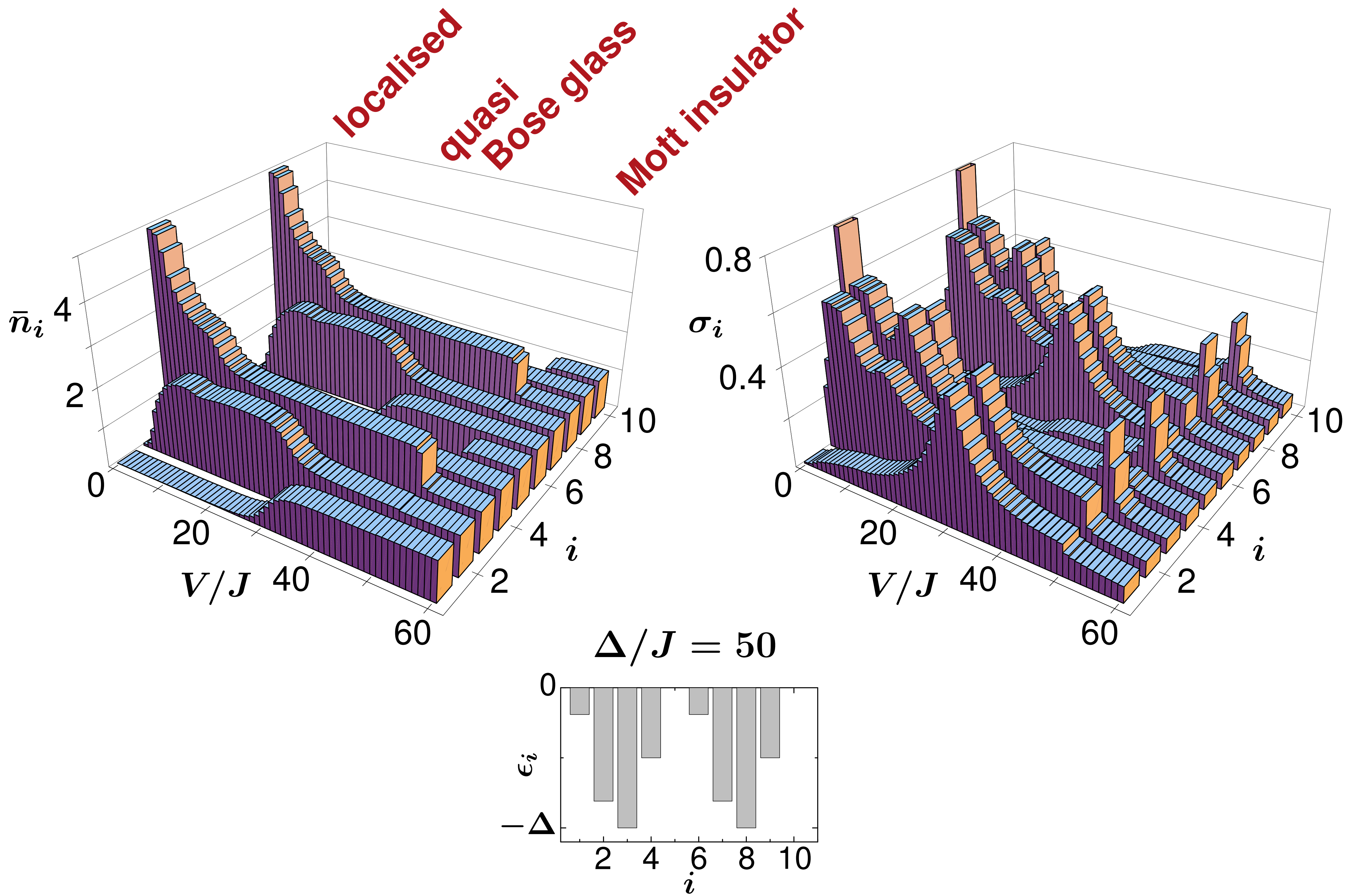
- add a second standing wave created by a laser with wavelength $\lambda_2 = \frac{5}{7}\lambda_1$ and much smaller intensity (here 4%)
- potential exhibits a periodic modulation of the well-depth with a period of 5 sites



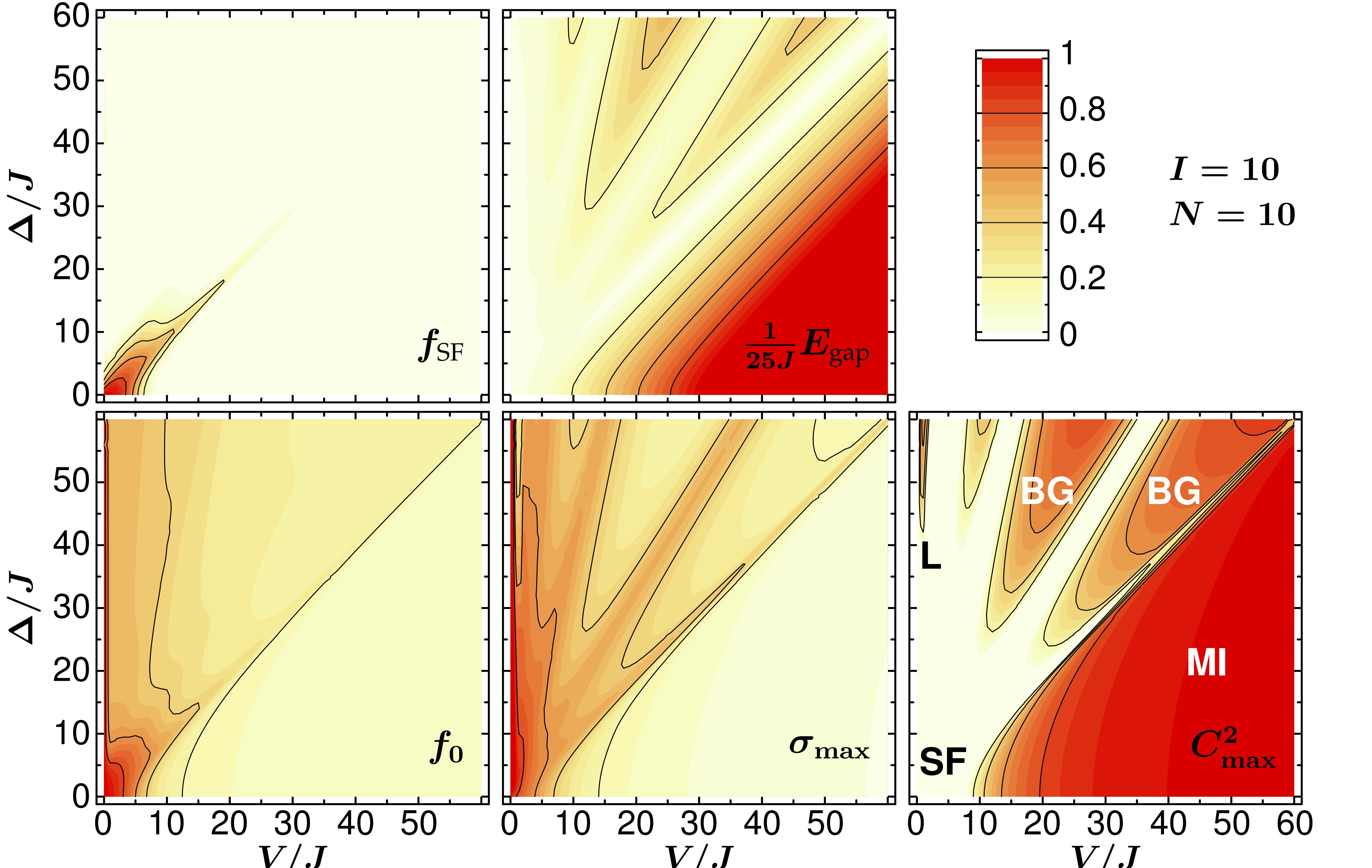
- Bose-Hubbard model: varying on-site energies $\epsilon_i \in [0, -\Delta]$

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

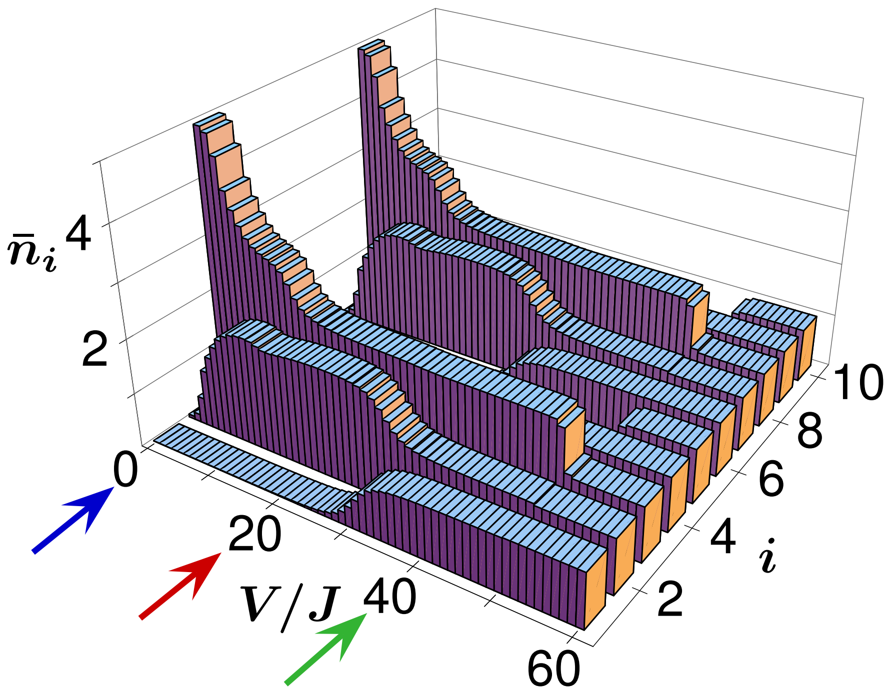
Interaction -vs- Lattice Irregularity



V-Δ Phase Diagrams

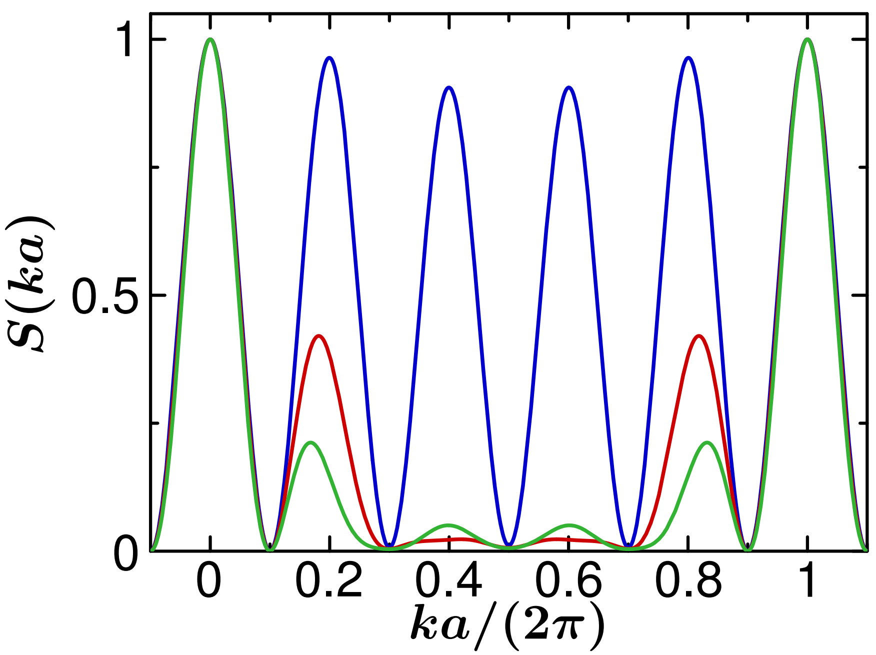


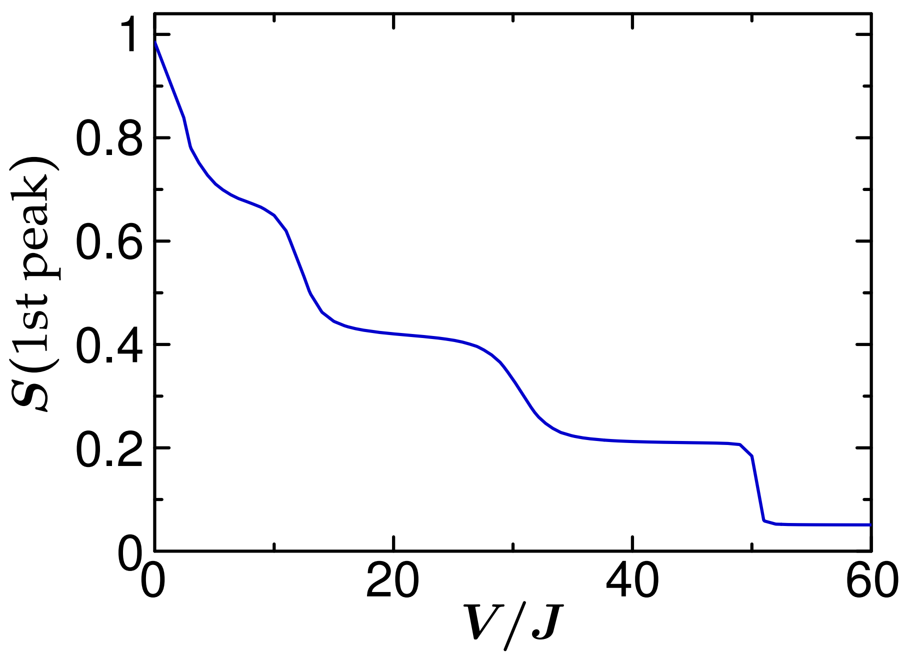
Experimental Signatures: Structure Factor



- Can one detect the structural changes?
- Bragg diffraction of light from trapped atoms provides information on the **static structure factor**

$$S(ka) = \frac{1}{I^2} \sum_{i,j=1}^{I} \mathrm{e}^{ika(i-j)} \langle \Psi_0 | \hat{n}_i \hat{n}_j | \Psi_0 \rangle$$





Conclusions

- **Superfluidity**
  - response of the system to a perturbation (phase variation)
  - depends crucially on the excitation spectrum
- **Condensate & Coherence**
  - properties of the one-body density matrix of the ground state
  - ground state quantities (interference pattern, fluctuations, etc.) cannot give direct information on the superfluid fraction or the phase transition
- **Two-Colour Superlattices**
  - rich phase diagram with several insulating phases: localised, quasi Bose-glass, Mott-insulator
  - distinct signatures in interference pattern and structure factor

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 and boson-fermion mixtures in lattices, spinor Bose gases
  - long-range interactions, molecules, dynamics,...

Epilogue

References

- R. Roth, K. Burnett; Phys. Rev. A 68 (2003), cond-mat/0304063
- R. Roth, K. Burnett; Phys. Rev. A 67 (2003) 031692(R)
- A. M. Rey, et al.; J. Phys. B 36 (2003) 825
- R. Roth, K. Burnett; J. Opt. B 5 (2003) S50

€ / £

- DFG, UK EPSRC, EU

Supplements

Commensurate / Incommensurate Filling

V-Δ Phase Diagrams