

# Non-equilibrium many-body dynamics and heating of cold atoms in optical lattices

Andrew Daley

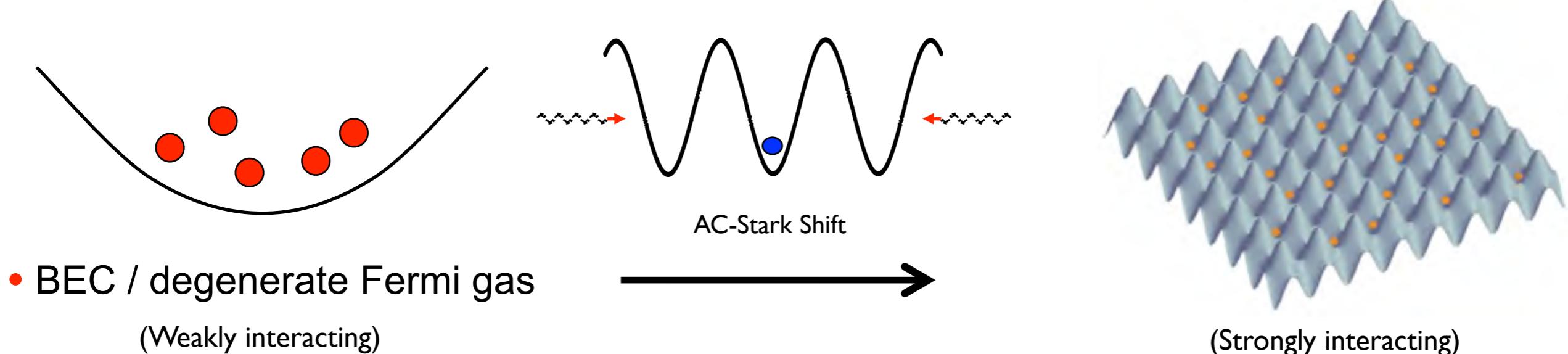
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# Atoms in 3D Optical Lattices:



Bose-Hubbard: D. Jaksch et al. PRL '98

A diagram showing two energy levels represented by black horizontal lines. A blue sphere is on the lower level, and two blue spheres are on the upper level. Orange wavy arrows between the levels represent hopping between sites. A double-headed vertical arrow between the levels is labeled  $U$ . A curved arrow below the lines is labeled  $J$ .

$$H = -J \sum_{\langle i,j \rangle} \hat{b}_i^\dagger \hat{b}_j + \frac{U}{2} \sum_i \hat{n}_i (\hat{n}_i - 1)$$

(Fermi-) Hubbard:

A diagram showing two energy levels represented by black horizontal lines. A green sphere with an upward arrow is on the lower level, and two green spheres with both upward and downward arrows are on the upper level. Orange wavy arrows between the levels represent hopping between sites. A double-headed vertical arrow between the levels is labeled  $U$ . A curved arrow below the lines is labeled  $J$ .

$$H = -J \sum_{\langle i,j \rangle, \sigma} c_{i,\sigma}^\dagger c_{j,\sigma} + U \sum_i c_{i,\uparrow}^\dagger c_{i,\downarrow}^\dagger c_{i,\downarrow} c_{i,\uparrow}$$

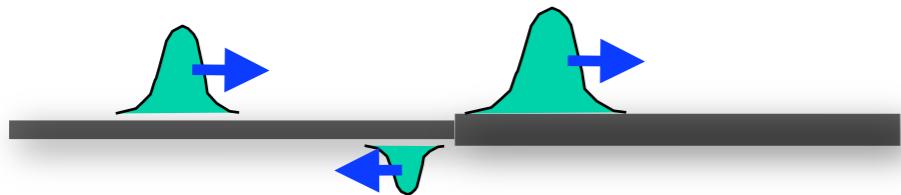
- Realise strongly correlated lattice models
- Microscopic understanding
- Study thermodynamics / quantum phases

Experiments:

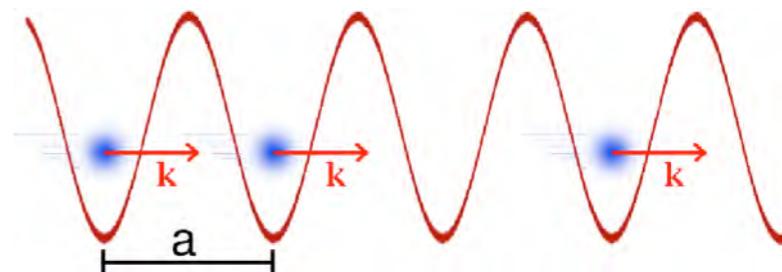
Munich, Zurich, NIST / JQI, MIT, Harvard,  
Innsbruck, Hamburg, Pisa, Florence, Oxford,  
Austin, Chicago, Penn State, Kyoto, Illinois, .....

# Coherent non-equilibrium dynamics:

- Transport dynamics

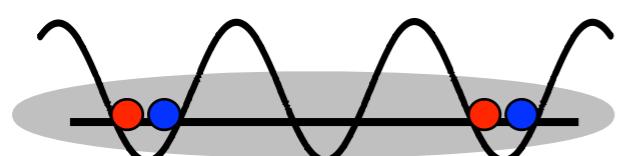
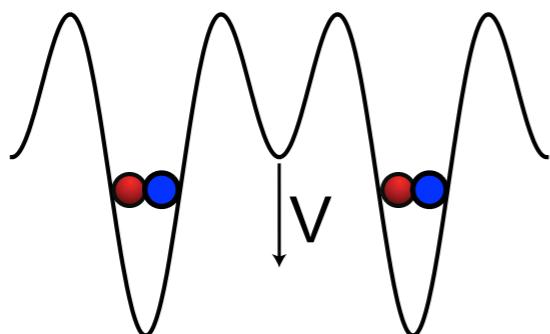


AJD, P. Zoller, and B. Trauzettel,  
PRL **100**, 110404 (2008)



J. Schachenmayer, G. Pupillo, and AJD,  
New J. Phys. **12**, 025014 (2010)

- Many-body State preparation (e.g., eta-pairs)



P. Rabl, AJD, P. O. Fedichev, J. I Cirac, and P. Zoller,  
PRL **91**, 110403 (2003)

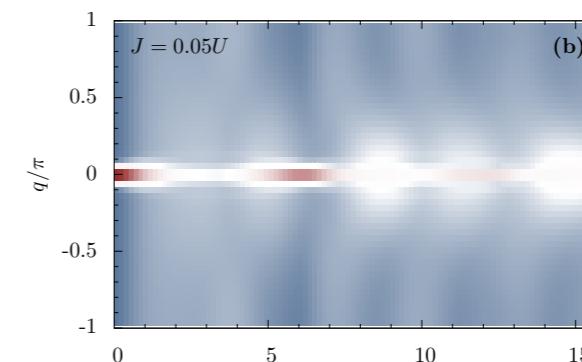
A. Kantian, AJD, and P. Zoller,  
PRL **104**, 240406 (2010)

- Dynamical crystal formation with Rydberg atoms / polar molecules



J. Schachenmayer, A. Micheli, I. Lesanovsky,  
and AJD, New J. Phys. **12**, 103044 (2010)

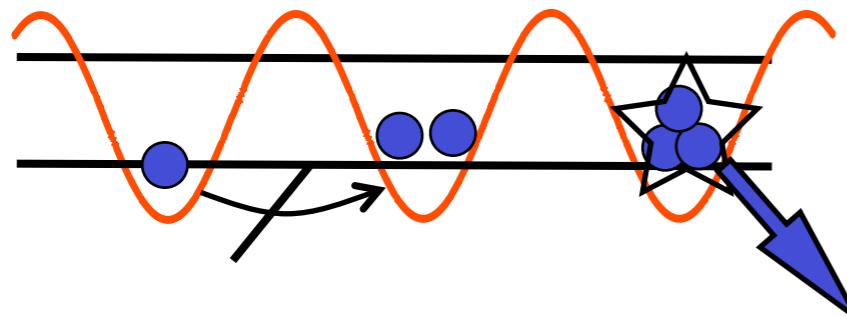
- Collapse/revival dynamics with fixed atom number



J. Schachenmayer, AJD, and P. Zoller,  
PRA in press, arXiv:1101.2385

# Dissipative non-equilibrium dynamics:

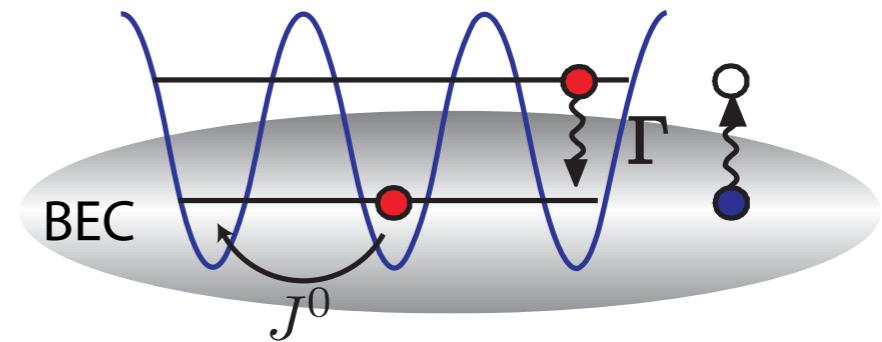
- Three-body loss



## Dimer superfluid of Bosons:

AJD, J. Taylor, S. Diehl, M. Baranov, and P. Zoller  
PRL **102**, 040402 (2009)  
S. Diehl, M. Baranov, AJD, and P. Zoller  
PRL **104**, 165301 (2010)

- State preparation by reservoir engineering



## Dark State Cooling:

A. Griessner, AJD, S. R. Clark, D. Jaksch, P. Zoller,  
PRL **97**, 220403 (2006)

## Colour superfluid in a 3-component Fermi gas:

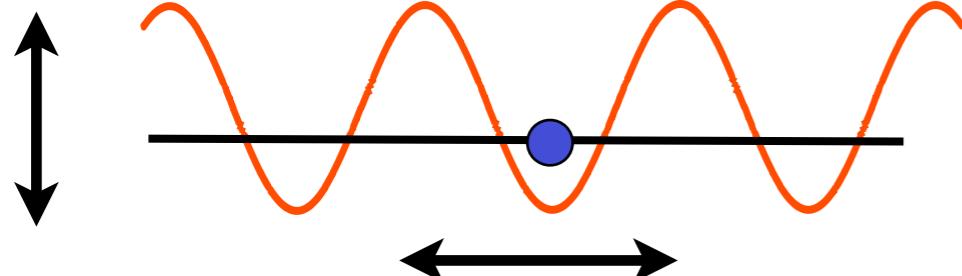
A. Kantian, M. Dalmonte, S. Diehl, W. Hofstetter,  
P. Zoller, and AJD, PRL **103**, 240401 (2009)

## Dissipative preparation of a d-wave paired state:

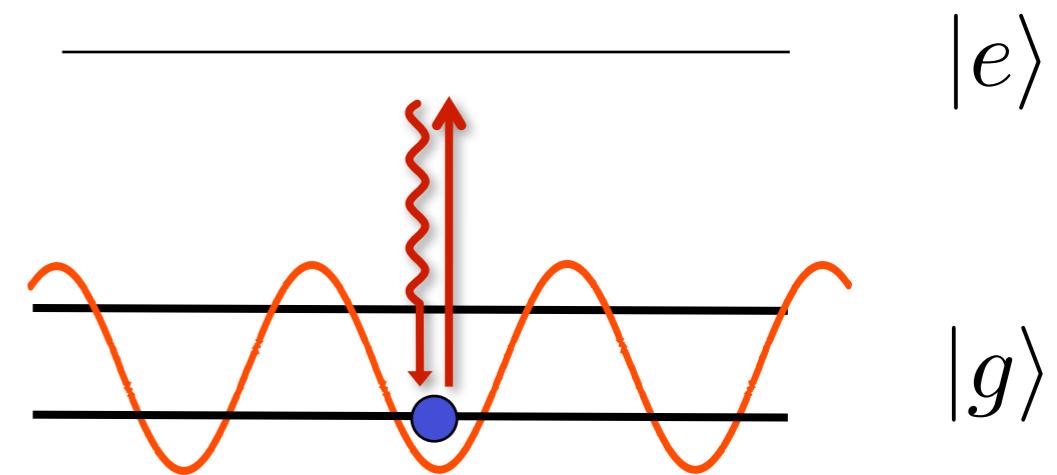
S. Diehl, W. Yi, AJD, P. Zoller  
PRL **105**, 227001 (2010)

# Heating:

Via “classical” noise:  
(e.g., lattice laser phase/amplitude noise)

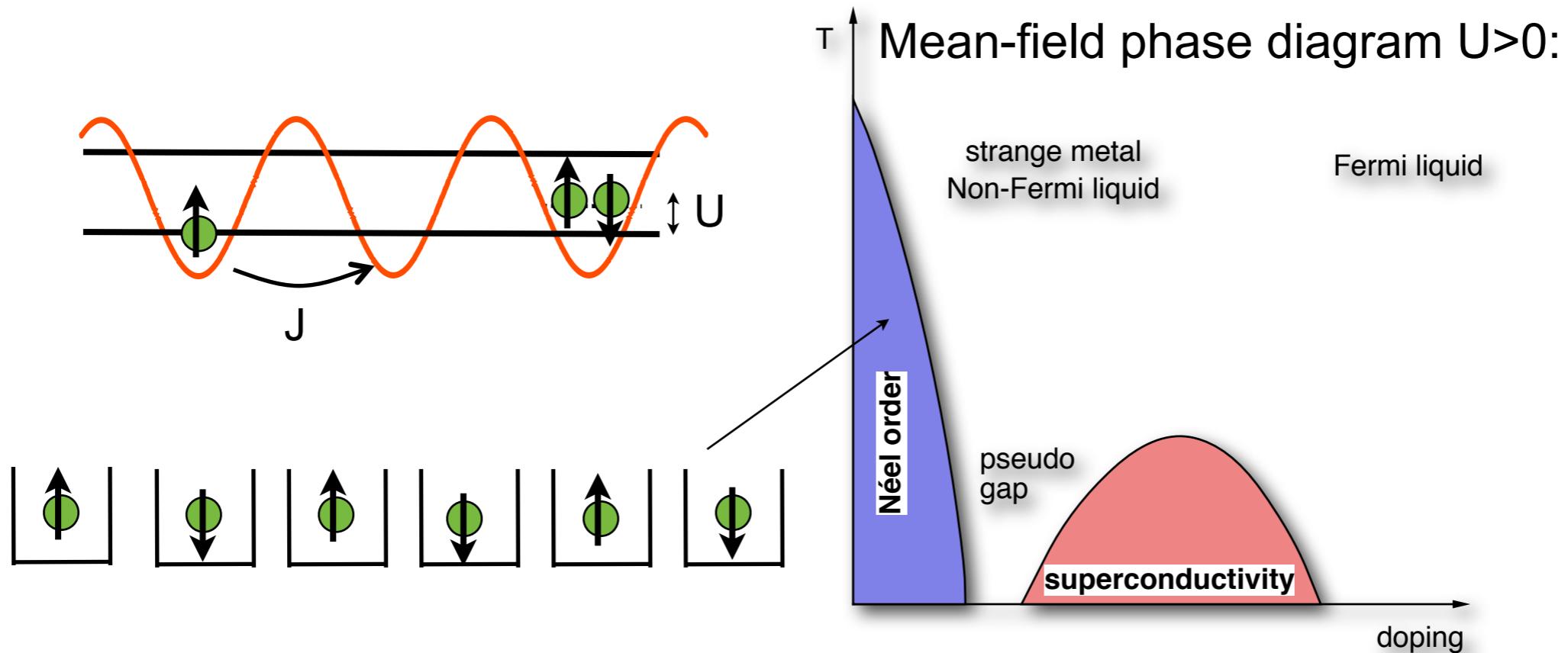


Via spontaneous emissions:



## Quantum Simulation:

- Ground state properties / quantum phases of important models from solid state physics  
e.g., Potential connection to high T<sub>c</sub> superconductivity:

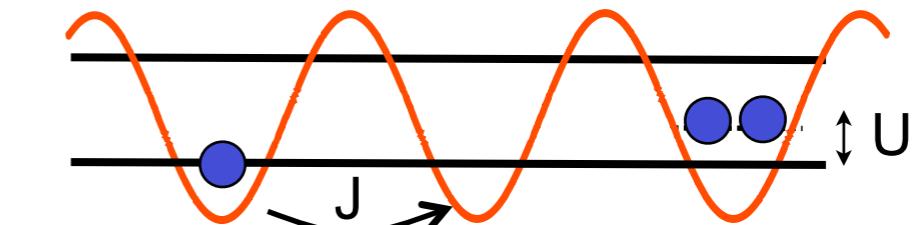
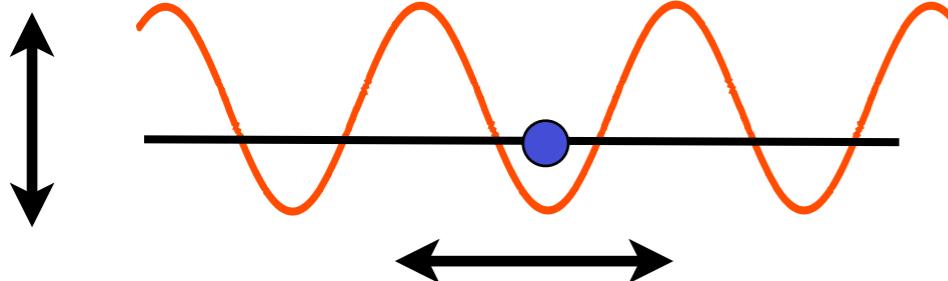


## Key challenges:

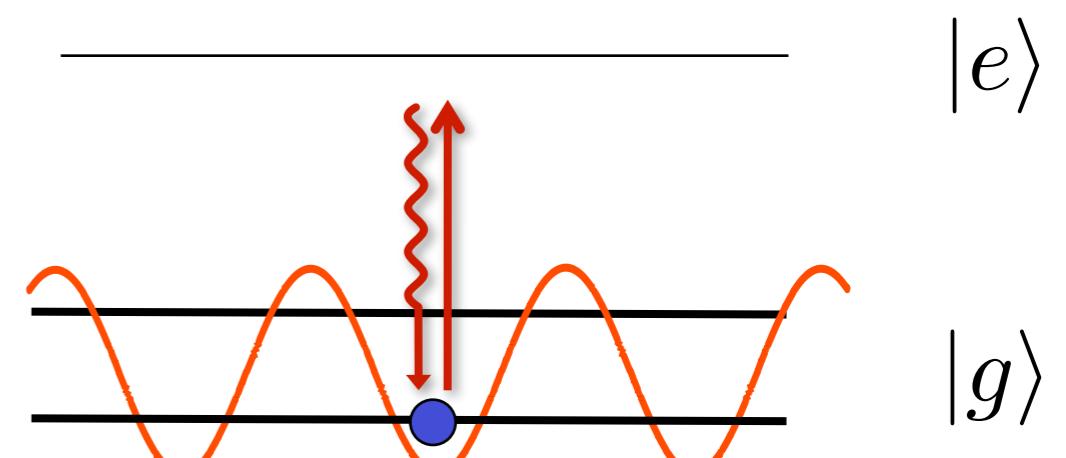
- State preparation / cooling to low temperatures
- Characterisation and control of heating processes

# Heating in an optical lattice

Via “classical” noise:  
(e.g., lattice laser phase/amplitude noise)



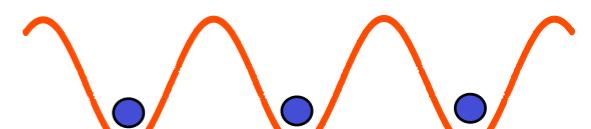
Via spontaneous emissions:



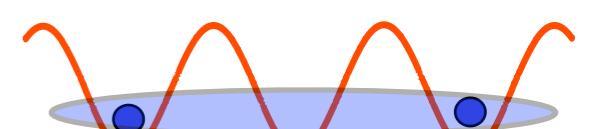
Also: collisional losses, background gas collisions....

Questions:

- Interplay: **heating with many-body physics**  
Are some strongly correlated states more/less sensitive?
- How do we control / minimise heating in experiments?  
(e.g., choice of red vs. blue detuning for lattices)



Mott Insulator ( $U \gg J$ )



Superfluid ( $J \gg U$ )

# Outline

## Heating of many bosons due to spontaneous emissions

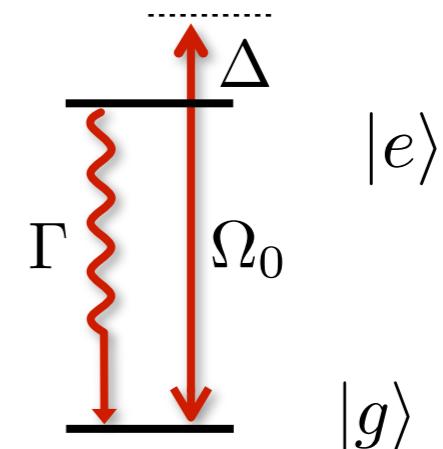
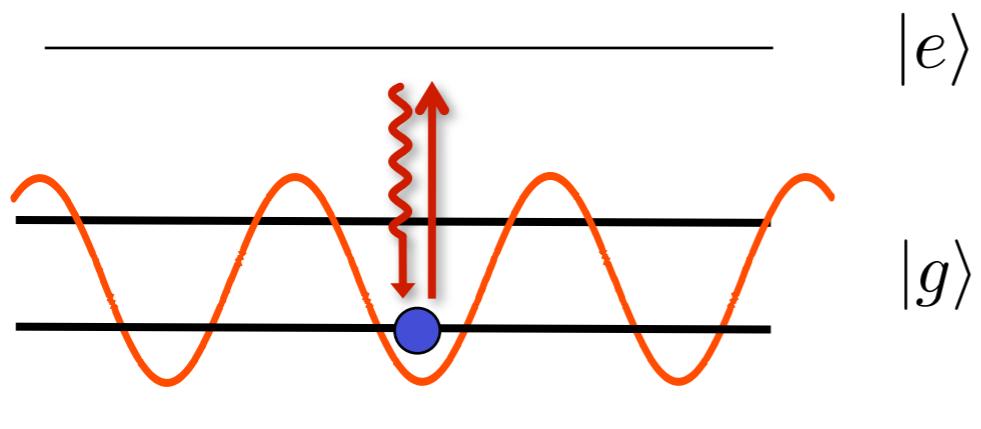
- Master equation
- Heating of single atoms
- Heating of many-body states
- Exact simulations in 1D

## Work in progress

- Thermalisation of bosons in the presence of heating
- Light-assisted collisions
- Heating of many fermions via spontaneous emissions
- Amplitude and position fluctuations and heating

**Heating of bosons via spontaneous emission**

# Theoretical Description (single atom)



- Spontaneous emissions from **two-level atoms**
- **Master equation** for spontaneous emissions in Born-Markov approximation

$$\dot{\rho} = -i [H, \rho] + \Gamma \int d^3 u N(\mathbf{u}) \left( C_{\mathbf{u}} \rho C_{\mathbf{u}}^\dagger - \frac{1}{2} C_{\mathbf{u}}^\dagger C_{\mathbf{u}} \rho - \frac{1}{2} \rho C_{\mathbf{u}}^\dagger C_{\mathbf{u}} \right)$$

$$C_{\mathbf{u}} = |g\rangle \langle e| e^{-ik_{eg}\mathbf{u} \cdot \hat{\mathbf{x}}}$$

$$H = \frac{\hat{\mathbf{p}}^2}{2m} - \Delta |e\rangle \langle e| - \left( |g\rangle \langle e| \frac{\Omega(\hat{\mathbf{x}})}{2} + \text{h.c.} \right)$$

Kinetic energy

Detuning of excited state

Coupling

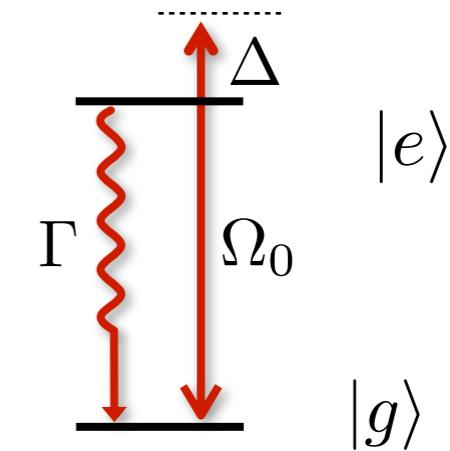
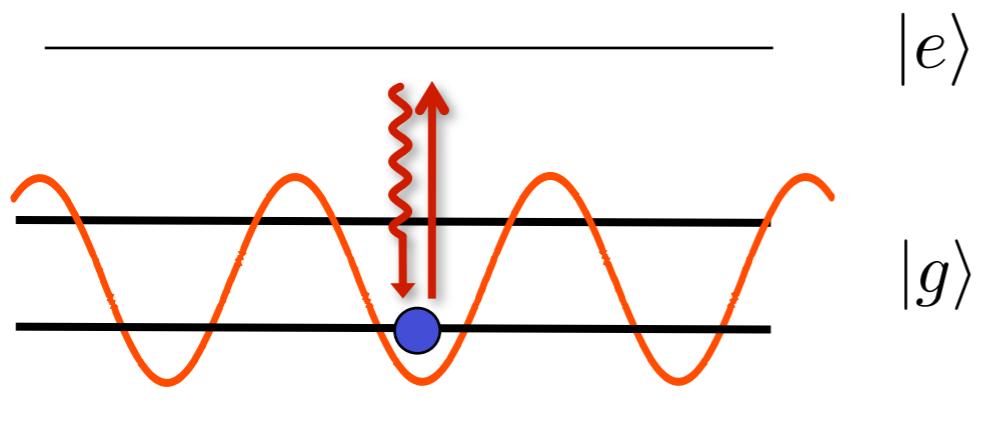
atomic lowering operator

$$N(\mathbf{u}) = \frac{3}{8\pi} \left( 1 - (\mathbf{u} \cdot \hat{\mathbf{d}})^2 \right)$$

Distribution of emitted photons

- Can be extended, e.g., with additional exit channels for internal state

## Theoretical Description (single atom)



- Limit of **large detuning** - can adiabatically eliminate excited state  $\Delta \gg \Gamma, \Omega_0$

$$\frac{d}{dt}\rho = -i(H_{\text{eff}}\rho - \rho H_{\text{eff}}^\dagger) + \mathcal{J}\rho$$

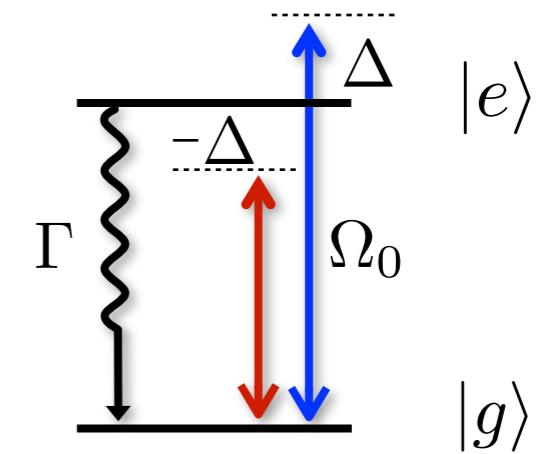
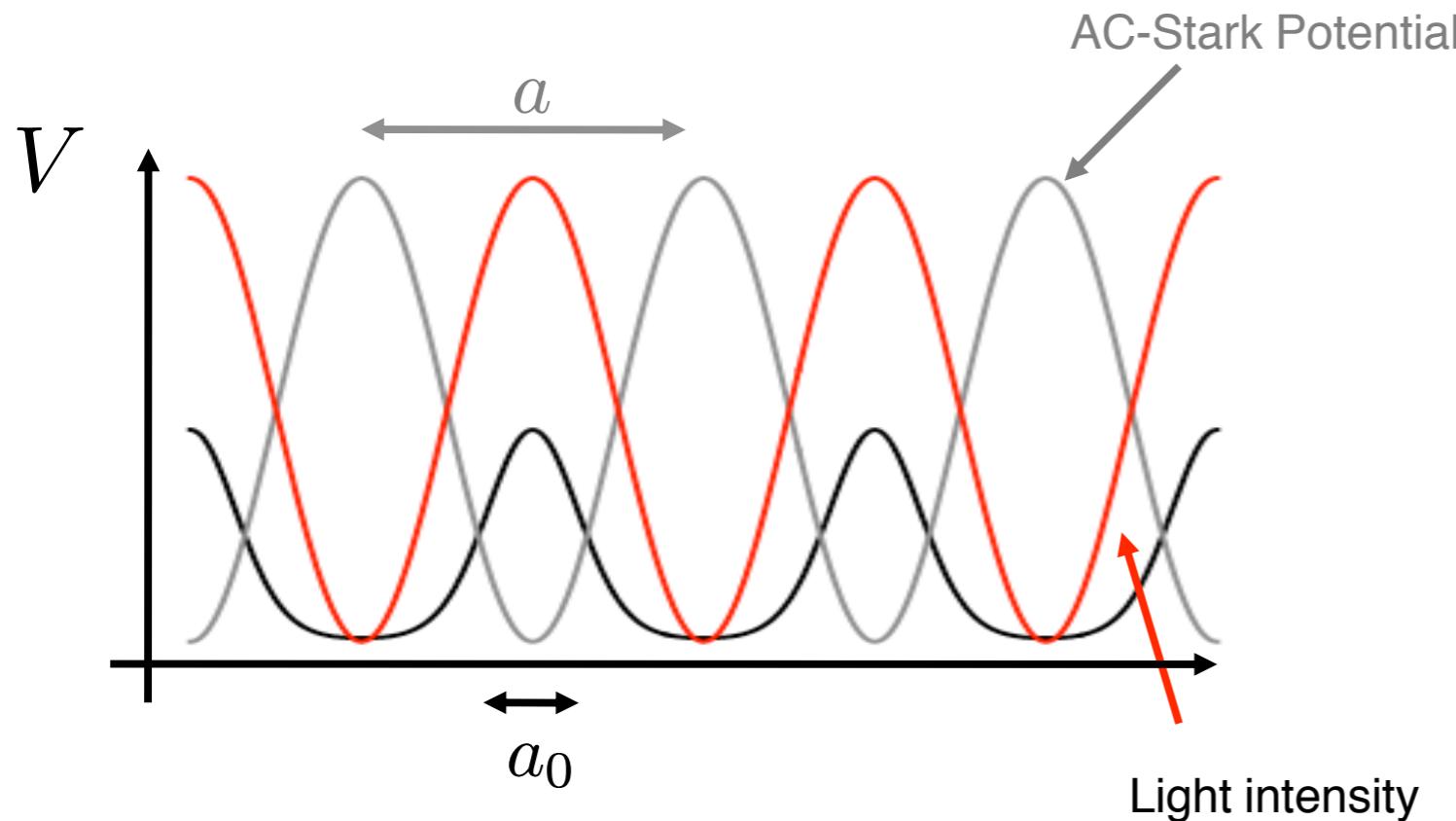
$$\begin{aligned} H_{\text{eff}} &= \frac{\hat{\mathbf{p}}^2}{2m} + \frac{|\Omega(\hat{\mathbf{x}})|^2}{4\Delta} - i\frac{1}{2}\frac{\Gamma|\Omega(\hat{\mathbf{x}})|^2}{4\Delta^2} \\ &\equiv \frac{\hat{\mathbf{p}}^2}{2m} + V_{\text{opt}}(\hat{\mathbf{x}}) - i\frac{\gamma(\mathbf{x})}{2}. \end{aligned}$$

AC-Stark shift      Decay

$$\mathcal{J}\rho = \Gamma \int d^2\mathbf{u} N(\mathbf{u}) \left[ e^{-ik_{eg}\mathbf{u}\cdot\hat{\mathbf{x}}} \frac{\Omega(\hat{\mathbf{x}})}{2\Delta} \right] \rho \left[ e^{ik_{eg}\mathbf{u}\cdot\hat{\mathbf{x}}} \frac{\Omega^*(\hat{\mathbf{x}})}{2\Delta} \right]$$

## Example: Red vs. Blue detuning, single atom

$$H = \frac{p^2}{2m} + \frac{|\Omega_0|^2}{4\Delta}$$



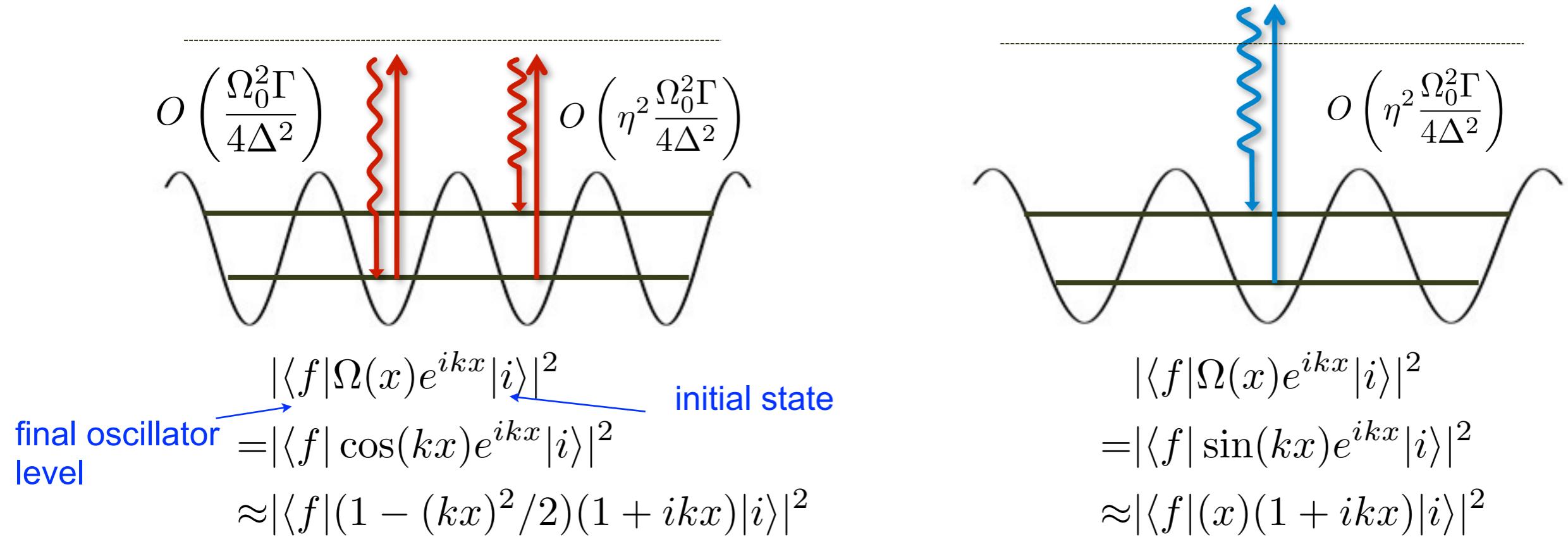
- Timescale for heating processes:

$$\Gamma_{\text{eff}} = \frac{\Omega_0^2}{4\Delta^2} \Gamma$$

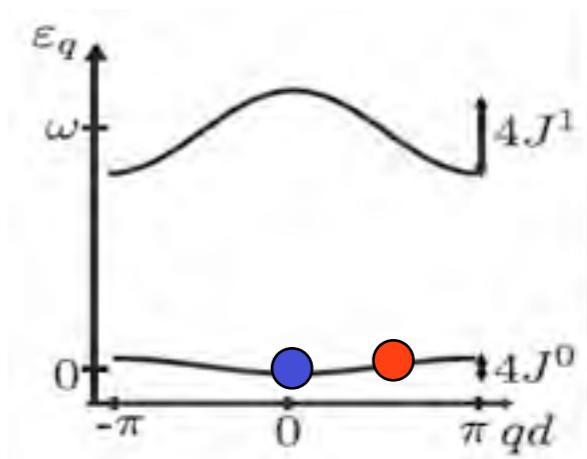
- Lamb-Dicke parameter:

$$\eta = \frac{\pi a_0}{a} = \left( \frac{1}{4V/E_R} \right)^{1/4}$$

- Harmonic oscillator approximation, Lamb-Dicke limit:  $\eta = \frac{\pi a_0}{a}$ ,  $kx = \eta(a + a^\dagger)$

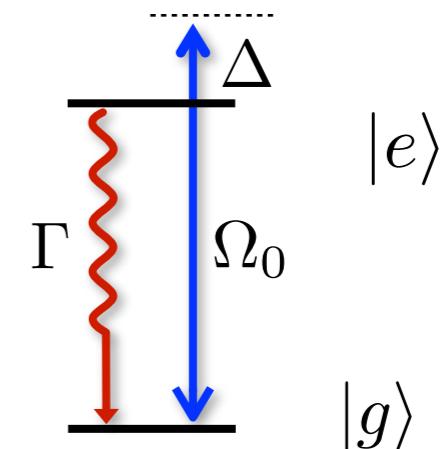
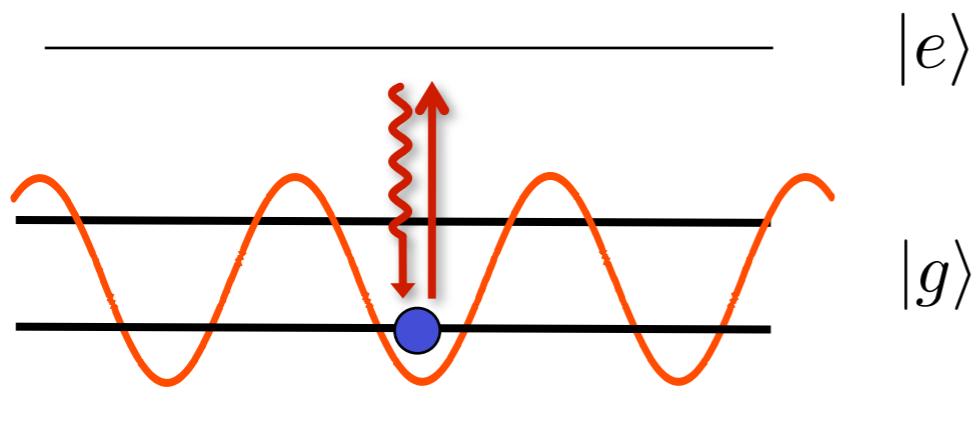


- General lattice: Lowest-band processes inelastic



- Time-dependence of the mean energy:  $\dot{E} = \frac{\Gamma |\Omega_0|^2}{4\Delta^2} E_R$

# Theoretical Description (many atoms)



- Spontaneous emissions from **two-level atoms**
- **Many-body** master equation for spontaneous emissions in Born-Markov approximation
- Limit of **large detuning** - eliminate excited state, obtain a description for motional states

$$\dot{\rho} = -i [\hat{H}, \rho] - \frac{1}{2} \frac{\Gamma}{4\Delta^2} \sum_{\mu} |\Omega_{0,\mu}|^2 \int d^3x \int d^3y F_{\mathbf{e}_\mu}(k(\mathbf{x} - \mathbf{y})) \epsilon_\mu(\mathbf{x}) \epsilon_\mu(\mathbf{y}) [\hat{\psi}^\dagger(\mathbf{x}) \hat{\psi}(\mathbf{x}), [\hat{\psi}^\dagger(\mathbf{y}) \hat{\psi}(\mathbf{y}), \rho]]$$

Many-body Hamiltonian  
(including optical potential)

multiple beams

bosonic field operator

$$F_{\mathbf{e}_\mu}(\xi) = \int d^2u \frac{3}{8\pi} (1 - (\mathbf{e}_\mu \cdot \mathbf{u})^2) e^{-i\mathbf{u}\cdot\xi}$$

- Can be extended, e.g., with additional exit channels for internal state

# Localisation due to spontaneous emission

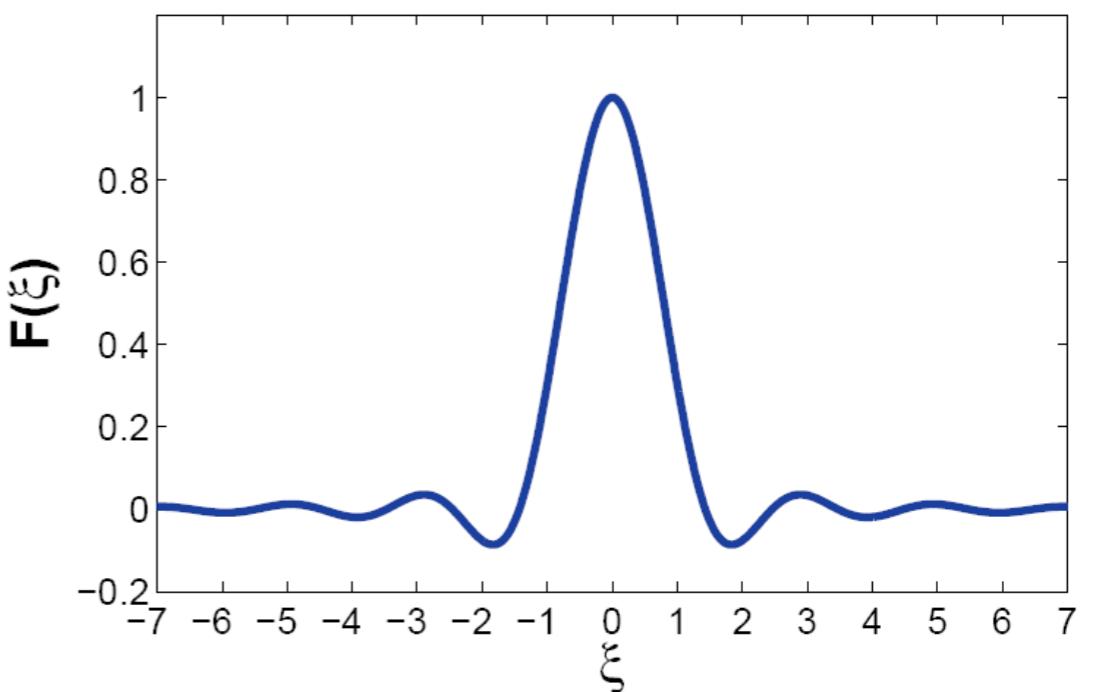
- Spontaneous emissions destroy long-range order by localising atoms



$$\dot{\rho} = -i [\hat{H}, \rho] - \frac{1}{2} \frac{\Gamma}{4\Delta^2} \sum_{\mu} |\Omega_{0,\mu}|^2 \int d^3x \int d^3y F_{\mathbf{e}_{\mu}}(k(\mathbf{x} - \mathbf{y})) \epsilon_{\mu}(\mathbf{x}) \epsilon_{\mu}(\mathbf{y}) [\hat{\psi}^{\dagger}(\mathbf{x}) \hat{\psi}(\mathbf{x}), [\hat{\psi}^{\dagger}(\mathbf{y}) \hat{\psi}(\mathbf{y}), \rho]]$$

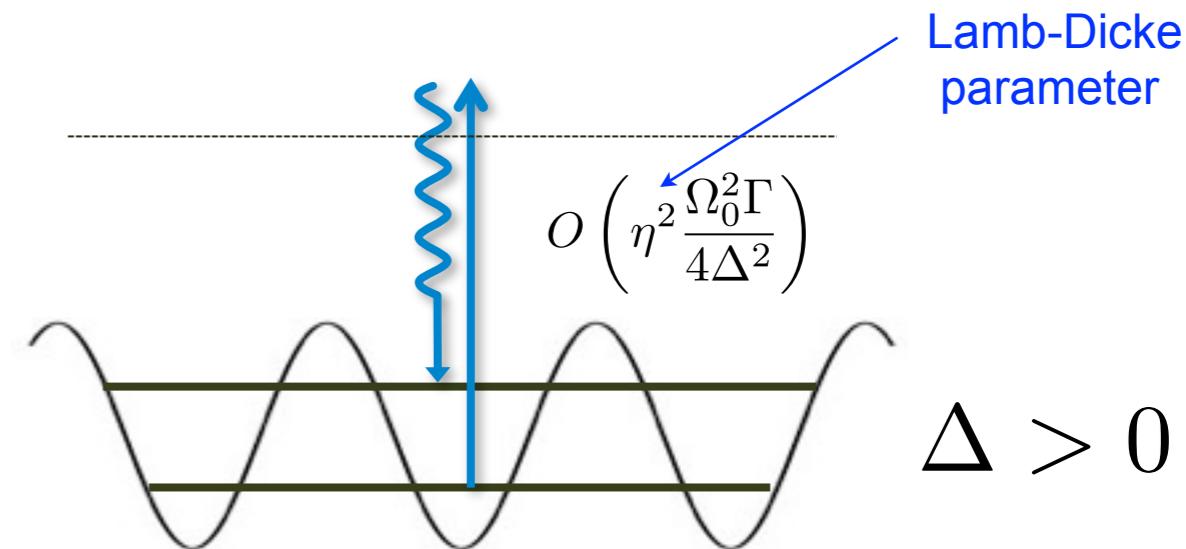
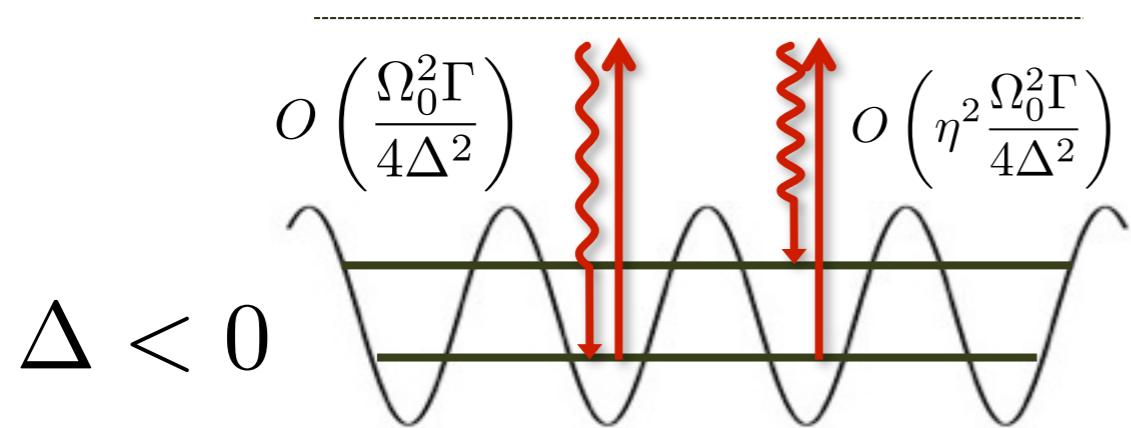
Many-body Hamiltonian  
(including optical potential)

$$F_{\mathbf{e}_{\mu}}(\xi) = \int d^2u \frac{3}{8\pi} (1 - (\mathbf{e}_{\mu} \cdot \mathbf{u})^2) e^{-i\mathbf{u} \cdot \xi}$$

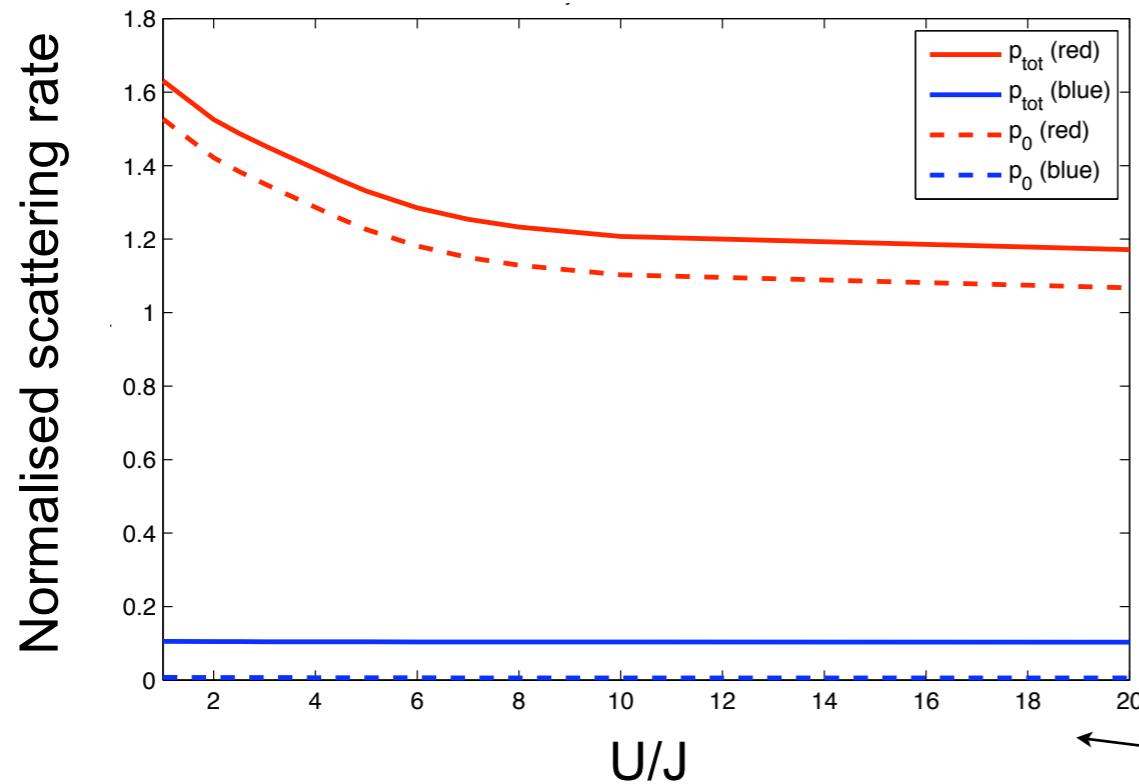


# Example: Red vs. Blue detuning

H. Pichler, A. J. Daley, P. Zoller, PRA 82, 063605 (2010)



- Red detuning gives rise to more spontaneous emission events in deep lattices
- Processes returning atoms to the lowest band are strongly suppressed for blue detuning
- Variation of total scattering rate with U/J  
(dashed lines: processes within lowest band)
- Total rate of energy increase is the same



$$\frac{d\langle \hat{H} \rangle}{dt} = \frac{\Gamma}{4\Delta^2} \sum_{\mu} |\Omega_{0,\mu}|^2 E_R N_{\text{tot}}$$

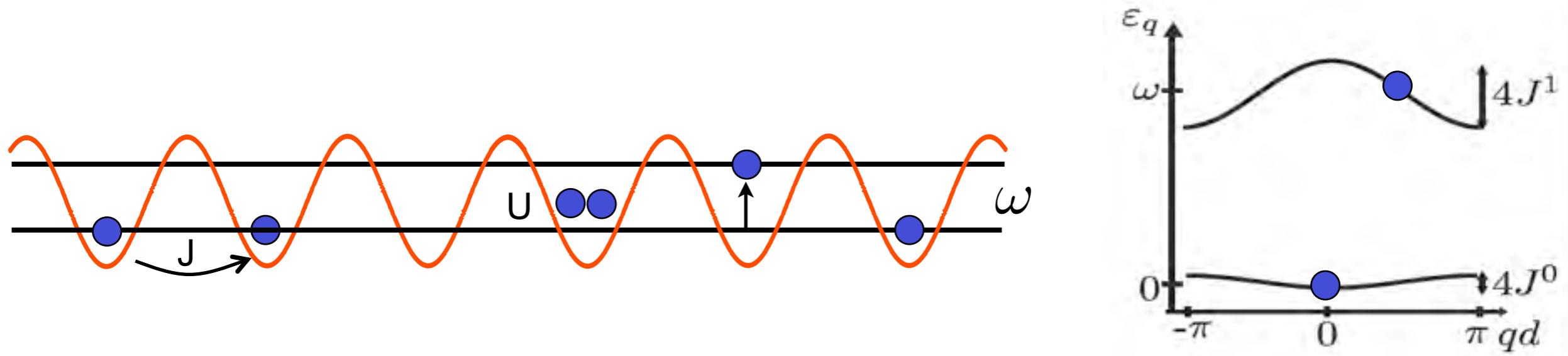
recoil energy      number of atoms

Estimates using many-body ground states from t-DMRG,  
typical parameters for Rb

# Heating of many-body states

H. Pichler, A. J. Daley, P. Zoller, PRA **82**, 063605 (2010)

- Rate of energy increase is not a complete characterisation, as the system will **not thermalise on experimental timescales**

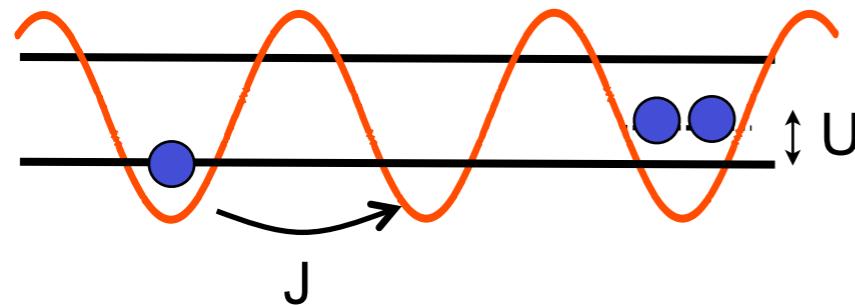


- This is particularly true of **atoms excited to higher bands**, where

$$\omega \gg U, J$$

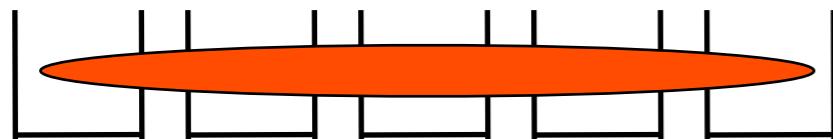
[possibility of thermalisation in the lowest band, see later, and also  
c.f. “thermal” momentum distributions in S. Trotzky et al., Nature Phys. **6**, 998 (2010)]

- To understand change in the many-body state we should examine the **characteristic correlation functions** and see how order is destroyed by heating



$$\hat{H} = -J \sum_{\langle i,j \rangle} b_i^\dagger b_j + \frac{U}{2} \sum_i \hat{n}_i (\hat{n}_i - 1)$$

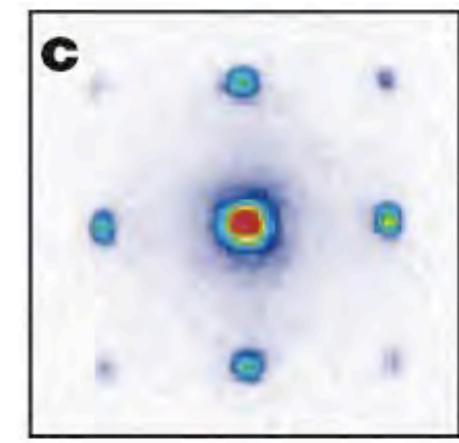
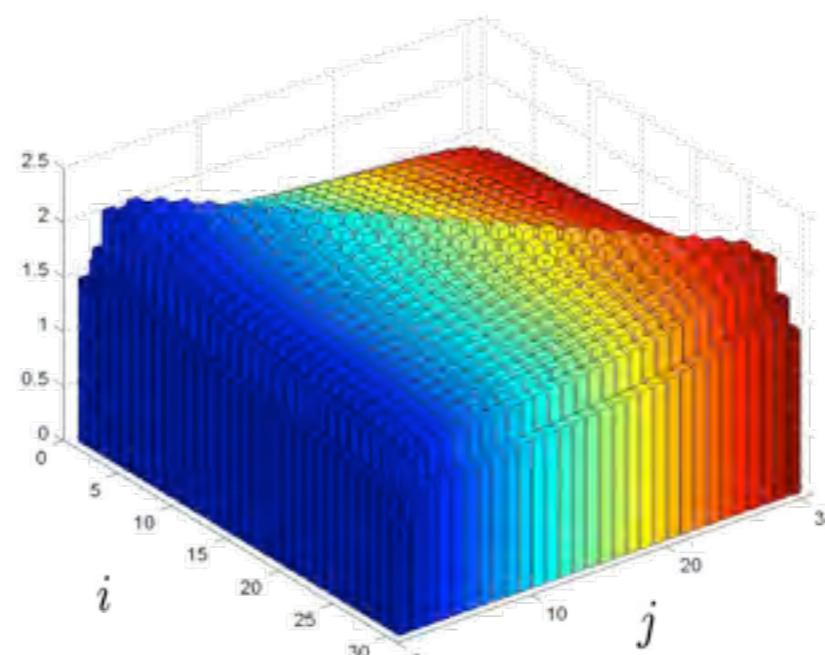
- **Superfluid**  $J \gg U$



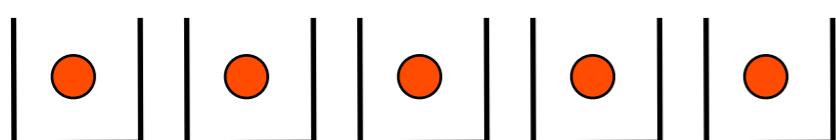
delocalised atoms: BEC

$$\langle b_i^\dagger b_j \rangle$$

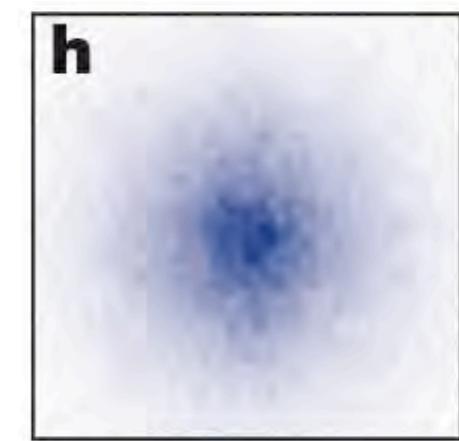
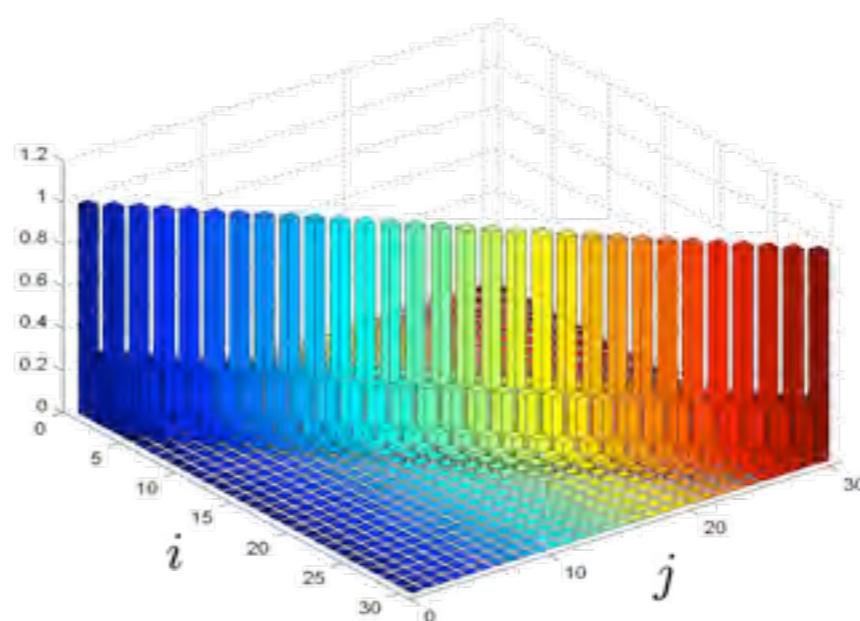
Momentum Distribution



- **Mott Insulator**  $J \ll U$



"atoms lower their energy by minimising the number of atoms per site"

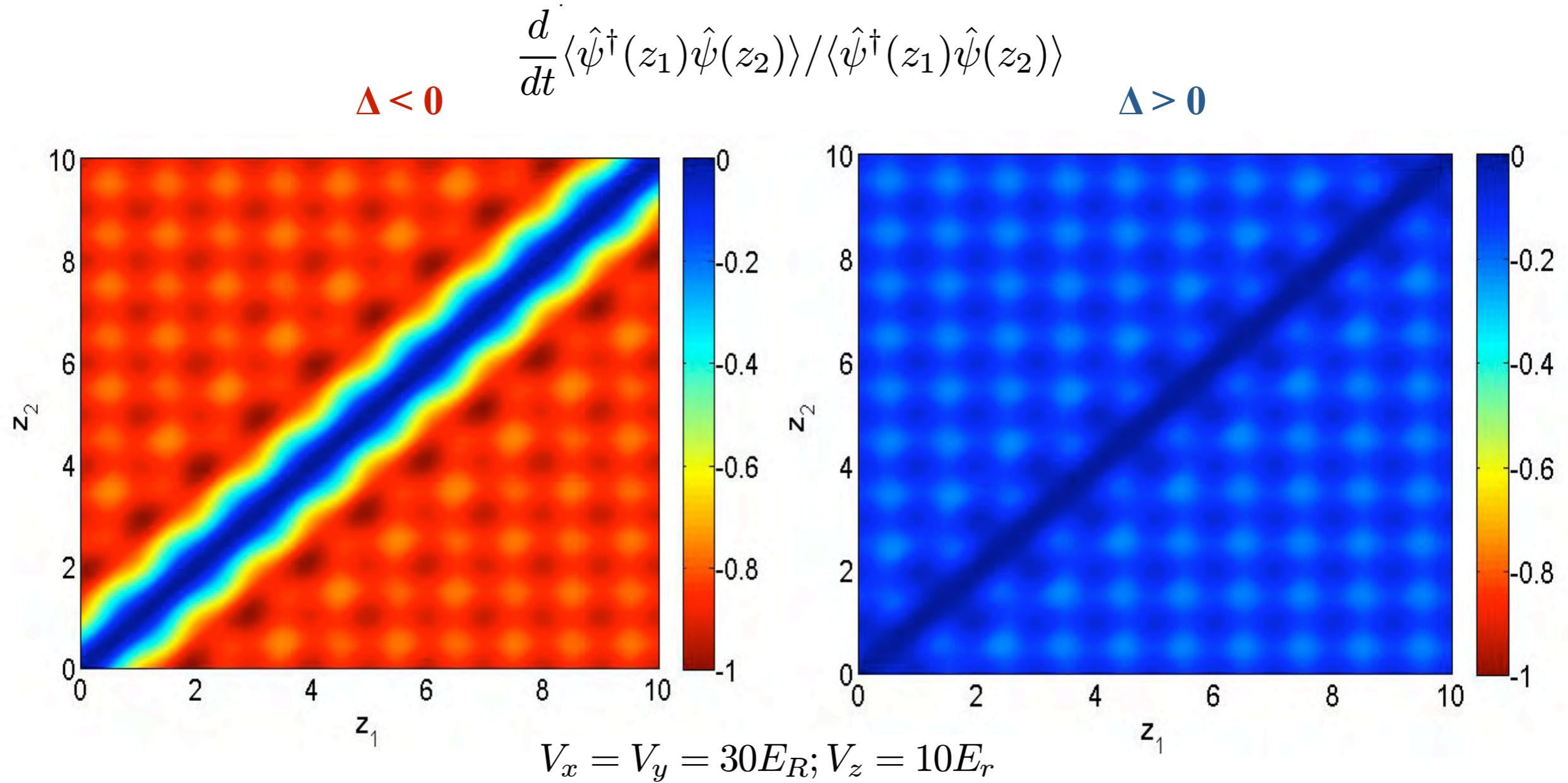


(Greiner et al., Nature '02)

# Decay of characteristic correlations

H. Pichler, A. J. Daley, P. Zoller, PRA **82**, 063605 (2010)

- 1st order perturbation theory calculation (in  $\Gamma_{\text{eff}}/J$ ), neglecting interactions after a spontaneous emission event:



- Red-detuned lattice: More scattering events, more rapid localisation
- Interaction dependence: Superfluid order strongly affected, Mott Insulator relatively robust

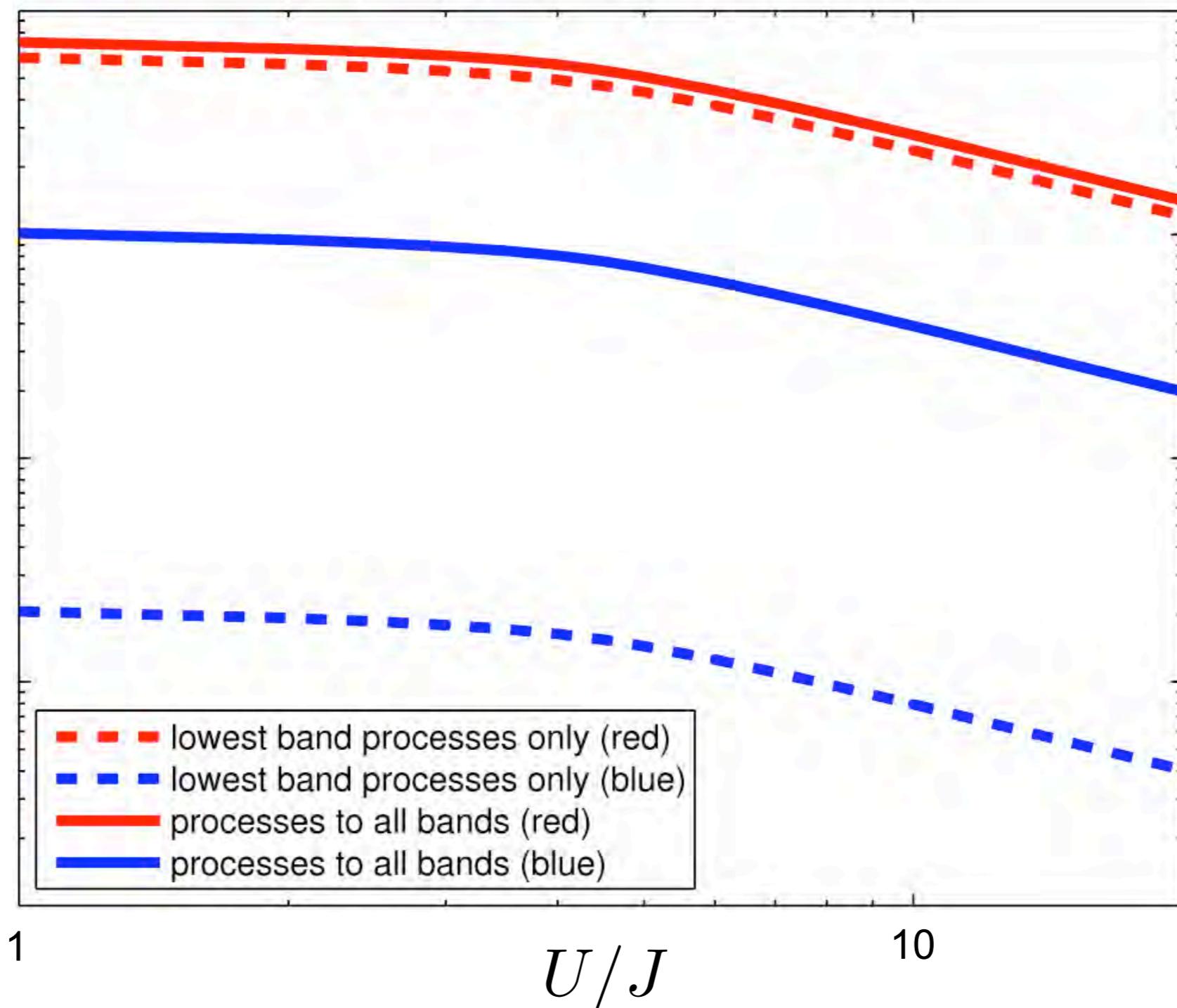
# Decay of characteristic correlations

H. Pichler, A. J. Daley, P. Zoller, PRA **82**, 063605 (2010)

- Interaction dependence: Superfluid order strongly affected, Mott Insulator relatively robust
- 1st order perturbation theory calculation (in  $\Gamma_{\text{eff}}/J$ ), neglecting scattering after loss:

$$\frac{d}{dt} \langle b_{0,i}^\dagger b_{0,i+1}^\dagger \rangle$$

(normalised to  
total decay rate,  
logarithmic scale)



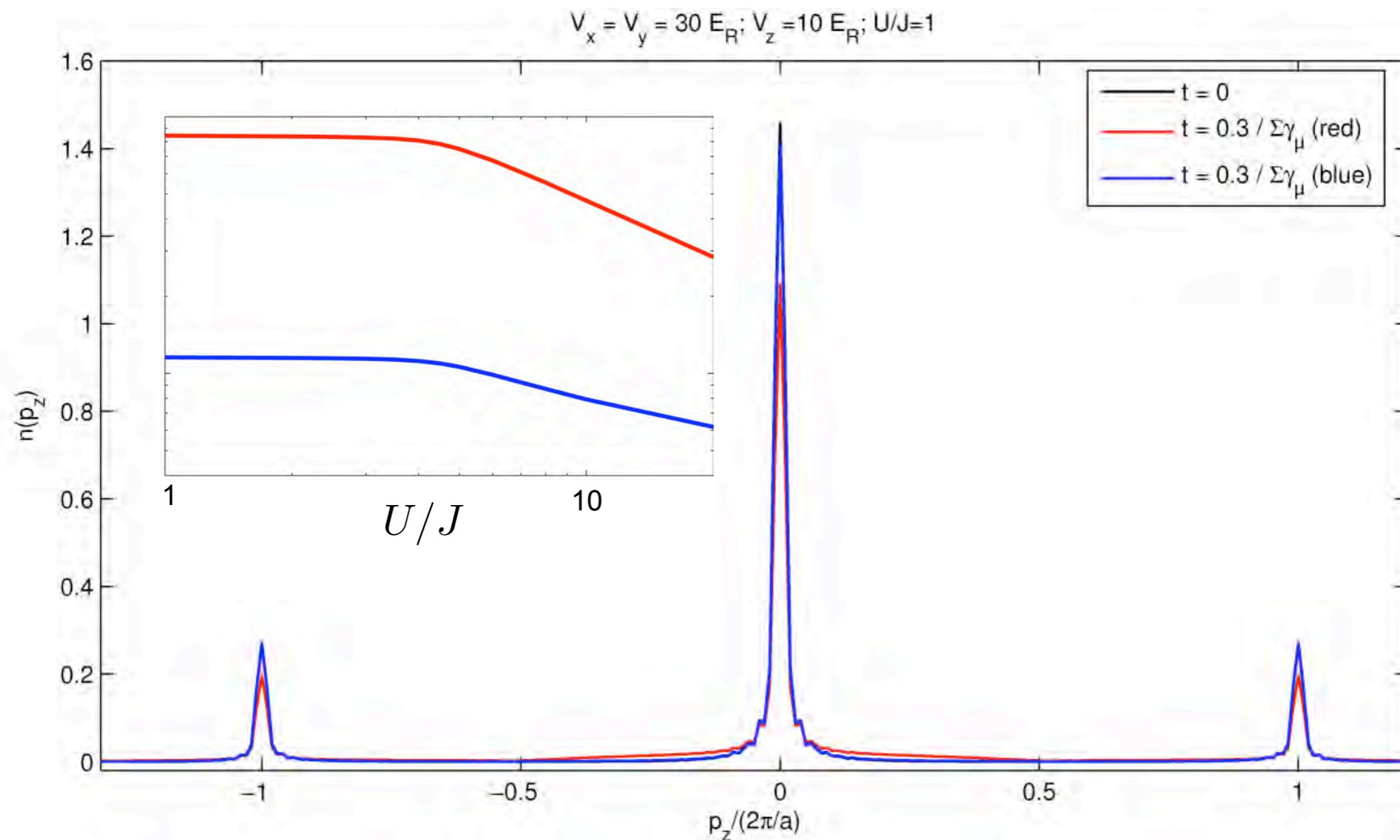
Computed using ground states in a quasi-1D lattice from t-DMRG calculations.

$V_x = V_y = 30 E_R$ ;  $V_z = 10 E_R$ ; ( $J_z = 0.0192 E_R$ )

# Momentum Distributions

H. Pichler, A. J. Daley, P. Zoller, PRA **82**, 063605 (2010)

- We compute the corresponding decay rates of the characteristic peaks in the momentum distributions from a superfluid state (inset: decay rate, central peak)

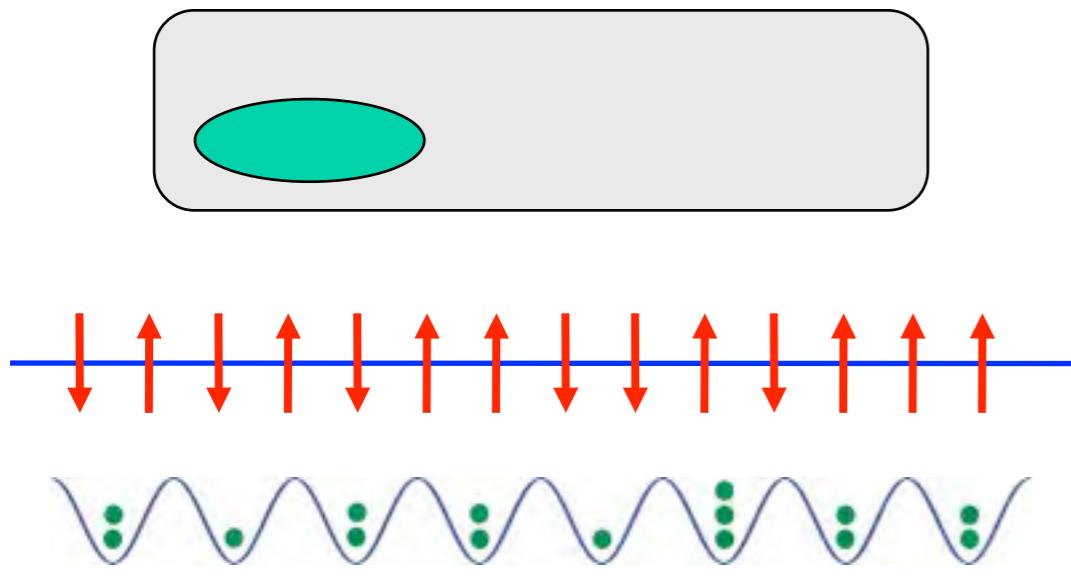


# Time-dependent dynamics in 1D: t-DMRG + Quantum Trajectories

A. J. Daley et al., Phys. Rev. Lett **102**, 040402 (2009).

## t-DMRG Algorithm

- Integration of many-body Schrödinger eq. in 1D on reduced Hilbert space.



- Works in 1D, near equilibrium
- Compute ground states / time evolution
- Direct determination of dynamics for typical experimental parameters

## Quantum Trajectories

$$\dot{\rho} = -i[H, \rho] - \frac{\Gamma}{2} \sum_m [c_m^\dagger c_m \rho + \rho c_m^\dagger c_m - 2c_m \rho c_m^\dagger]$$

- Developed to treat master equations (H. Carmichael; K. Mølmer, Y. Castin, J. Dalibard; C. Gardiner & P. Zoller)
- Evolve stochastic trajectories (states)

$$H_{\text{eff}} = H - i \frac{\Gamma}{2} \sum_m c_m^\dagger c_m$$

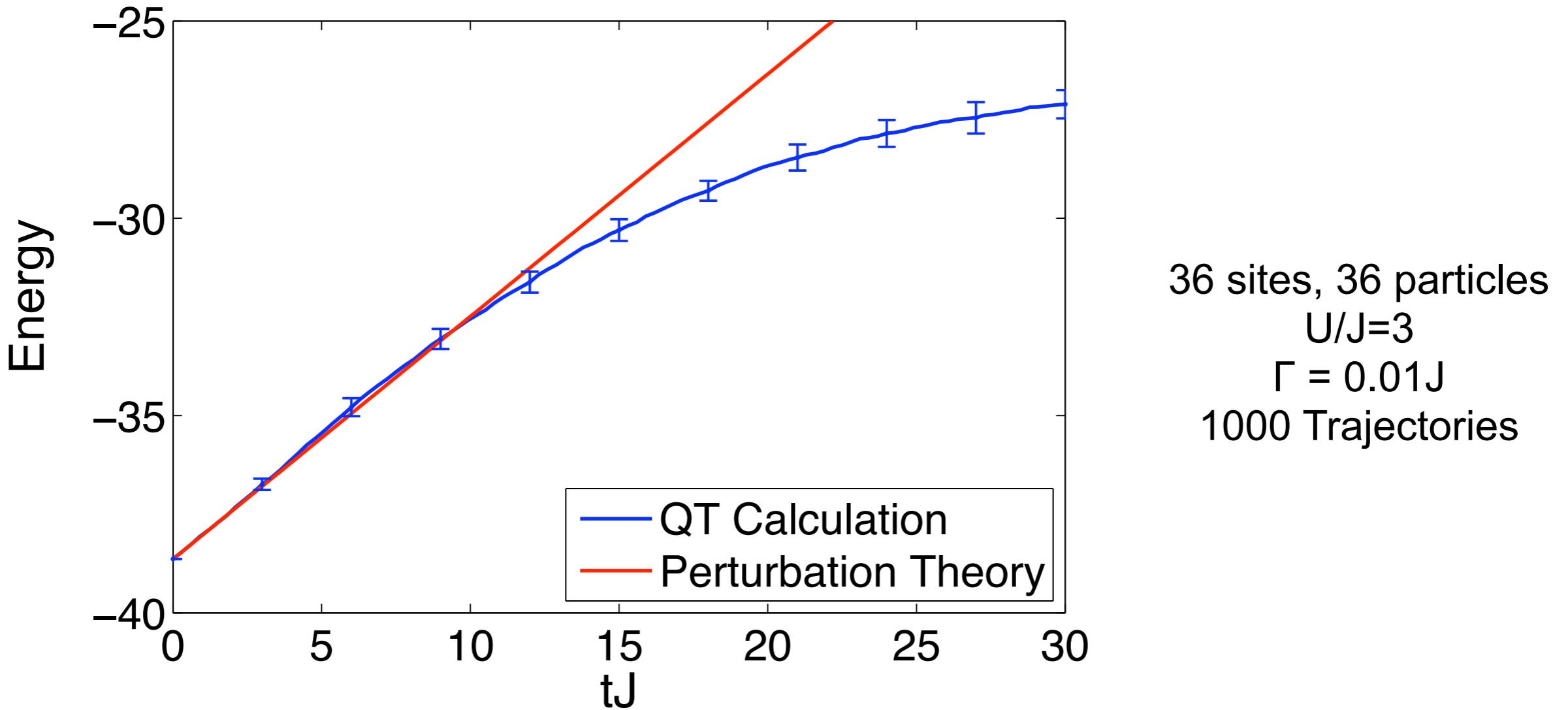
- Quantum Jumps

$$|\psi\rangle = \frac{c_m |\psi\rangle}{||c_m |\psi\rangle||}$$

- Norm decays below random threshold
- Jump operator chosen randomly
- Expectation values by stochastic average.

## Full time-dependent calculation for heating (here: lowest band)

- Time-dependent DMRG + Quantum trajectories calculation



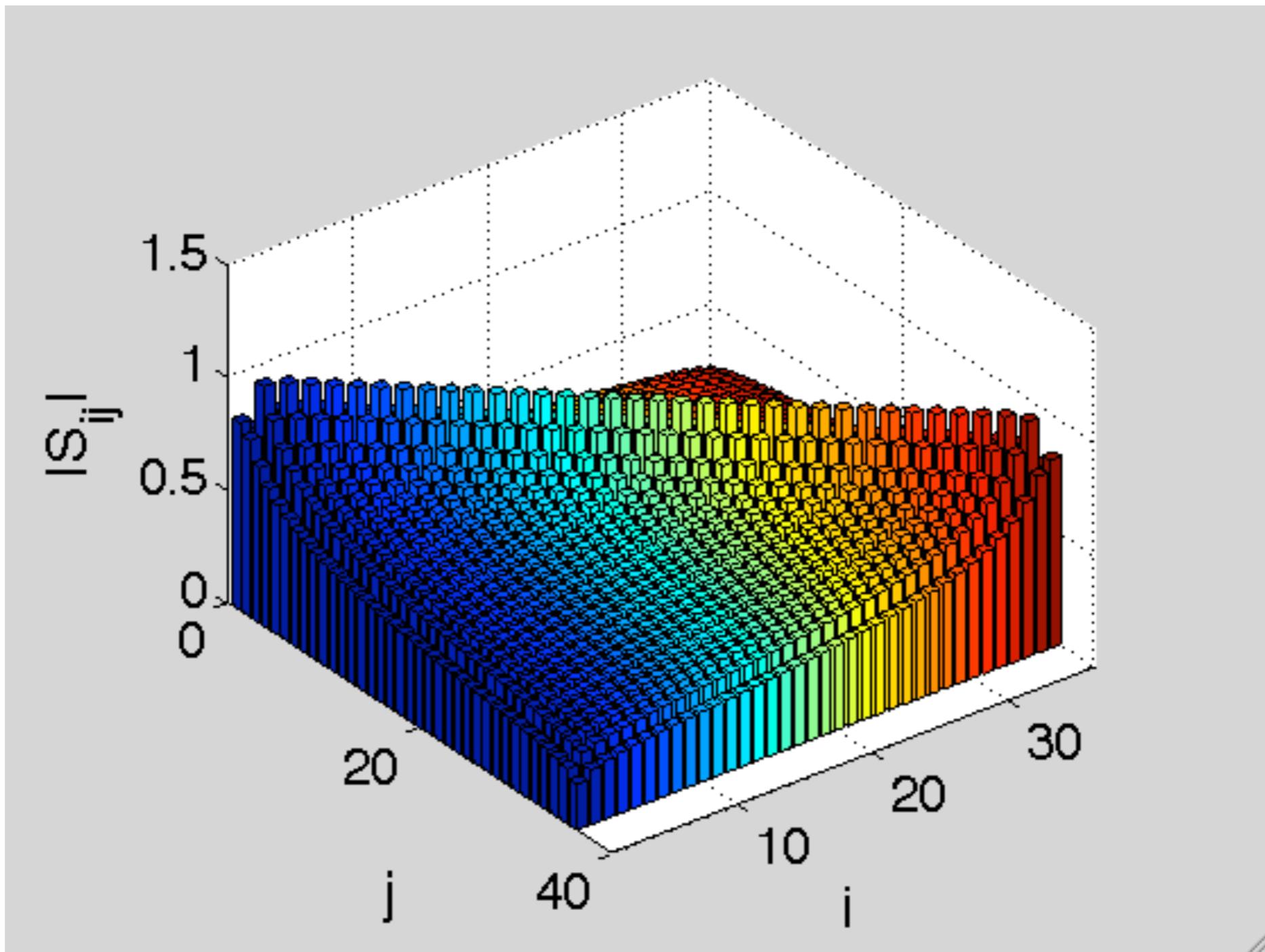
Here: we use master equation in lowest order approximation, neglecting off-diagonal terms

$$\dot{\rho} = -i [\hat{H}, \rho] + \sum_{\mathbf{n}, \mu} \gamma_{\mathbf{n}, \mu} \left( b_{\mathbf{n}, i}^\dagger b_{0, i} \rho b_{0, i}^\dagger b_{\mathbf{n}, i} - \frac{1}{2} b_{0, i}^\dagger b_{\mathbf{n}, i} b_{\mathbf{n}, i}^\dagger b_{0, i} \rho - \rho \frac{1}{2} b_{0, i}^\dagger b_{\mathbf{n}, i} b_{\mathbf{n}, i}^\dagger b_{0, i} \right)$$

band      site

## Decay of correlations during heating

$$\langle |b_{0,i}^\dagger b_{0,j}| \rangle$$

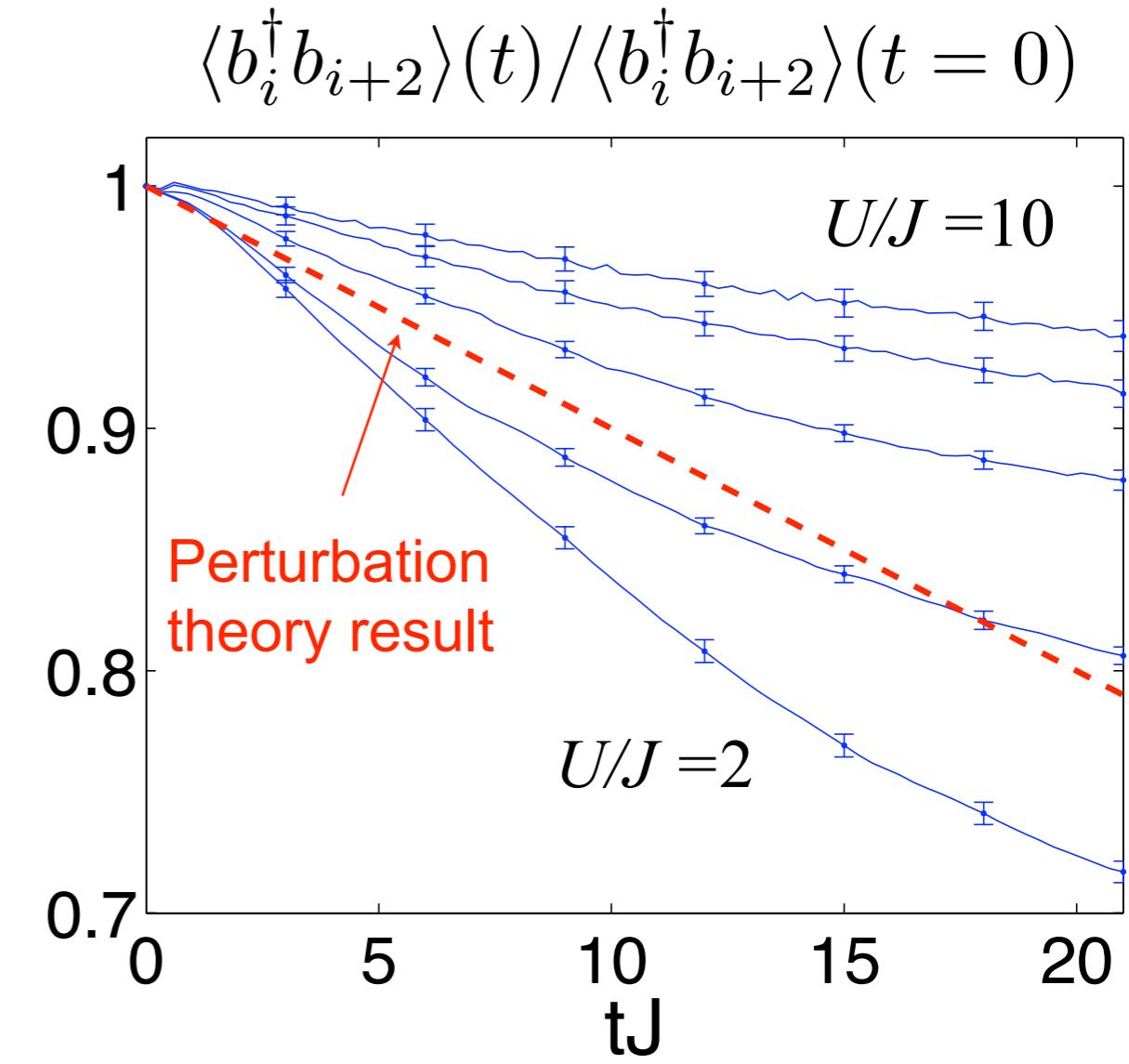
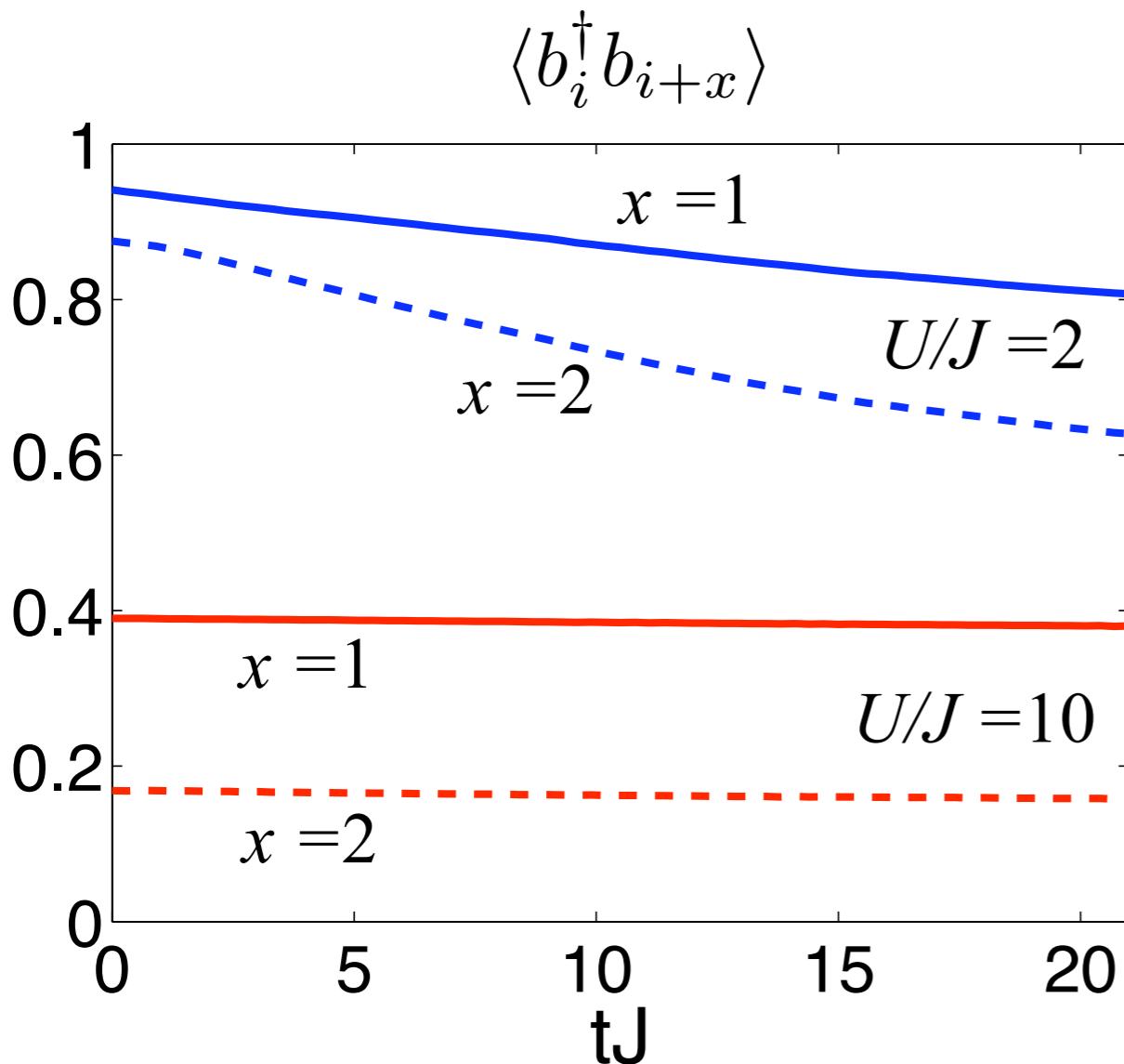


36 sites, 36 particles,  $U/J=3$ ,  $\Gamma = 0.01J$   
1000 Trajectories, total time  $tJ=30$

# Decay of correlations during heating

H. Pichler, A. J. Daley, P. Zoller, PRA **82**, 063605 (2010)

- Time-dependent DMRG + Quantum trajectories calculation:  
Dynamics beyond the perturbation theory result, including (partial) thermalisation
- (Partial) thermalisation leads to more rapid decay of correlations in SF
- Mott Insulator is even more robust



36 sites, 36 particles  
 $U/J=3, \Gamma = 0.01J$   
 1000 Trajectories

## Work in progress...

- Thermalisation of Bosons
- Light-assisted collisions
- Heating of Fermions via spontaneous emissions
- Amplitude and position fluctuations and heating

# Heating due to spontaneous emissions - further work in progress.....

## Light-assisted collisions for Bosons

- Trade-off between heating due to spontaneous emissions, and light assisted collisions in blue-detuned lattices.

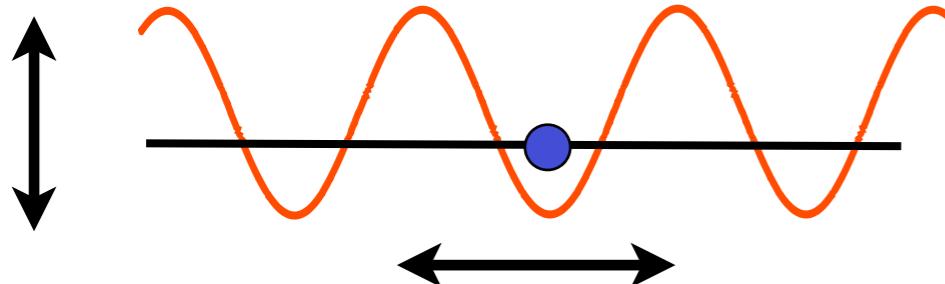
## Heating of Fermions via spontaneous emissions

- Additional physics of internal states, spin flips / spin coherence in spontaneous emissions (coherence of nuclear spins in Li / Sr / Yb can be preserved if laser is far-detuned)
- Robustness of Mott insulator is probably good news for quantum magnetism (e.g., AF phase), *provided spontaneous emissions do not affect spin coherence*

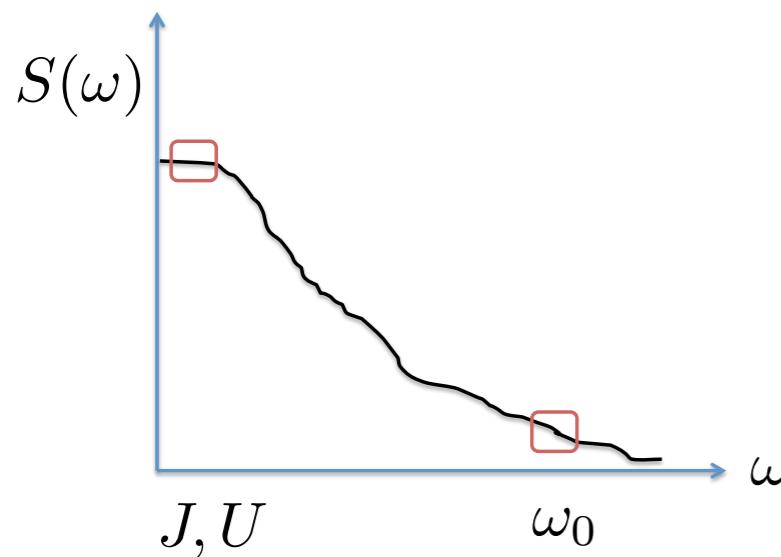


- Example Questions:
  - What happens in the weakly-interacting limit?
  - What happens away from half-filling?
  - What happens when spin coherence is not perfectly maintained?

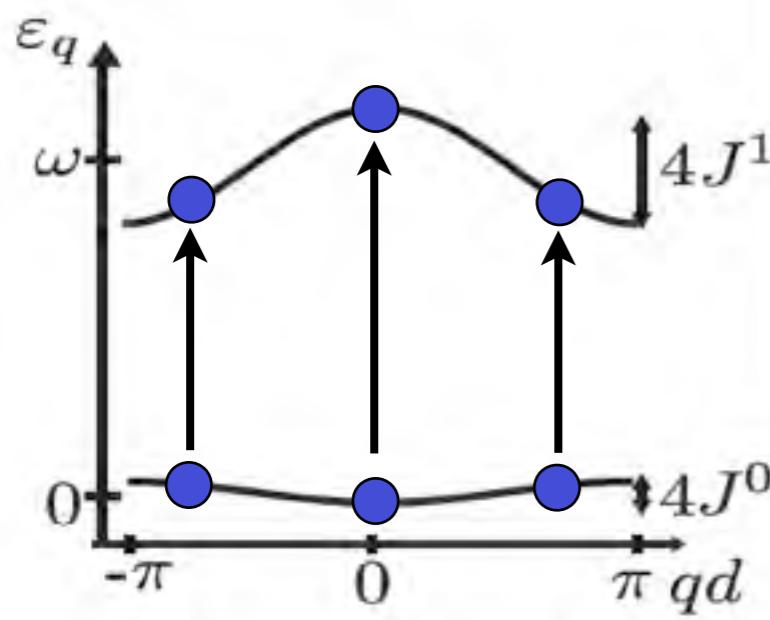
# Heating due to classical noise on the lattice potential



- Amplitude noise from intensity fluctuations
- Position noise, e.g., from jittering optics



- Form of the noise spectrum dependent on experiment.
- Transitions/heating determined by noise spectrum around  $J, U$  (intraband) and the bandgap ( $\omega_0$ , interband)



- Spatially uniform noise - single particle transitions do not change the quasimomentum
- Heating of the system due to interband transitions relies on thermalisation between bands
- In progress: Stochastic differential equation + t-DMRG analysis

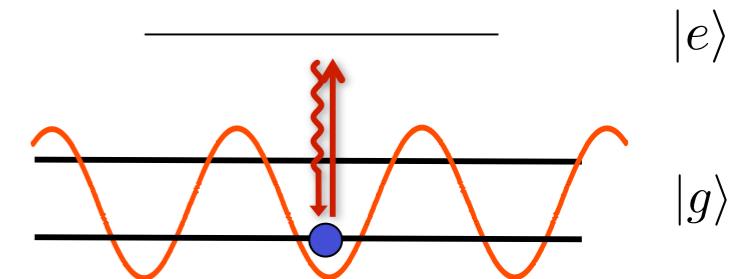
# Summary / Outlook

## Heating of many-body states

- Depends strongly on the **many-body state**
- Intrinsically **non-equilibrium system**
- **Mean energy is not sufficient** to characterise change in many-body properties

## Heating of bosons due to spontaneous emissions

- Breakdown of long-range order in SF due to localisation
- Stronger in red-detuned lattices (more scattering events)
- MI affected only by (rare) transitions to higher bands



## Outlook:

- Thermalisation in the presence of heating (?)
- Potential for trade-off with light-assisted collisions in blue-detuned lattice
- Investigation of heating due to amplitude/phase fluctuations on lattice
- Heating of Fermions