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Oxford Summer School on Ultracold Atoms

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QIPEST

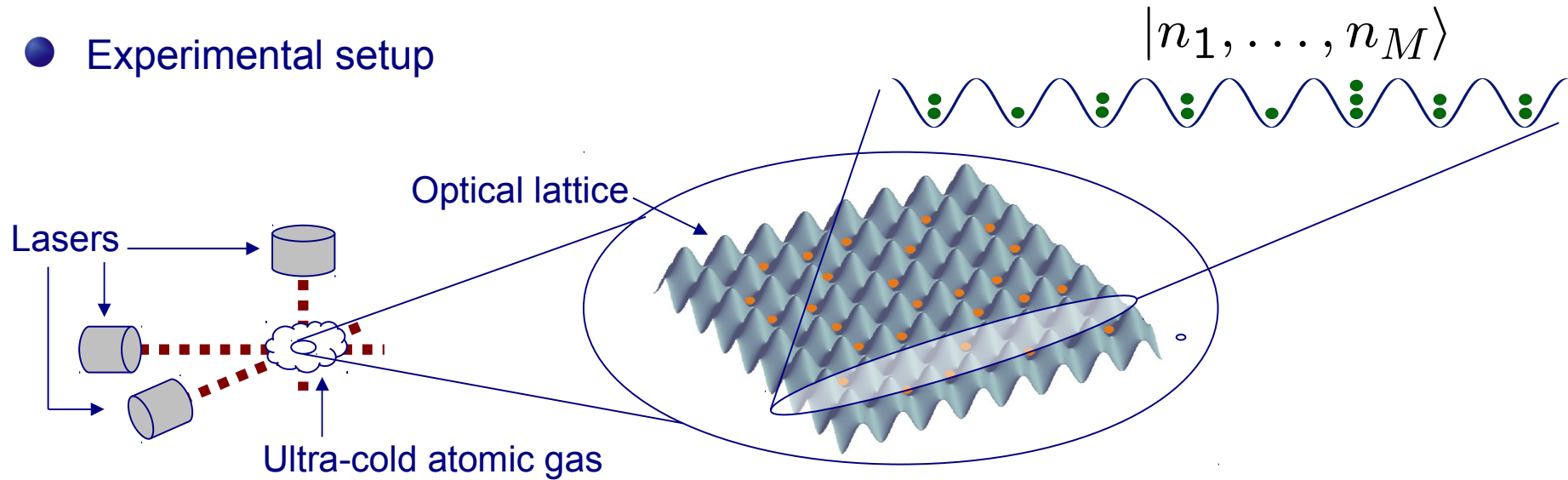


Aims and Goals

- Matrix product states for 1D quantum systems
 - ⇒ Understand the basic ideas behind using matrix product states (MPS) for describing strongly correlated systems
 - ⇒ Acquire mathematical techniques for handling MPS
 - ⇒ Understand the connection between MPS and graphical representation of tensor networks
 - ⇒ Investigate the Bose-Hubbard model using simple MPS states
- The Bose-Hubbard model – numerical studies
 - ⇒ Dynamics of ultracold lattice atoms when ramping or shaking the lattice
- Optical lattices immersed into degenerate quantum gases
 - ⇒ Explain techniques for loading an optical lattice from a degenerate gas
 - ⇒ Describe how phononic excitations in the background gas can be used to cool lattice atoms and discuss the main differences to optical cooling
 - ⇒ Study the effects of a background Bose-Einstein condensate on the dynamics of atoms in the lowest band of an optical lattice

Optical lattice

- Experimental setup



- Described by the Bose-Hubbard model (BHM)

$$H = -J \sum_{\langle \alpha, \beta \rangle} (a_{\alpha}^{\dagger} a_{\beta} + \text{h.c.}) - \mu_{\alpha} a_{\alpha}^{\dagger} a_{\alpha} + \frac{U}{2} a_{\alpha}^{\dagger} a_{\alpha}^{\dagger} a_{\alpha} a_{\alpha},$$

Hopping term J and interaction U are adjustable via the lattice depth V_0

- a_{α} bosonic destruction operator for atoms in site α .
- The chemical potential μ_{α} contains the lattice site offset

Matrix product states for 1D quantum systems

1D lattice with short range interactions

- The quantum state is written as
$$|\psi\rangle = \sum_{n_1=0}^{\infty} \cdots \sum_{n_M=0}^{\infty} c_{n_1 \dots n_M} |n_1, \dots, n_M\rangle,$$
- and for short range interactions
$$\hat{H} = \sum_{i=1}^M \hat{H}_i^{[1]} + \sum_{i=1}^{M-1} \hat{H}_{i,i+1}^{[2]}$$
- The size of the Hilbert space increases exponentially with size and thus an exact numerical treatment is only possible for up to 12 particles in 12 sites for which we need to keep track of 1,352,078 contributions to the quantum state.
- We can make progress by making use of generic properties of 1D quantum systems with nearest neighbour interactions. Here we illustrate these properties using the exactly solvable Ising chain in a transverse magnetic field as an example.
- There is a large body of literature. For more details see e.g.
 - ⇒ G. Vidal, *Phys. Rev. Lett.* **91**, 147902 (2003); *ibid.* **93**, 040502 (2004); *ibid.* **98**, 070201 (2007).
 - ⇒ A.J. Daley, C. Kollath, U. Schollwoeck, G. Vidal, *J. Stat. Mech.* P04005 (2004).
 - ⇒ U. Schollwoeck, *Rev. Mod. Phys.* **77**, 259 (2005).
 - ⇒ F. Verstraete, D. Porras, J. I. Cirac, *Phys. Rev. Lett.* **93**, 227205 (2004).
 - ⇒ S.R. White, *Phys. Rev. Lett.* **69**, 2863 (1992).

Ising chain in transverse magnetic field

- Hamiltonian
$$H_{\text{Ising}} = -J \left(\sum_{i=1}^{M-1} \sigma_i^x \sigma_{i+1}^x + g \sum_{i=1}^M \sigma_i^z \right)$$
- for $g \gg g_c$
$$|\psi_{\text{gs}}\rangle_{g \rightarrow \infty} \approx \prod_i |\uparrow\rangle_i$$
- for $g \ll g_c$
$$|\psi_{\text{gs}}^+\rangle_{g \rightarrow 0} \approx \prod_i |\rightarrow\rangle_i \quad \text{or} \quad |\psi_{\text{gs}}^-\rangle_{g \rightarrow 0} \approx \prod_i |\leftarrow\rangle_i$$

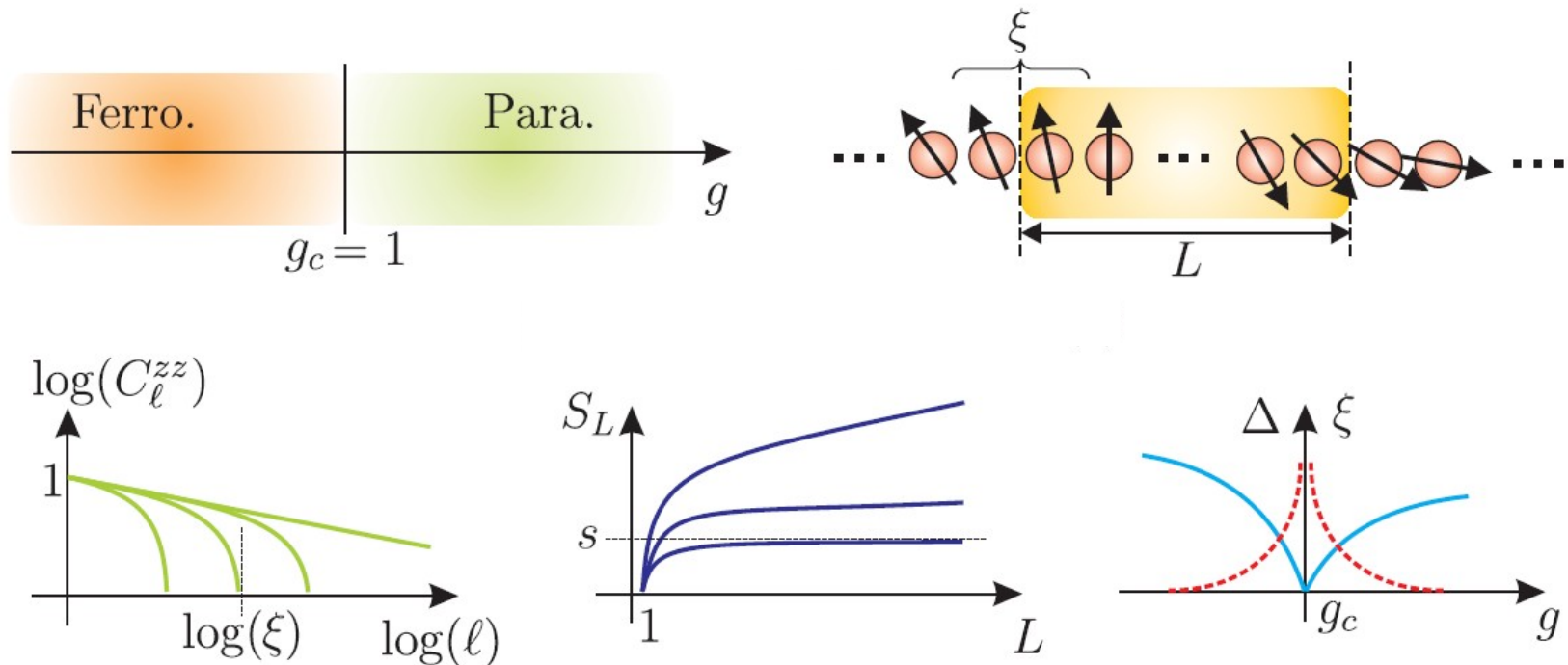
- We consider the correlation functions
$$C_\ell^{ab} = \langle \sigma_i^a \sigma_{i+\ell}^b \rangle = \langle \sigma_i^a \rangle \langle \sigma_{i+\ell}^b \rangle$$

- and the entropy of a block of L spins which is a measure of the entanglement of this block with the rest of the chain

$$\rho_L = \text{tr}_{M-L} (|\psi_{\text{gs}}\rangle \langle \psi_{\text{gs}}|)$$

$$S_L = -\text{tr}(\rho_L \log_2 \rho_L)$$

Ising chain in transverse magnetic field



- The growth of S_L with L is exponentially smaller than it could be in principle.
 - ⇒ when $g \neq g_c$ the entropy $S_L \rightarrow s = \text{const.}$ for large L
 - ⇒ at criticality when $g = g_c$ the entropy $S_L \rightarrow k \log_2 L$ for large L
- This is a generic property of 1D systems with nearest neighbour interactions

The Schmidt decomposition

- We divide the system into subsystem A containing the L particles and subsystem B consisting of the other particles. We write the state as

$$|\psi\rangle = \sum_{i=1}^{d^L} \sum_{j=1}^{d^{M-L}} C_{ij} |i\rangle_A \otimes |j\rangle_B$$

- C_{ij} is interpreted as a matrix and via a singular value decomposition can be written as $C=UDV$ with U,V unitary and D a diagonal matrix with semipositive elements λ_α so-called Schmidt coefficients. This allows writing the state as

$$\begin{aligned} |\psi\rangle &= \sum_{\alpha=1}^{\chi} \lambda_\alpha \left(\sum_{i=1}^{d^L} U_{i\alpha} |i\rangle_A \right) \otimes \left(\sum_{j=1}^{d^{M-L}} V_{\alpha j} |j\rangle_B \right) \\ &= \sum_{\alpha=1}^{\chi} \lambda_\alpha |\phi_\alpha^{[A]}\rangle \otimes |\phi_\alpha^{[B]}\rangle. \end{aligned}$$

- The sum goes up to the number of non-zero elements in D, called χ , whose upper limit is the dimension of the smaller of Hilbert spaces of A,B.

Examples

- A superposition state $|\psi\rangle = \frac{1}{\sqrt{2}}(|1, 0\rangle + |0, 1\rangle)$

is written as $|\psi\rangle = \sum_{\mu=1}^2 \lambda_{\mu} \phi_{\mu}^A \phi_{\mu}^B$

with $\lambda_{\mu} = 2^{-1/2}$, $\phi_1^A = |1\rangle$, $\phi_2^A = |0\rangle$, $\phi_1^B = |0\rangle$, $\phi_2^B = |1\rangle$

- A superposition state $|\psi\rangle = \frac{1}{\sqrt{2}}(|0, 0\rangle + |0, 1\rangle)$

is written as $|\psi\rangle = \sum_{\mu=1}^1 \lambda_{\mu} \phi_{\mu}^A \phi_{\mu}^B$

with $\lambda_{\mu} = 1$, $\phi_1^A = |0\rangle$, $\phi_1^B = 2^{-1/2}(|0\rangle + |1\rangle)$

The Schmidt decomposition

- So far we have not gained anything. We calculate the entropy of subsystems A,B and find

$$\rho_A = \sum_{\alpha=1}^{\chi} \lambda_{\alpha}^2 \left| \phi_{\alpha}^{[A]} \right\rangle \left\langle \phi_{\alpha}^{[A]} \right| \quad \rho_B = \sum_{\alpha=1}^{\chi} \lambda_{\alpha}^2 \left| \phi_{\alpha}^{[B]} \right\rangle \left\langle \phi_{\alpha}^{[B]} \right|$$

$$S_{[A|B]} = - \sum_{\alpha=1}^{\chi} \lambda_{\alpha}^2 \log_2(\lambda_{\alpha}^2)$$

- By keeping χ_L^{ϵ} terms such that
$$\sum_{\alpha=1}^{\chi_L^{\epsilon}} \lambda_{\alpha}^2 \geq 1 - \epsilon$$

ρ_A and ρ_B can be approximated to and accuracy $1-\epsilon$.

- The previous observation on the saturation of S_L indicates that χ_L^{ϵ} also saturates for 1D systems with nearest neighbour interactions
- We find numerically that λ_{α} decays exponentially in many cases of interest.
- Good accuracy can then be achieved by choosing $\chi_L^{\epsilon} \ll \chi$ and thus significantly reducing the number of parameters for describing the state.

Matrix product states

- We can write the state of the optical lattice as

$$|\psi\rangle = \sum_{\mathbf{j}_{[1,M]}} f(\mathbf{A}^{[1]j_1} \mathbf{A}^{[2]j_2} \dots \mathbf{A}^{[M]j_M}) |\mathbf{j}_{[1,M]}\rangle$$

where for periodic boundary conditions we usually choose

$$|\Psi\rangle = \sum_{\mathbf{j}_{[1,M]}} \text{tr}(\mathbf{A}^{[1]j_1} \mathbf{A}^{[2]j_2} \dots \mathbf{A}^{[M]j_M}) |\mathbf{j}_{[1,M]}\rangle$$

and for open boundary conditions (with boundary states $|\Phi_0\rangle$ and $|\Phi_M\rangle$)

$$|\psi\rangle = \sum_{\mathbf{j}_{[1,M]}} \langle \Phi_0 | \mathbf{A}^{[1]j_1} \mathbf{A}^{[2]j_2} \dots \mathbf{A}^{[M]j_M} | \Phi_M \rangle |\mathbf{j}_{[1,M]}\rangle$$

- We leave the matrices $\mathbf{A}$ general for the moment and will now investigate the connection of MPS and the Schmidt decomposition.
- Note that in this generality matrix product states can be used to describe bond-site and PEPS methods.
 - ⇒ U. Schollwoeck, Rev. Mod. Phys. **77**, 259 (2005).
 - ⇒ F. Verstraete, D. Porras, J. I. Cirac, Phys. Rev. Lett. **93**, 227205 (2004).

MPS and Schmidt decompositions

- It can be shown that by making use of the gauge freedom

$$\mathbf{A}^{[m]j_m} \mathbf{A}^{[m+1]j_{m+1}} = (\mathbf{A}^{[m]j_m} \mathbf{X}^{-1}) (\mathbf{X} \mathbf{A}^{[m+1]j_{m+1}})$$

the matrix product can be rewritten as

$$\prod_{m=1}^M \mathbf{A}^{[m]j_m} = (\prod_{m=1}^L \mathbf{A}^{[m]j_m}) \mathbf{D} (\prod_{m=L+1}^M \mathbf{A}^{[m]j_m})$$

where $\mathbf{D}$ is a diagonal matrix with entries λ_{α_L} which satisfies

$$\text{tr}(\mathbf{D}^2) = 1 = \sum_{\alpha_L} \lambda_{\alpha_L}^2 = 1$$

$|\alpha_L\rangle$ are the corresponding eigenvectors and

$$\sum_{j_m=1}^d (\mathbf{A}_{\leftarrow}^{[m]j_m})^\dagger \mathbf{A}_{\leftarrow}^{[m]j_m} = \mathbb{1} \quad \text{for } 1 < m \leq L \quad \sum_{j_1=1}^d (\mathbf{A}_{\leftarrow}^{[1]j_1})^\dagger |\Phi_0\rangle \langle \Phi_0| \mathbf{A}_{\leftarrow}^{[1]j_1} = \mathbb{1}$$

$$\sum_{j_m=1}^d \mathbf{A}_{\rightarrow}^{[m]j_m} (\mathbf{A}_{\rightarrow}^{[m]j_m})^\dagger = \mathbb{1} \quad \text{for } M > m > L \quad \sum_{j_M=1}^d \mathbf{A}_{\rightarrow}^{[M]j_M} |\Phi_M\rangle \langle \Phi_M| (\mathbf{A}_{\rightarrow}^{[M]j_M})^\dagger = \mathbb{1}$$

MPS and Schmidt decompositions

- The Schmidt decomposition at L is then easily accessible as

$$\begin{aligned}
 |\psi\rangle &= \sum_{\alpha_L=1}^{\chi_L} \lambda_{\alpha_L} |\varphi_{\alpha_L}^{[A]}\rangle |\varphi_{\alpha_L}^{[B]}\rangle, \text{ where} \\
 |\varphi_{\alpha_L}^{[A]}\rangle &= \sum_{\mathbf{j}_{[1,L]}} \langle \Phi_0 | \mathbf{A}^{[1]j_1} \dots \mathbf{A}^{[L]j_L} | \alpha_L \rangle |\mathbf{j}_{[1,L]}\rangle, \\
 |\varphi_{\alpha_L}^{[B]}\rangle &= \sum_{\mathbf{j}_{[L+1,M]}} \langle \alpha_L | \mathbf{A}^{[L+1]j_{L+1}} \dots \mathbf{A}^{[M]j_M} | \Phi_M \rangle |\mathbf{j}_{[L+1,M]}\rangle
 \end{aligned}$$

- It is possible to impose an additional shifting constrained

$$\begin{aligned}
 \sum_{j_m=1}^d \mathbf{A}_{\leftarrow}^{[m]j_m} \mathbf{\Lambda}^{[m]} (\mathbf{A}_{\leftarrow}^{[m]j_m})^\dagger &= \mathbf{\Lambda}^{[m-1]} \\
 \sum_{j_m=1}^d (\mathbf{A}_{\rightarrow}^{[m]j_m})^\dagger \mathbf{\Lambda}^{[m-1]} \mathbf{A}_{\rightarrow}^{[m]j_m} &= \mathbf{\Lambda}^{[m]}
 \end{aligned}$$

so that all Schmidt decompositions become easily accessible through

$$\mathbf{A}_{\leftarrow}^{[m]j_m} \sqrt{\mathbf{\Lambda}^{[m]}} = \sqrt{\mathbf{\Lambda}^{[m-1]}} \mathbf{A}_{\rightarrow}^{[m]j_m}$$

If the matrices A fulfil all these conditions the MPS is said to be of *canonical form*.

Density matrices

- The density matrix (PBC) can be written as

$$\rho = \sum_{\mathbf{j}_{[1,M]}} \sum_{\mathbf{i}_{[1,M]}} \text{tr} \left(\prod_{m=1}^M \mathbf{A}^{[m]j_m} \right) \text{tr} \left(\prod_{m=1}^M \mathbf{A}^{*[m]i_m} \right) |\mathbf{j}_{[1,M]}\rangle \langle \mathbf{i}_{[1,M]}|$$

$$\rho = \sum_{\mathbf{j}_{[1,M]}} \sum_{\mathbf{i}_{[1,M]}} \text{tr} \left(\prod_{m=1}^M \mathbf{E}^{[m]j_m i_m} \right) |\mathbf{j}_{[1,M]}\rangle \langle \mathbf{i}_{[1,M]}|$$

- We use the following definitions

$$\mathbf{E}^{[m]j_m i_m} = \mathbf{A}^{[m]j_m} \otimes \mathbf{A}^{*[m]i_m}$$

$$\mathbf{I}^{[m]} = \sum_{j_m=1}^d \mathbf{E}^{[m]j_m j_m}$$

- This allows us to e.g. work out the reduced density matrix for site k

$$\rho_k = \sum_{j_k=1}^d \sum_{i_k=1}^d \text{tr} \left(\left[\prod_{m=1}^{k-1} \mathbf{I}^{[m]} \right] \mathbf{E}^{[k]j_k i_k} \left[\prod_{m'=k+1}^M \mathbf{I}^{[m']} \right] \right) |j_k\rangle \langle i_k|$$

Graphical representation

- The contraction of indices is denoted by connecting corresponding tensor legs
- The full density matrix

Diagram illustrating a quantum circuit structure for a density matrix ρ . The circuit consists of two horizontal bars representing gates. The top bar has inputs $i_1, i_2, \dots, i_m, \dots, i_M$ and outputs $j_1, j_2, \dots, j_m, \dots, j_M$. The bottom bar has inputs $j_1, j_2, \dots, j_m, \dots, j_M$ and outputs $i_1, i_2, \dots, i_m, \dots, i_M$. The output of the top bar is labeled $\rho = (\dots)^*$ and the output of the bottom bar is labeled $|\psi\rangle$. An arrow points from the label $\mathbf{A}^{[m]j_m}$ to the m -th gate in the bottom bar.

- The reduced density matrix of the m-th site

Diagram illustrating the structure of the m -th layer of the quantum state, denoted as ρ_m . The circuit is represented by two horizontal lines (qubits) and a sequence of operations enclosed in large parentheses with a superscript $*$.

The circuit consists of M stages, labeled 1, 2, ..., M . Each stage involves a pair of blue triangles (representing gates) connected by a dashed line. The first stage is labeled 1, the second stage is labeled 2, and the final stage is labeled M .

The input to the circuit is labeled $\mathbf{I}[2]$ (top line) and $\mathbf{E}[m]j_m i_m$ (bottom line). The output of the circuit is labeled i_m (top line) and j_m (bottom line).

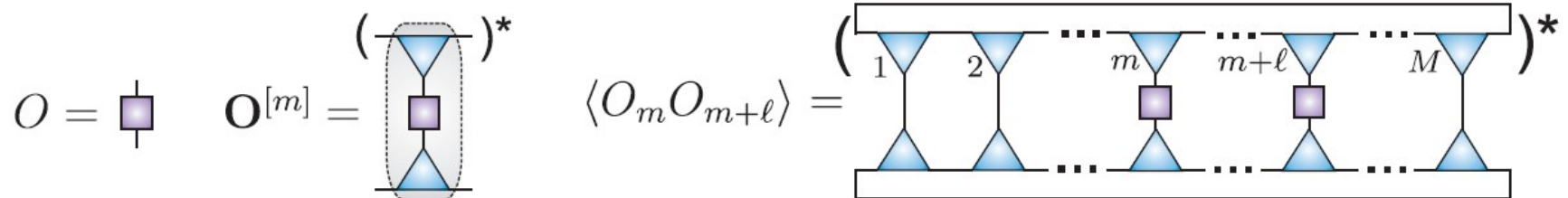
Observables

- Similarly we can work out

$$\langle \psi | O_1 \otimes O_2 \otimes \cdots \otimes O_M | \psi \rangle = \text{tr} \left(\prod_{m=1}^M \mathbf{o}^{[m]} \right)$$

$$\mathbf{o}^{[m]} = \sum_{j_m=1}^d \sum_{i_m=1}^d \langle j_m | O_m | i_m \rangle \mathbf{E}^{[m]j_m i_m}$$

- This can be visualized as



Two-site gates

- For applying a gate to two nearest neighbour sites we write (OBC)

$$|\psi\rangle = \sum_{\mathbf{j}_{[1,M]}} \langle \Phi_0 | \left(\prod_{m=1}^{k-1} \mathbf{A}_{\leftarrow}^{[m]j_m} \right) \Xi^{j_k j_{k+1}} \left(\prod_{m'=k+2}^M \mathbf{A}_{\rightarrow}^{[m']j_{m'}} \right) | \Phi_M \rangle | \mathbf{j}_{[1,M]} \rangle$$

$$|\psi\rangle = \sum_{\mathbf{j}_{[k,k+1]}} \sum_{\alpha_{k-1}=1}^{\chi_{k-1}} \sum_{\alpha_{k+1}=1}^{\chi_{k+1}} \langle \alpha_{k-1} | \Xi^{j_k j_{k+1}} | \alpha_{k+1} \rangle | \mathbf{L}_{\alpha_{k-1}}^{[k-1]} \rangle | j_k \rangle | j_{k+1} \rangle | \mathbf{R}_{\alpha_{k+1}}^{[k+1]} \rangle$$

- The central two sites are described by

$$\Xi^{j_k j_{k+1}} = \begin{cases} \sqrt{\Lambda^{[k-1]}} \mathbf{A}_{\rightarrow}^{[k]j_k} \mathbf{A}_{\rightarrow}^{[k+1]j_{k+1}} & (a) \quad \text{Left} \\ \mathbf{A}_{\leftarrow}^{[k]j_k} \sqrt{\Lambda^{[k]}} \mathbf{A}_{\rightarrow}^{[k+1]j_{k+1}} & (b) \quad \text{Centre} \\ \mathbf{A}_{\leftarrow}^{[k]j_k} \mathbf{A}_{\leftarrow}^{[k+1]j_{k+1}} \sqrt{\Lambda^{[k+1]}} & (c) \quad \text{Right} \end{cases}$$

Two-site gates

- An arbitrary two-site gate applied to gates $k, k+1$ is given by

$$\mathcal{G} = \sum_{\mathbf{j}_{[k,k+1]}} \sum_{\mathbf{i}_{[k,k+1]}} G_{i_k i_{k+1}}^{j_k j_{k+1}} |j_k\rangle |j_{k+1}\rangle \langle i_k| \langle i_{k+1}|$$

- The application of the gate turns the state into

$$\Theta^{j_k j_{k+1}} = \sum_{\mathbf{i}_{[k,k+1]}} G_{i_k i_{k+1}}^{j_k j_{k+1}} \Xi^{j_k j_{k+1}}$$

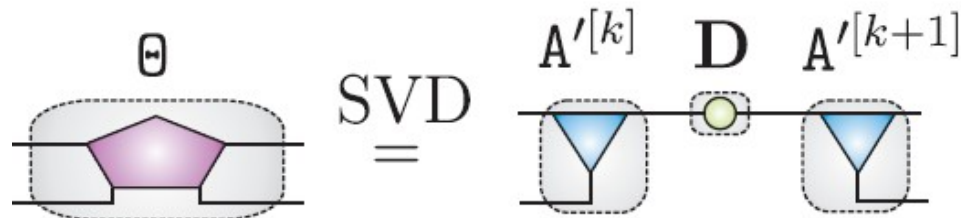
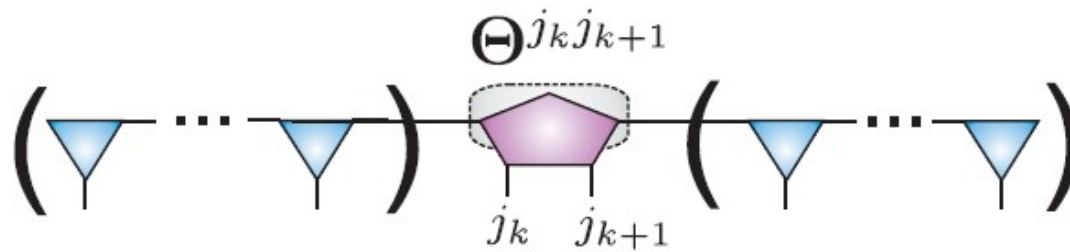
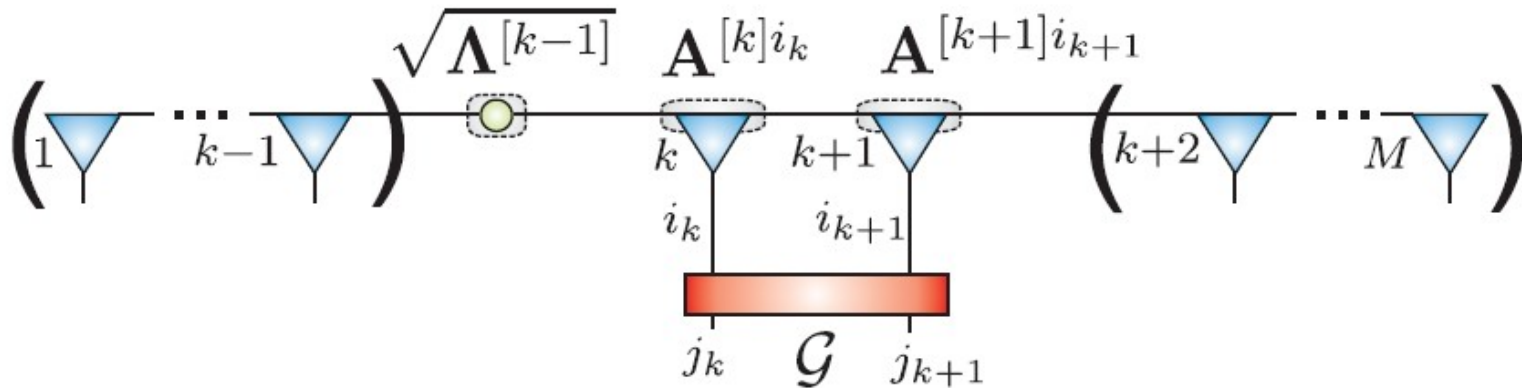
$$|\psi'\rangle = \sum_{\mathbf{j}_{[k,k+1]}} \sum_{\alpha_{k-1}=1}^{\chi_{k-1}} \sum_{\alpha_{k+1}=1}^{\chi_{k+1}} \langle \alpha_{k-1} | \Theta^{j_k j_{k+1}} | \alpha_{k+1} \rangle |L_{\alpha_{k-1}}^{[k-1]}\rangle |j_k\rangle |j_{k+1}\rangle |R_{\alpha_{k+1}}^{[k+1]}\rangle$$

- By an SVD the theta tensor can be turned into

$$\Theta^{j_k j_{k+1}} = \bar{\mathbf{A}}_{\leftarrow}^{\prime[k]j_k} \mathbf{D} \mathbf{A}_{\rightarrow}^{\prime[k+1]j_{k+1}}$$

where $\mathbf{D}$ might have to be renormalized (for non-unitary gates only)

Graphical representation of a two-site gate



Time evolution via Trotter expansion

- We consider a Hamiltonian of the form

$$\hat{H}(t) = \sum_{j=1}^M \sum_{\nu=1}^{k_1} c_j^\nu(t) \hat{h}_j^\nu + \sum_{j=1}^{M-1} \sum_{\nu=1}^{k_2} c_j^\nu(t) \hat{h}_{j,j+1}^\nu = \sum_{j=1}^{M-1} \hat{H}_{j,j+1}(t)$$

- This is split up into two-sites parts

for $1 < j < M$

$$1 < j < M - 1$$

and for OBC we also define

$$\hat{H}_{1,2}(t) = \sum_{\nu=1}^{k_1} c_1^\nu(t) \hat{h}_1^\nu + \sum_{\nu=1}^{k_2} c_1^\nu(t) \hat{h}_{1,2}^\nu + \frac{1}{2} \sum_{\nu=1}^{k_1} c_2^\nu(t) \hat{h}_2^\nu$$

$$\hat{H}_{M-1,M}(t) = \frac{1}{2} \sum_{\nu=1}^{k_1} c_{M-1}^\nu(t) \hat{h}_{M-1}^\nu + \sum_{\nu=1}^{k_2} c_{M-1}^\nu(t) \hat{h}_{M-1,M}^\nu + \sum_{\nu=1}^{k_1} c_M^\nu(t) \hat{h}_M^\nu$$

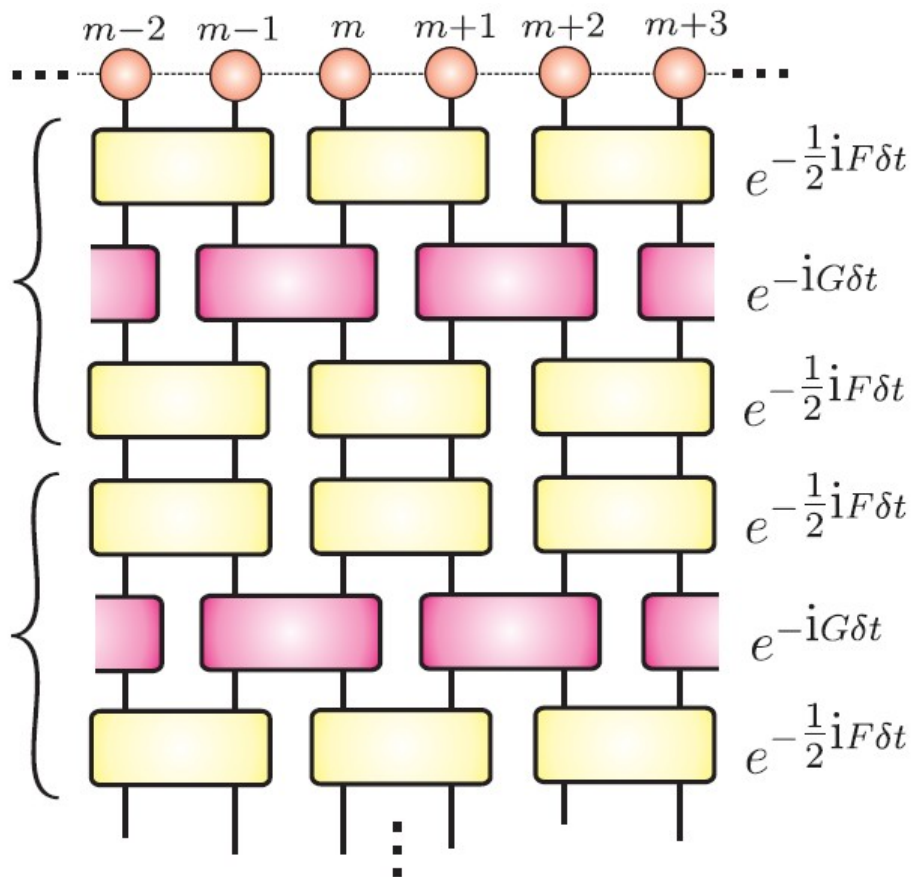
Time evolution via Trotter expansion (TEBD)

- A Trotter expansion is used to divide the time evolution operator corresponding to this Hamiltonian into a product of small time steps of nearest neighbour operators. These are then applied as two-site quantum gates to the initial state to simulate the time evolution.
- There are many different ways for doing this. They vary in accuracy (i.e. how the error depends on the chosen time step) but also in how the product is ordered.
- For doing the numerics it is desirable to keep the matrix product state in canonical form. The splitting of the evolution operator into 'Left and Right zips' is well suited for achieving this

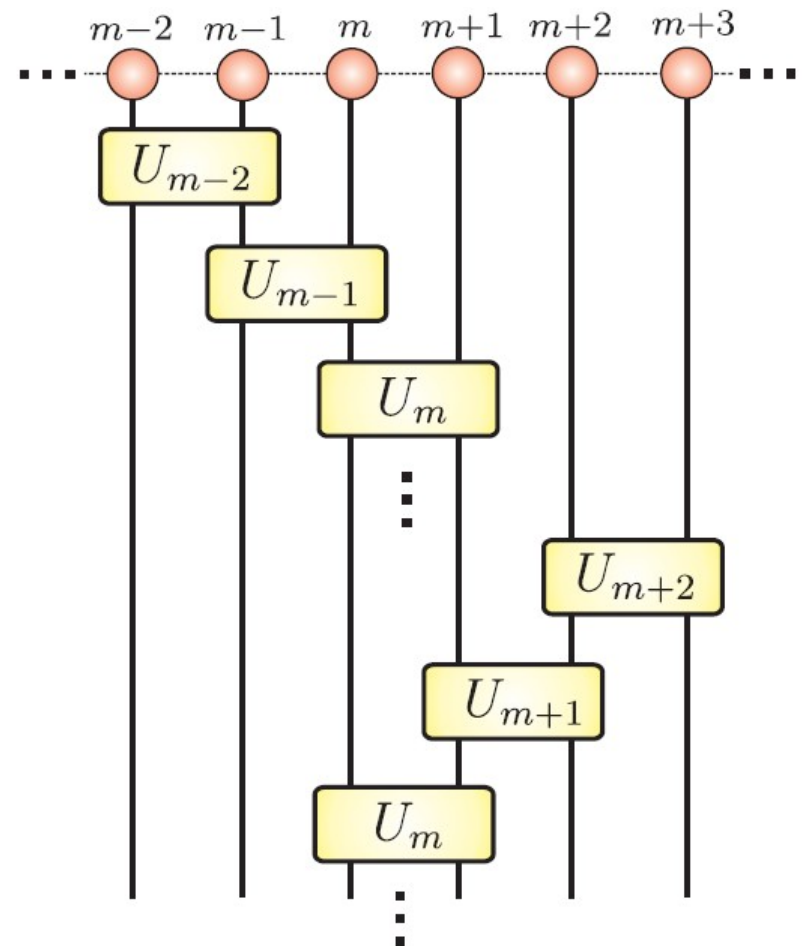
$$\begin{aligned} e^{-iH(t_n)\delta t} &= \mathcal{P}_{1 \rightarrow M} \left(\prod_{j=1}^M e^{-\frac{1}{2}iH_{j,j+1}(t_n)\delta t} \right) \times \mathcal{P}_{M \rightarrow 1} \left(\prod_{j=1}^M e^{-\frac{1}{2}iH_{j,j+1}(t_n)\delta t} \right) + O(\delta t^3), \\ &= \underbrace{e^{-\frac{1}{2}iH_{1,2}(t_n)\delta t} \dots e^{-\frac{1}{2}iH_{M-1,M}(t_n)\delta t}}_{\text{Left zip}} \times \underbrace{e^{-\frac{1}{2}iH_{M-1,M}(t_n)\delta t} \dots e^{-\frac{1}{2}iH_{1,2}(t_n)\delta t}}_{\text{Right zip}} + O(\delta t^3) \end{aligned}$$

Graphical representation

● 'Standard' Trotter steps



● Left – Right Trotter zips



Finding the ground state

- Use imaginary time evolution:
 - ⇒ Replace time t by imaginary time $-i\beta$
 - ⇒ The evolution operator is not unitary anymore
 - ⇒ To achieve good accuracy the time steps are reduced as the simulation proceeds
 - ⇒ When the time step size tends towards 0 the state gets “re-canonicalized”
 - ⇒ This method is known to converge slowly!
- Implement finite size DMRG
 - ⇒ Method can be based on TEBD discussed above
 - ⇒ Use variant of Trotter splits to minimize energy, for details see
 - ⊗ U. Schollwoeck, *Rev. Mod. Phys.* **77**, 259 (2005)
 - ⇒ DMRG and TEBD are fully compatible i.e. ground states worked out via DMRG can be used as initial conditions for TEBD calculations

Simulation of mixed states

- Arrange the $N \times N$ matrix ρ as a vector with N^2 elements
- Introduce superoperators $\mathcal{L}$ on these matrices of dimension $N^2 \times N^2$
- The evolution equation is then formally equivalent to the Schrödinger equation.

- For a typical master equation of Lindblad type

$$\begin{aligned}\dot{\rho} &= -i[H, \rho] + \frac{\gamma}{2} (2A\rho A^\dagger - A^\dagger A\rho - \rho A^\dagger A) \\ &\equiv \mathcal{L}[\rho]\end{aligned}$$

- If $\mathcal{L}$ decomposes into single site and two site operations the same techniques as discussed for pure states and unitary evolution can be applied
- Alternatively quantum Monte Carlo simulation techniques can be used
- It is known that methods based on MPS are inaccurate for large times
⇒ see: N. Schuch, *et al.* [arXiv:0801.2078](https://arxiv.org/abs/0801.2078)

Strong correlations

- MPS allow to describe systems in 1D where the correlations at long distances are mean field like or scale like

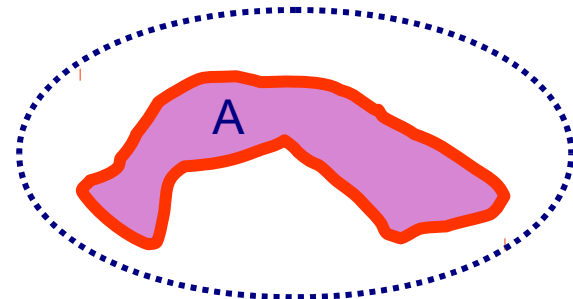
$$\langle \psi^\dagger(x) \psi(x') \rangle \propto e^{-\zeta|x-x'|}$$

- Systems at criticality with long range strong correlations of the form

$$\langle \psi^\dagger(x) \psi(x') \rangle \propto |x - x'|^\zeta$$

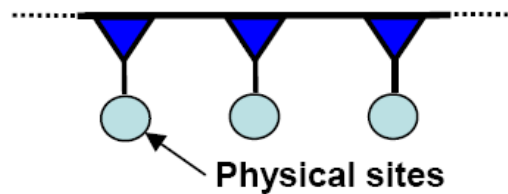
require $\chi \rightarrow \infty$ and are thus not appropriately described

- In higher than one dimension χ scales badly with the size of the system
 - ⇒ The amount of entanglement and thus χ scales with the size of the boundary of the system. In 1D this is constant leading to $\chi \propto \log(L)$ at most while in 2D and 3D the boundary increases with the system size

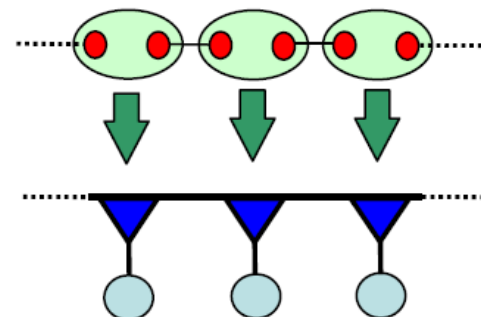


Towards higher dimensions

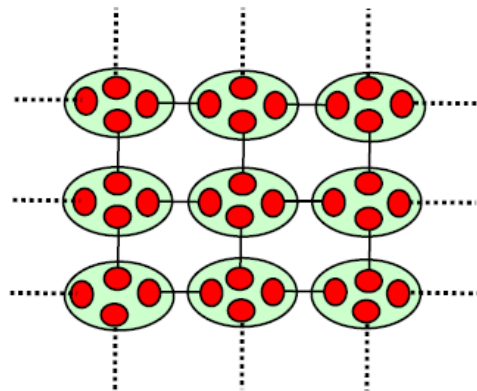
(a) MPS



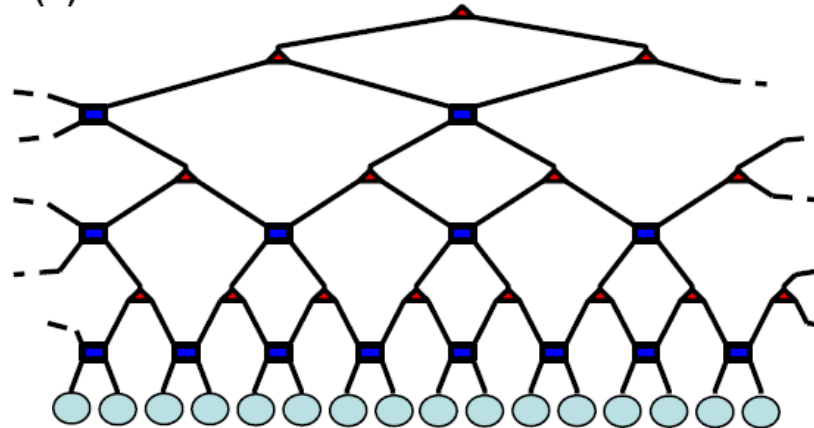
(b) PEPS - 1D



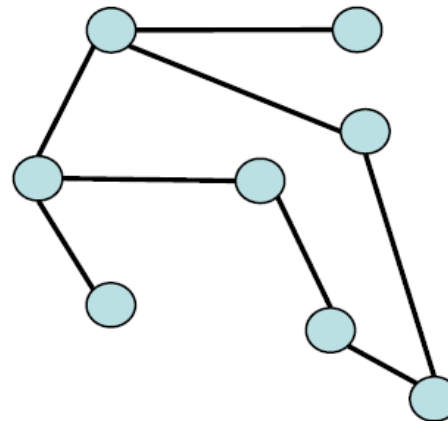
(c) PEPS - 2D



(d) MERA - 1D



(e) WGS



MPS and MERA: G. Vidal
PEPS: F. Verstraete and J.I. Cirac
WGS: M. Plenio and H. Briegel

MPS: Gutzwiller approximation

- Not number conserving ansatz

lattice site

$$|G\rangle = \prod_{\alpha} \left(\sum_n f_n^{(\alpha)} |n\rangle_{\alpha} \right)$$

occupation α

→ Remarks:

- ☒ not number preserving (i.e. the superfluid will have a phase)
- ☒ number preserving version

$$P_N |G\rangle$$

- Variational method

$$\langle G | H | G \rangle \rightarrow \min \quad \text{for} \quad \{f_n^{(\alpha)}\}$$

Time dependent Gutzwiller

- Time-dependent ansatz

$$|G(t)\rangle = \prod_{\alpha} \left(\sum_n f_n^{(\alpha)}(t) |n\rangle_{\alpha} \right)$$

- Variational method

$$\langle G(t) | i\hbar \frac{d}{dt} - H | G(t) \rangle \rightarrow \min \quad \text{for} \quad \{f_n^{(\alpha)}(t)\}$$

- Resulting equations

$$i \frac{d}{dt} f_n^{(\alpha)} = - \left(\sqrt{n} \sum_{\beta} f_{n-1}^{(\alpha)} J_{\alpha,\beta} \langle a_{\beta} \rangle + \text{c.c.} \right) + \frac{U}{2} n(n-1) f_n^{(\alpha)}$$

- Only nearest neighbour hopping $\langle \alpha, \beta \rangle$

$$\Rightarrow J_{\alpha,\beta} = J \text{ for } \langle \alpha, \beta \rangle$$

$$\Rightarrow J_{\alpha,\beta} = 0 \text{ otherwise}$$

$$\langle a_{\beta} \rangle = \sum_n \sqrt{n} f_{n-1}^{(\beta)*} f_n^{(\beta)}$$

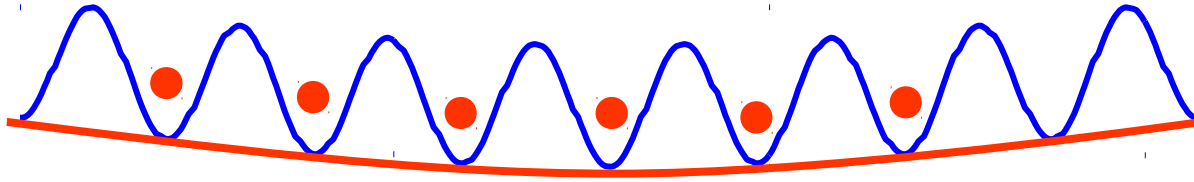
superfluid parameter

Ramping an optical lattice

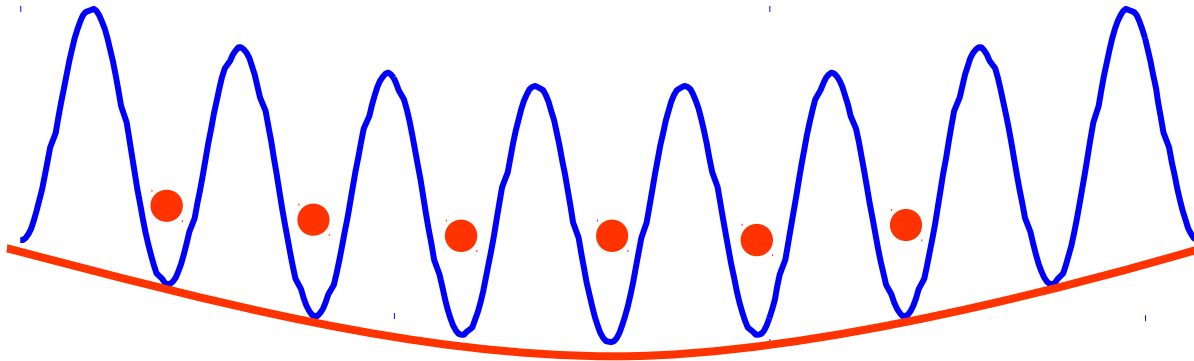
S.R. Clark and D.J, Phys. Rev. A **70**, 043612 (2004)

System

- By changing the laser intensity we go slowly from a shallow lattice $U \geq J$



- to a deep lattice with $U \gg J$

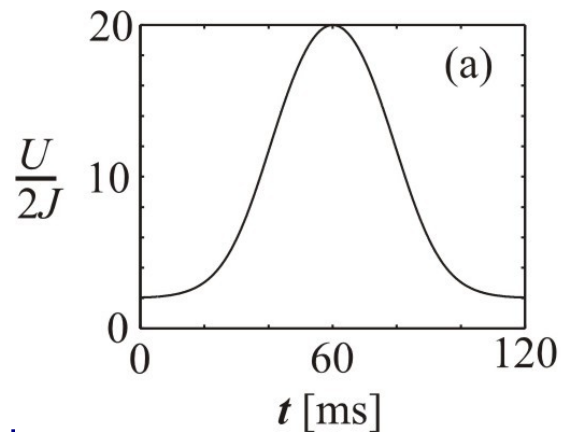


- Time dependent Hamiltonian

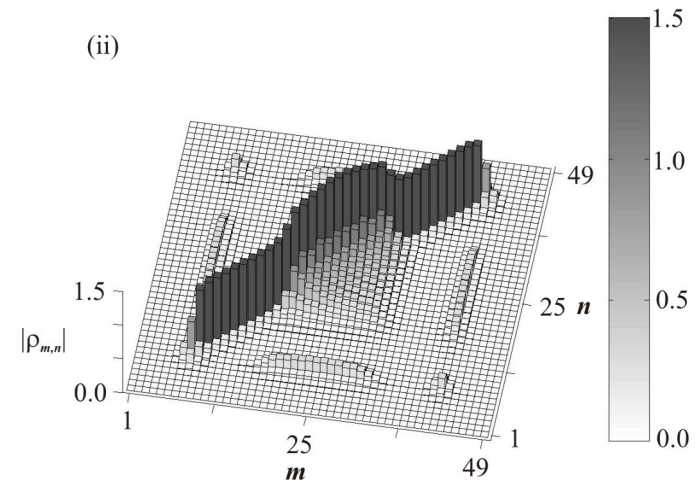
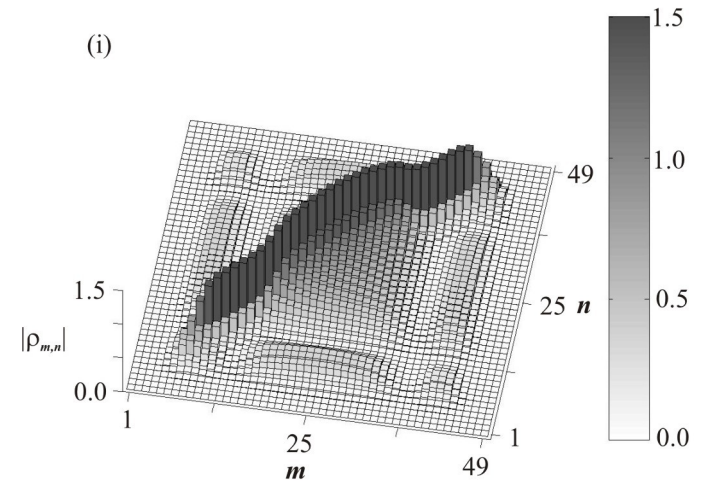
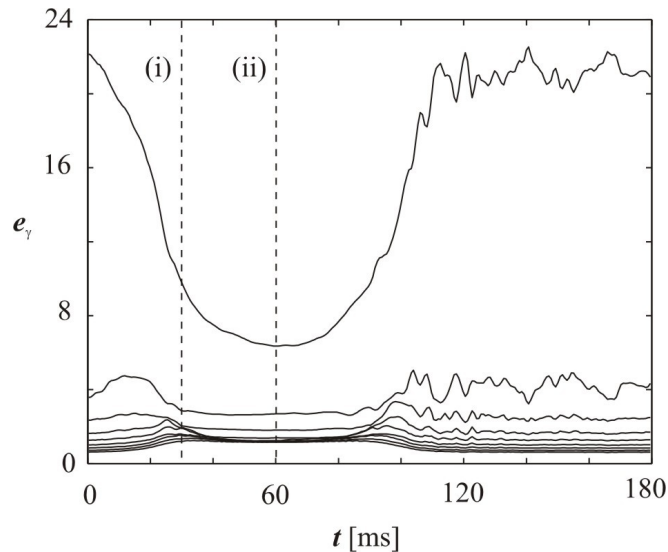
$$H(t) = -J(t) \sum_{\langle \alpha, \beta \rangle} (a_{\alpha}^{\dagger} a_{\beta} + \text{h.c.}) - \sum_{\alpha} \mu_{\alpha} a_{\alpha}^{\dagger} a_{\alpha} + \frac{U(t)}{2} \sum_{\alpha} (\hat{n}_{\alpha} - 1) \hat{n}_{\alpha},$$

Slow dynamics

- We consider “slowly” ramping the lattice for $M = 49$

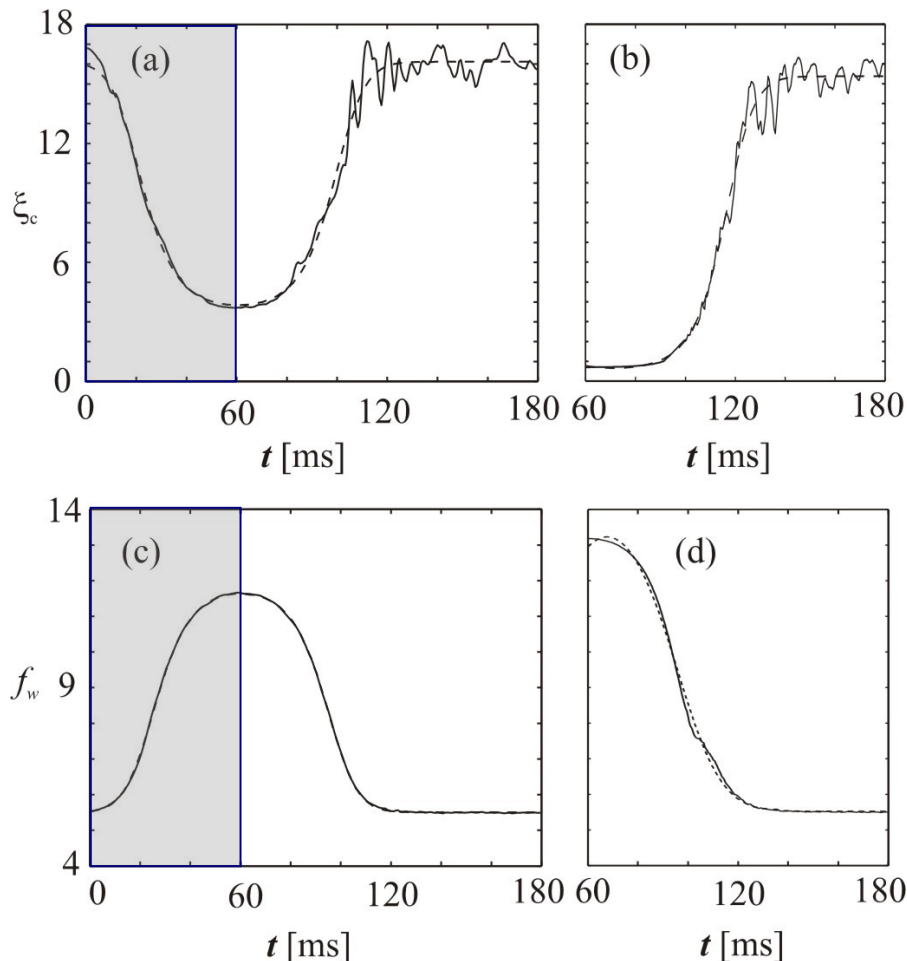


- Eigenvalues of the single particle density matrix



Slow dynamics cont.

- Correlation length cut-off length and momentum distribution width



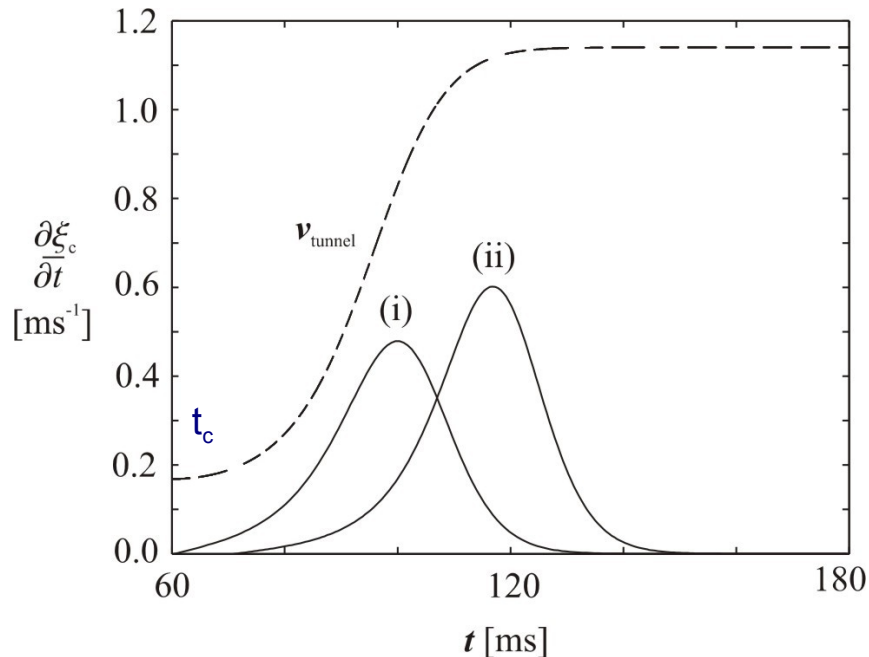
- Define a correlation cut-off length

$$|\rho_{25,25+\xi_c}| = 1/e \approx 0.37$$

- And also consider the momentum distribution width f_w
- Starting from the MI ground state at $t=60$ ms yields similar results.

Slow dynamics cont.

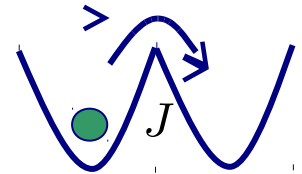
- We also computed the correlation cut-off speed $\frac{\partial \xi_c}{\partial t}$ for $t > t_c$



- (i) = dynamically driven
- (ii) = MI ground-state

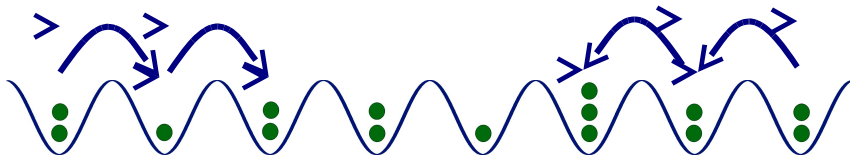
$$\tau_{\text{tunnel}}(t) = \frac{\pi}{2J(t)}$$

$$v_{\text{tunnel}}(t) = \frac{1}{\tau_{\text{tunnel}}(t)}$$



- Note that neither correlation speed exceeds the instantaneous tunnelling speed.

- Consistent with the growth of correlations being caused by a single atom hopping to the centre.



Greiner *et al* Nature (2002)
Batrouni *et al* PRL (2002)

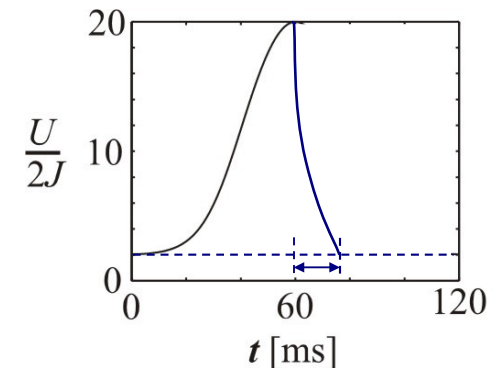
$$t_{\text{restore}} = \frac{M\tau_{\text{tunnel}}}{2} \approx 23 \text{ ms}$$

Fast dynamics

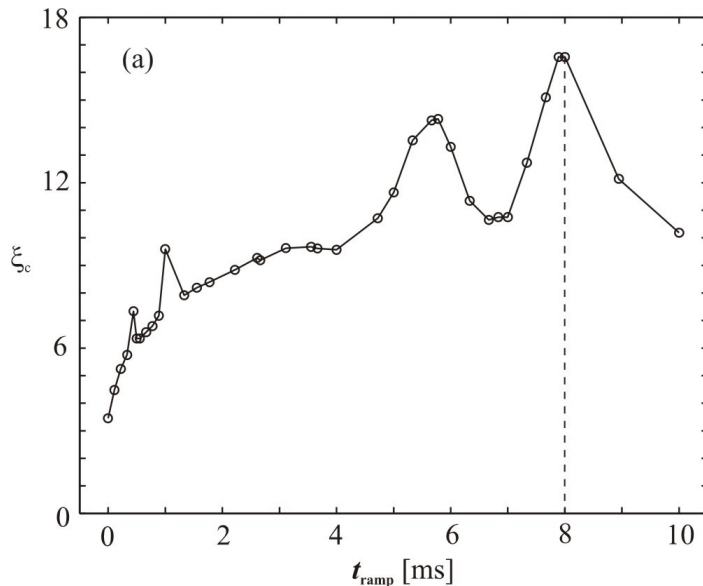
- Replace the latter half with rapid linear decay of the form $t > t_c$

$$V_0(t) = V_{\text{MI}} - \frac{(V_{\text{MI}} - V_{\text{SF}})}{t_{\text{ramp}}}(t - t_c)$$

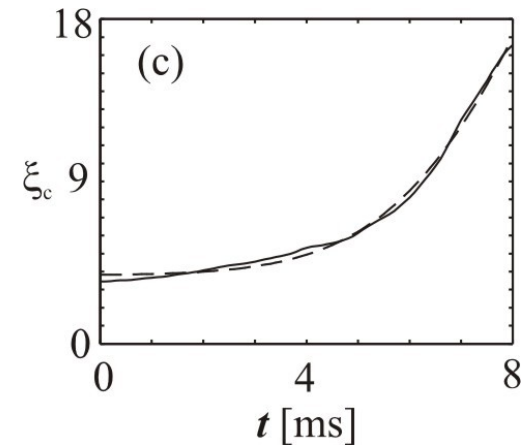
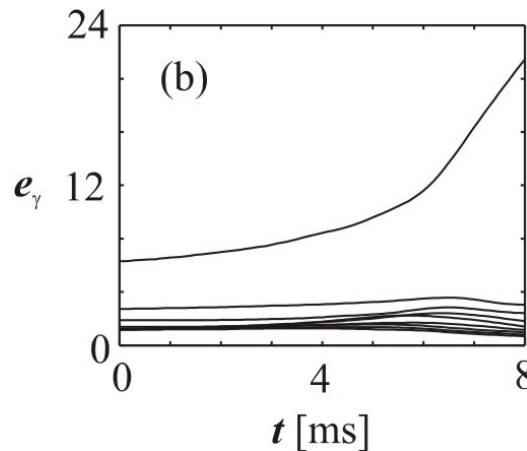
where t_{ramp} is the total ramping time.



- We considered t_{ramp} between 0.1 ms and 10 ms.



- Focussing on $t_{\text{ramp}} = 8$ ms



Fast dynamics cont.

- Here we plot (a) the final momentum distribution width for each rapid ramping.

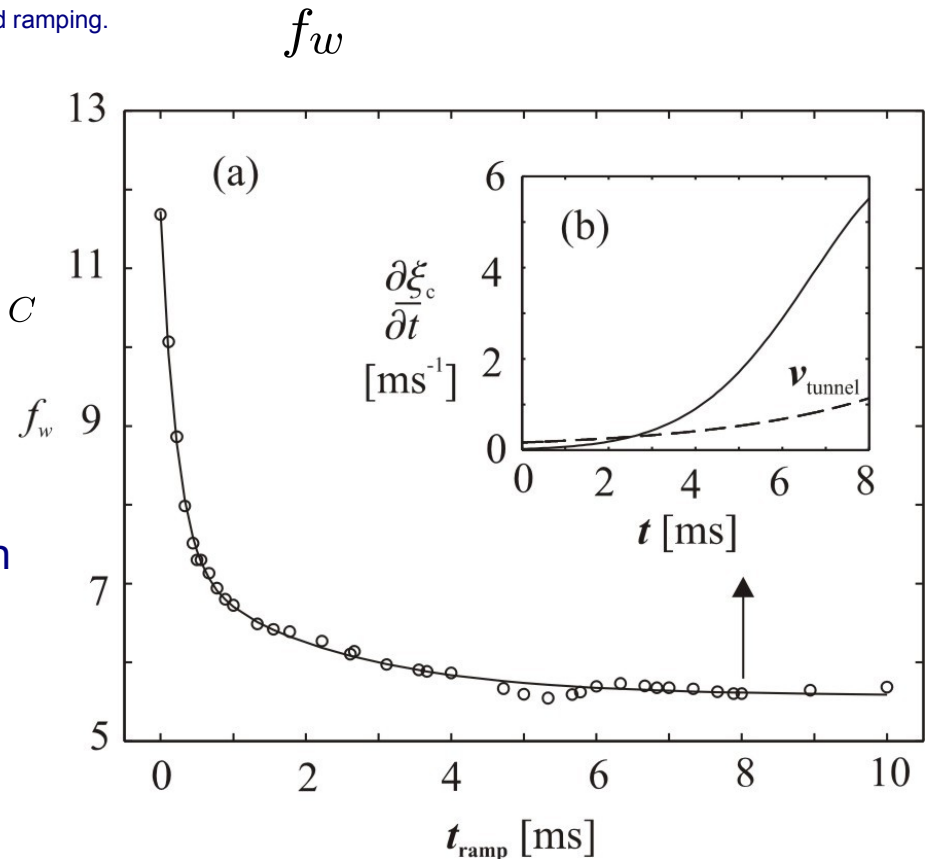
- The fitted curve is a double exponential decay

$$f_w(t_{\text{ramp}}) = A_1 e^{-t_{\text{ramp}}/\tau_1} + A_2 e^{-t_{\text{ramp}}/\tau_2} + C$$

with $\frac{\tau_2}{\tau_1} \approx 10$

- The steady state SF width is acquired in approx. 4 ms.

- For the 8 ms ramping we plot (b) the correlation speed.



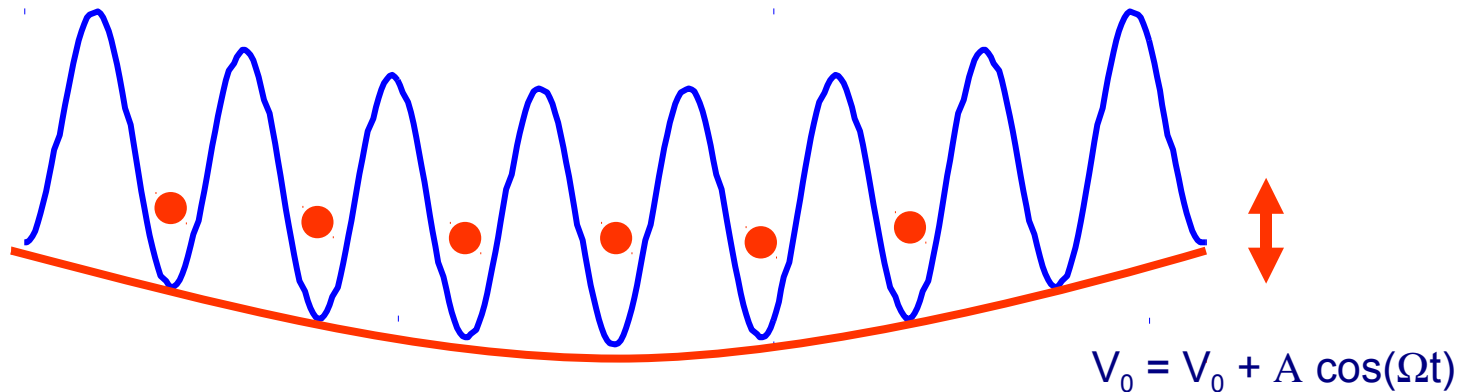
- Rapid restoration explicable with BHM alone, and occurs in 1D.
- Higher order correlation functions are important – **how do they contribute?**

Excitation spectrum of a 1D lattice

S.R. Clark and DJ, New J. Phys. **8**, 160 (2006)

System

- Periodically changing the laser intensity induces periodic changes in U , J .



- Time dependent Hamiltonian

$$H = -(J - \Delta J \cos(\Omega t)) \sum_{\langle \alpha, \beta \rangle} (a_{\alpha}^{\dagger} a_{\beta} + \text{h.c.}) - \sum_{\alpha} \mu_{\alpha} a_{\alpha}^{\dagger} a_{\alpha} + \frac{(U + \Delta U \cos(\Omega t))}{2} \sum_{\alpha} (\hat{n}_{\alpha} - 1) \hat{n}_{\alpha},$$

Probing the excitation spectrum

- The lattice depth is modulated according to

$$V_{OL}(x, t) = V_0[1 + A \sin(\Omega t)] \sin^2(q_B x)$$

where ideally A is small enough to stay in the regime of linear response.

- Linear response probes the hopping part of the Hamiltonian; in first order

$$P_{0 \rightarrow n}^{(1)}(\tau, \Omega) = \left| t_{0 \rightarrow n}^{(1)} \right|^2 = \kappa^2 \left| \langle n | H_J | 0 \rangle I_n^{(1)}(\tau, \Omega) \right|^2$$

$$I_n^{(1)}(\tau, \Omega) = \int_0^\tau dt e^{i\omega_{n0}t} \sin(\Omega t)$$

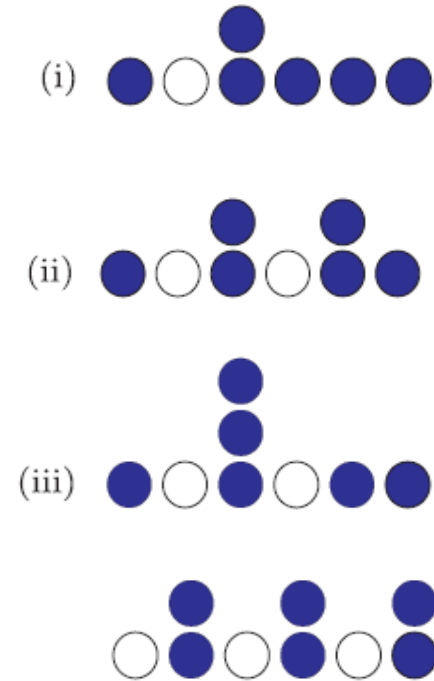
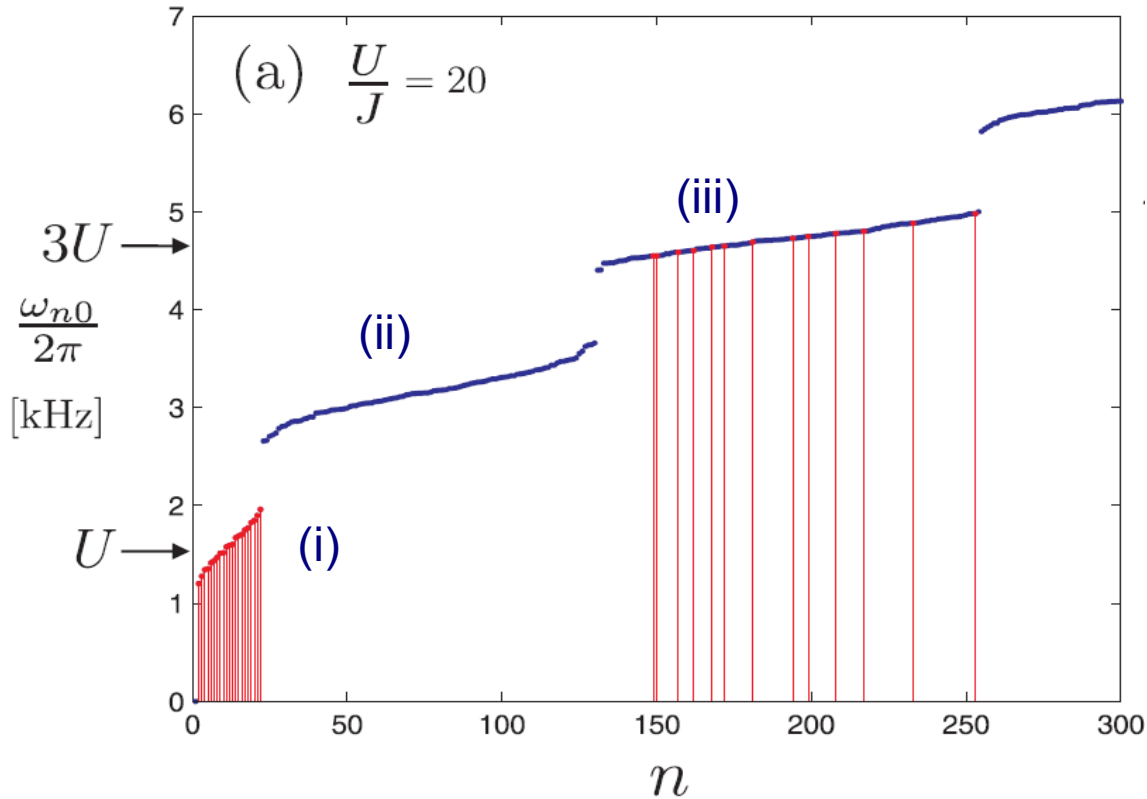
- and in second order quadratic response

$$P_{0 \rightarrow n}^{(2)}(\tau, \Omega) = \left| t_{0 \rightarrow n}^{(1)} - \kappa^2 \sum_m \langle n | H_J | m \rangle \langle m | H_J | 0 \rangle I_{nm}^{(2)}(\tau, \Omega) \right|^2$$

$$I_{nm}^{(2)}(\tau, \Omega) = \int_0^\tau dt \int_0^t dt' e^{i\omega_{nm}t} e^{i\omega_{m0}t'} \sin(\Omega t) \sin(\Omega t')$$

- The total energy absorbed by the system is $E(\tau, \Omega) = \sum_n \epsilon_n P_{0 \rightarrow n}(\tau, \Omega) - \epsilon_0$.
- In the experiment $A \approx 0.2$ and response calculations thus not applicable

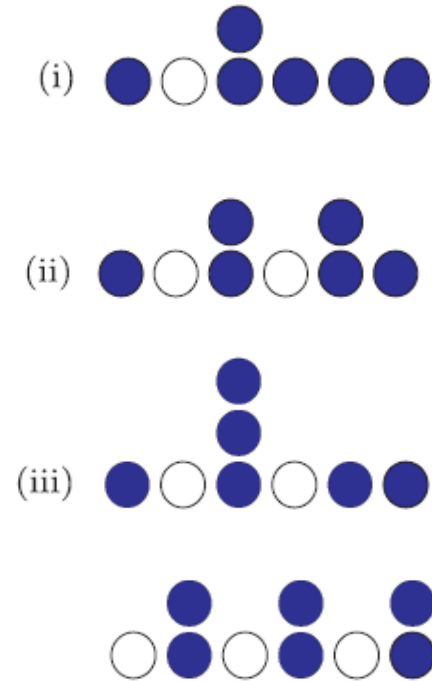
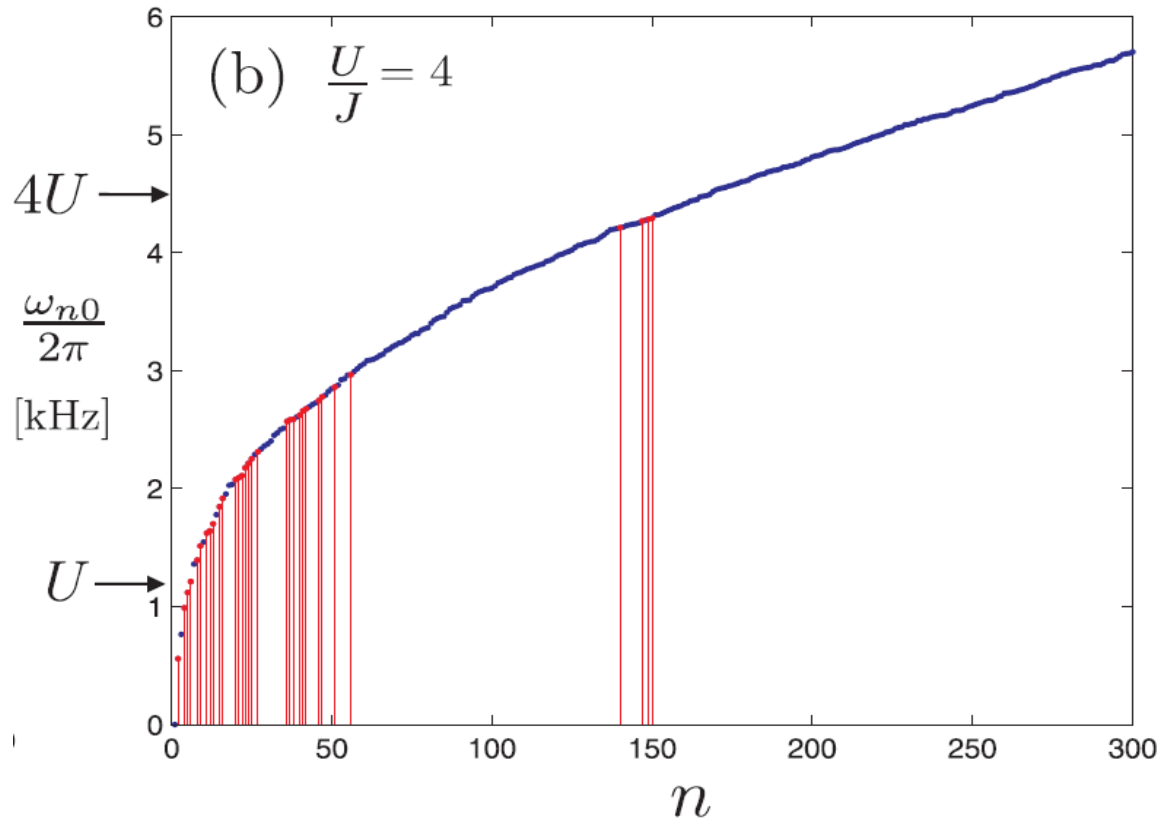
Exact calculation



Spectrum for $U/J=20$ for commensurate filling

Vertical lines denote major matrix elements from ground state

Exact calculation



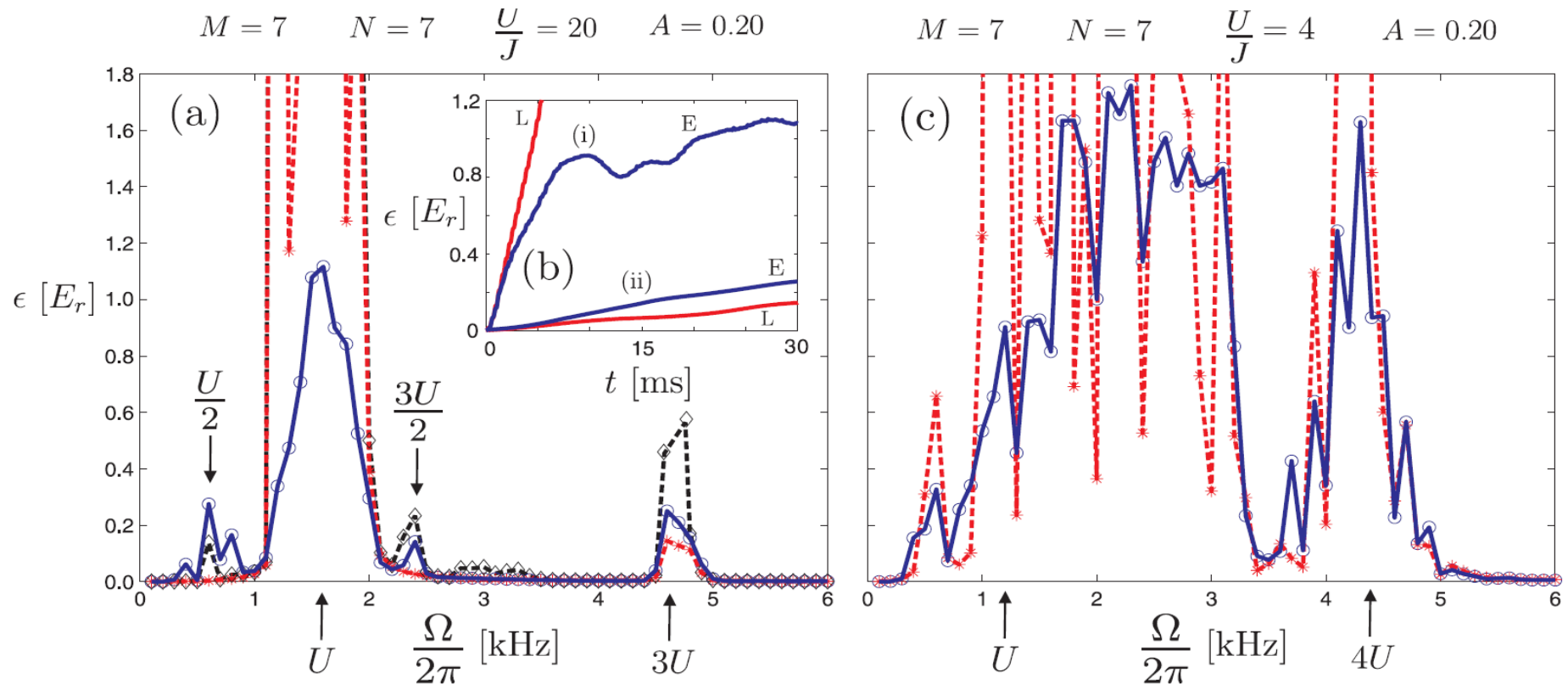
Spectrum for $U/J=4$ for commensurate filling

Vertical lines denote major matrix elements from ground state

How does the energy spectrum change as a function of U/J ?

Validity of linear response

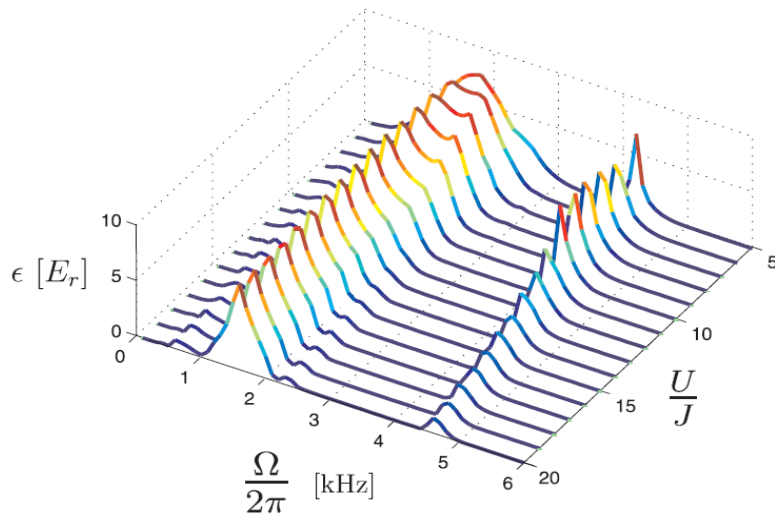
- Small system, comparison to exact calculation



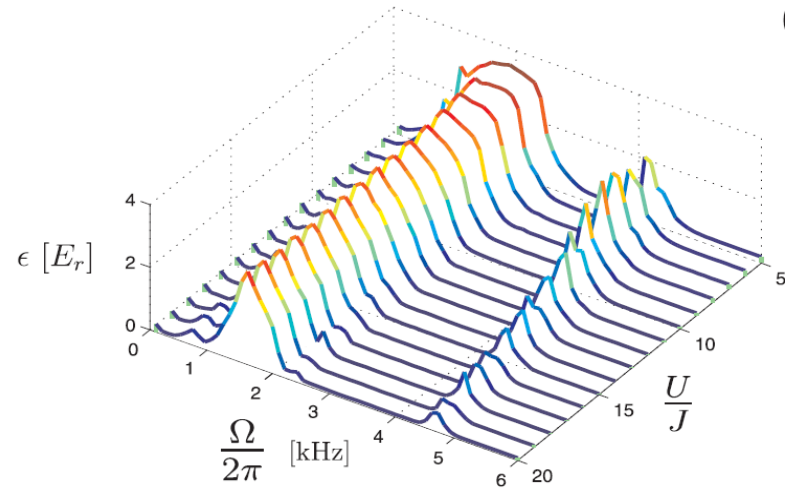
Linear response: red curve
Exact calculation: blue curve

Numerical simulations

- Using the TEBD algorithm to obtain results for larger system of $M=40$ lattice sites and $N=40$ atoms for no trap and $M=25$, $N=15$ with trap



NO trap

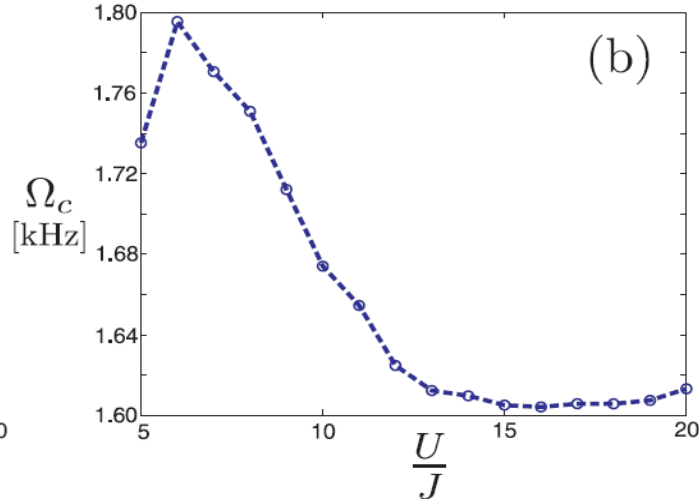
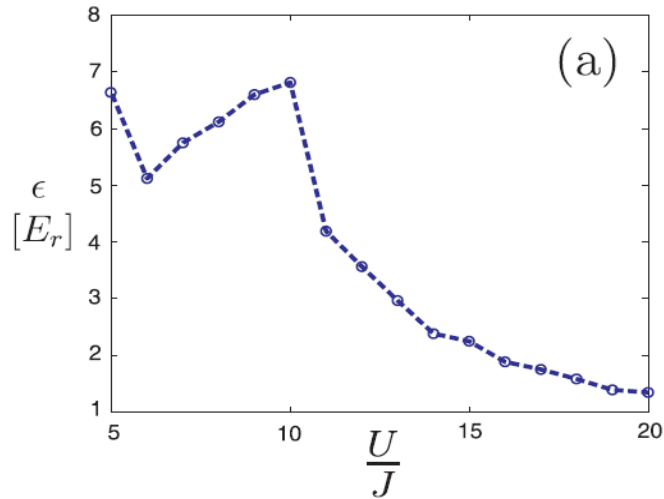


Harmonic trap

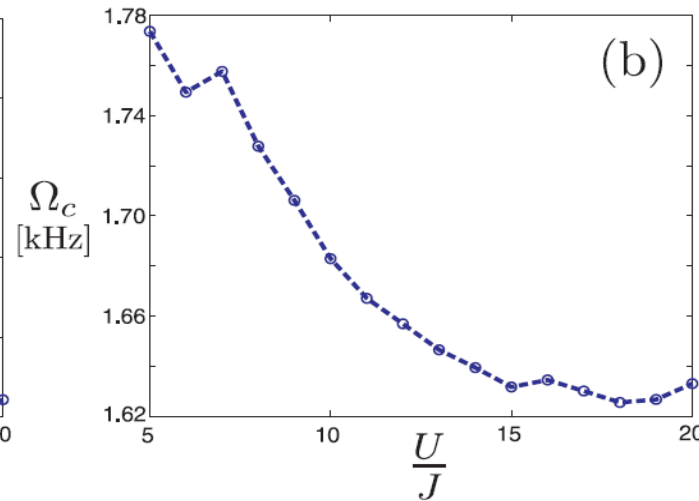
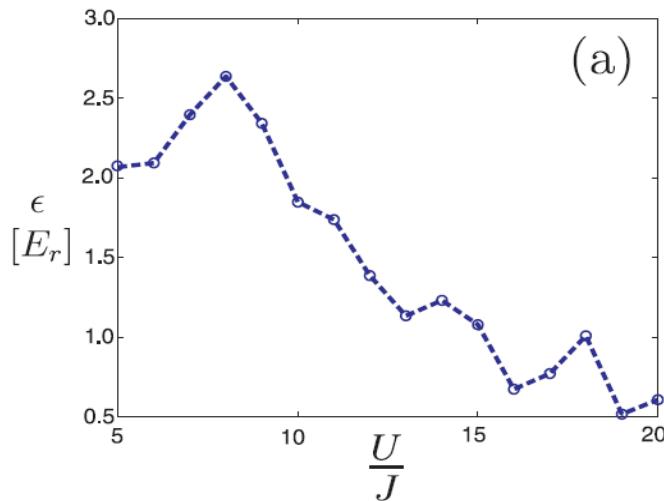
Signatures of SF-MI transition

Energy in $3U \rightarrow 4U$ peak

Centre position of U peak



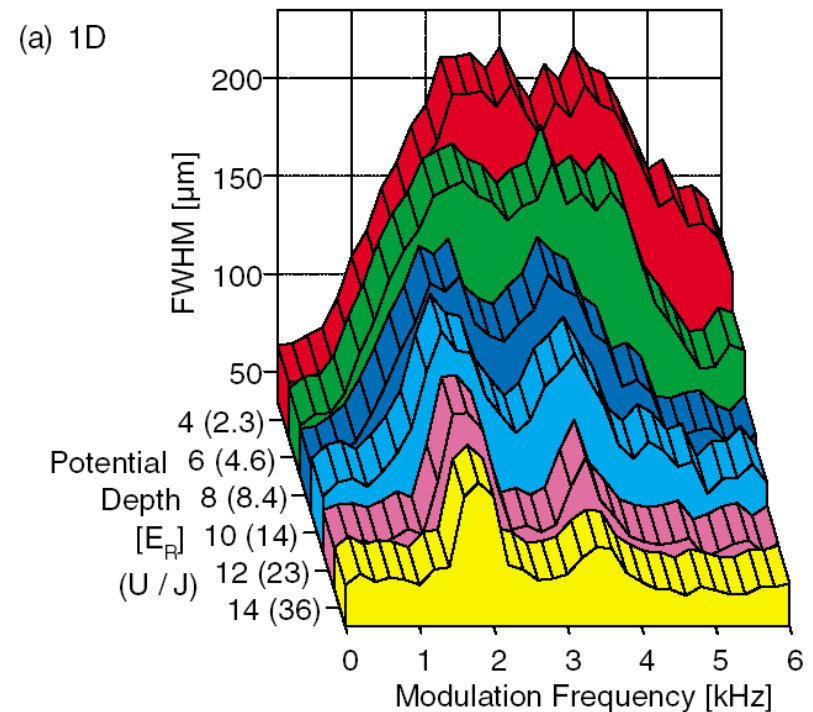
NO trap



Harmonic trap

Comparison with the experiment

- We obtain very good agreement with the experimental data
 - ➡ broad spectrum in the superfluid region
 - ➡ split up into several peaks when going to the MI regime
 - ➡ Shift of the MI peaks from U by approximately 10%
- Differences compared to the experiment
 - ➡ Different relative heights of the peaks
 - ➡ Transition between SF and MI region at a different value of U/J
- Signatures in peak height not visible in the experiment



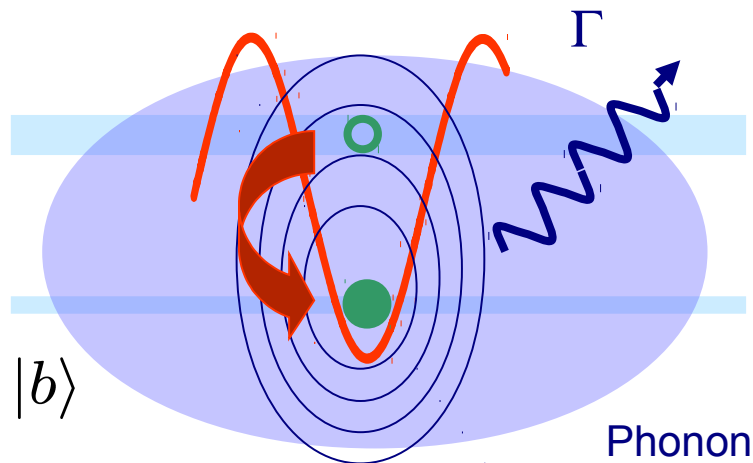
exp. Stoferle et al PRL (2004)

Loading and Cooling

A. Griessner *et al.*, Phys. Rev. A **72**, 032332 (2005).
A. Griessner *et al.*, Phys. Rev. Lett. **97**, 220403 (2006).

Emission of a particle into background

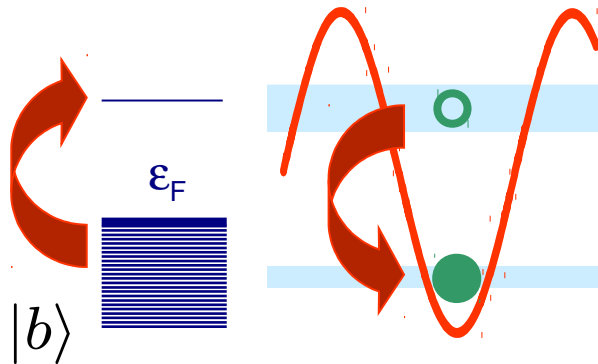
- Interband transitions by spontaneous emission of a phonon (particle like)



$$\hat{H}_{\text{int}} = \sum_{\alpha, \alpha'} \sum_{\mathbf{k}, \mathbf{q}} \left(G_{\alpha, \alpha'}^{\mathbf{k}} \hat{b}_{\mathbf{k}} (\hat{A}_{\mathbf{q}}^{\alpha})^{\dagger} \hat{A}_{\mathbf{q}-\mathbf{k}}^{\alpha'} + \text{h.c.} \right)$$

$$G_{\alpha, \alpha'}^{\mathbf{k}} \approx g_{ab} (S(\mathbf{k}) \rho_b / V)^{1/2} \int d^3x e^{i\mathbf{k}\mathbf{x}} w^{\alpha}(\mathbf{x}) w^{\alpha'}(\mathbf{x})$$

- Interband transition by exciting a Fermi gas atom

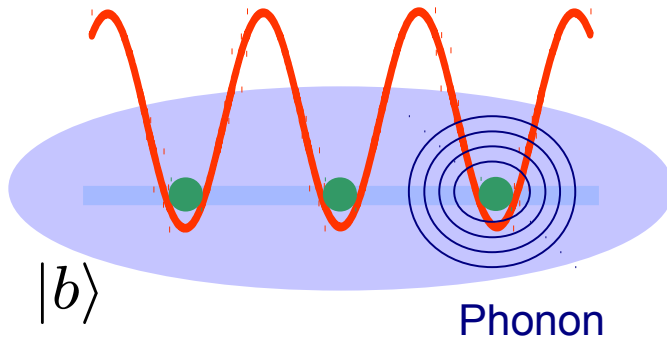


$$H_{\text{int}} = \sum_{\substack{\mathbf{k}, \mathbf{k}' \\ \alpha, \mathbf{n}, \mathbf{n}'}} g_{\alpha, \mathbf{n}, \mathbf{n}'}^{\mathbf{k}, \mathbf{k}'} b_{\mathbf{k}}^{\dagger} b_{\mathbf{k}'} a_{\alpha, \mathbf{n}}^{\dagger} a_{\alpha, \mathbf{n}'}$$

$$g_{\alpha, \mathbf{n}, \mathbf{n}'}^{\mathbf{k}, \mathbf{k}'} = \frac{g}{V} e^{i\mathbf{x}_{\alpha}(\mathbf{k}' - \mathbf{k})} \int d^3x e^{i\mathbf{x}(\mathbf{k}' - \mathbf{k})} w_{\mathbf{n}}(\mathbf{x}) w_{\mathbf{n}'}(\mathbf{x})$$

Intraband interactions

- BEC background gas at finite temperature



$$\hat{H}_I = \sum_j \sum_{\mathbf{q} \neq 0} \hat{n}_j \hbar \omega_{\mathbf{q}} (M_{j,\mathbf{q}} \hat{b}_{\mathbf{q}} + M_{j,\mathbf{q}}^* \hat{b}_{\mathbf{q}}^\dagger)$$

$$M_{j,\mathbf{q}} = \kappa \int d\mathbf{r} \sqrt{n_0(\mathbf{r})} |w_j(\mathbf{r})|^2 [u_{\mathbf{q}}(\mathbf{r}) - v_{\mathbf{q}}(\mathbf{r})] / \hbar \omega_{\mathbf{q}}$$

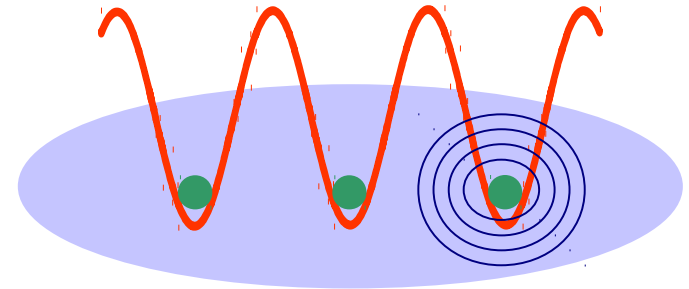
- The BEC is deformed by the presence of the lattice atoms
 - ⇒ Deformation energy E_p
 - ⇒ The deformation affects nearby lattice sites; attractive potential V_{ij}
- Only elastic collisions are energetically allowed
 - ⇒ These cause dephasing of the lattice wave function
 - ⇒ They also lead to thermally induced incoherent hopping

Irreversible loading and cooling schemes?

- Can we combine irreversible processes with repulsive and/or Fermi blocking for irreversible loading schemes?

→ Spontaneous emission of photons

- ❑ Large momentum kick → heating
- ❑ Large energies → no selectivity
- ❑ Reabsorption → heating



Phonon

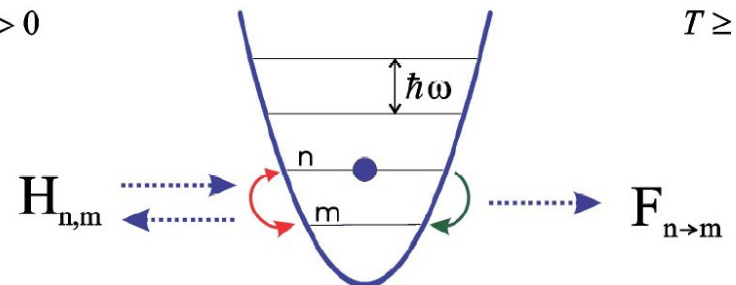
~~N~~
PHOTONS

→ Spontaneous emission of phonons

- ❑ Loading of atoms into lattices
- ❑ Cooling within the lowest Bloch band
- ❑ Destroy spatial correlations
- ❑ Mediate interactions between sites

$T > 0$

$T \geq 0$



A.J. Daley, *et al.* Phys. Rev. A **69**, 022306 (2004).

Current loading methods

- Adiabatic loading in one sweep with almost no disorder

⇒ Arrange atoms by repulsion between bosons

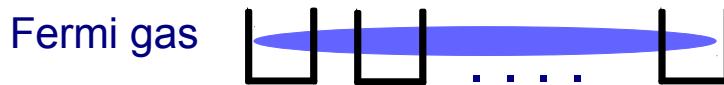


D. J., C. Bruder, J. I. Cirac, C. W. Gardiner, and P. Zoller, Phys. Rev. Lett. **81**, 3108 (1998).



M. Greiner, O. Mandel, T. Esslinger, T.W. Hänsch, and I. Bloch, Nature **415**, 39 (2002).

⇒ Arrange atoms by Fermi blocking

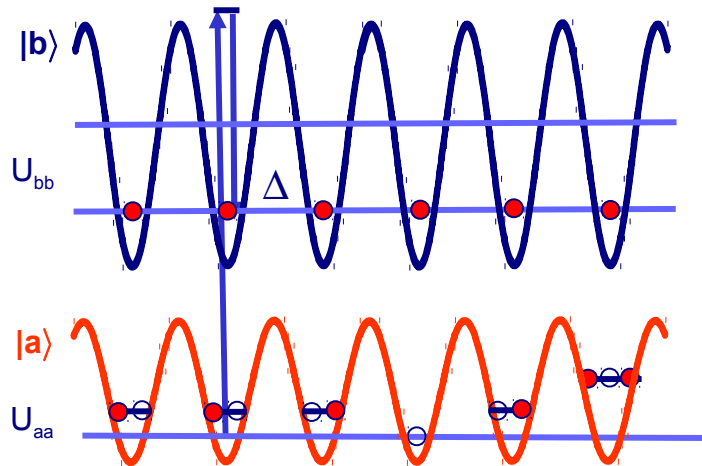


L. Viverit, C. Menotti, T. Calarco, A. Smerzi, Phys. Rev. Lett. **93**, 110401 (2004)



Possible Improvements

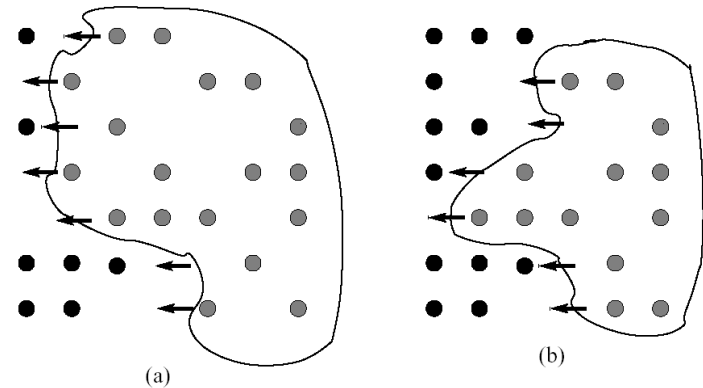
● Defect suppressed lattices



irregular $\rightarrow$ regular filling, i.e., mixed state $\rightarrow$ pure state $\rightarrow$ cooling

P. Rabl, A. J. Daley, P. O. Fedichev, J. I. Cirac, and P. Zoller, Phys. Rev. Lett. **91**, 110403 (2003).

● Measurement based schemes



Selective shift operations to close gaps

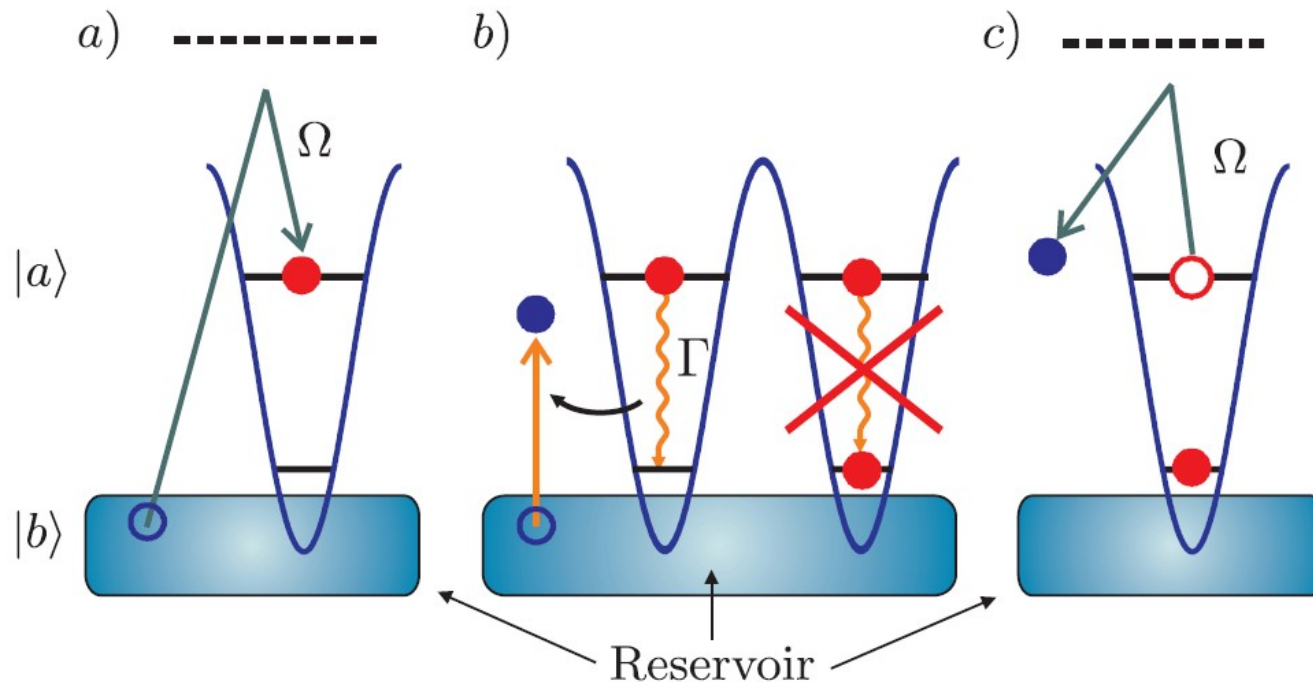
J. Vala, A.V. Thapliyal, S. Myrgren, U. Vazirani, D.S. Weiss, K.B. Whaley, Phys. Rev. A **71**, 032324 (2005).

Selective measurements of double occupancies

G.K. Brennen, G. Pupillo, A.M. Rey, C.W. Clark, C.J. Williams, Journal of Physics B **38**, 1687 (2005).

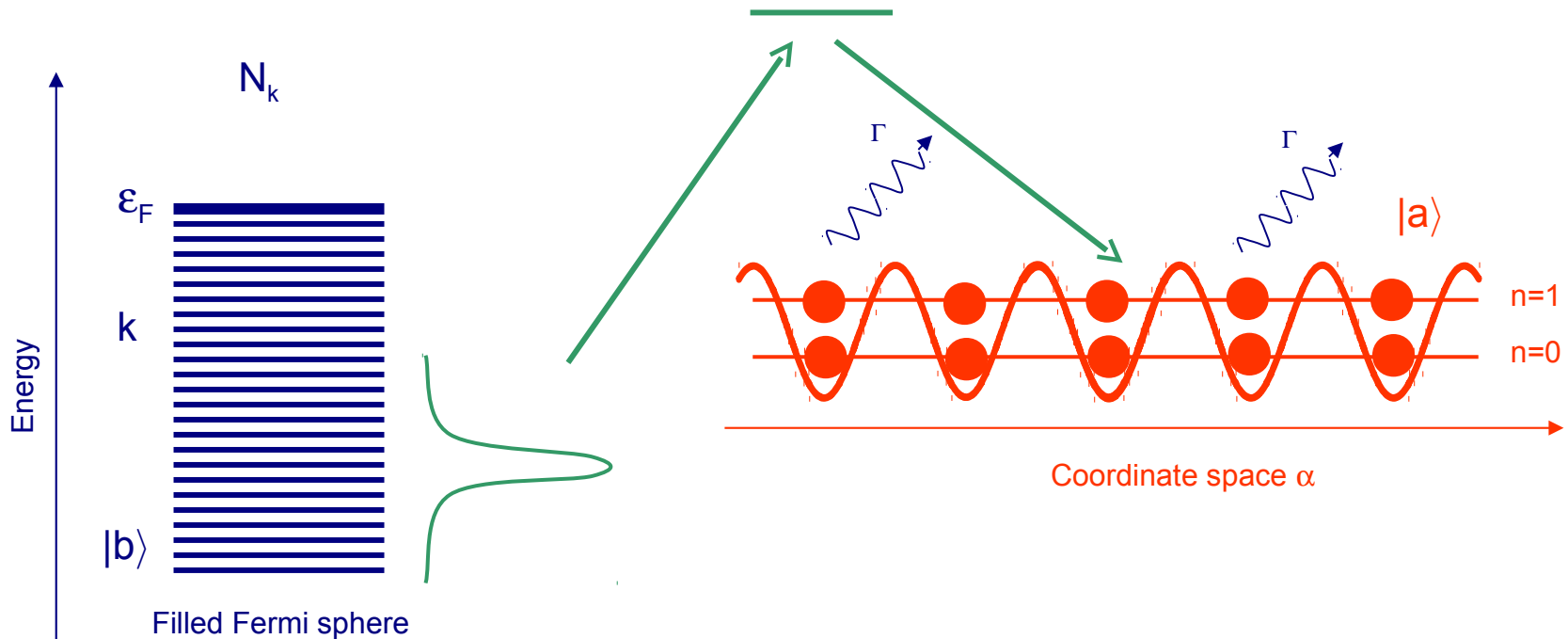
Initialization of a fermionic register

- We consider an optical lattice immersed in an ultracold Fermi gas



- ➡ a) Load atoms into the first band
- ➡ b) incoherently emit phonons into the reservoir
- ➡ c) remove remaining first band atoms

Linear sweep to load the whole lattice



Not drawn to scale

- We change the laser detuning dynamically
 - Sweep through the Fermi sea to load the first band
 - Spontaneously emit phonons
 - Empty remaining atoms by tuning above the Fermi sea

Loading regimes

- Fast loading regime: Motion of atoms in background gas is frozen
 ⇒ Simple Rabi oscillations

$$\langle a_{\alpha,\mathbf{n}}^\dagger a_{\beta,\mathbf{m}}(t) \rangle = \delta_{\alpha,\beta} \delta_{\mathbf{n},\mathbf{m}} \sin^2 \frac{\Omega}{2} t$$

- Slow loading regime: Background atoms move significantly during loading
 ⇒ Coherent loading

$$\dot{a}_{\alpha,1} = -i \frac{\Omega}{2} \sum_{\mathbf{q}} R_{\mathbf{q},1}^* e^{i\mathbf{k}\mathbf{x}_\alpha} b_{\mathbf{q}} - i\epsilon a_{\alpha,1},$$

$$\dot{b}_{\mathbf{k}} = -i \frac{\Omega}{2} \sum_{\mu,n} R_{\mathbf{k},n} e^{-i\mathbf{k}\mathbf{x}_\mu} a_{\mu,n} - i\epsilon_{\mathbf{k}} b_{\mathbf{k}},$$

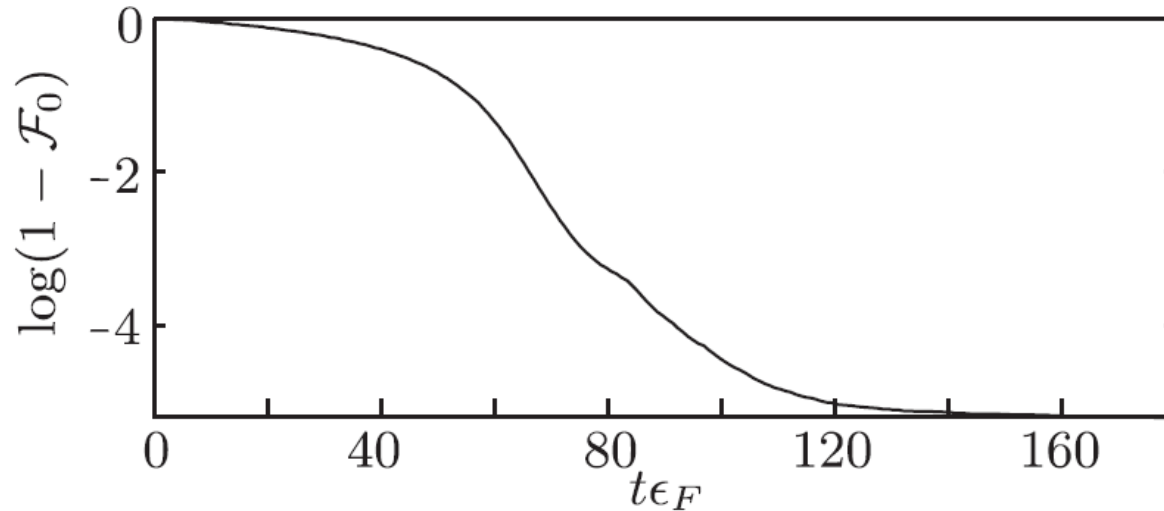
$$\dot{a}_{\alpha,0} = -i \frac{\Omega}{2} \sum_{\mathbf{q}} R_{\mathbf{q},0}^* e^{i\mathbf{k}\mathbf{x}_\mu} b_{\mathbf{q}} + i(\omega - \epsilon) a_{\alpha,0}$$

⇒ Dissipative transfer

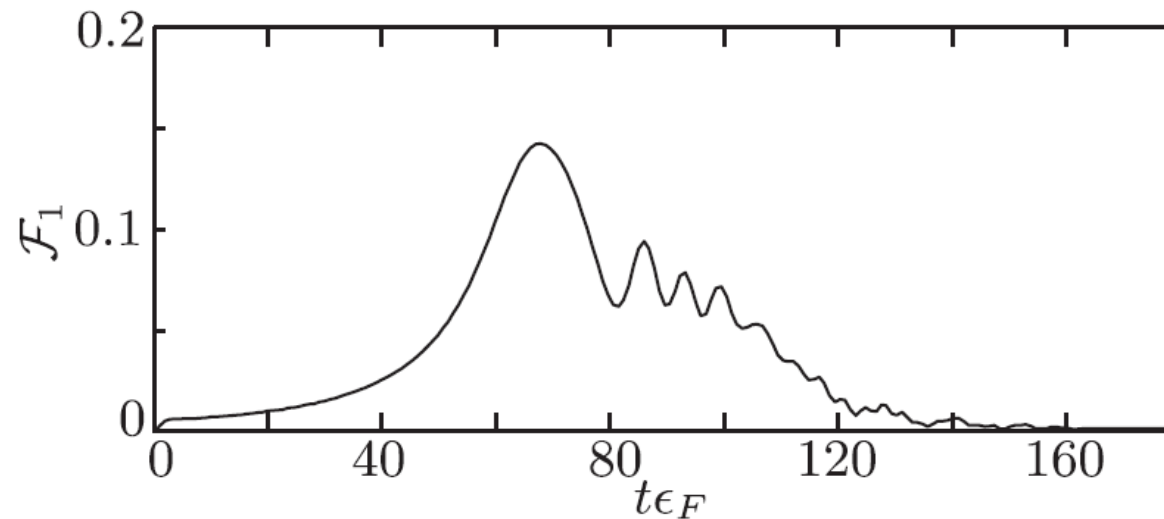
$$\dot{\rho} = \sum_{\alpha,\beta,\mathbf{n}} \frac{\Gamma_{\alpha,\beta,\mathbf{n}}}{2} \left(2A_{\alpha,\mathbf{n}} \rho A_{\beta,\mathbf{n}}^\dagger - A_{\alpha,\mathbf{n}}^\dagger A_{\beta,\mathbf{n}} \rho - \rho A_{\alpha,\mathbf{n}}^\dagger A_{\beta,\mathbf{n}} \right)$$

$$A_{\alpha,\mathbf{n}} = a_{\alpha,0}^\dagger a_{\alpha,\mathbf{n}}$$

Result



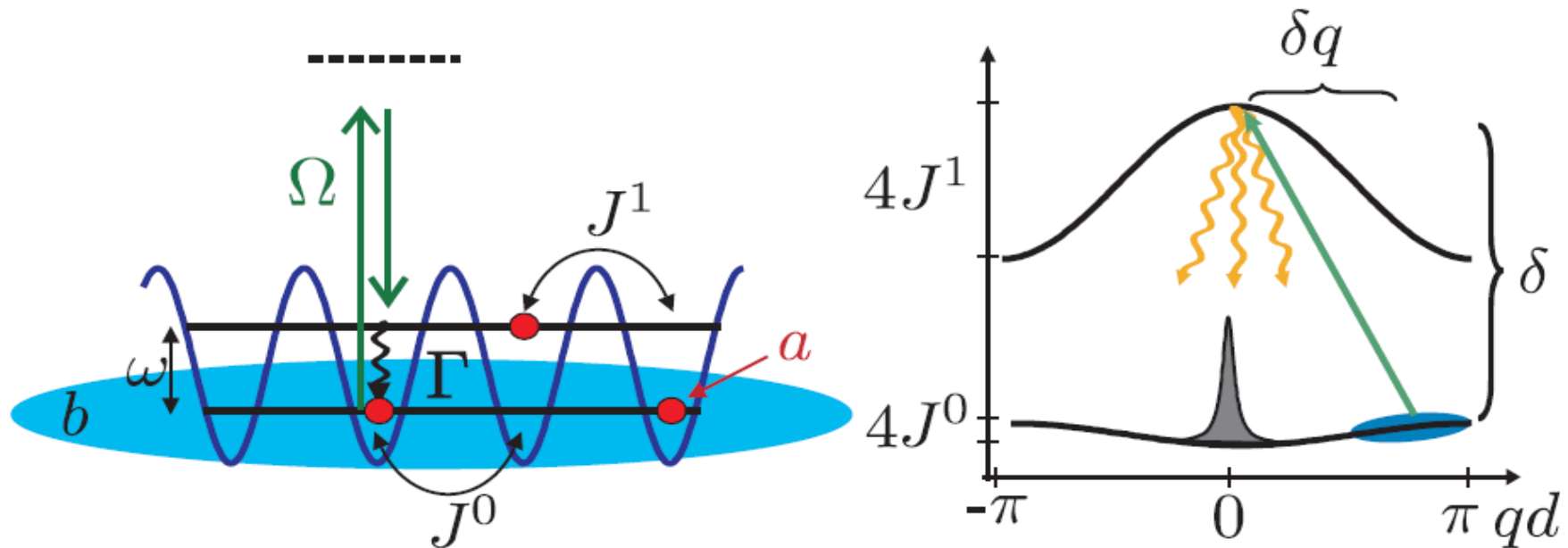
- $\mathcal{F}_0$ is the filling in the lower Bloch band



- $\mathcal{F}_1$ is the filling in the first excited Bloch band

$$N = 101, M = 5, \Omega/2 = 0.45\epsilon_F, n_{1D}\lambda/2 = 1.4, \omega = 10\epsilon_F \text{ and } \Gamma = 0.1\epsilon_F$$

Cooling by superfluid immersion

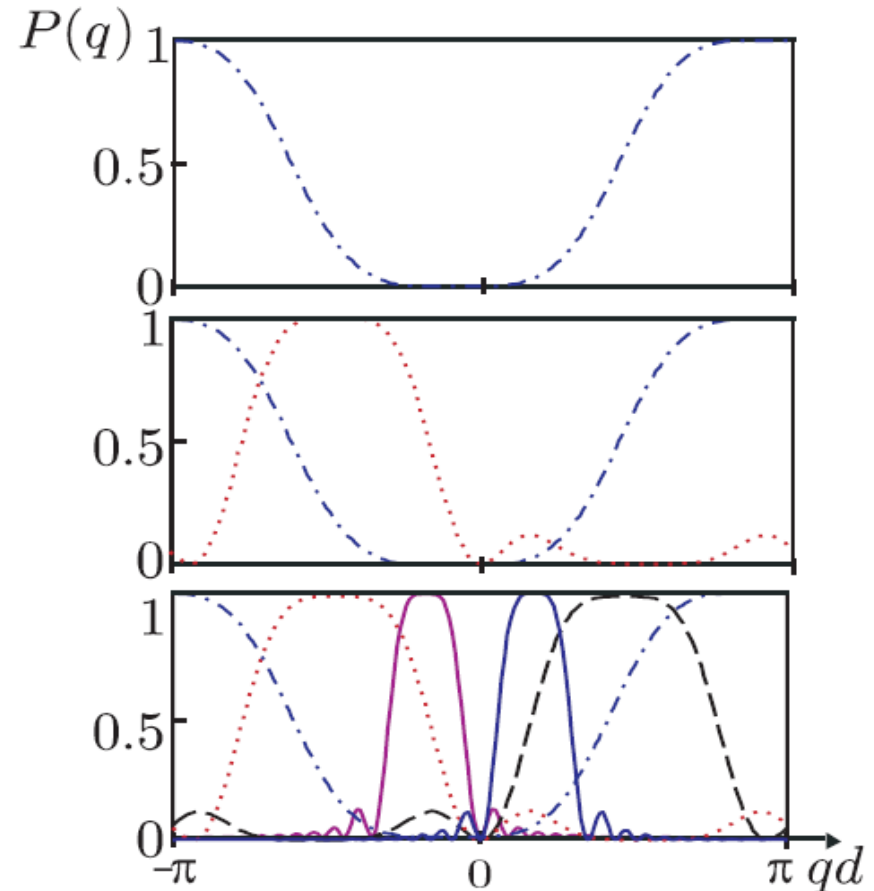


- Lattice immersed in a BEC
- Atoms with higher quasi-momentum q are excited
- They decay via the emission of a phonon into the BEC
- They are collected in a dark state in the region $q \approx 0$
- Analysis using an iterative map in terms of Levy statistics

$$\mathcal{M}_j : \hat{\rho}_j \rightarrow \hat{\rho}_{j+1} \equiv \left(\hat{\mathcal{D}} \circ \hat{E}_j \right) \hat{\rho}_j$$

Excitation steps E_j

- In analogy to Raman cooling schemes we choose square pulses with Rabi frequency Ω_j and duration $\tau_j = \pi / \Omega_j$. This leads to an excitation probability $P(q)$ shown right.
- With increasing pulse duration the region of excitation is narrowed down.
- All momenta q except those with $q \approx 0$ are excited.
- By using Blackman pulses a more box like (inverted Fermi profile) of excitation probabilities can be obtained.



$$\delta q = (0.16, -1.75, 1.75, -2.63, 2.63)/d$$

$$\Omega = (27.9, 13.7, 13.7, 2.37, 2.37)J^0$$

$$(\delta - \omega) = -(28.4, 25.8, 25.8, 24.7, 24.7)J^0$$

Dissipative steps D

- Decay according to master equation with Liouvillian (in the momentum basis)

$$\mathcal{L}[\rho] = \sum_k \Gamma_k \left(2c_k \rho c_k^\dagger - c_k^\dagger c_k \rho - \rho c_k^\dagger c_k \right) / 2$$

$$c_k = \sum_q A_{q-k,0}^\dagger A_{q,1}$$

This approach is valid for a single particle only as it neglects quantum statistics

- For many particles: Quantum Boltzmann master equation (QBME)

- ⇒ Define occupation vectors $\mathbf{m} = [\{\mathbf{m}_q^0\}_q, \{\mathbf{m}_q^1\}_q]$
- ⇒ Project the density operator onto its diagonal elements

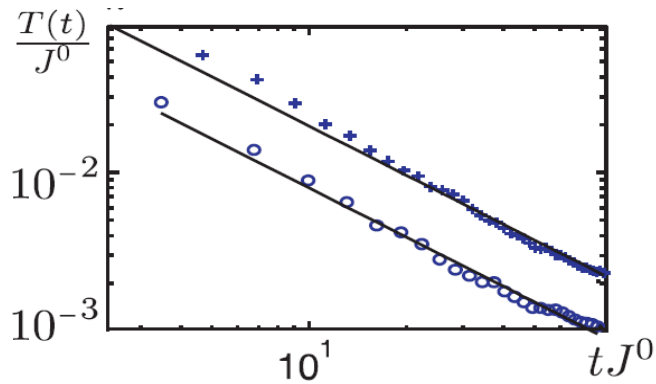
$$\mathcal{P} \hat{\rho} \mathcal{P} = \sum_{\mathbf{m}} w_{\mathbf{m}} |\mathbf{m}\rangle \langle \mathbf{m}|$$

- ⇒ We obtain the QBME as the evolution equation for the $w_{\mathbf{m}}$

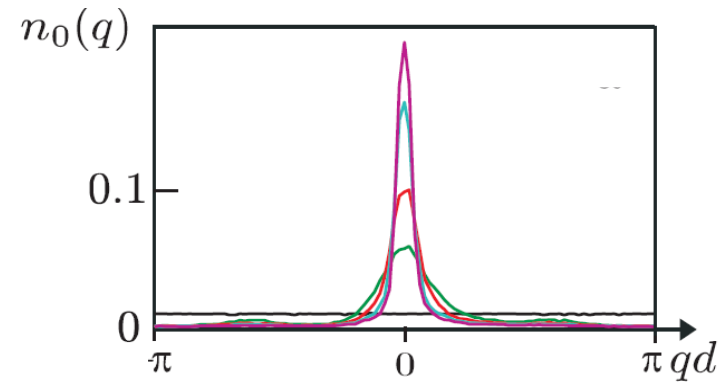
$$\dot{w}_{\mathbf{m}} = \sum_{k,q} \Gamma_k \left[m_{q-k}^0 (1 \pm m_q^1) w_{\mathbf{m}'} - m_q^1 (1 \pm m_{q-k}^0) w_{\mathbf{m}} \right]$$

$$\mathbf{m}' = \mathbf{m} - \mathbf{e}_{q-k,q}$$

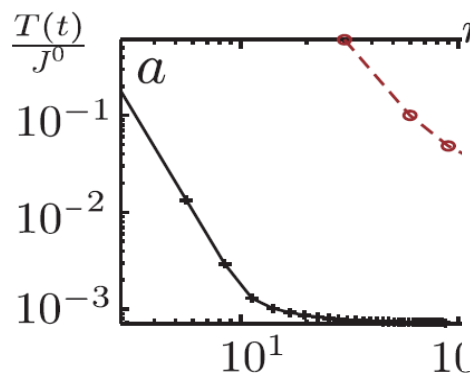
Results



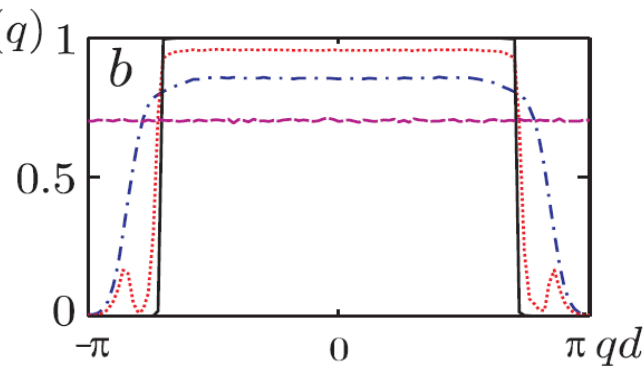
Single particle, comparison with Levy statistics result



Single particle momentum distribution during cooling



Bosons (black) and Fermions (red) cooling



Fermion momentum distribution during cooling

$J_0 \approx 100\text{Hz}$ and this corresponds to $T \approx 5\text{nK} \rightarrow$ we can reach the few pK regime

Immersed optical lattices

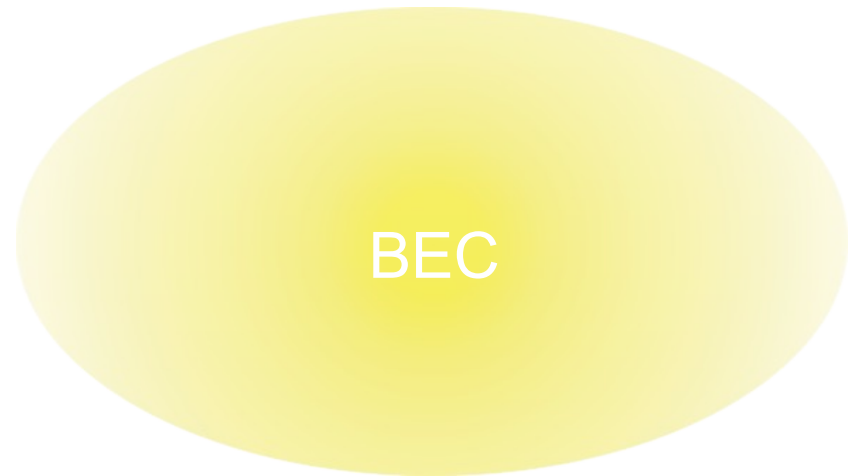
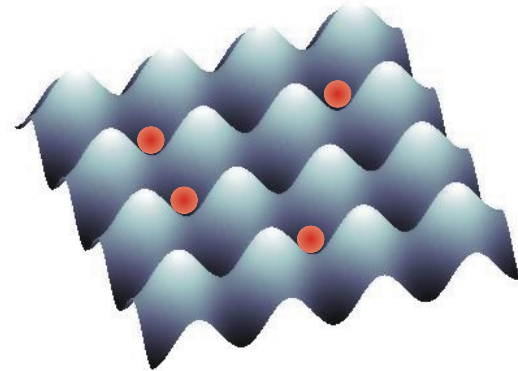
Lattice immersed in a BEC

- A BEC with interaction strength g exhibits phonons, which are well understood.
- Coupling κ between BEC phonons and lattice atoms is controllable by Feshbach resonances.

⇒ Introduce phonons into an optical lattice

- Study their influence on the dynamics of lattice atoms
- Phonon properties can be manipulated by the trapping of the BEC.

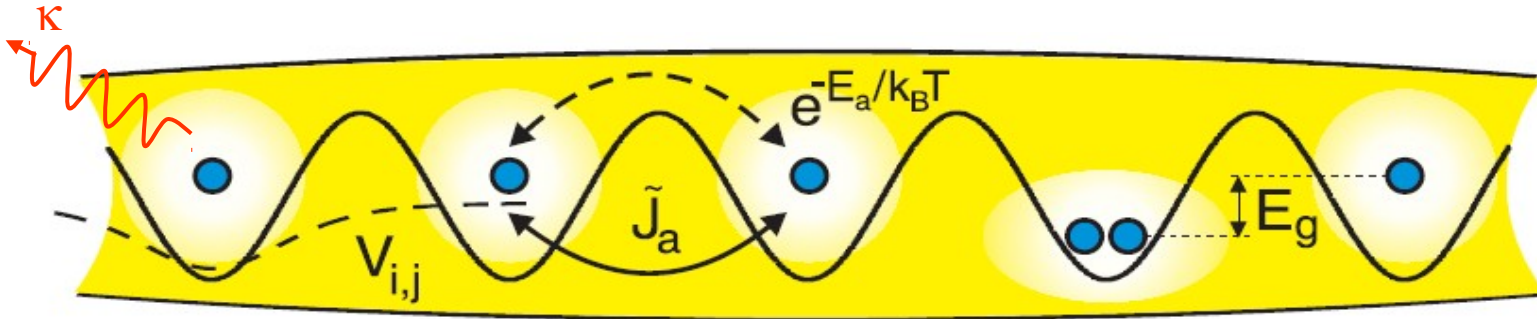
⇒ Simulate dynamics of condensed matter systems



Theory work on immersed atoms

- A single atomic impurity in a BEC
 - ⇒ Atomic quantum dot, A. Recati et al., PRL **94**, 040404 (2005)
 - ⇒ Dephasing of a single atom, M. Bruderer et al., New J. Phys. **8**, 87 (2006)
- Two atomic impurities immersed in a BEC
 - ⇒ Impurity – Impurity interactions, A. Klein et al., PRA **71**, 033605 (2005)
- Quantum state engineering by superfluid immersion
 - ⇒ Lattice loading, A. Griessner et al., Phys. Rev. A **72**, 032332 (2005).
 - ⇒ Raman cooling, A. Griessner et al., Phys. Rev. Lett. **97**, 220403 (2006)
 - ⇒ Open system engineering, A. Micheli et al., in progress
- Lattice dynamics in BEC immersion
 - ⇒ Polaron physics, M. Bruderer et al., Phys. Rev. A **76**, 011605(R) (2007)
 - ⇒ Dephasing and cluster formation, A. Klein et al., New J. Phys. **9**, 411 (2007)
 - ⇒ Transport, M. Bruderer, New J. Phys. **10**, 033015 (2008)
 - ⇒ Self trapping, M. Bruderer et al., EuroPhys. Lett. **82**, 30004 (2008)

Coherent atom hopping

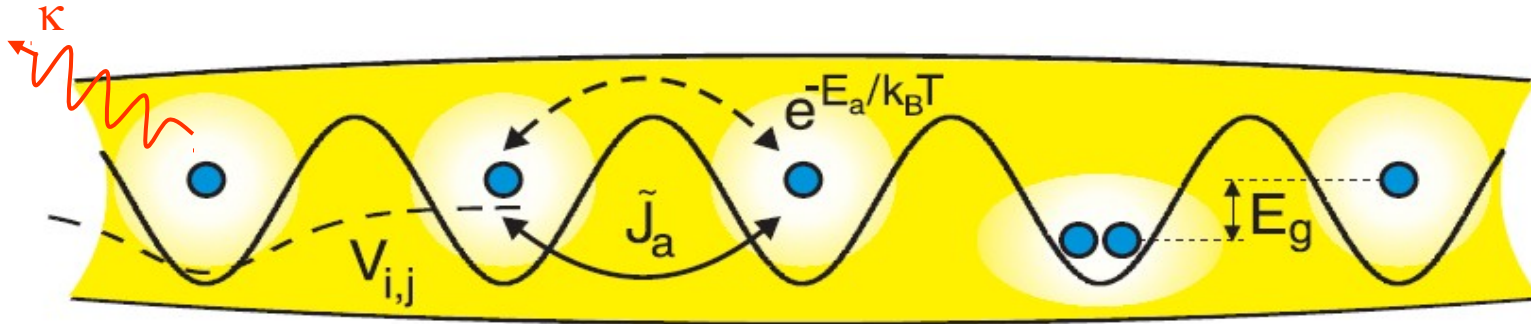


- When hopping from one site to the next the deformation needs to be dragged along
 - ➡ Reduction of coherent hopping rate
 - ☒ Exponential decrease with BEC temperature T
 - ☒ Exponential decrease with coupling κ
 - ☒ Details depend on the phonon dispersion relation

$$\tilde{J}_a \approx J e^{-C\kappa^2 T}$$

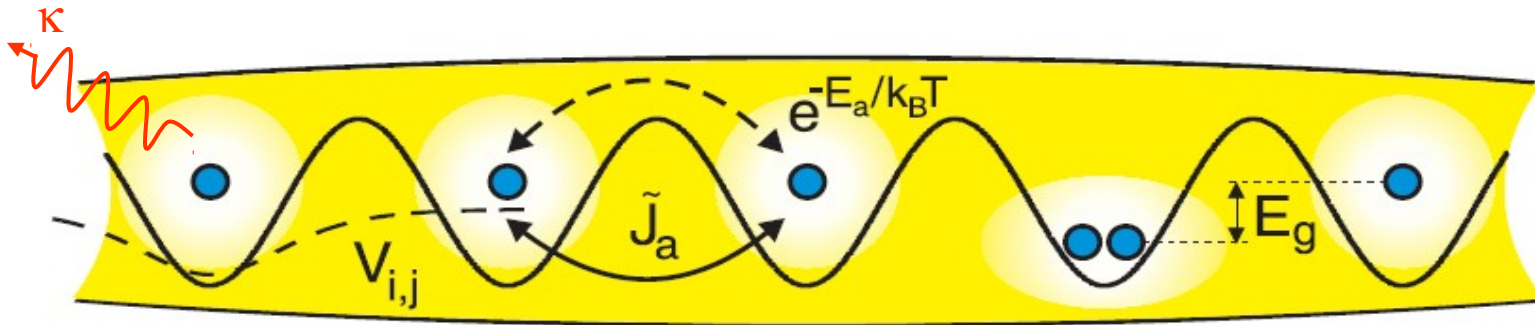
Experiment: J Catani et al., PRA **77**, 011603(R) (2008)

Thermally activated atom hopping

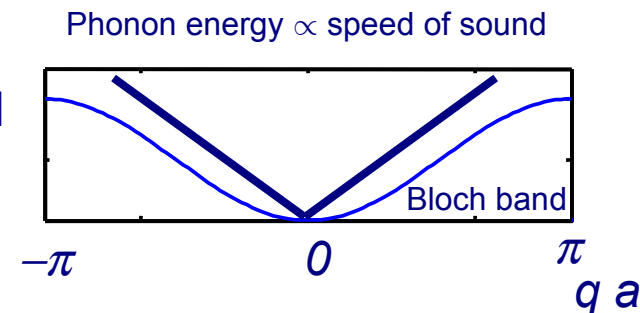


- At higher BEC temperatures phonon collisions thermally induce hopping
 - ➡ Diffusive atom hopping
 - ➡ Phase coherence lost in hopping process
- The equation describing the dynamics of lattice atoms transforms from a wave equation at small T to a diffusion equation at higher T

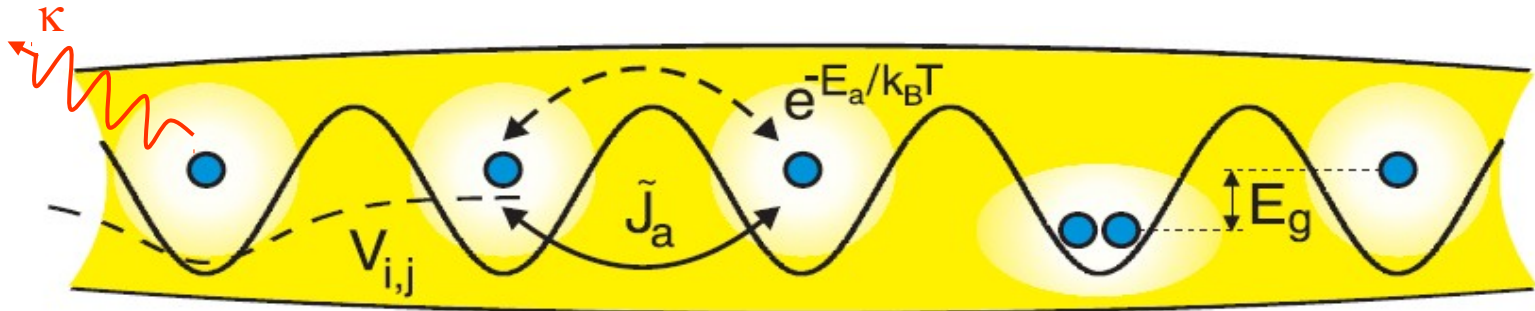
Dephasing



- Energy and momentum conservation laws do not allow for energy to be dissipated
- The interaction between lattice atoms and BEC still leads to dephasing of the atomic wave function which can e.g. be seen in atomic interferometry
- The dephasing properties depend on the properties of the BEC
 - ⇒ 1D: phase coherence reduces exponentially fast
 - ⇒ 2D: phase coherence goes down polynomially
 - ⇒ 3D: phase coherence is (almost) fully preserved



BEC deformation – Off site interactions

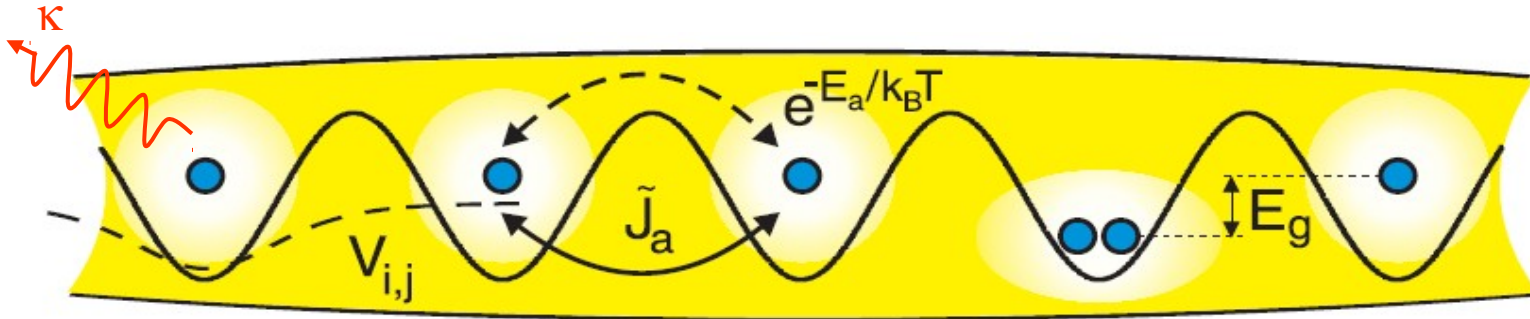


- The presence of a lattice atom will deform the BEC
 - ➡ Size of the deformation is the healing length ξ usually bigger than lattice spacing a
 - ☒ Attractive term for the on-site interaction
 - ☒ Attractive off-site interaction, e.g. for a 1D BEC

$$V_{i,j} = \frac{\kappa^2}{\xi g} e^{-2|i-j|\frac{a}{\xi}}$$

- ➡ Extended Bose-Hubbard model
- ➡ Formation of atom clusters

Self trapping



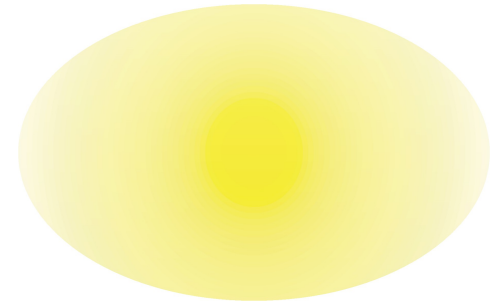
- Self trapping may alter the picture if it affects the lattice atom wave functions
 - ➡ For repulsive interactions $\kappa > 0$ we find self trapping to have negligible effects
 - ☒ 3D and 2D self trapping only occurs above a certain interaction threshold
 - ☒ 1D self trapping will always occur
 - ☒ Self trapping will not compress the atomic wave function far beyond ξ
 - ➡ For attractive interactions $\kappa < 0$ the solutions may be unstable
 - ☒ 3D: finite width solutions with $\kappa < 0$ are unstable
 - ☒ 2D: finite width solutions with $\kappa < \kappa_2$ are unstable
 - ☒ 1D: finite width solutions are stable

Immersed lattices: model

Model: BEC

- Full BEC Hamiltonian

$$\hat{H}_B = \int d\mathbf{r} \hat{\phi}^\dagger(\mathbf{r}) \left[-\frac{\hbar^2 \nabla^2}{2m_b} + V_{\text{ext}}(\mathbf{r}) + \frac{g}{2} \hat{\phi}^\dagger(\mathbf{r}) \hat{\phi}(\mathbf{r}) \right] \hat{\phi}(\mathbf{r})$$



- Use mean field and Bogoliubov ansatz

$$\hat{\phi} \rightarrow \phi_0 + \sum_{\nu}' u_{\nu}(\mathbf{r}) \hat{b}_{\nu} - v_{\nu}^*(\mathbf{r}) \hat{b}_{\nu}^{\dagger}$$

- This yields a simple description of the BEC in terms of Bogoliubov phonons

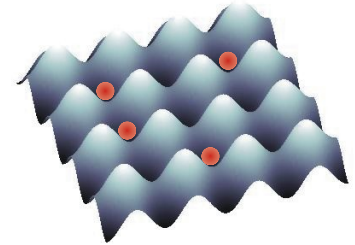
$$\hat{H}_B = \sum_{\nu}' \hbar \omega_{\nu} \hat{b}_{\nu}^{\dagger} \hat{b}_{\nu}$$

- Dispersion relation $\hbar \omega_{\nu}$ depends on dimensionality of BEC and trapping.

Model: Lattice atoms

- Full lattice Hamiltonian

$$\hat{H}_\chi = \int d\mathbf{r} \hat{\chi}^\dagger(\mathbf{r}) \left[-\frac{\hbar^2 \nabla^2}{2m} + V_{\text{lat}}(\mathbf{r}) + \frac{u}{2} \hat{\chi}^\dagger(\mathbf{r}) \hat{\chi}(\mathbf{r}) \right] \hat{\chi}(\mathbf{r})$$



- Expand field operator in terms of localized Wannier functions

$$\hat{\chi}(\mathbf{r}) = \sum_i \eta_i(\mathbf{r}) \hat{a}_i$$

- Neglect higher bands and get the Bose-Hubbard model

$$\hat{H}_\chi = -J \sum_{\langle i,j \rangle} \hat{a}_i^\dagger \hat{a}_j + \frac{1}{2} U \sum_j \hat{n}_j (\hat{n}_j - 1) + \mu \sum_j \hat{n}_j$$

- Note: The procedure works for any H_χ decomposed into localized modes

Model: Interaction

- Interaction Hamiltonian $|\kappa|/gn_0(\mathbf{r})\xi^D(\mathbf{r}) \ll 1$

$$\hat{H}_I = \kappa \int d\mathbf{r} \hat{\chi}^\dagger(\mathbf{r}) \hat{\chi}(\mathbf{r}) \hat{\phi}^\dagger(\mathbf{r}) \hat{\phi}(\mathbf{r})$$

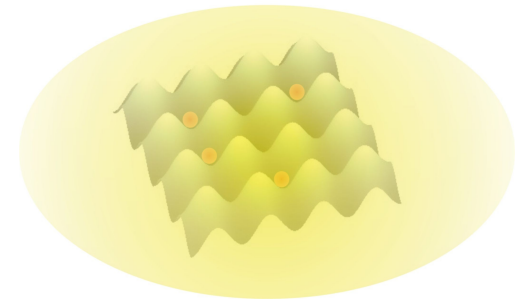
- Do the same expansions as before

$$\hat{H}_I = \sum_{j,\nu} \hbar\omega_\nu \left[M_{j,\nu} \hat{b}_\nu + M_{j,\nu}^* \hat{b}_\nu^\dagger \right] \hat{n}_j$$

- The matrix elements are essentially overlaps of the Wannier functions and the Bogoliubov modes

$$M_{j,\nu} = \frac{\kappa}{\hbar\omega_\nu} \int d\mathbf{r} \phi_0 |\eta_j|^2 [u_\nu - v_\nu]$$

➡ Total Hamiltonian is analogous to the Hamiltonian $\hat{H} = \hat{H}_B + \hat{H}_\chi + \hat{H}_I$



Lang-Firsov transformation

- We apply a unitary Lang-Firsov transformation

$$\hat{H}_{\text{LF}} = e^{\hat{S}} \hat{H} e^{-\hat{S}} \quad \hat{S} = - \sum_{\nu, \mu} \left(M_{\nu, \mu} \hat{b}_{\mu} - \text{h.c.} \right) \hat{n}_{\nu}$$

- We specialize to the case where H_{χ} is a BHM (parameters U_a and J_a) and find the transformed Hamiltonian

$$\begin{aligned} \hat{H}_{\text{LF}} = & -J_a \sum_{\langle i, j \rangle} (\hat{X}_i \hat{a}_i)^{\dagger} (\hat{X}_j \hat{a}_j) + \left(\frac{U_a}{2} - E_P \right) \sum_j \hat{n}_j (\hat{n}_j - 1) \\ & + (\mu - E_P) \sum_j \hat{n}_j - \sum_{i \neq j} V_{i, j} \hat{n}_i \hat{n}_j + \sum_{\mathbf{q}} \omega_{\mathbf{q}} \hat{b}_{\mathbf{q}}^{\dagger} \hat{b}_{\mathbf{q}} \end{aligned}$$

- X_{ν} is a unitary Glauber displacement operator for the phonon cloud

$$\hat{X}_{\nu}^{\dagger} = \exp \left[\sum_{\mu} \left(M_{\nu, \mu}^* \hat{b}_{\mu}^{\dagger} - M_{\nu, \mu} \hat{b}_{\mu} \right) \right]$$

- For a sufficiently deep lattice $V_{i, j} = (\kappa^2 / \xi g) e^{-2|i-j|a/\xi}$ and $E_p = V_{i, i}/2$, where a is the lattice spacing in a 1D BEC

Immersed lattices: transport

Small hopping term and low BEC temperature

- For $J/E_p \ll 1$ and $k_B T/E_p \ll 1$ we treat the hopping term as a perturbation trace out the BEC and find

$$\hat{H}^{(1)} = -\tilde{J} \sum_{\langle i,j \rangle} \hat{a}_i^\dagger \hat{a}_j + \tilde{\mu} \sum_j \hat{n}_j + \frac{1}{2} \tilde{U} \sum_j \hat{n}_j (\hat{n}_j - 1) - \frac{1}{2} \sum_{i \neq j} V_{i,j} \hat{n}_i \hat{n}_j$$

where $\tilde{\mu} = \mu - E_p$, $\tilde{U} = U - 2E_p$ and $\tilde{J} = J \langle\langle \hat{X}_i^\dagger \hat{X}_j \rangle\rangle$.

- $\langle\langle . \rangle\rangle$ denotes the average over the thermal phonon bath and gives

$$\langle\langle \hat{X}_i^\dagger \hat{X}_j \rangle\rangle = \exp \left\{ - \sum_{\mathbf{q} \neq 0} |M_{0,\mathbf{q}}|^2 [1 - \cos(\mathbf{q} \cdot \mathbf{a})] (2N_{\mathbf{q}} + 1) \right\}$$

⇒ $N_{\mathbf{q}}$ is the thermal occupation of the Bogoliubov excitation $\mathbf{q}$

⇒ The hopping bandwidth thus decreases exponentially with T and κ .

Coherent and diffusive hopping

- Use the Nakajima-Zwanzig method to derive a Generalised Master Equation

$$\frac{\partial P_i(t)}{\partial t} = \int_0^t ds \sum_j [W_{i,j}(s)P_j(t-s) - W_{j,i}(s)P_i(t-s)]$$

P_j : Probability of finding atom at site j
 $W_{i,j}$: Memory function, only nearest neighbours

- For $W = \text{const}$ GME simplifies to $\frac{\partial^2 P_i(t)}{\partial t^2} = W[P_{i-1}(t) - 2P_i(t) + P_{i+1}(t)]$

⇒ Discrete wave equation, coherent evolution

- For $W = c\delta(t)$ GME simplifies to $\frac{\partial P_i(t)}{\partial t} = c[P_{i-1}(t) - 2P_i(t) + P_{i+1}(t)]$

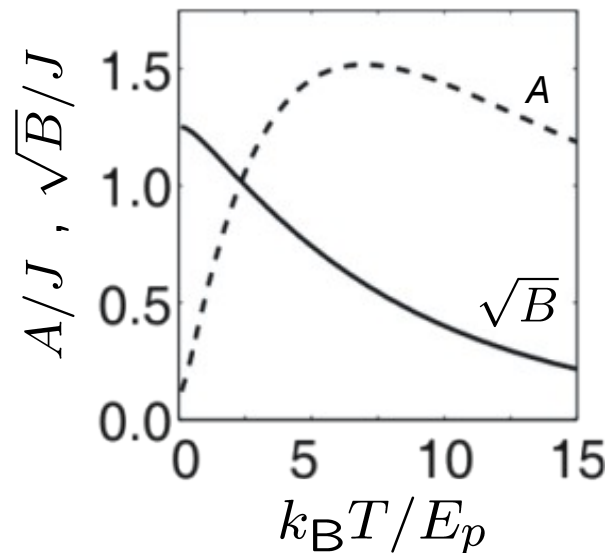
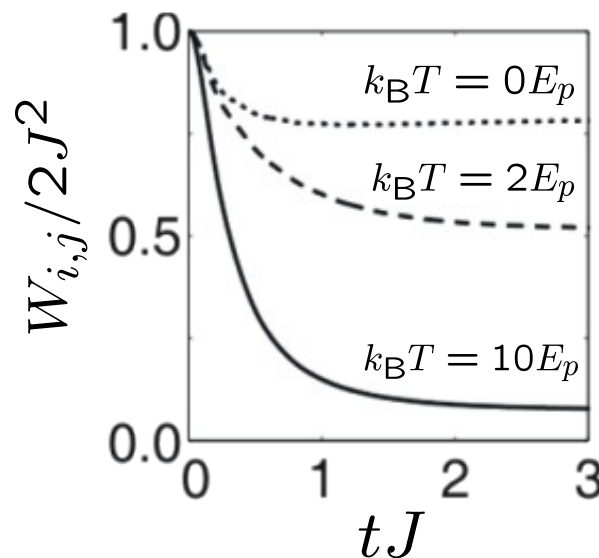
⇒ Discrete diffusion equation, incoherent evolution

Coherent and diffusive hopping

- Rates are given by A (diffusive) and $\sqrt{B}$ (coherent). The spread of an initially localized atom is given by

$$\overline{l^2}(t) = At + Bt^2$$

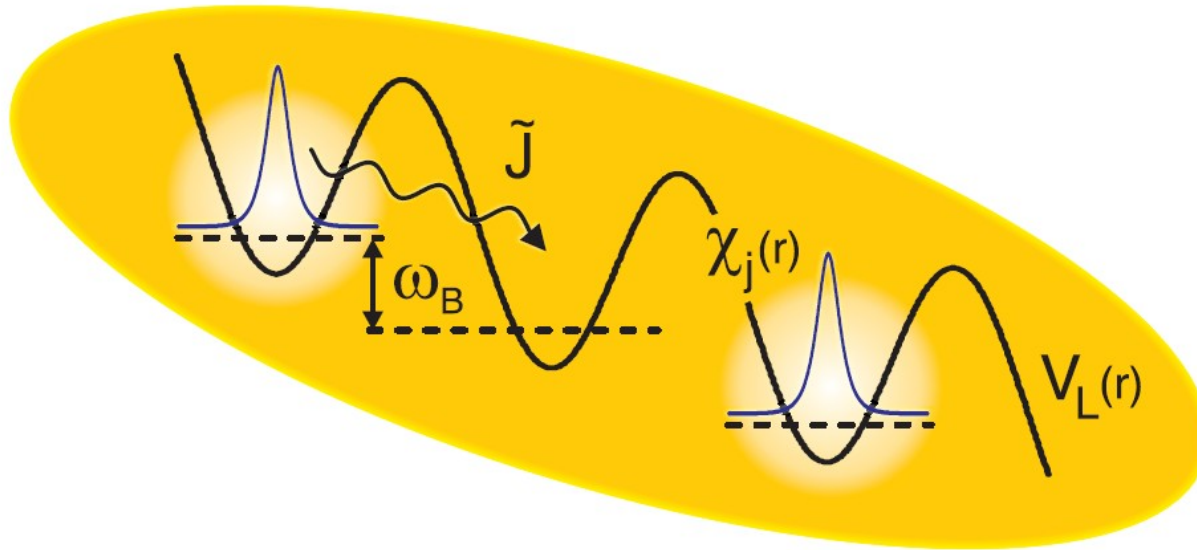
➡ Crossover from coherent to diffusive hopping occurs at realistic temperatures



$$E_p \approx 11 \text{ nK}$$

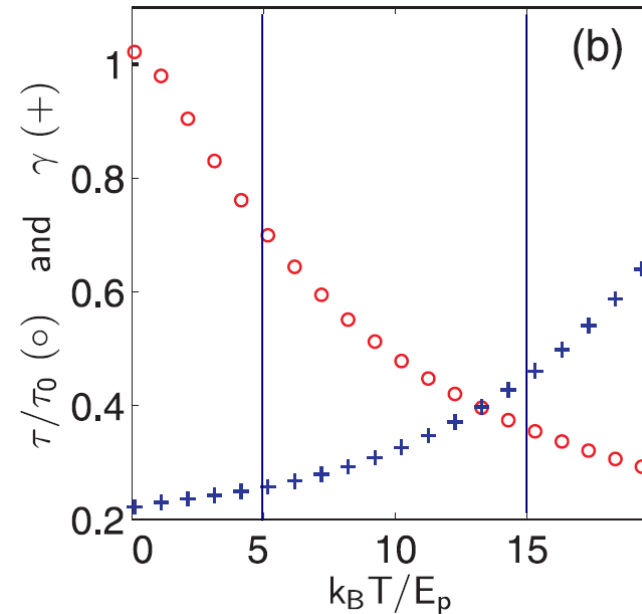
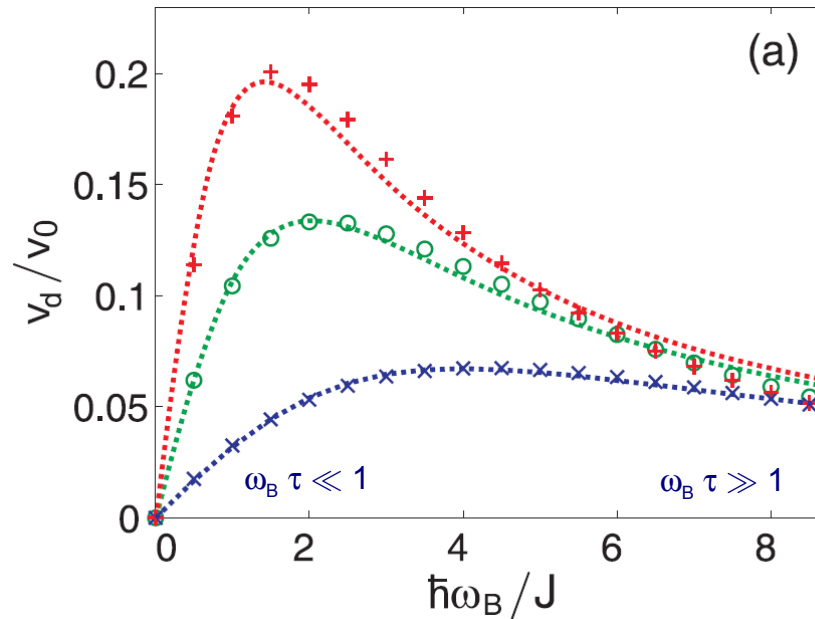
Transport through a tilted lattice

- Coherent vs. incoherent hopping



- Tilting the lattice $\propto$ voltage
 - ⇒ Acceleration
 - ⇒ Electric fields
- Atoms flowing through the lattice $\rightarrow$ current

Conductivity and relaxation time



- The current can be described by the Esaki-Tsui relation

$$v_d = 2 \gamma \tilde{v}_0 \frac{\omega_B \tau}{1 + (\omega_B \tau)^2}$$

➡ Negative differential conductivity

$\tau \dots$ relaxation time
 $v_0 = Ja \dots$ Lattice speed
 $\tau_0 = 1/gn_0 \dots$ BEC timescale
 $\gamma \dots$ dimensionless parameter

A.V. Ponomarev et al.,
Phys. Rev. Lett. **96**, 050404 (2006)

Dephasing

Dephasing of a single impurity (J=0)

- With $H_\chi=0$ and

$$\hat{H}_B = \frac{1}{2} \int d^D \mathbf{x} \left(\frac{n_0}{m} (\nabla \hat{\varphi})^2 + g \hat{n}^2 \right)$$

⇒ The temporal correlation function of the impurity is given by

$$\langle \hat{a}^\dagger(0) \hat{a}(\tau) \rangle \propto \left\langle \exp \left(-i \frac{\kappa}{g} \int d\mathbf{x} |\eta(\mathbf{x})|^2 \{ \hat{\varphi}(\mathbf{x}, \tau) - \hat{\varphi}(\mathbf{x}, 0) \} \right) \right\rangle$$

- ☒ Turn the dephasing into fringe visibility by Ramsey interferometry
- ☒ Measure coarse grained phase correlations
- ☒ Spatial and temporal correlations accessible

⇒ In terms of Bogoliubov excitations the resulting Hamiltonian is an independent boson model (solvable)

$$H = \left(\kappa n_0 + \sum_{\mathbf{k}} (g_{\mathbf{k}} b_{\mathbf{k}}^\dagger + \text{h.c.}) \right) \hat{a}^\dagger \hat{a} + \sum_{\mathbf{k}} \omega_{\mathbf{k}} \left(b_{\mathbf{k}}^\dagger b_{\mathbf{k}} + \frac{1}{2} \right) + \text{const}$$

with $g_{\mathbf{k}}$ overlap matrix elements for the impurity-Bogoliubov excitations coupling

Measuring properties of the BEC

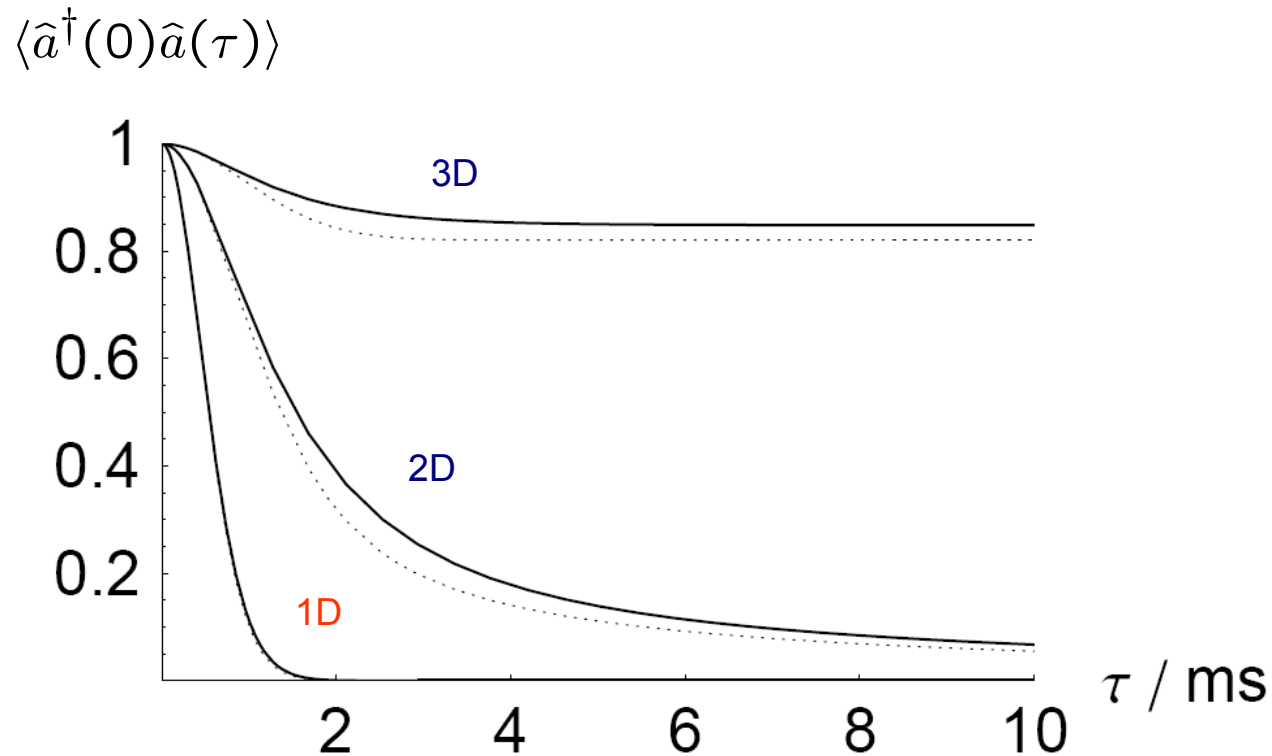
- We obtain for a D dimensional BEC and long waiting time $\tau \rightarrow \infty$

$$\langle \hat{a}^\dagger(0) \hat{a}(\tau) \rangle \propto \begin{cases} C_T \exp \left[- \left(\frac{\kappa}{g} \right)^2 \frac{m c k_B T}{2 \hbar^2 n_0} \tau \right] & \text{for } D = 1 \\ C'_T \left(\frac{\sigma}{c \tau} \right)^\nu & \text{for } D = 2 \\ \exp \left[- \left(\frac{\kappa}{g} \right)^2 \frac{m k_B T}{(2\pi)^{3/2} \hbar^2 n_0 \sigma} \right] & \text{for } D = 3 \end{cases}$$

$$\nu = (\kappa/g)^2 m k_B T / (2\pi \hbar^2 n_0)$$

- ⇒ Measure temperature, speed of sound, ...
- ⇒ A SAT in a 1D BEC cannot be used as a qubit
- ⇒ The frequencies of the Bogoliubov excitations are not changed by the presence of the impurity

BEC properties

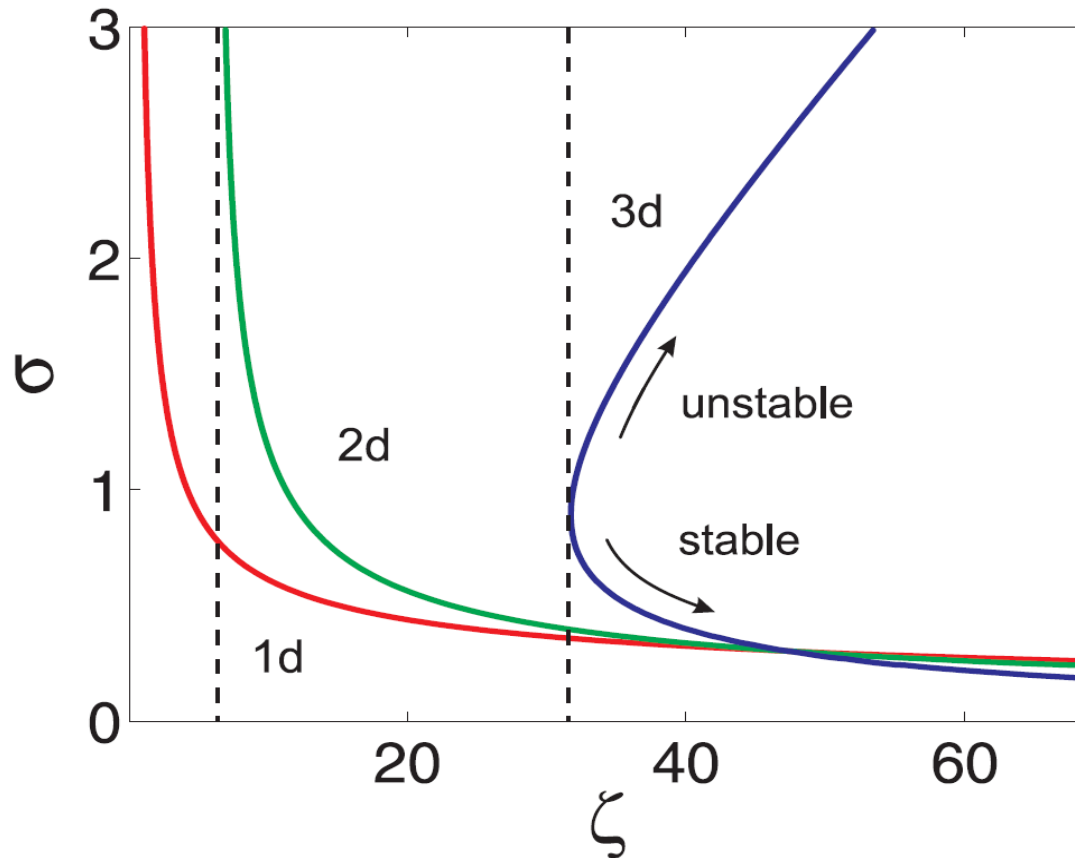


$$m = 10^{-25} \text{kg}, l_0 = 2 \times 10^6 \text{m}^{-1}, c = 10^{-3} \text{ms}^{-1}$$
$$\sigma = 10^{-6} m \quad \kappa = g \quad T = 2 \times 10^{-7} \text{K}$$

Immersed lattices: self-trapping

Self-trapping - perturbation theory

- We consider a single self-trapped impurity atom immersed in a BEC. For interaction strength ζ the width of the impurity wave function is σ given by



Self trapping for

$$\zeta > 2\pi \text{ in 2d}$$

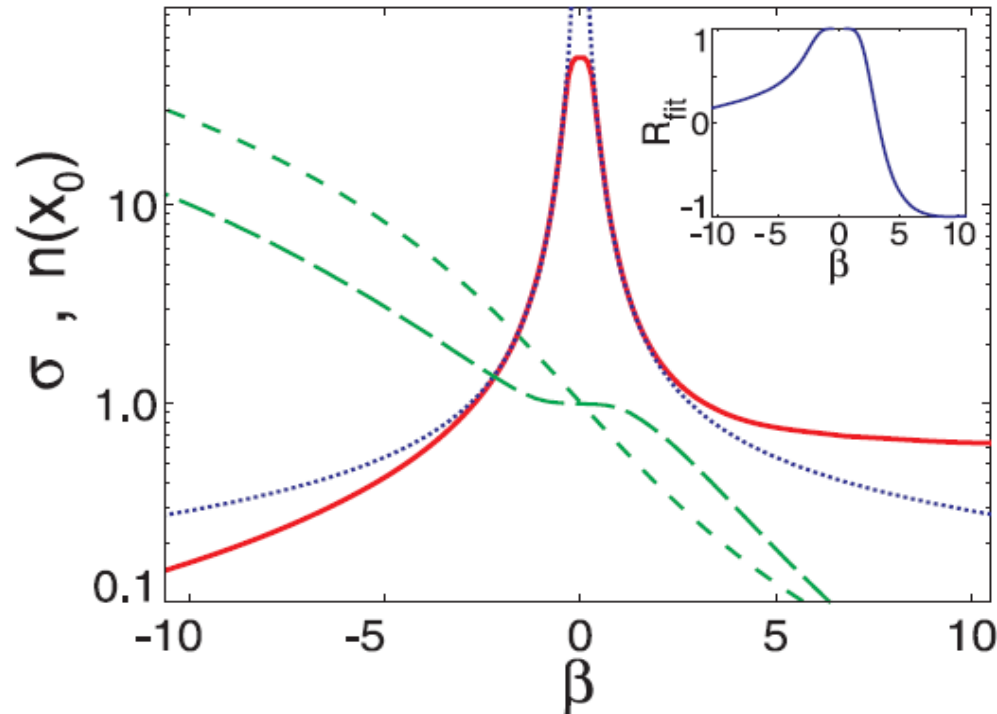
$$\zeta \gtrsim 31.7 \text{ in 3d}$$

$$\zeta = (\kappa/g)^2 m_a/m_b \xi^d n_0$$

$$\varepsilon' \chi = -\frac{1}{2} \nabla^2 \chi - \zeta |\chi|^2 \chi$$

Self-trapping beyond perturbation theory

- One spatial dimension



Red curve: width of the impurity wave function σ

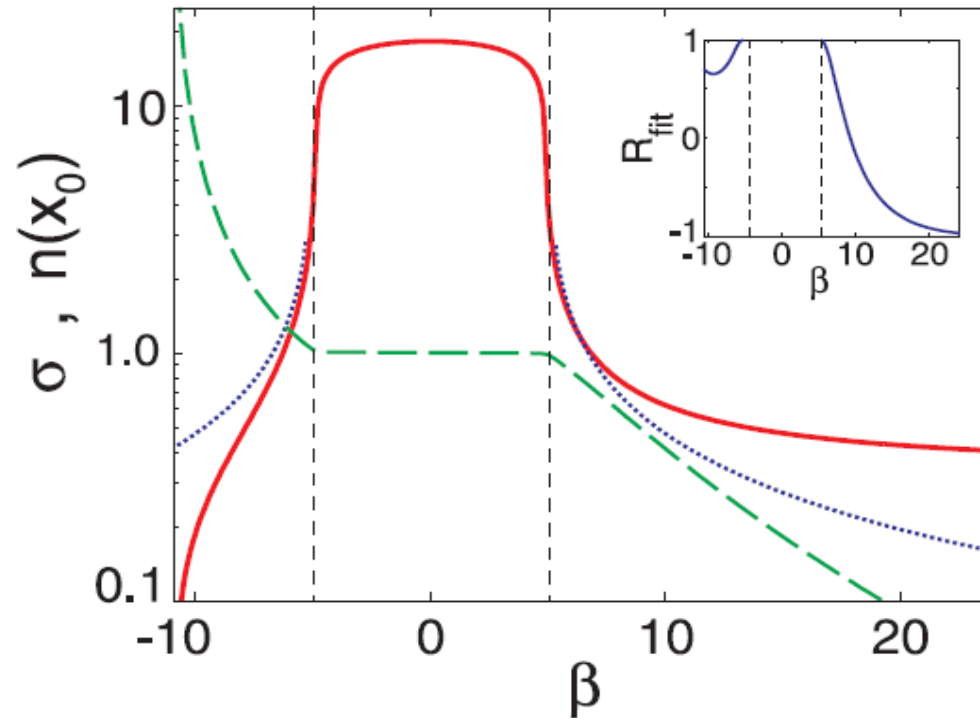
Long dashed green curve: density of the BEC at the impurity position

Short dashed green curve: δ approximation

Blue dotted curve: Weak coupling approximation

Self-trapping beyond perturbation theory

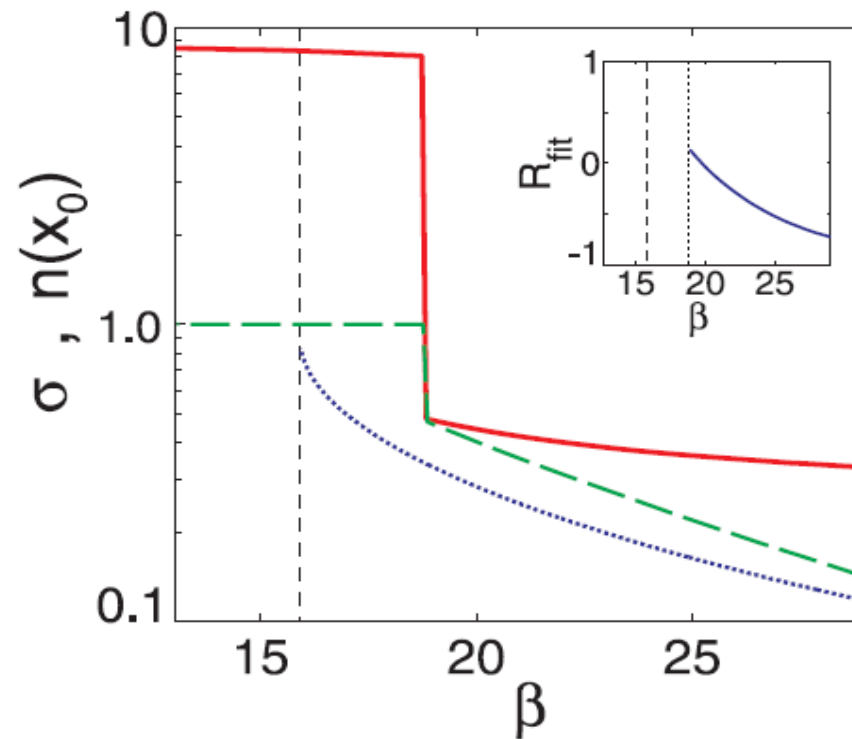
- Two spatial dimensions



Red curve: width of the impurity wave function σ
Long dashed green curve: density of the BEC at the impurity position
Short dashed green curve: δ approximation
Blue dotted curve: Weak coupling approximation

Self-trapping beyond perturbation theory

- Three spatial dimensions



Red curve: width of the impurity wave function σ

Long dashed green curve: density of the BEC at the impurity position

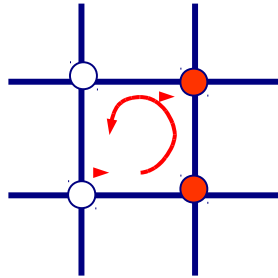
Short dashed green curve: δ approximation

Blue dotted curve: Weak coupling approximation

Rotating lattice immersions

Artificial magnetic fields

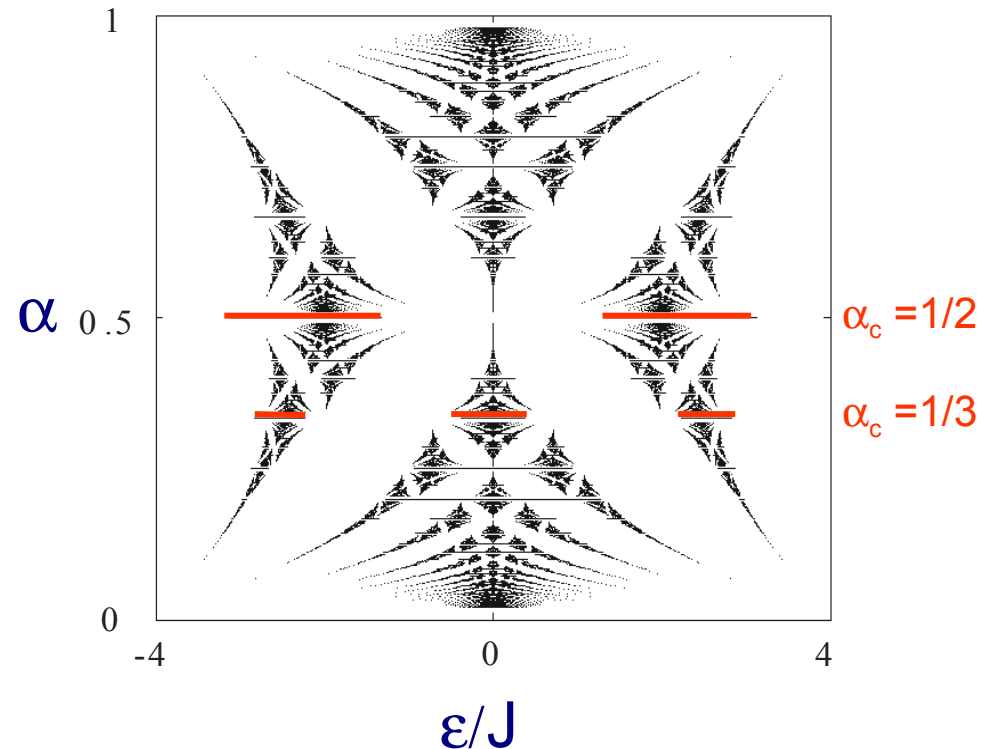
● Effect of a magnetic field



$$e^{\oint \mathbf{A} \cdot d\mathbf{l}} = e^{i2\pi\alpha}$$

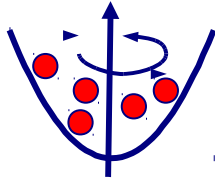
- ➡ The wave function accumulates a phase characterized by α when hopping around plaquette.
- ➡ Phase proportional to enclosed magnetic flux

● Resulting energy spectrum



Ultracold atoms in rotating lattices

- Effective magnetic field via rotation



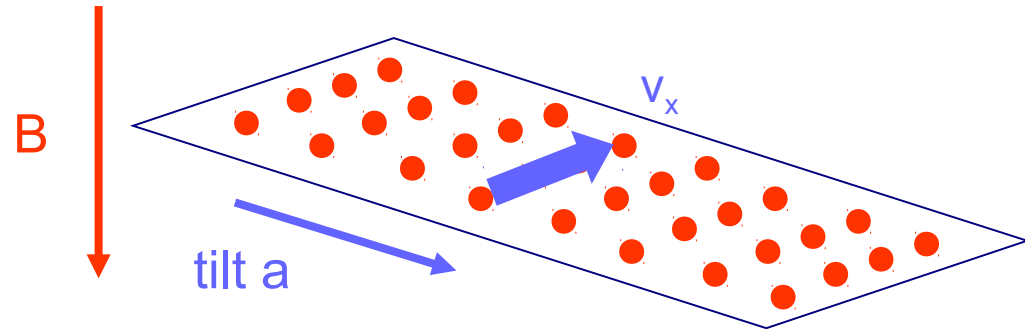
- ⇒ N.K. Wilkin *et al.* PRL 1998
- ⇒ B. Paredes *et al.* PRL 2001
- ⇒ Experiment: E. Cornell, JILA
- ⇒ Experiment: J. Dalibard, ENS
- ⇒ Experiment: C. Foot, Oxford

- Alternative ways for realizing artificial magnetic fields, e.g.

- ⇒ A.S. Sorensen *et al.* PRL 2005
- ⇒ G. Juzeliunas *et al.* PRL 2004
- ⇒ E.J. Mueller, PRA 2004
- ⇒ DJ *et al.*, New J. Phys. 2003
- ⇒ A. Klein and DJ, preprint

Hall current

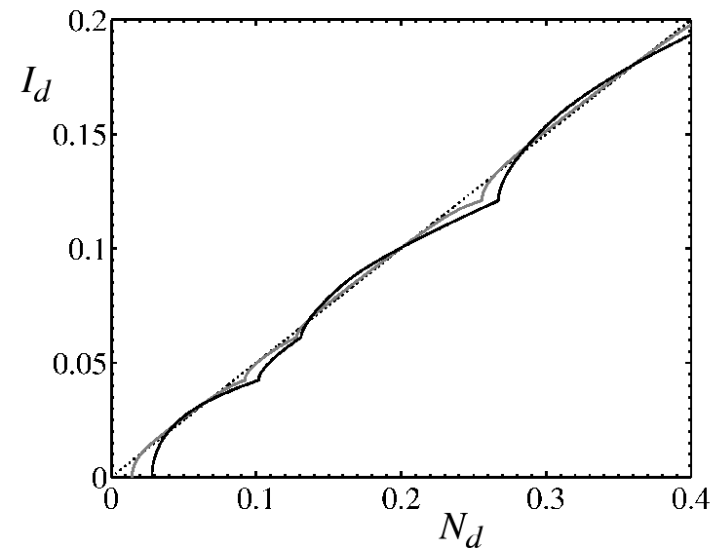
- Hall current visible in harmonic trap geometry
- Plateaus turn into corners
- Hall flow of particles



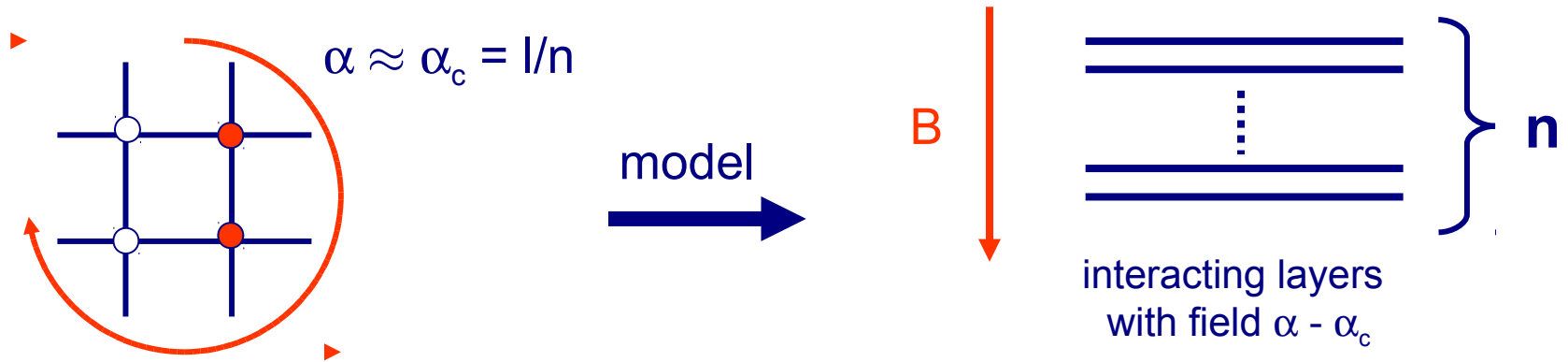
$$\tilde{v}_x = \frac{2a\tilde{\Omega}}{4\tilde{\Omega}^2 + \omega^2/C}$$

$$\tilde{\Omega} \equiv (\alpha - \alpha_c)\pi/md^2$$

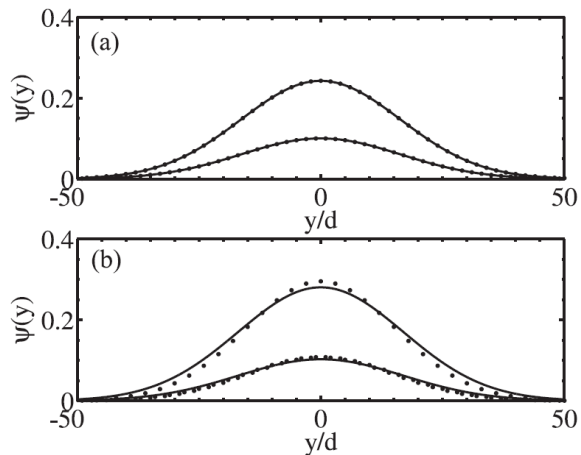
- Negative currents for $\alpha < \alpha_c$



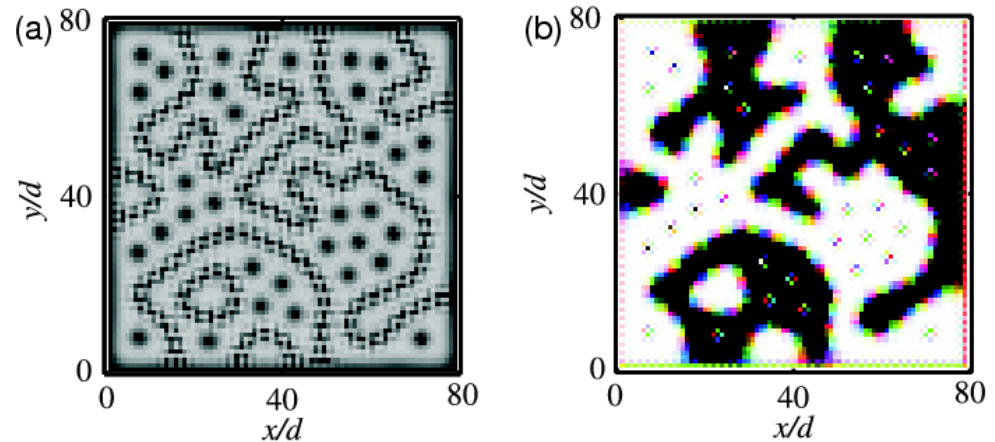
Huge artificial fields: n layers near $\alpha = l/n$



Wave function

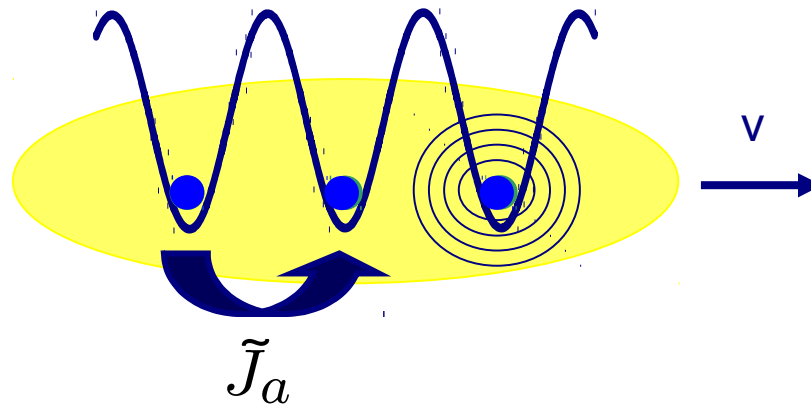


Vortex lattice



Rotating lattice immersion

- Optical lattice in a moving BEC at very low temperature



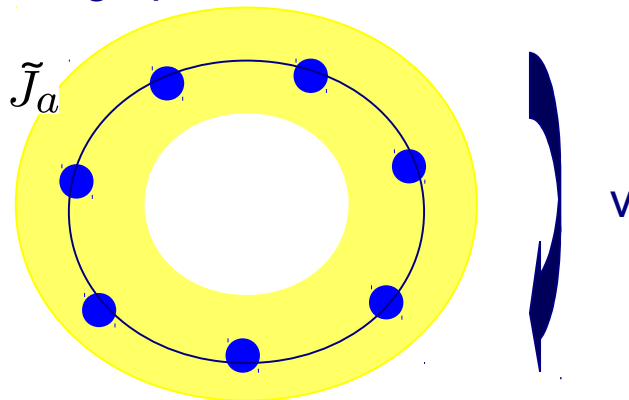
$$q \rightarrow q - mv$$

$$\tilde{J}_a \rightarrow \tilde{J}_a e^{i2\pi\alpha}$$

$$\alpha \propto v$$

⇒ In lowest order for $v \ll c$ this leads to a phase α proportional to v

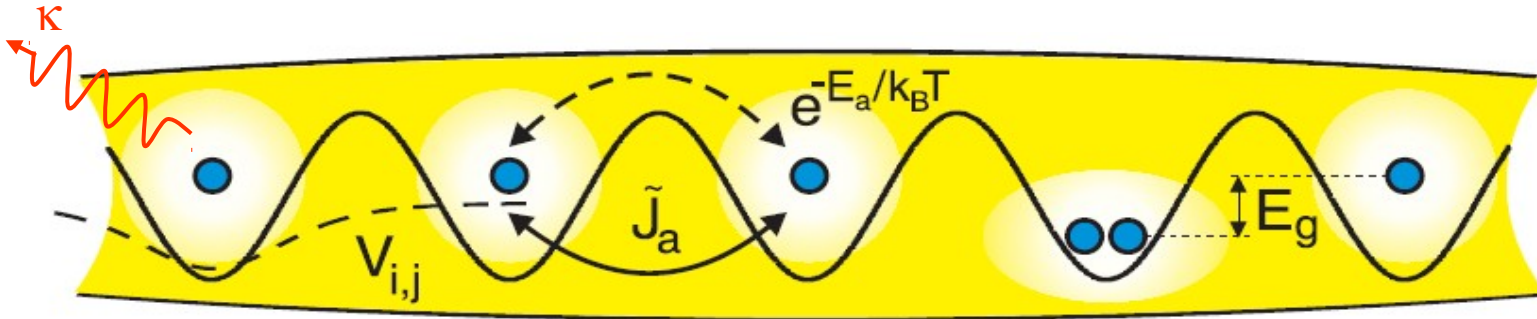
- Rotating optical lattice immersions



Rotating BEC
Rotating lattice

→ No need to balance
centrifugal terms

Coherent atom hopping



- When hopping from one site to the next the deformation needs to be dragged along $\rightarrow$ hopping matrix element is affected

$$\tilde{J} = J \langle\langle \hat{X}_i^\dagger \hat{X}_j \rangle\rangle.$$

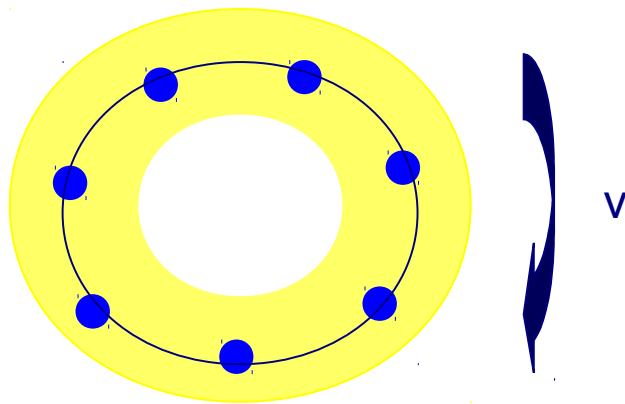
$$\langle\langle \hat{X}_i^\dagger \hat{X}_j \rangle\rangle = \exp \left\{ - \sum_{\mathbf{q} \neq 0} |M_{0,\mathbf{q}}|^2 [1 - \cos(\mathbf{q} \cdot \mathbf{a})] (2N_{\mathbf{q}} + 1) \right\}$$

Experiment: J Catani et al., PRA **77**, 011603(R) (2008)

Moving BEC

- A BEC moving at velocity v relative to the lattice induces a phase

$$\alpha_a = \frac{1}{2\pi i} \frac{1}{2} \sum_q' M_{i,q} M_{j,q}^* - M_{i,q}^* M_{j,q} \propto \kappa^2 n_0 v$$



$$\tilde{J}_a = |\tilde{J}_a| e^{i\alpha_a}$$

