Phase Diagram of Bosons in Optical Superlattices

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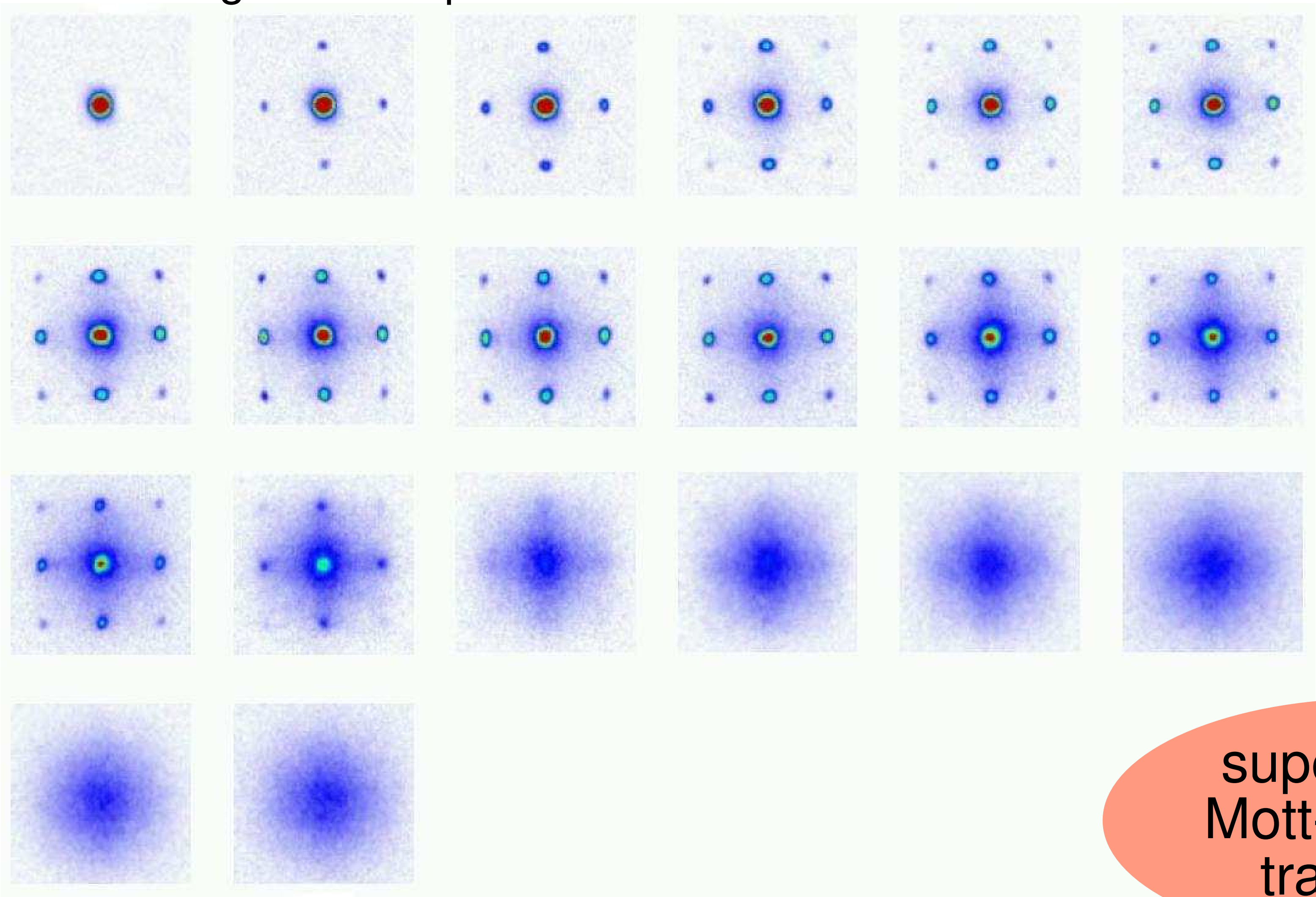
Overview

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

Interference Pattern

increasing lattice depth $\longrightarrow$



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** $|\{n_1, ..., n_I\}_\alpha\rangle$

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

- 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)]

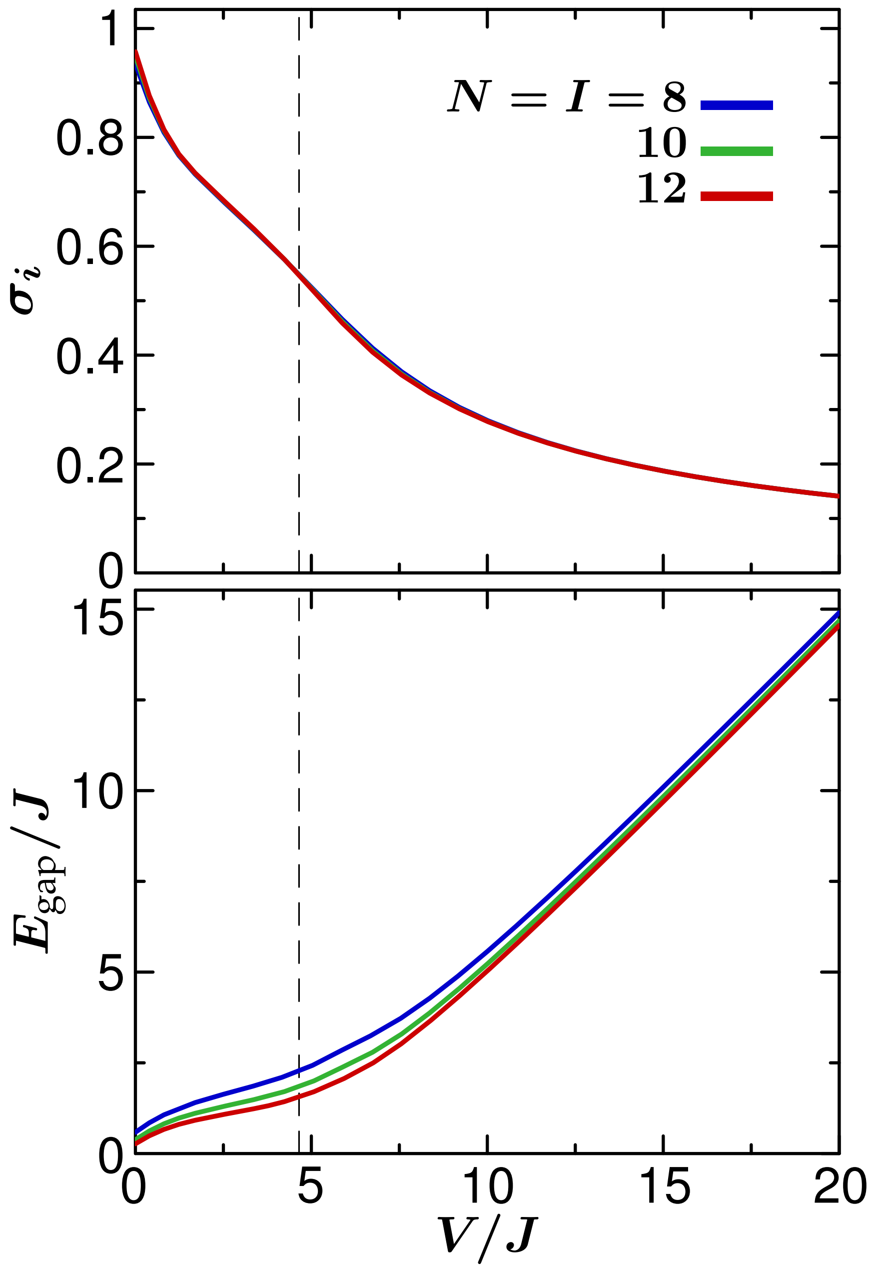
$$\hat{\mathrm{H}}_0 = \underbrace{-J \sum_{i=1}^{I} (\hat{\mathrm{a}}_{i+1}^\dagger \hat{\mathrm{a}}_i + \mathrm{h.a.})}_{\text{tunnelling between adjacent lattice sites}} + \underbrace{\sum_{i=1}^{I} \epsilon_i \, \hat{\mathrm{n}}_i}_{\text{single-particle energy}} + \underbrace{\frac{V}{2} \sum_{i=1}^{I}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

- 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 number**

$$\bar{n}_i = \left\langle \Psi_0 \right| \hat{\mathrm{n}}_i \left| \Psi_0 \right\rangle$$

- **number fluctuations**

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

- **energy gap**

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

Condensate & Superfluidity

Bose-Einstein Condensate

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

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

defines natural orbitals and the corresp. occupation numbers

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

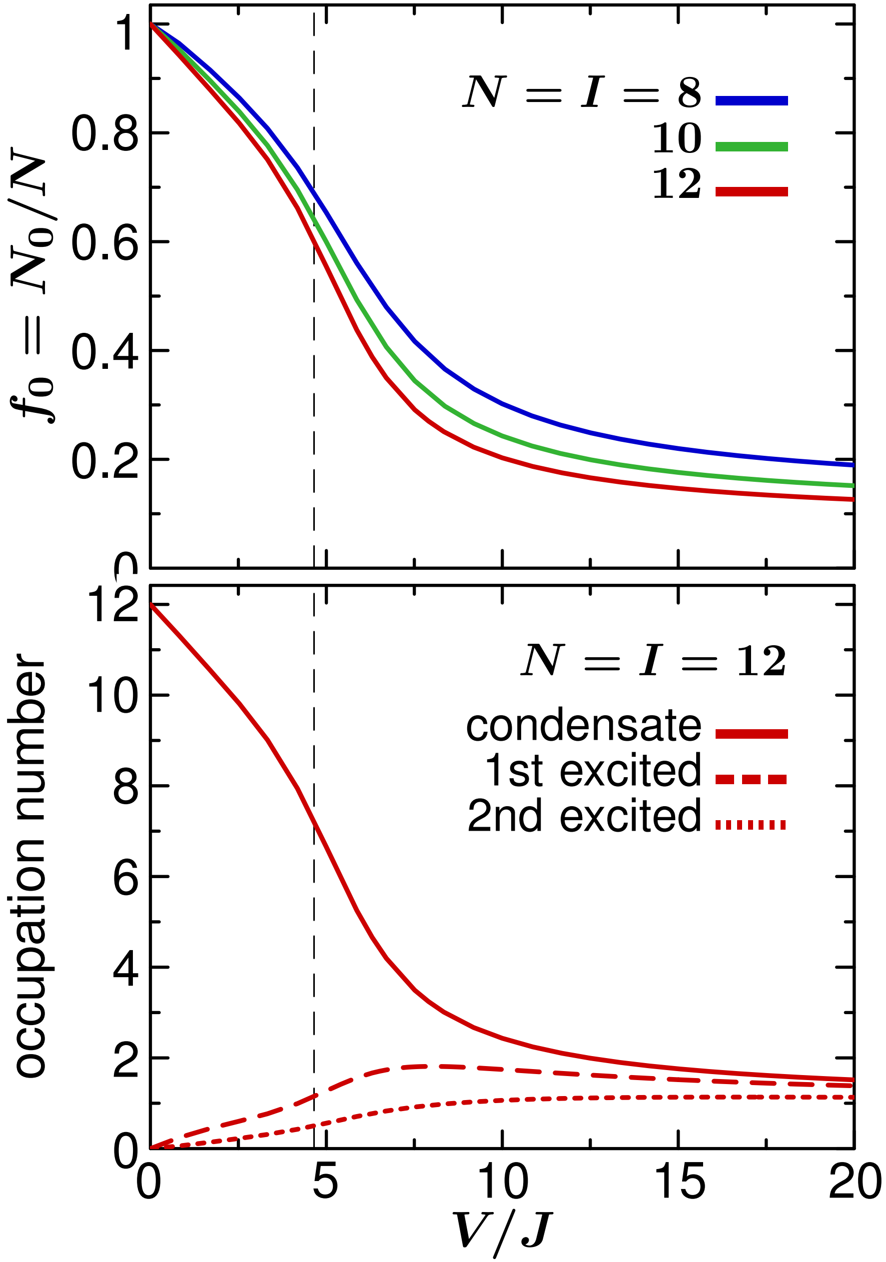
$$\begin{array}{rcll} \text{eigenvalue} & \longrightarrow & N_0 & : \ \text{number of condensed particles} \\ \text{eigenvector} & \longrightarrow & \phi_{0,i} & : \ \text{condensate wave function} \end{array}$$

- existence of a condensate implies **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 & 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**

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

► 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 $\phi_0(\vec{x})$

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

- 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**

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

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

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

Superfluidity on the Lattice

- by a unitary transformation the phase twist can be mapped onto the Hamiltonian ➔ **twisted Hamiltonian** containing Peierls 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 compute the **superfluid fraction**

$$f_{\mathrm{SF}} = \frac{I^2}{JN} \frac{E_{\Theta} - E_{0}}{\Theta^2} \qquad\qquad \Theta \ll \pi$$

- closely related to helicity modulus [Fisher, Barber, Jasnow (1973)] and winding number [Pollock, Ceperley (1987)]

- this is not the Landau picture of superfluidity ➔ we do not consider the stability of the superflow (critical velocity)

Superfluid Fraction

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

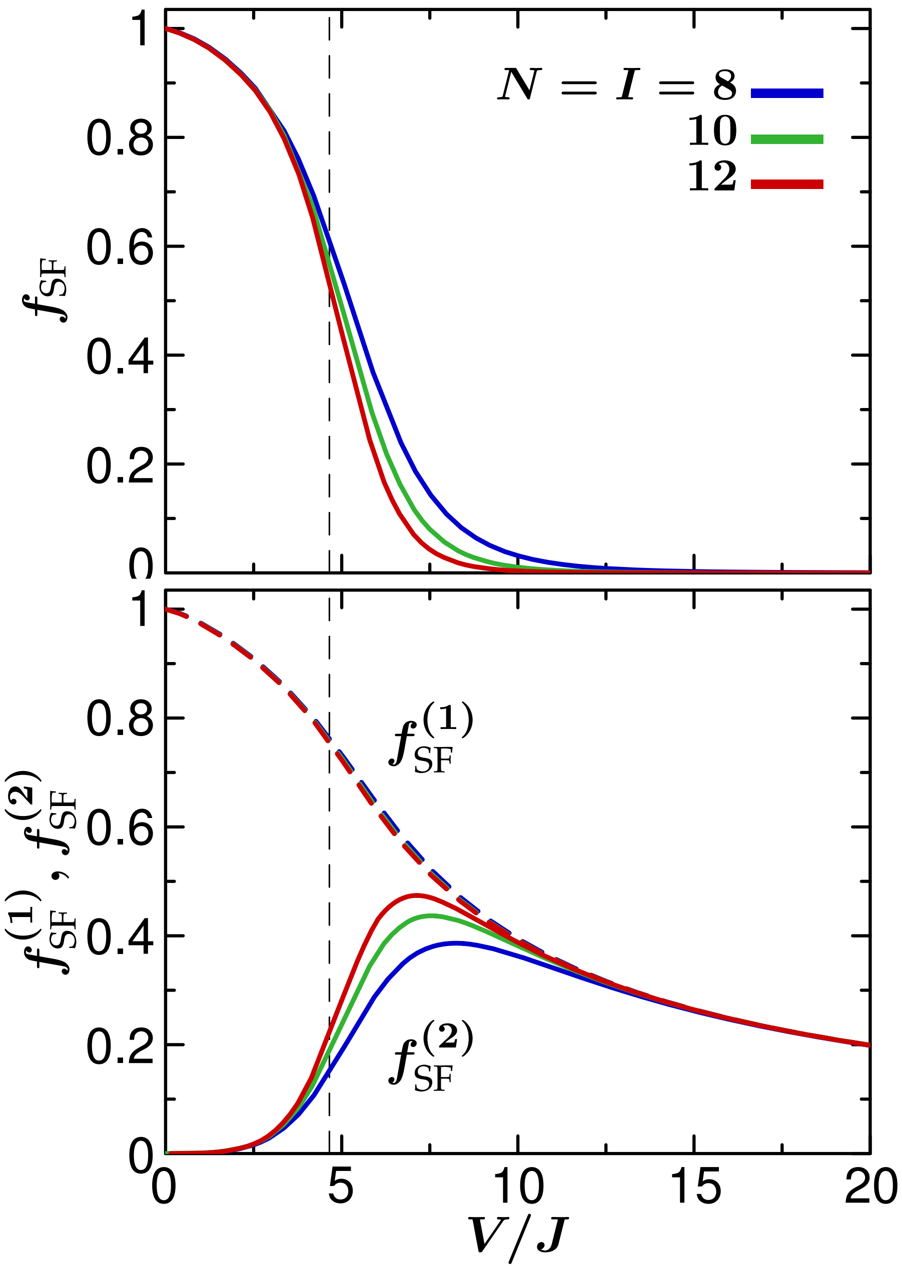
$$f_{\text{SF}} = f_{\text{SF}}^{(1)} - f_{\text{SF}}^{(2)}$$

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

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

- **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
- $f_{\text{SF}}^{(1)}$ decreases only very slowly
- vanishing of f_{SF} is due to a cancellation between $f_{\text{SF}}^{(1)}$ and $f_{\text{SF}}^{(2)}$
- 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

$f_0 < f_{SF}$

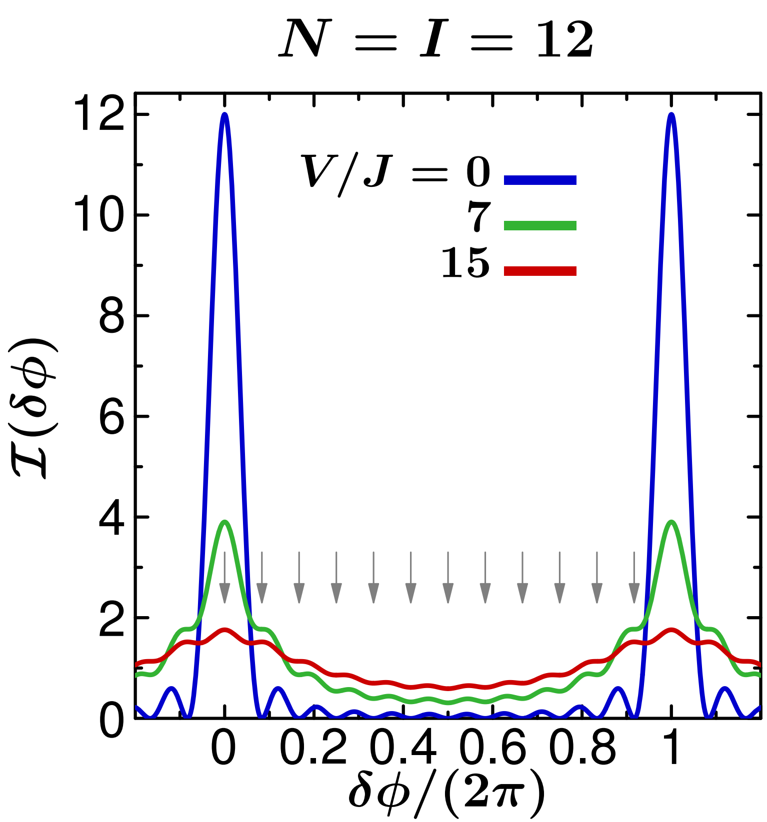
- non-condensed particles are dragged along with condensate
- liquid ^{4}He at $T = 0$K:

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

$f_0 > f_{SF}$

- 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?



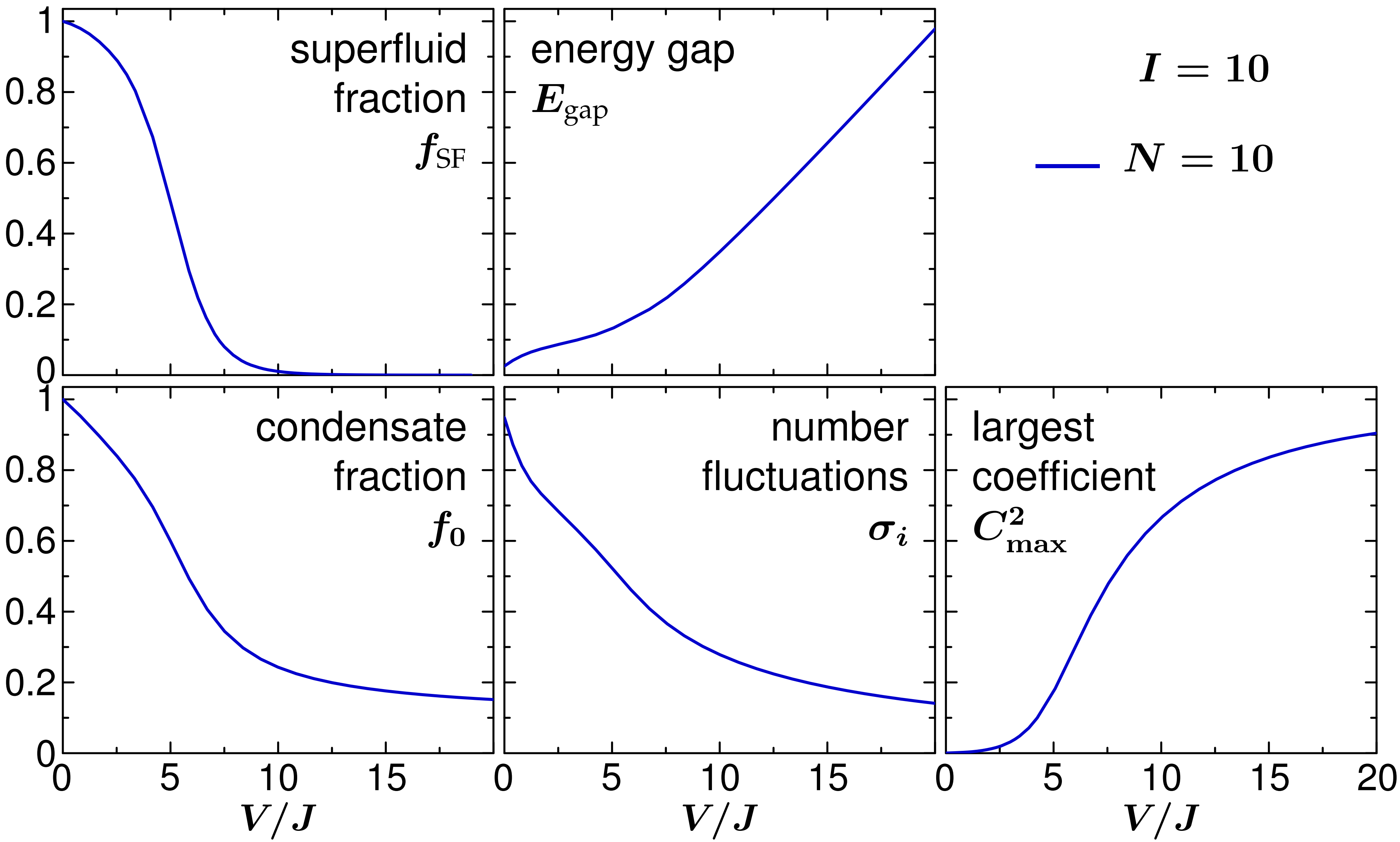
- interference fringes are a measure for the coherence properties
- intensity in the far-field as function of phase difference $\delta\phi$

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

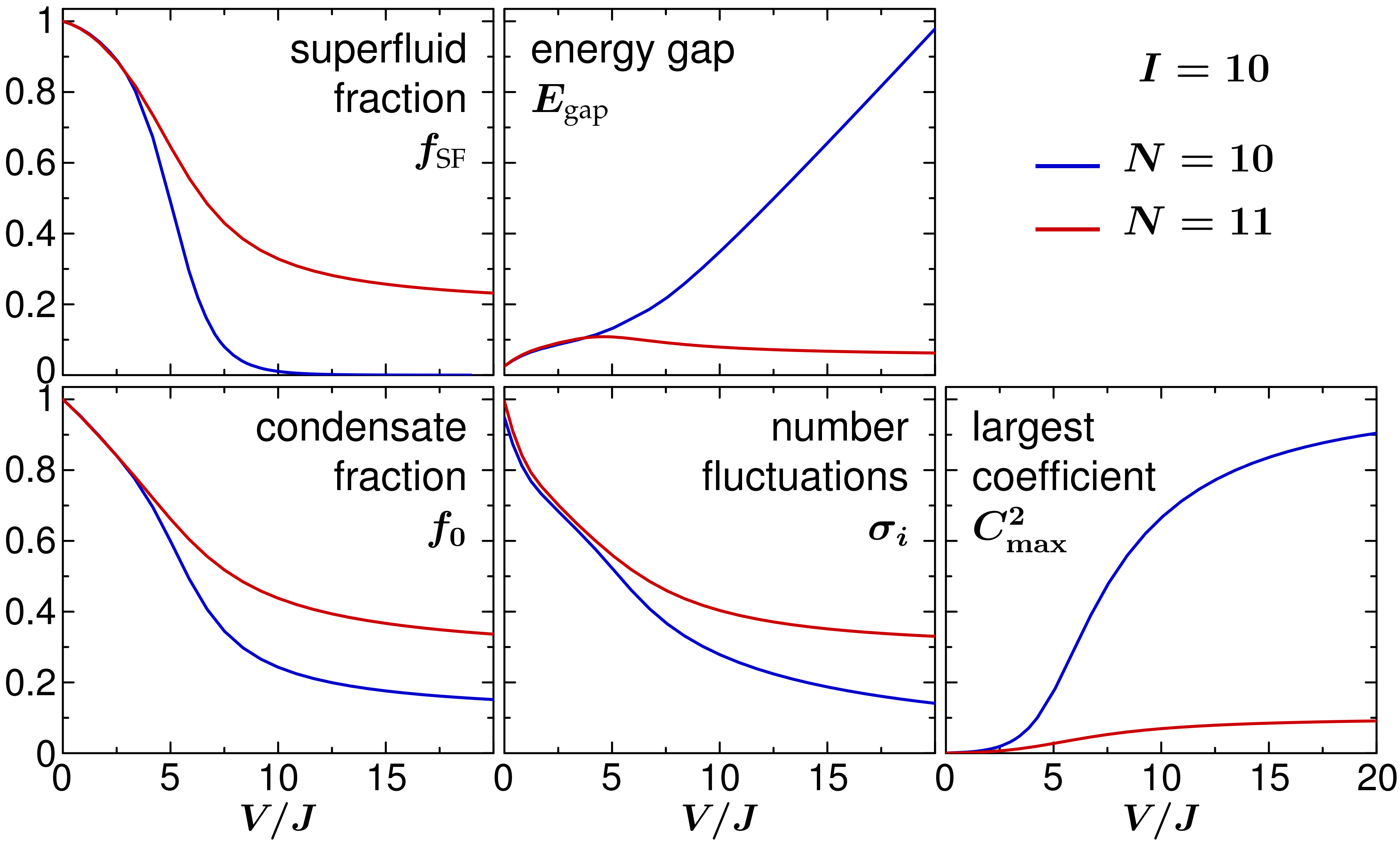
- determined entirely by the one-body density matrix of the ground state

► 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

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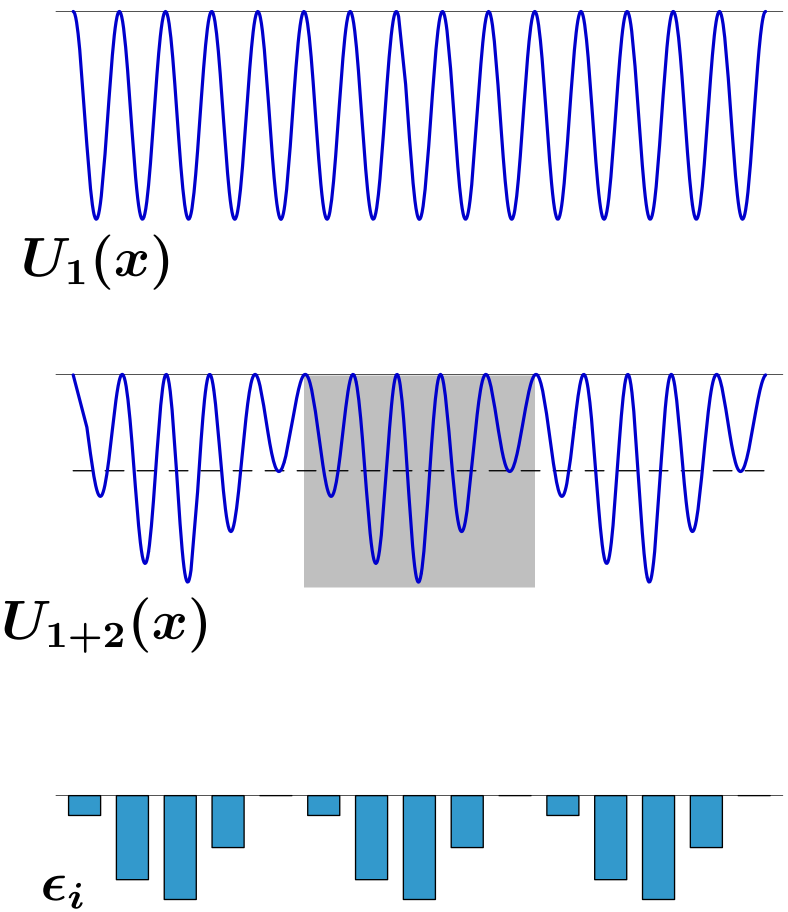
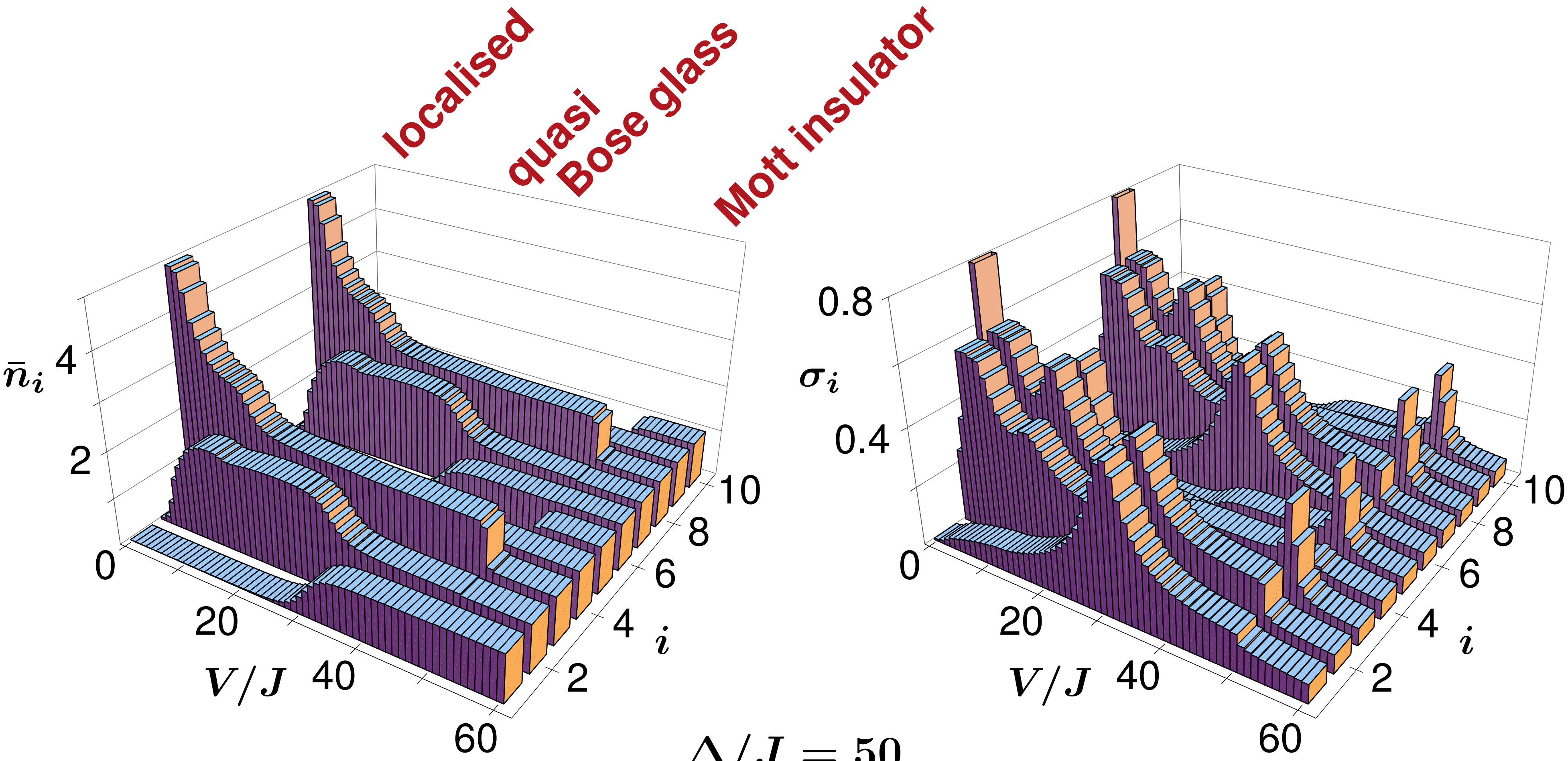
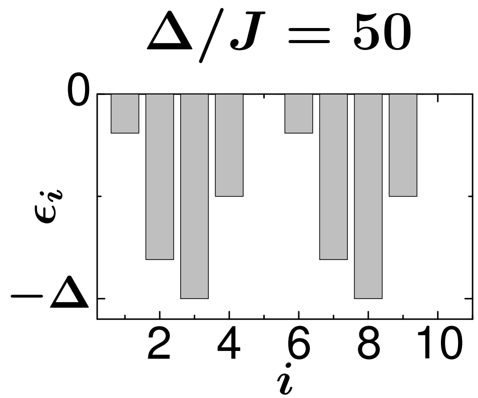


- start with a standing wave created by a laser with wavelength λ_1
- add a second standing wave created by a laser with wavelength $\lambda_2 = \frac{5}{7}\lambda_1$ and much smaller intensity (here 4%)
- potential exhibits a periodic modulation of the well-depth with a period of 5 sites
- Bose-Hubbard model: varying on-site energies $\epsilon_i \in [0, -\Delta]$

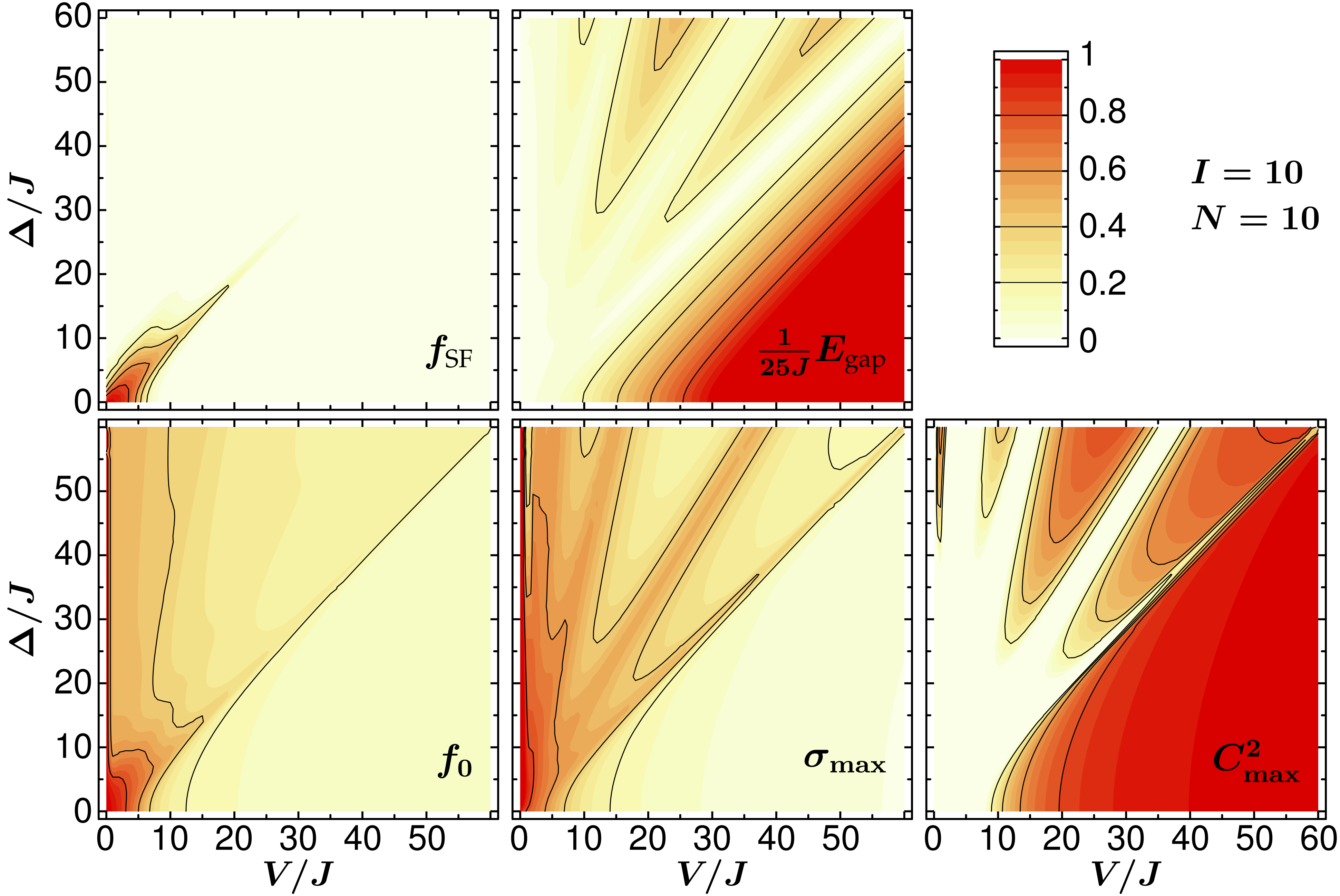
► **controlled lattice irregularities** open novel possibilities to study "disorder" related effects; more complex topologies easily possible

Interaction -vs- Lattice Irregularity





V-Δ Phase Diagrams



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

- **References**
  - R. Roth, K. Burnett; 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