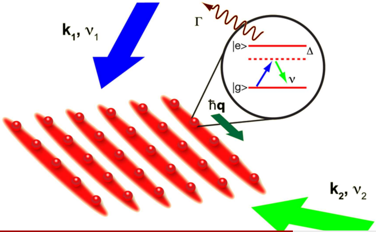
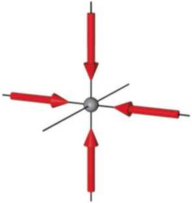
QMC Simulations of Systems of Cold Atoms

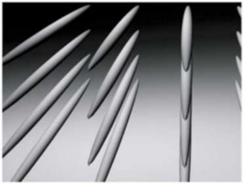
Peter Pippan

TU Graz

Hallstatt 28.9.2009



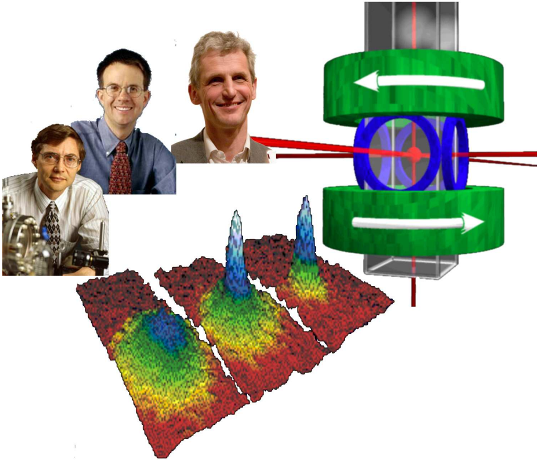




What experimentalists can do:

Cooling atom cloud in magneto-optical-traps (MOTs)

- Bose Einstein condensation
  Nobel Prize 2001, Cornell, Ketterle & Wieman



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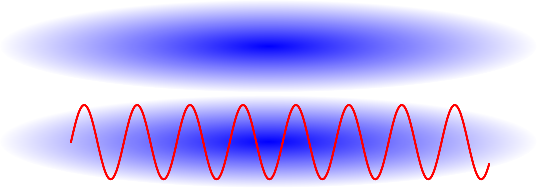
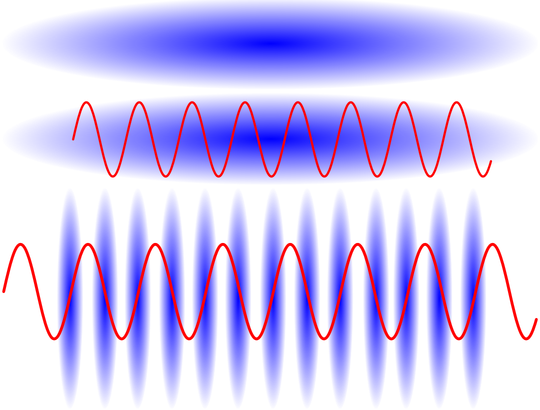
- two counterpropagating laser beams



What experimentalists can do:

- Bose-Einstein condensate in a MOT
- two counterpropagating laser beams
- act as lattice potential



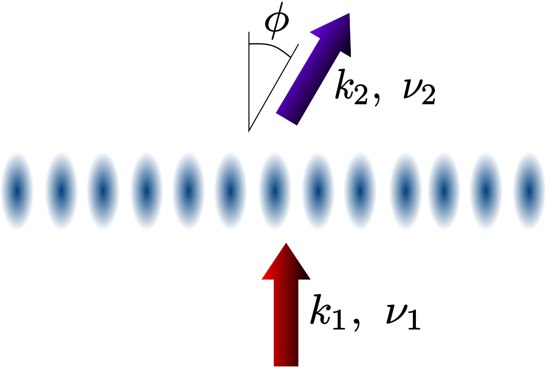
- Simulation of lattice models.
- Mott insulator to superfluid transition

Greiner et al., Nature 415, 39 (2002)

- Ultimate goal: Simulation of fermionic Hubbard model.

What experimentalists can do:

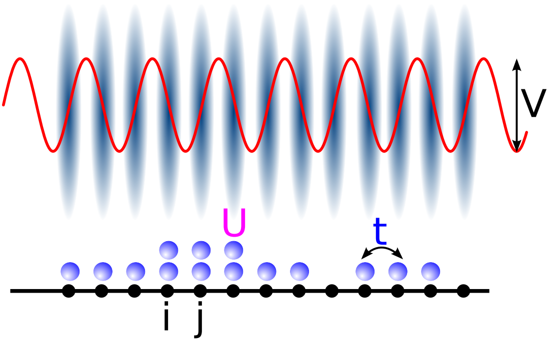
- Basic Excitations of quantum systems can be studied.
- e.g. by 2 photon Bragg spectroscopy.



Clément *et al.*, PRL 102, 155301 (2009)

Fabbri *et al.*, PRA 79, 043623 (2009)

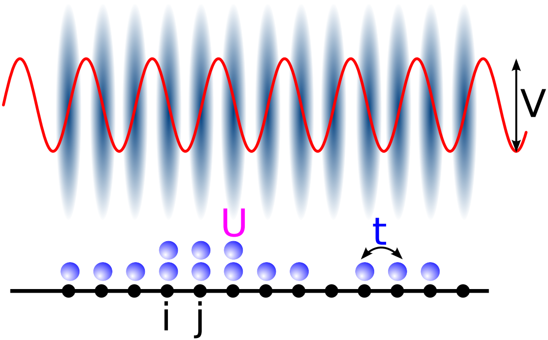
The Bose Hubbard model



- $a_i^\dagger, a_j$: bosonic creation and annihilation operators $[a_i, a_j^\dagger] = \delta_{i,j}$

$$H^{BH} = -t \sum_{\langle i,j \rangle} (a_i^\dagger a_j + h.c) + \frac{U}{2} \sum_i n_i(n_i - 1) + \sum_i \mu n_i$$

The Bose Hubbard model

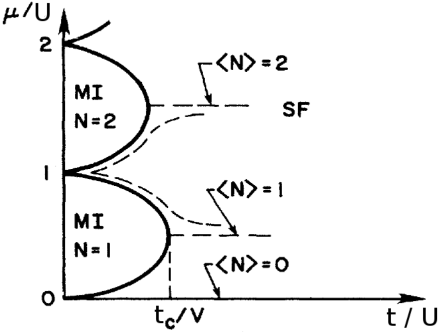


- $a_i^\dagger, a_j$: bosonic creation and annihilation operators $[a_i, a_j^\dagger] = \delta_{i,j}$
- parameters t and U can be well controlled by potential depth V.

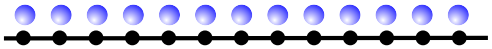
$$H^{BH} = -t \sum_{\langle i,j \rangle} (a_i^\dagger a_j + h.c) + \frac{U}{2} \sum_i n_i(n_i - 1) + \sum_i \mu n_i$$

Phase Transition: Superfluid to Mott insulator

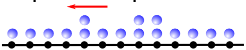
$$H^{BH} = -t \sum_{\langle i,j \rangle} (a_i^\dagger a_j + h.c) + \frac{U}{2} \sum_i n_i(n_i - 1) - \sum_i \mu n_i$$



- Mott insulator: $\langle n_i \rangle$ = const



- Superfluid phase:



- Lobe tips: particle hole symmetry, $z = 1$

Fisher *et al.*, PRB **40**, 546 (1989)

Stochastic series expansion (SSE)

- Evaluation of partition sum $Z = \text{Tr}\exp(-\beta H)$

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- Taylor expansion: $Z = \sum_\alpha \sum_{n=0}^{\infty} \frac{(-\beta)^n}{n!} \langle\alpha|H^n|\alpha\rangle$
- $H = \sum_b H_b$ with H_b acting on one bond.
- e.g.: $H = \hat{a} + \hat{b}$, $H^2 = \hat{a}\hat{a} + \hat{a}\hat{b} + \hat{b}\hat{a} + \hat{b}\hat{b}$
- Denote each term in H^n as index sequence $S_n = (b_1, \ldots, b_n)$

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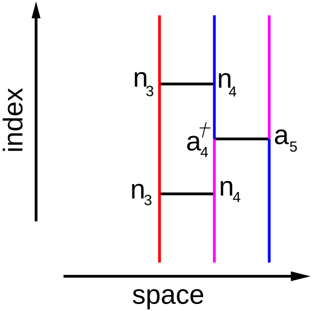
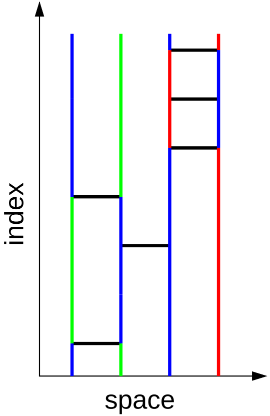
$$Z = \sum_\alpha \sum_{n=0}^{\infty} \sum_{S_n} \frac{(-\beta)^n}{n!} \langle\alpha| \prod_{i=1}^{n} H_{b_i} |\alpha\rangle$$

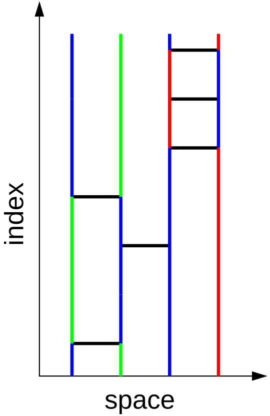


Resembles path integral in space and time.

Efficient sampling of partition sum

$$Z = \sum_{\alpha} \sum_{n=0}^{\infty} \sum_{S_n} \frac{(-\beta)^n}{n!} \langle \alpha | \prod_{i=1}^{n} H_{b_i} | \alpha \rangle$$





Directed loop algorithm

Sandvik, Syljuasen, PRE 66,046701 (2002)

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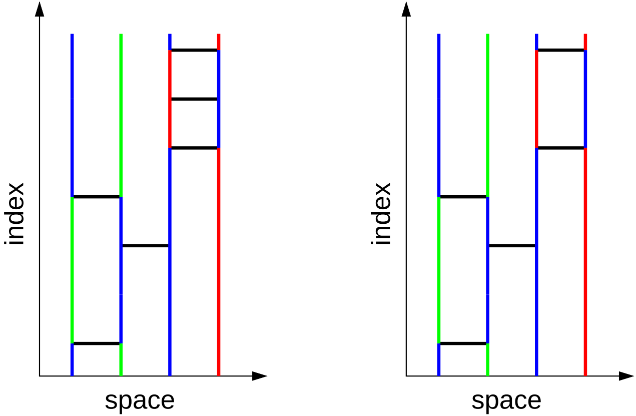

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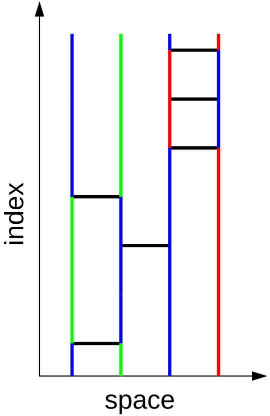

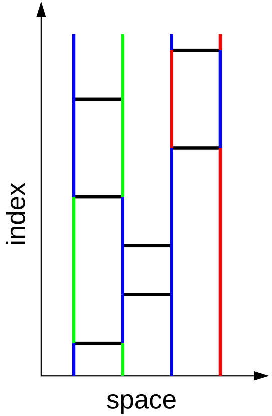

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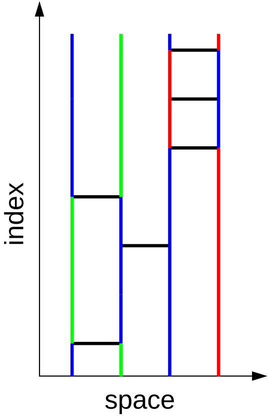

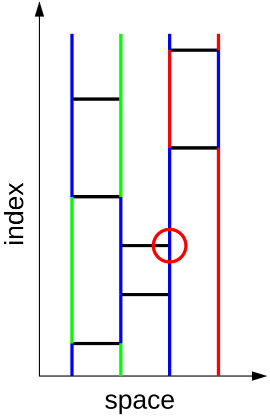

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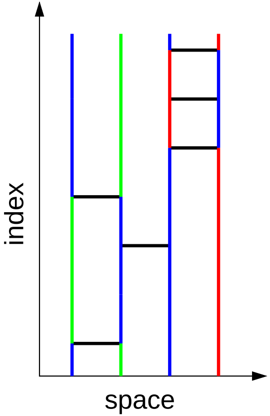

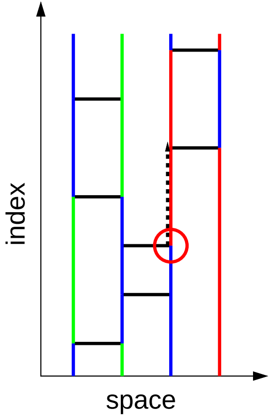

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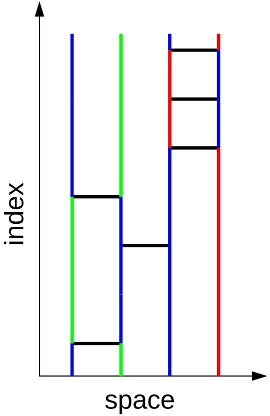

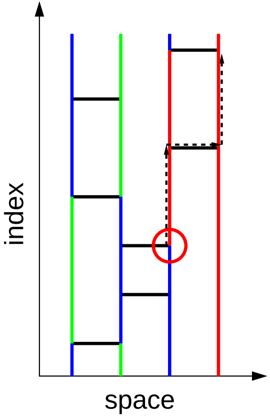

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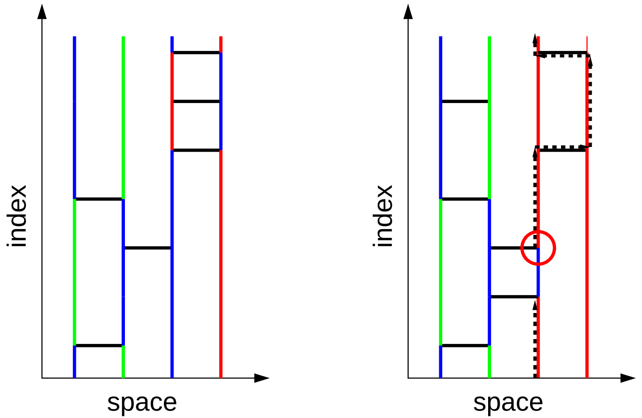

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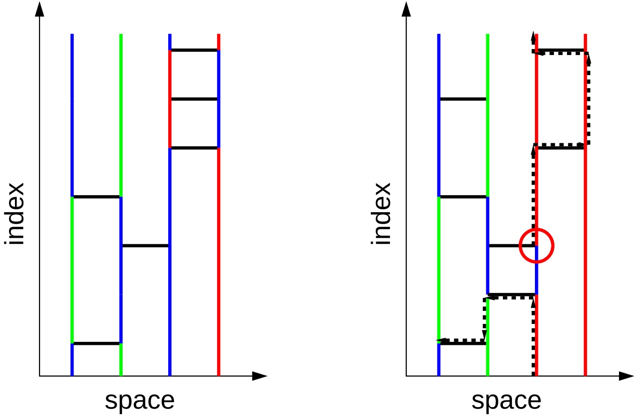

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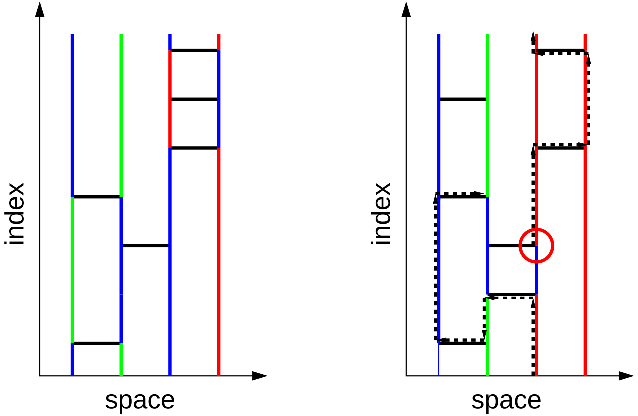

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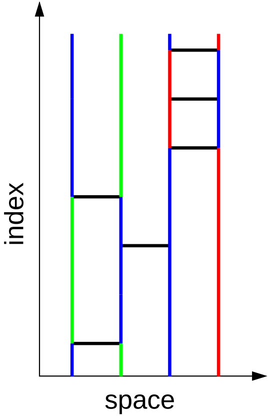

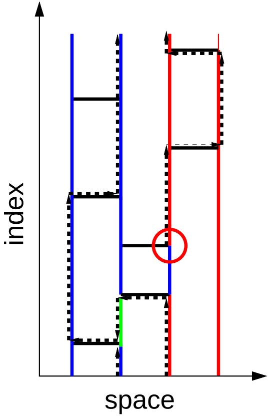

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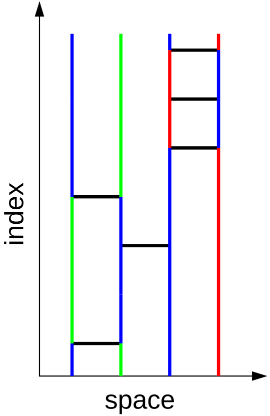

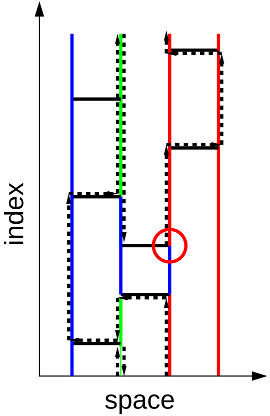

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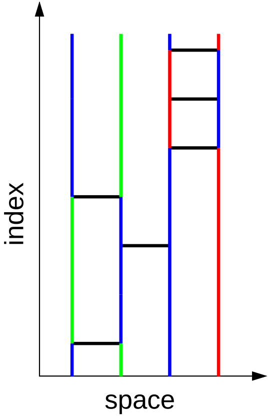

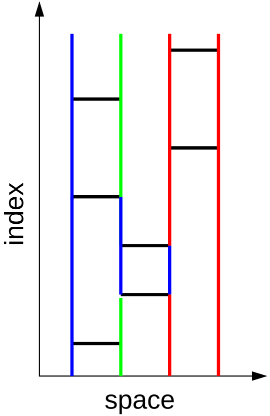

Directed loop algorithm

Sandvik, Syljuasen, PRE 66,046701 (2002)

Other non local update schemes:

- Loop Algorithm

  H.G. Evertz, Adv.Phys. 52, 1-66 (2003)

- Worm algorithm

  Worms: Prokof'ev *et al* JETP 87, 311 (1998)

What can be done?

- No Critical Slowing Down
  1 million sites instead of O(100), $T = t/1000$ instead of $t/10$
- Ground state and thermodynamic properties, Quantum Phase transitions, Dynamical properties, ...

Limitations

- Frustration
- Fermions $d > 1$ ($\rightarrow$ det-QMC)

Dynamics

Dynamical quantities

- Dynamic structure factor

$$S(k,\omega) = \frac{1}{L}\sum_{n,m}\frac{e^{-\beta E_n}}{Z}\left|\langle m|\,\hat{n}_k\,|0\rangle\right|^2\delta[\omega-(E_m-E_n)]$$

describes propagation of particle – hole pairs.

- Single particle spectral function

$$A(k,\omega) = \sum_{m,n}\frac{e^{-\beta E_n}}{Z}\left|\langle m|\,\hat{a}_k^\dagger\,|0\rangle\right|^2\delta[\omega-(E_m-E_n)]$$

describes propagation of particle (or holes)

Dynamics

QMC measurement of $S(k,\omega)$ and $A(k,\omega)$

- Measurement of correlation functions
  $\langle \hat{n}_i(\tau)\hat{n}_j(0)\rangle$, and $\langle \hat{a}_i(\tau)\hat{a}_j^\dagger(0)\rangle$
- Inversion of

$$\langle \hat{n}_k(\tau)\hat{n}_{-k}(0)\rangle = \int d\omega S(k,\omega)\frac{\exp(-\tau\omega)}{1+\exp(-\omega\beta)}$$

via Maximum entropy method

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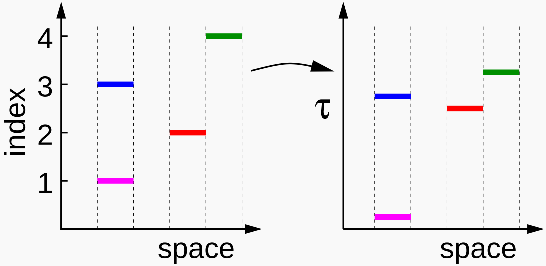
But:

- It is cumbersome to measure time dependent correlations in the SSE representation.

Mapping to imaginary time

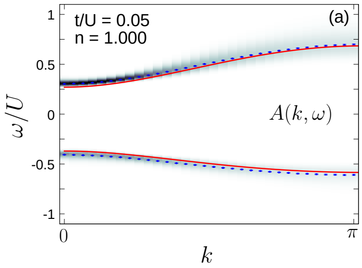
Equivalence: SSE – worldline picture

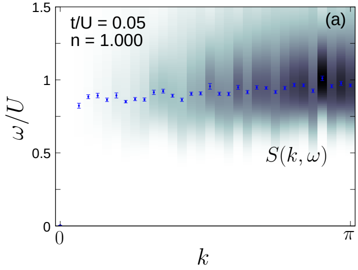


Michel and Evertz, arxiv:07050799

- Measurement of $n_i(\tau) \rightarrow \langle n_k(\tau) n_{-k}(0)\rangle$ in Fourier space
- Measurement of $\langle a_i(\tau) a_j^\dagger(0)\rangle$ during loop update.

Excitations in 1 spacial dimension





1D chain $L = 64$, $\beta = 3L$

PP, Evertz, Hohenadler, PRA 80, 033612 (2009)

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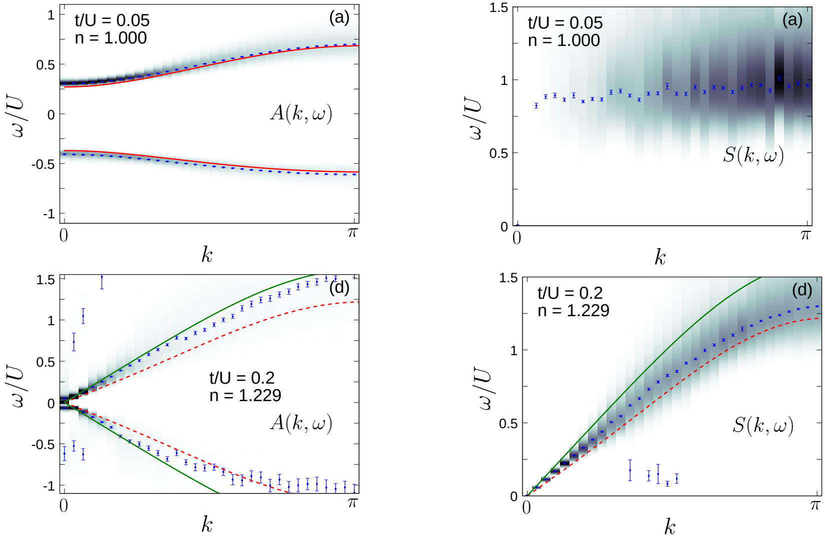

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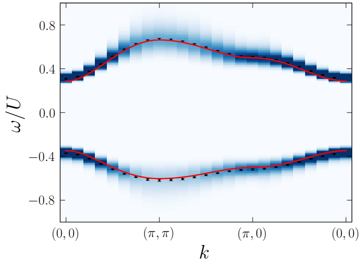
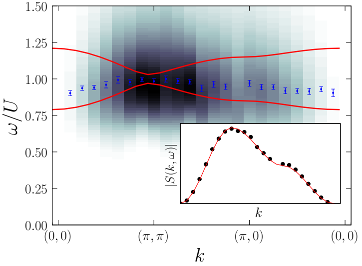
Excitations: 2 spacial dimensions

2D square, periodic boundary conditions
$L \times L = 16 \times 16$, $\beta = 40$



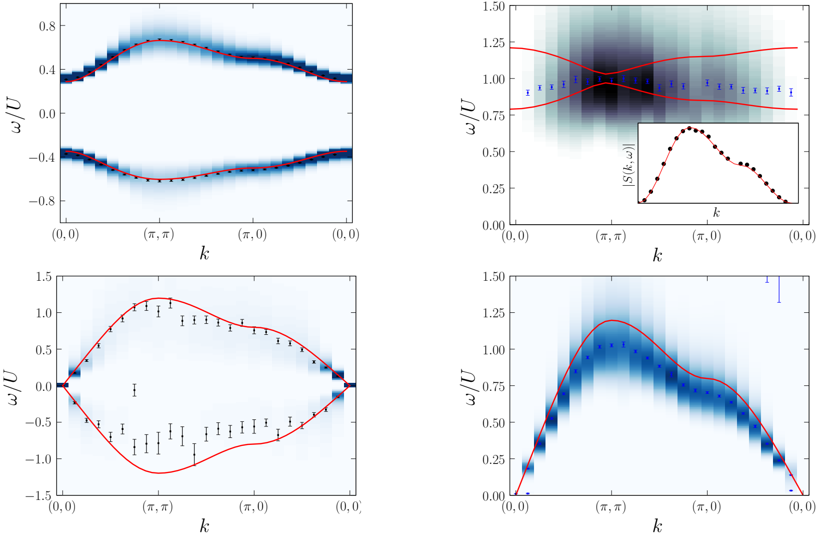
Mott insulator:
$t/U = 0.015$



Excitations: 2 spacial dimensions

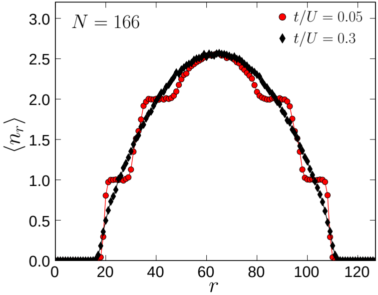
2D square, periodic boundary conditions
$L \times L = 16 \times 16$, $\beta = 40$

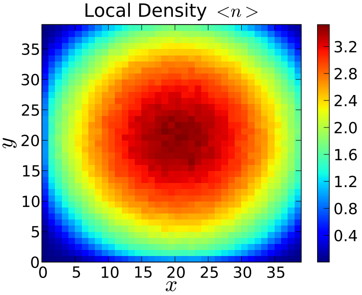
superfluid
$t/U = 0.07$



Trapped Bose Einstein condensates

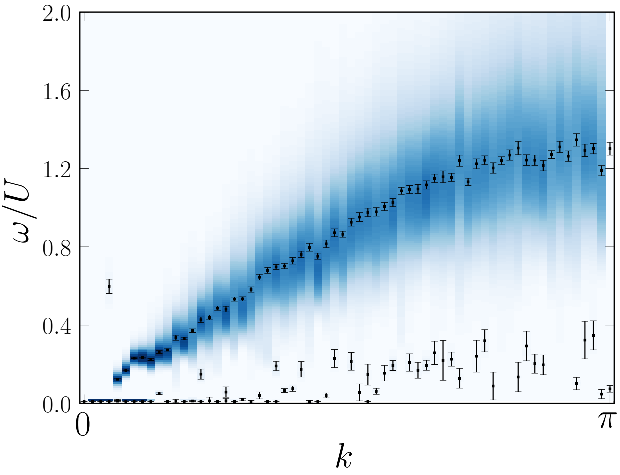
$$H^{BH} = -t \sum_{\langle i,j \rangle} (a_i^\dagger a_j \quad + \quad h.c) + \frac{U}{2} \sum_i n_i(n_i - 1)$$
$$- \quad \sum_i (\mu_0 + K \mathbf{r_i}^2) n_i$$





Excitations: trapped condensates

- Structure factor $S(k,\omega)$ 1D chain, L128



Conclusions

- Bose Einstein condensates serve as quantum simulators.
  Also excitations can be studied experimentally
- SSE representation + directed loops allows to study large systems at low temperatures, also close to the phase transition.
- Mapping to continous time $\longrightarrow$ excitations can be calculated.