Ultracold Bose Gases in Optical Superlattices:

Superfluidity, Interference, Disorder

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Overview

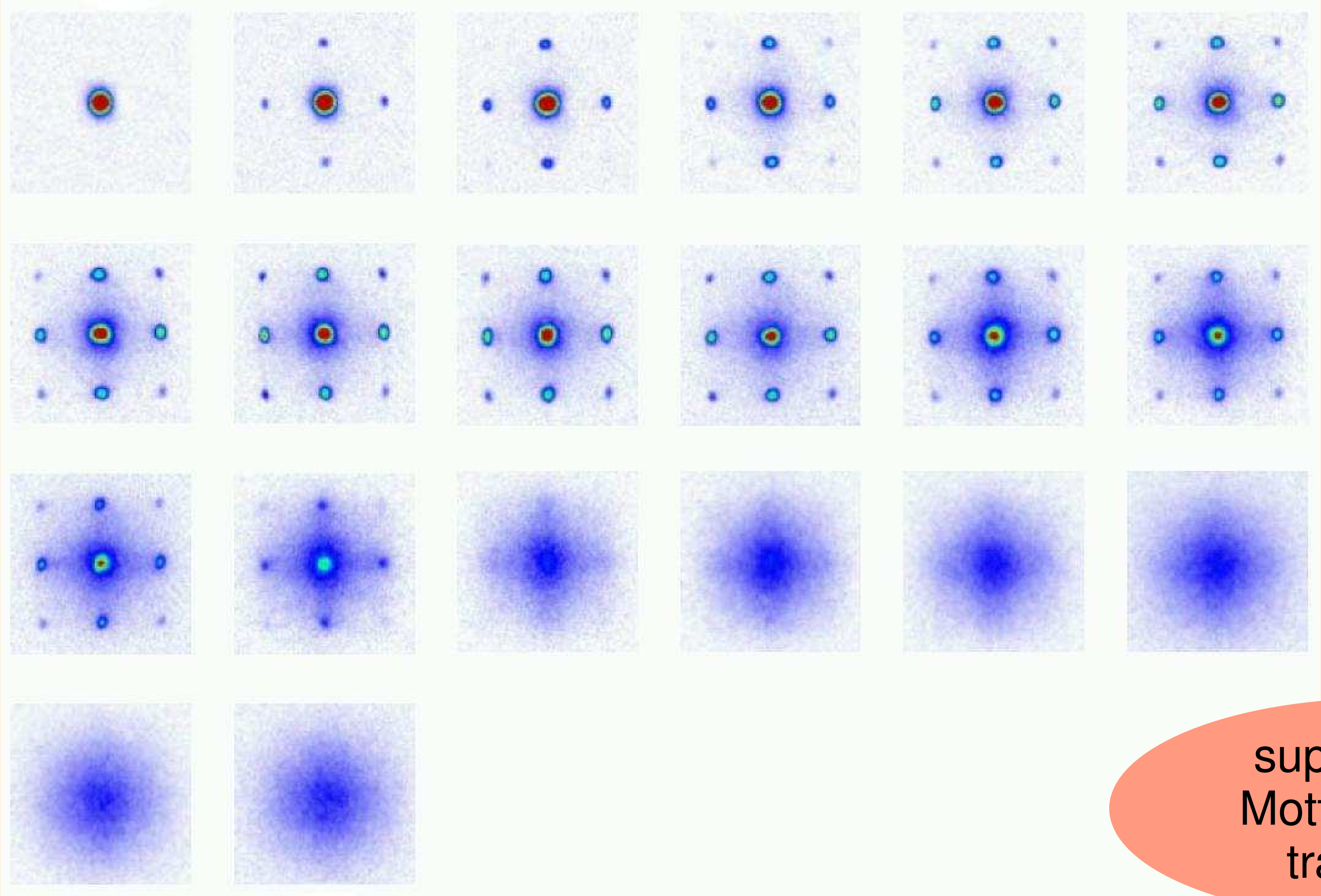
- Introduction
- Bose-Hubbard Model
- Condensate & Superfluidity
- Matter-Wave Interference Pattern
- Superfluid to Mott-Insulator Transition
- Two-Colour Lattices

The Experiment

- produce a **Bose-Einstein condensate** of atoms in a conventional magnetic trap
- load the condensate into an **optical standing-wave lattice** created by counter-propagating laser beams of variable intensity
- the loading process should be **adiabatic** such that only the lowest band is populated
- 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
- vary the **lattice depth** and possibly the **interaction strength** to 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 $\longrightarrow$



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

Many Questions

- How to describe ultracold Bose gases 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
- describe interacting many-body system in a restricted Hilbert space which comprises the **lowest energy band** only
- complete basis of single-particle **Wannier functions** $w(x - \xi_i)$ which are localised at the individual lattice sites $i = 1, ..., I$
- 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

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

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

Bose-Hubbard Hamiltonian

- second quantised many-body Hamiltonian in restricted Hilbert space

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

- 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**

▶ it goes far **beyond** the realm of the mean-field **Gross-Pitaevskii equation**

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

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

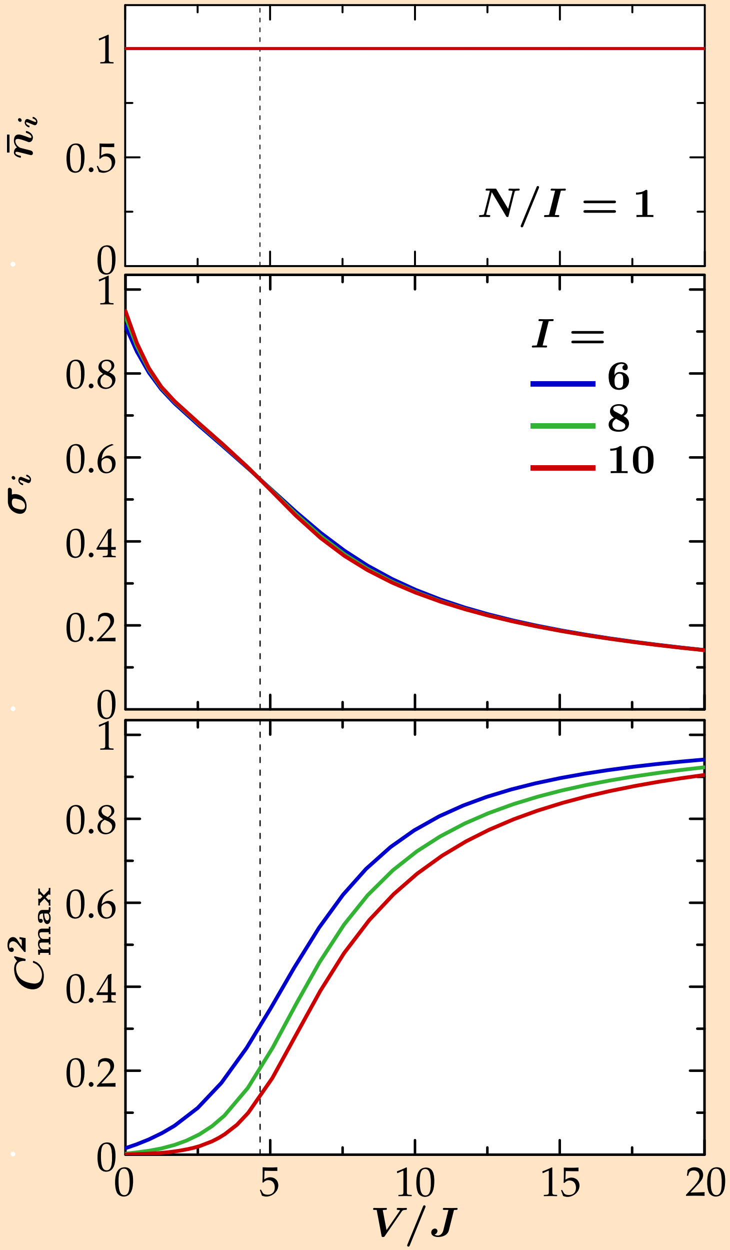
- problem: the number D of basis states **grows dramatically**

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
- there are several **approximation methods**, each applicable in very restricted parameter regimes only; none can describe phase transition regions
  - mean-field, discrete non-linear Schrödinger equation
  - Bogoliubov approximation
  - Gutzwiller ansatz

Simple Quantities



- calculate ground state $|\Psi_0\rangle$ for a sequence of values for V/J
- **mean occupation number**

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

- **number fluctuations**

$$\sigma_i = \Big[\langle\Psi_0|\,\hat{\mathrm{n}}_i^2\,|\Psi_0\rangle - \langle\Psi_0|\,\hat{\mathrm{n}}_i\,|\Psi_0\rangle^2\Big]^{1/2}$$

- **largest coefficient**

$$C^2_{\mathrm{max}} = \max(C^2_\alpha)$$

▶ 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

Bose-Einstein Condensate

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

- **Onsager-Penrose criterion**: if the one-body density matrix

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

  has an eigenvalue N_0 of order N, such that N_0/N stays finite in the thermodynamic limit, then a Bose-Einstein condensate is present and

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

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

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

  as can be seen from the spectral decomposition $\rho^{(1)}_{ij} = N_0\, \phi_{0,i}\, \phi^\star_{0,j} + \tilde{\rho}^{(1)}_{ij}$

- one can define condensation with respect to higher-order density matrices

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

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

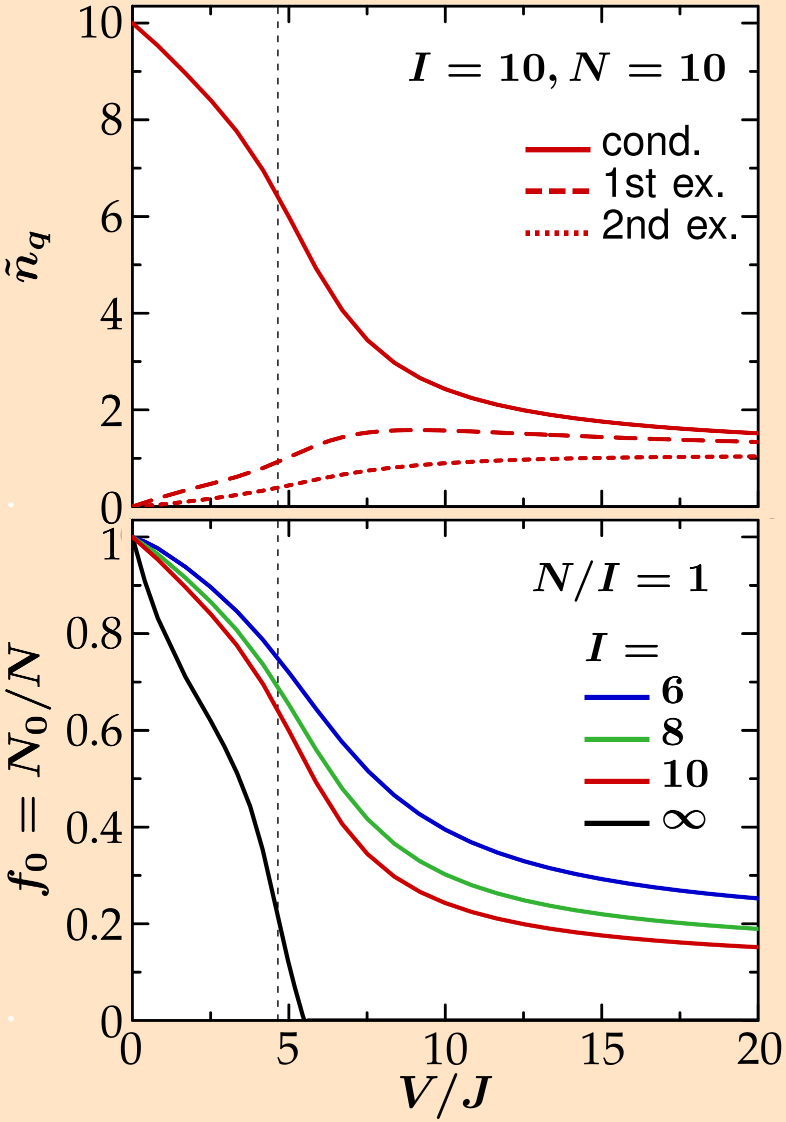
- occupation numbers for the Bloch states, i.e., **quasi-momentum distribution**

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

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

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

Quasi-Momentum Distribution



- noninteracting system: only the $q = 0$ condensate state is populated
- with increasing V/J condensate is depleted and larger q are successively populated
- uniform population of the band in the strong interaction limit

- strong finite size effects: condensate fraction in a finite lattice always $\geq 1/I$
- not possible to decide whether there is a condensate in the Penrose-Onsager sense
- rough extrapolation to $I \to \infty$ leads to vanishing condensate fraction for $V/J \gtrsim 5$

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 approach does not consider the stability of the superflow (critical velocity) as in the Landau definition

Definition of Superfluidity

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

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

- 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

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

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

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

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

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

- 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

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

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

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

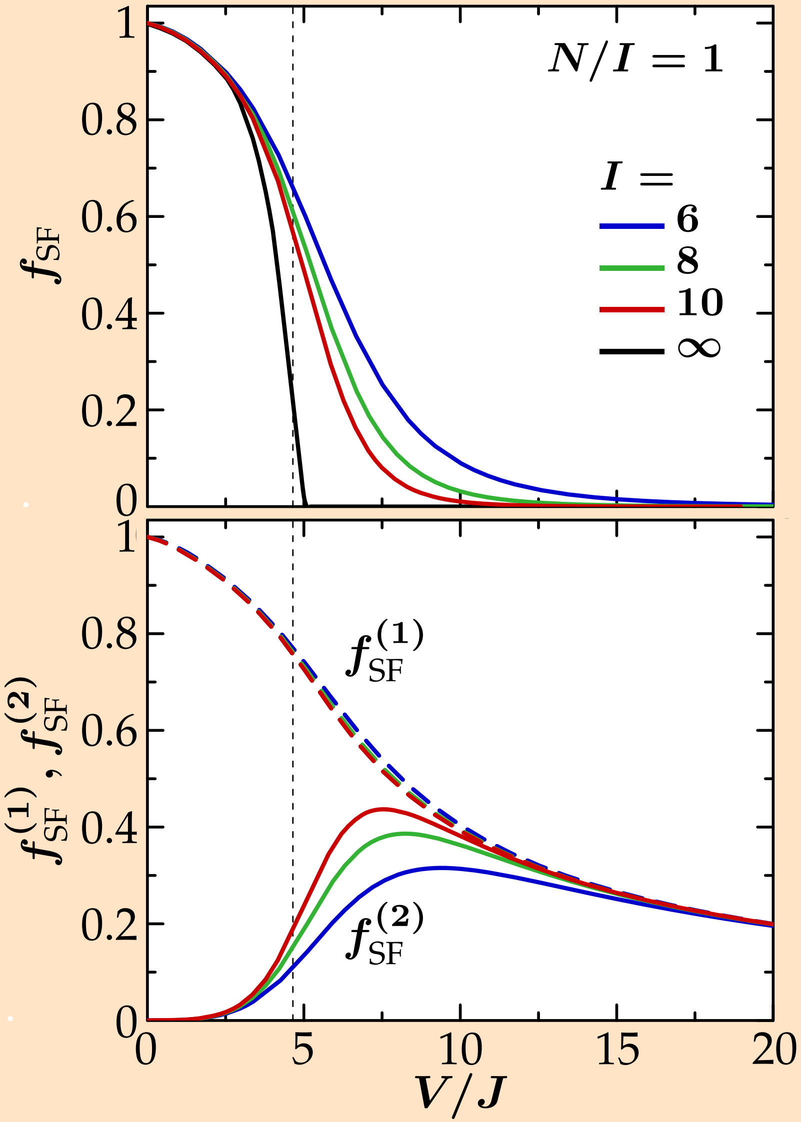
- including all contributions to the energy difference up to order Θ^2 gives for the superfluid fraction

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

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

- ▶ **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
- extrapolation: good agreement with Monte Carlo calculations for critical V/J
- first order contribution $f_{SF}^{(1)}$ 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

condensate

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

superfluid

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

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

- some of the non-condensed particles exhibit a net flow behaviour like the condensate
- prime example: liquid ^4He at $T = 0\text{K}$

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

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

- part of the (quasi-) condensate is not superfluid, i.e. it does not react to the phase twist with an energy change
- seems to appear in systems with disorder / fragmentation

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 $\chi_i(\vec{y}, t)$
- intensity $\mathcal{I}(\vec{y})$ observed at a point $\vec{y}$ after expansion time τ

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

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

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

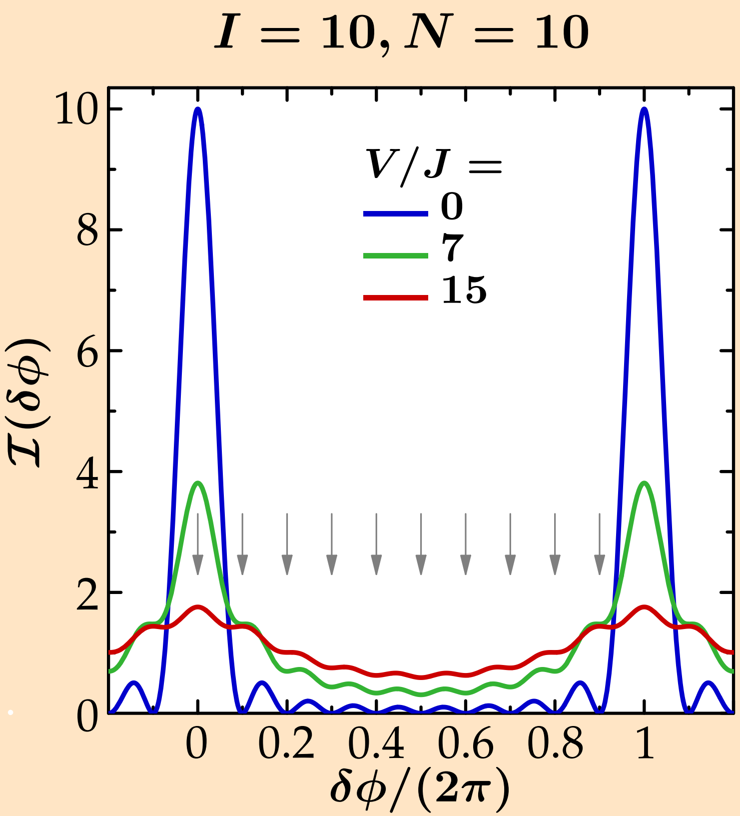
- intensity as function of phase difference $\delta\phi$

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

► exactly the same equation that determines the **quasi-momentum distribution**

$$\tilde{n}_q \;=\; \mathcal{I}(\delta\phi = qa)$$

Interference Pattern

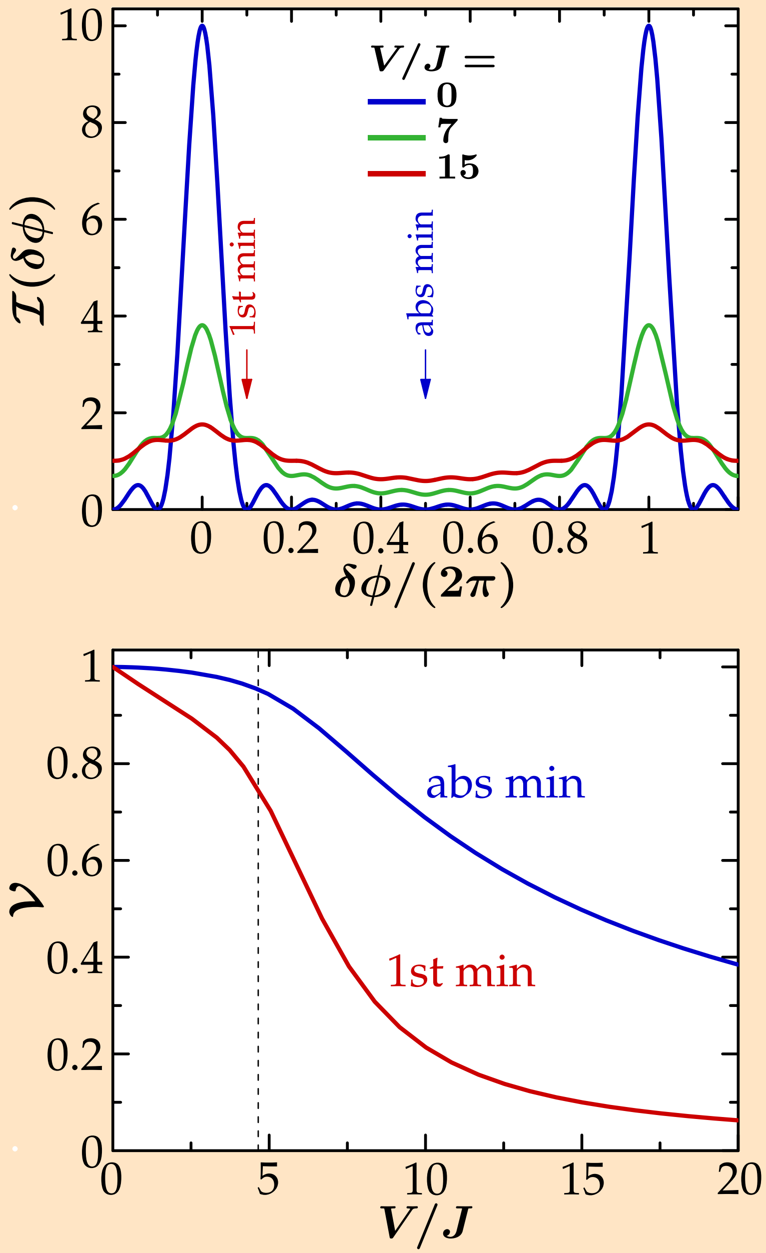


- peaks at $\delta\phi = 0, \pm 2\pi, \ldots$ correspond to the principal interference peaks seen in experiment
- with increasing V/J principal peaks are depleted and broadened; background emerges
- equivalently: with increasing V/J the condensate is depleted and the band is filled successively

▶ pronounced fringes still visible in the insulating phase

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

Interference Pattern & Visibility



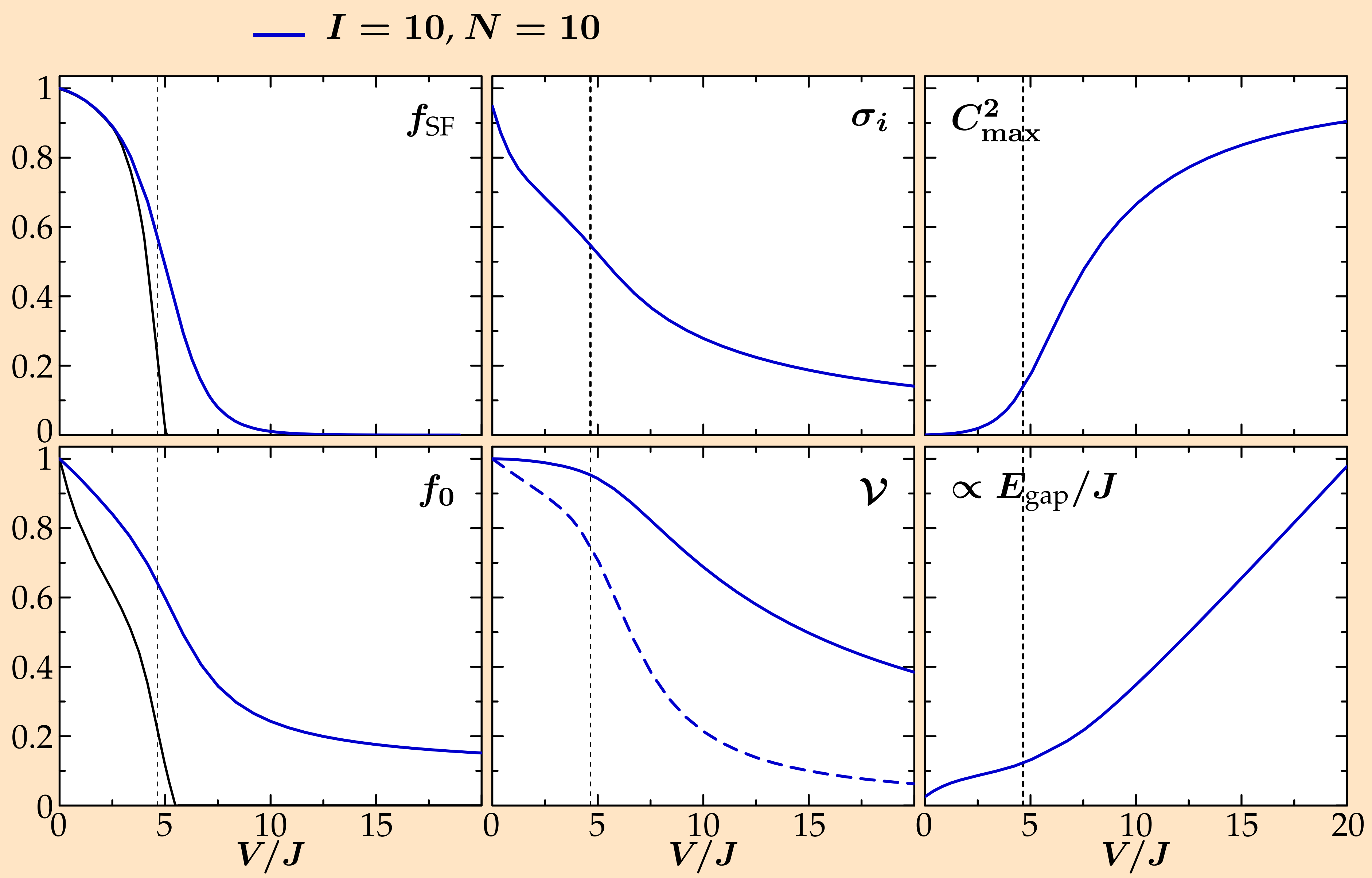
- wanted: simple measure for the presence or absence of fringes
- standard definition of fringe visibility

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

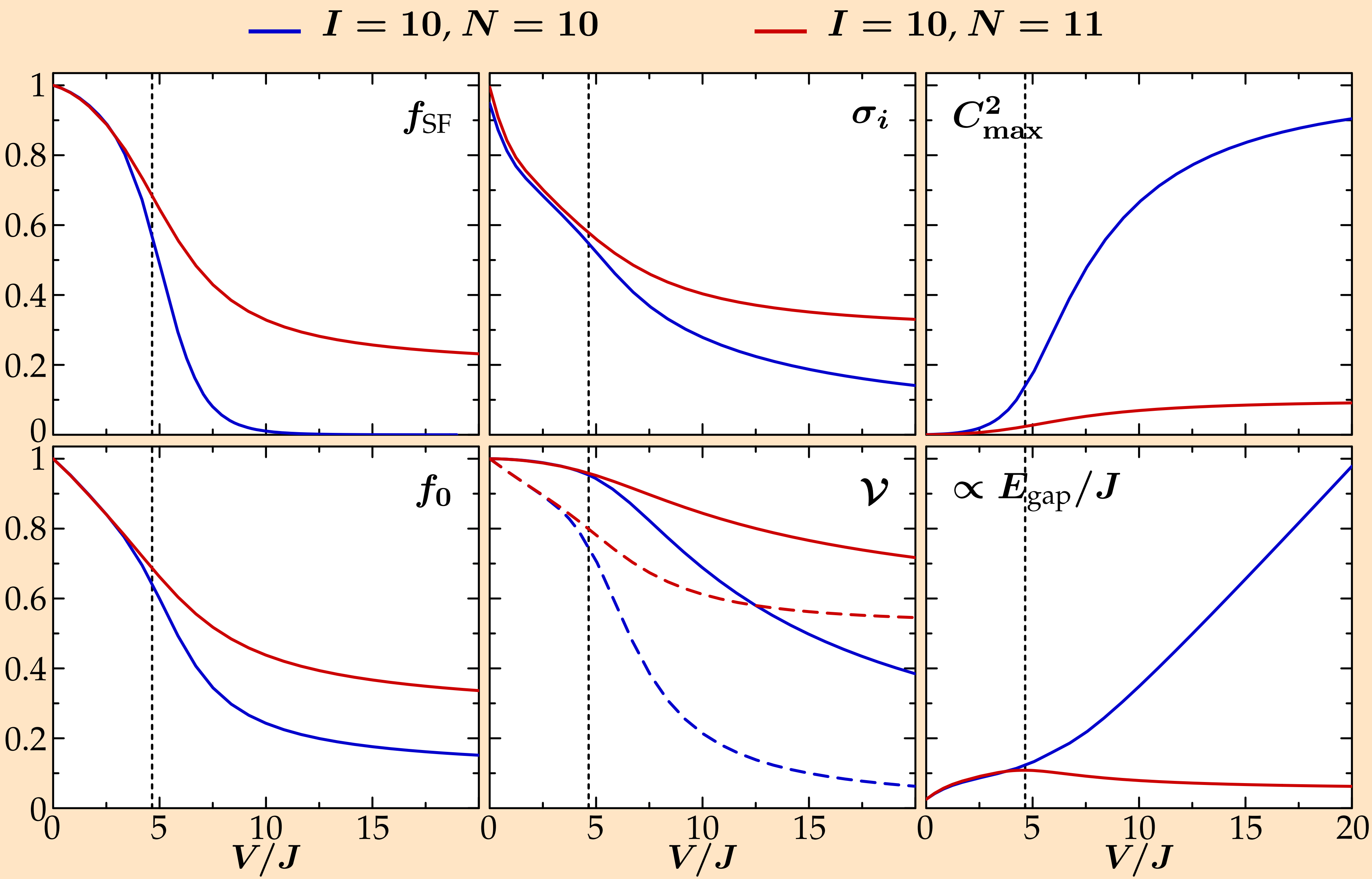
- $\mathcal{I}_{\min}$ = absolute minimum
  - measures non-uniformity of quasi-momentum distribution
  - very insensitive
- $\mathcal{I}_{\min}$ = first minimum
  - measures occupation difference between condensate and 1st excited Bloch state
  - better sensitivity but problematic experimentally

Superfluid to Mott-Insulator Transition

Relevant Quantities



Relevant Quantities



Superfluid to Mott-Insulator Transition

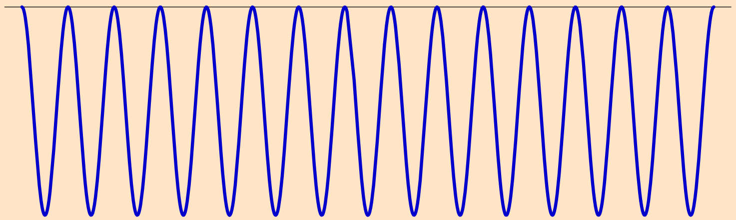
- **quantum phase transition** for commensurate fillings governed by the competition between kinetic energy (large fluctuations) and repulsive interactions (small occupation numbers)

	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 significantly 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 experimental schemes that probe superfluidity directly

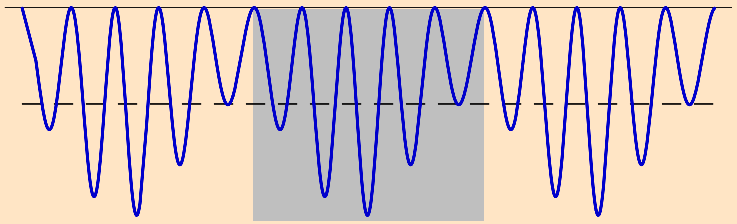
Two-Colour Superlattices

Two-Colour Superlattices



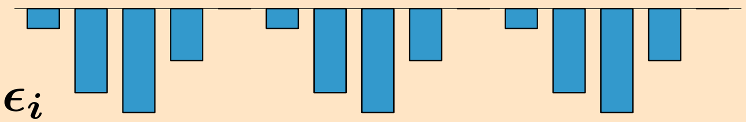
$U_1(x)$

- 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

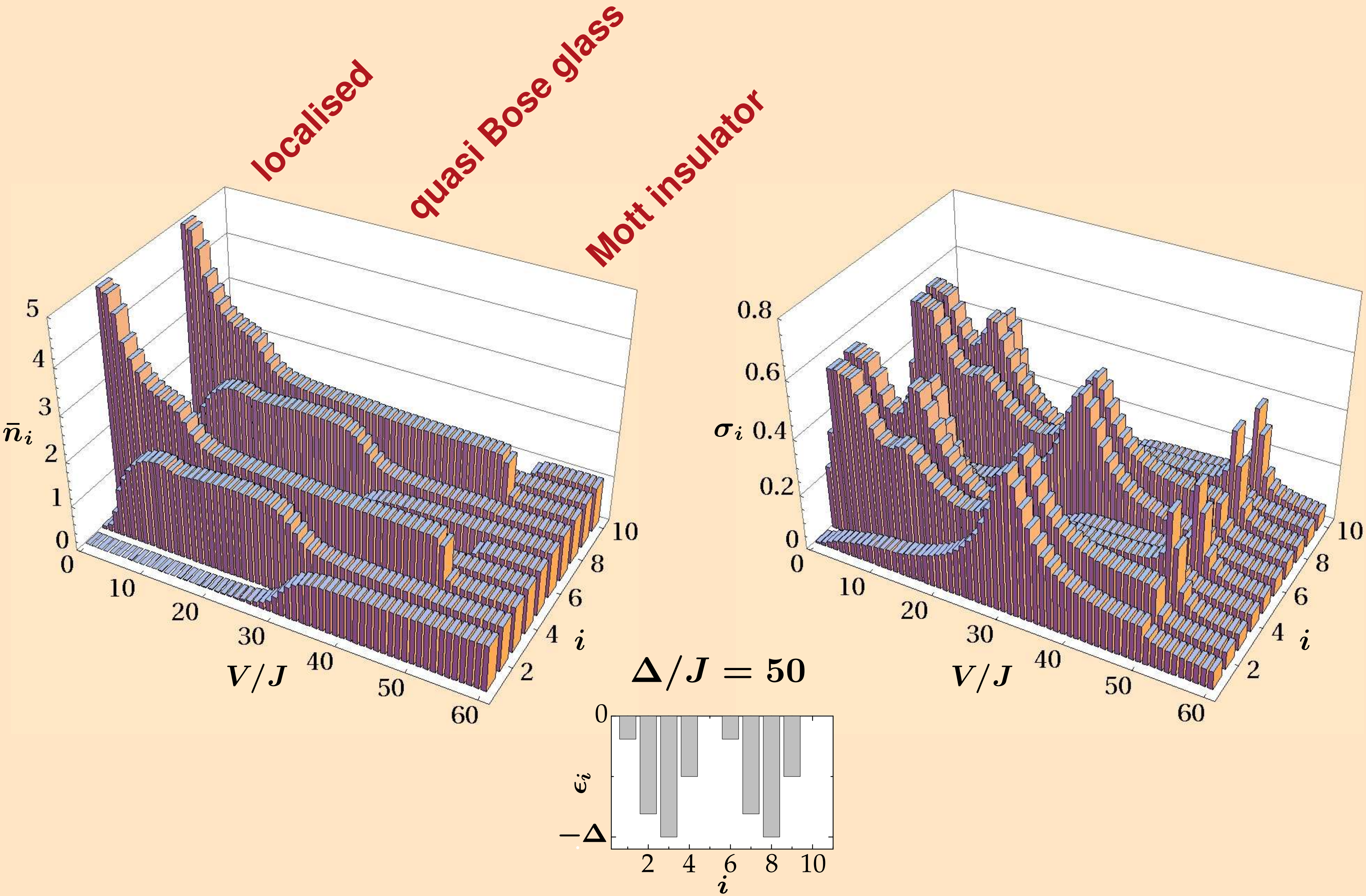


ϵ_i

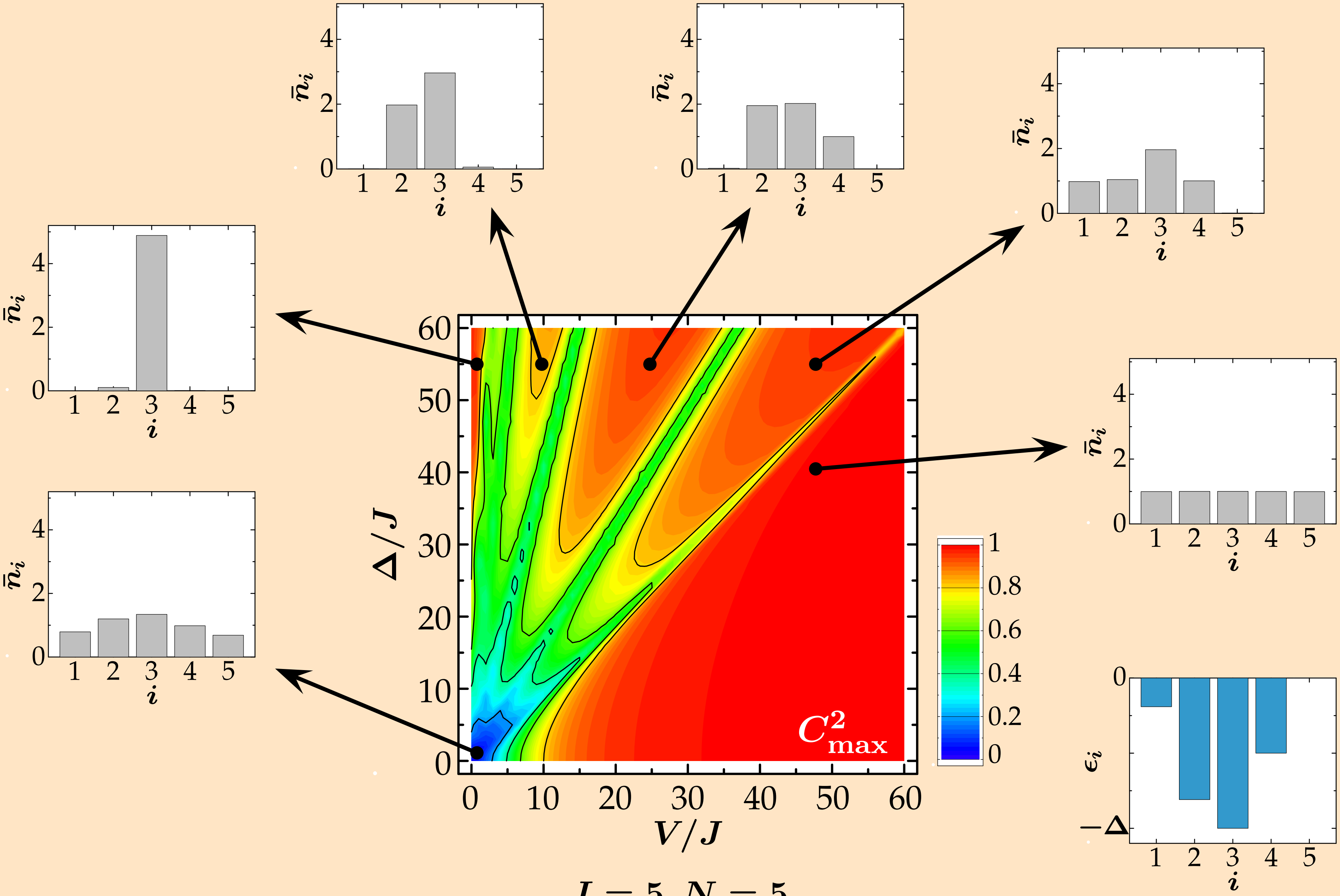
- in the language of the Bose-Hubbard model this means varying on-site energies ϵ_i
- amplitude Δ of the modulation is controlled by the intensity of the second laser

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

Interaction -vs- Lattice Irregularity

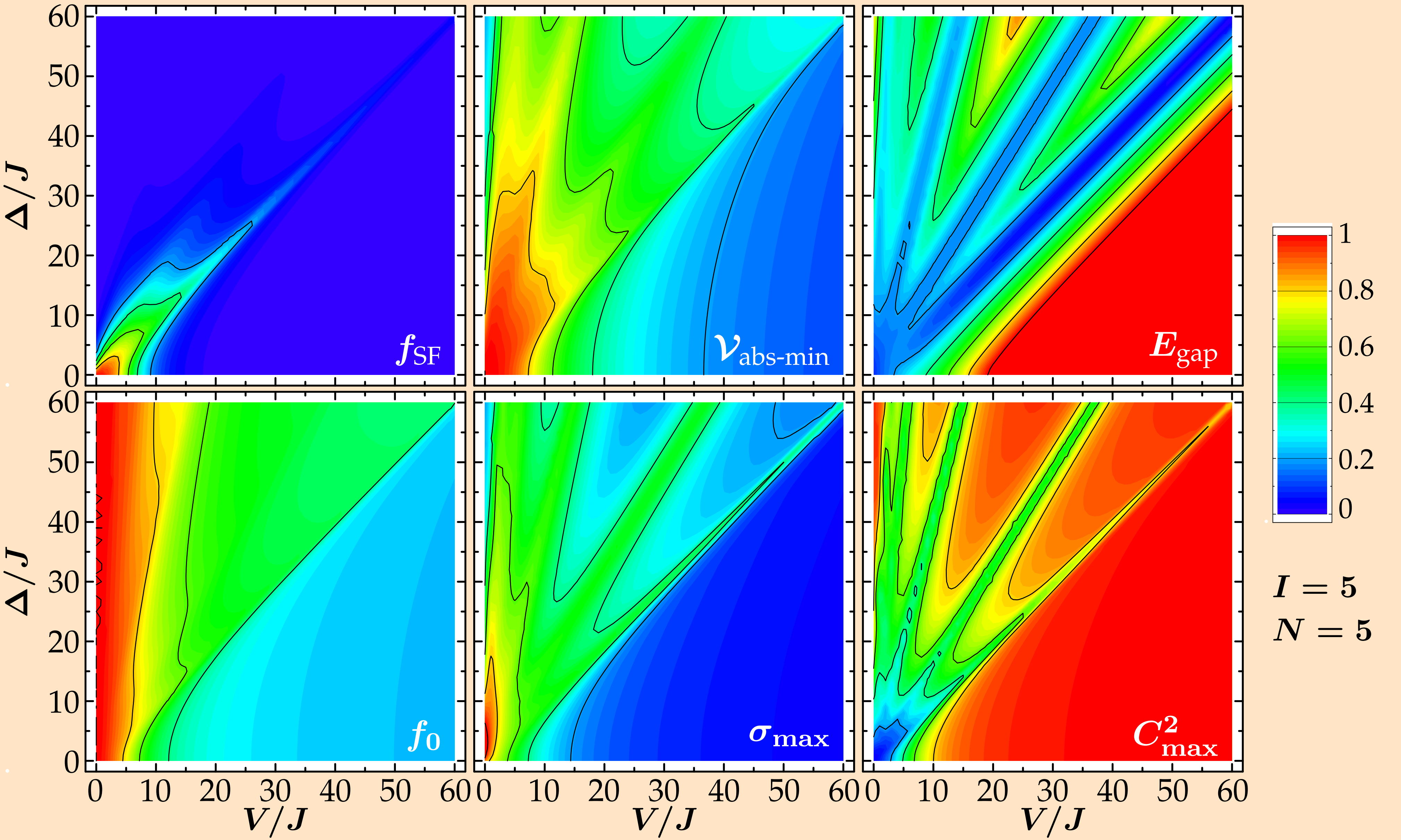


V-Δ Phase Diagram



$I = 5, N = 5$

More Phase Diagrams



$I = 5$

$N = 5$

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