Beyond Gutzwiller: Corrections to mean-field expansion patterns of interacting bosonic atoms in optical lattices

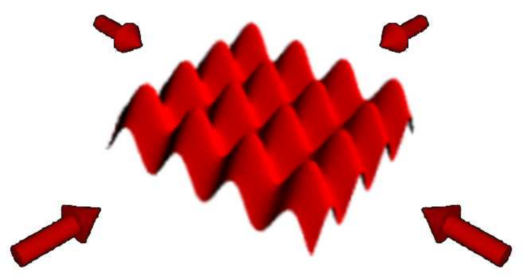
Christian Schroll[1], Florian Marquardt[2], Christoph Bruder[1]

[1]Department of Physics and Astronomy, University of Basel, Klingelbergstr. 82, 4056 Basel, Switzerland
[2] Yale University, Department of Physics PO Box 208284, New Haven, CT 06511, USA

We consider the Mott-insulator transition in optical lattices, studying in particular short-range correlations that determine the momentum distribution and the experimentally observed expansion patterns. There are many different numerical approaches based on the Gutzwiller ansatz, DMRG[1], Exact Diagonalization[2] or QMC techniques[3,4].

We are using a Gutzwiller ansatz and study in particular the corrections arising from the inclusion of short-range inter-lattice correlations. As the Gutzwiller approach does not correctly describe the spatial decay of the one-particle density matrix, we improve the Gutzwiller approach in a perturbative way by including nearest-neighbor and next-nearest neighbor correlations. We present results for 2D- and 3D optical lattices and study the modifications of the density fluctuations and the density matrix.

Optical Lattices

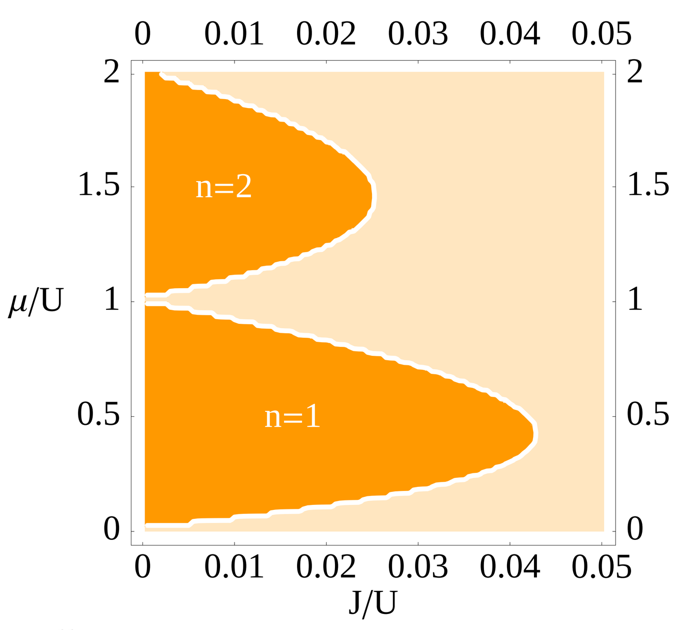


- retro-reflected lasers in $\hat{x}$, $\hat{y}$, and $\hat{z}$ directions form a 3D lattice of intensity maxima and minima
- condensed atoms are loaded into the off-resonant laser field
- the 3D-standing wave forms an periodic lattice potential for the condensate with the ratio of the hopping element J to on-site repulsion U as a tunable parameter.

Mott-Hubbard model

Mott-Hubbard Hamiltonian:

$$H = \sum_{i=1}^{M} \frac{U}{2} n_i(n_i-1) + \sum_{i=1}^{M} (\epsilon_i - \mu)\, n_i - \sum_{\langle i,j\rangle} J_{ij} a_i^\dagger a_j$$



Gutzwiller ansatz:

$$|G_0\rangle = \prod_{i=1}^{M} \left(\sum_{n=0}^{\infty} f_n^{(i)} |n_i\rangle \right)$$

Mean Field Approximation:

$$H_{\mathrm{MF}} = \sum_{i=1}^{M} \frac{U}{2} n_i(n_i-1) + \sum_{i=1}^{M} (\epsilon_i - \mu)\, n_i - J \sum_{\langle i,j\rangle} \left(a_i^\dagger \Psi_j + \Psi_i^* a_j \right)$$

where the mean field is obtained from the Gutzwiller result: $\Psi_i = \langle G_0 | a_i | G_0 \rangle$

Perturbative Approach

Rewriting the Hamiltonian:

$$H = H_{\mathrm{MF}} + (H - H_{\mathrm{MF}}) = H_{\mathrm{MF}} + \sum_{\langle i,j\rangle} \Psi_i^* \Psi_j \underbrace{- J \sum_{\langle i,j\rangle} (\Psi_i^* - a_i^\dagger)(\Psi_j - a_j)}_{V}$$

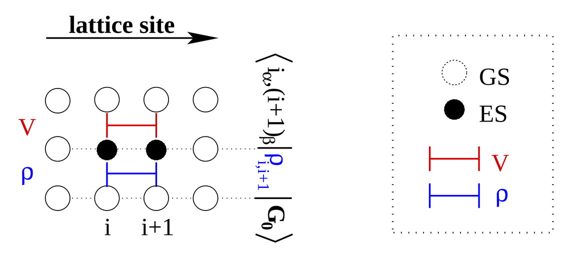
Using the mean field solution obtained from the Gutzwiller ansatz, $|G_0\rangle$, as a starting point we do perturbation theory in V:

$$|G_l\rangle = \frac{V|G_{l-1}\rangle - \sum_{n=1}^{l-1} \epsilon_n |G_{l-n}\rangle}{\epsilon_0 - \epsilon^\alpha}$$

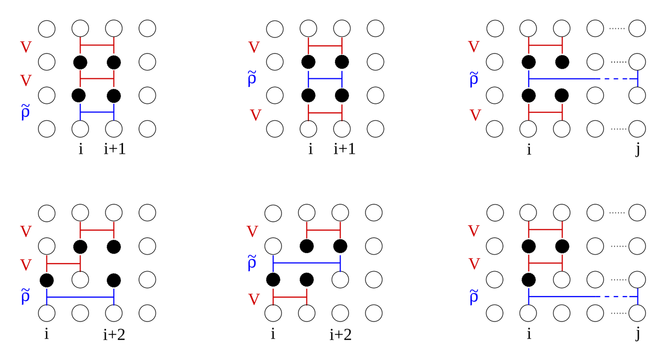
$\Longrightarrow$ Inclusion of short-range inter-lattice correlations!

Corrections to $\rho_{ij} = \langle a_i^\dagger a_j \rangle$

1[st] order corrections:



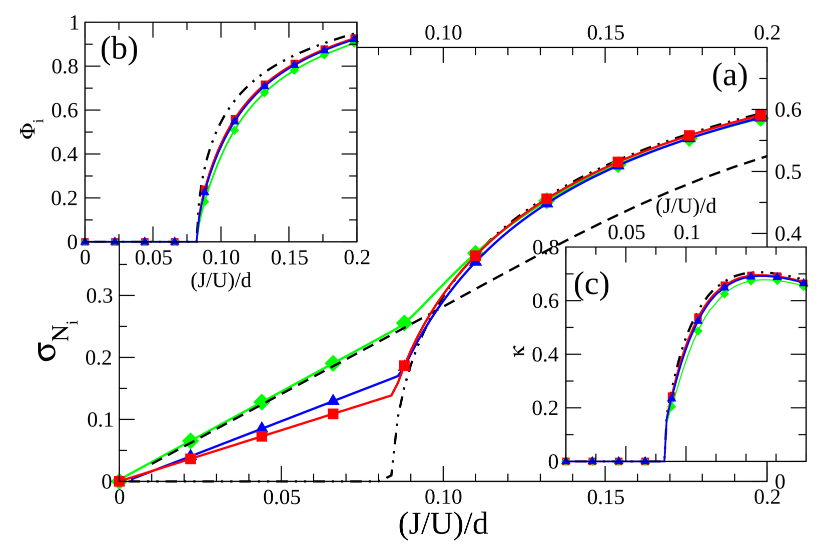
2[nd] order corrections:



Numerical Results

- computing the Gutzwiller wavefunction $|G_0\rangle$
- computing the MF-excitation spectrum for all lattice sites
- computing the corrections using perturbation theory up to second order in V

Single Lattice Site Observables



Results for GW (dashed-dotted line), and PT for a d = 1D,2D, and 3D lattice. (fix $N = 7^d$ in (a) and ED (dashed line), $\mu/U = 0.5$ in (b),(c)).

(a) number fluctuations: $\sigma_{N_i} = \sqrt{\langle n_i^2 \rangle - \langle n_i \rangle^2}$

(b) order parameter: $\Phi_i = \langle a_i \rangle$

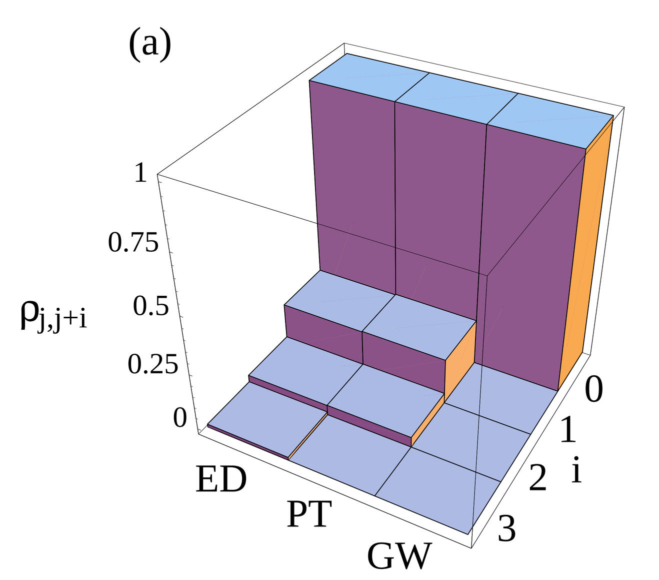
(c) compressibility: $\kappa = \frac{M}{N^2} \sum_{i=1}^{M} \frac{\partial \langle n_i \rangle}{\partial \mu}$

The Correlation Function

Comparing with exact diagonalization results:

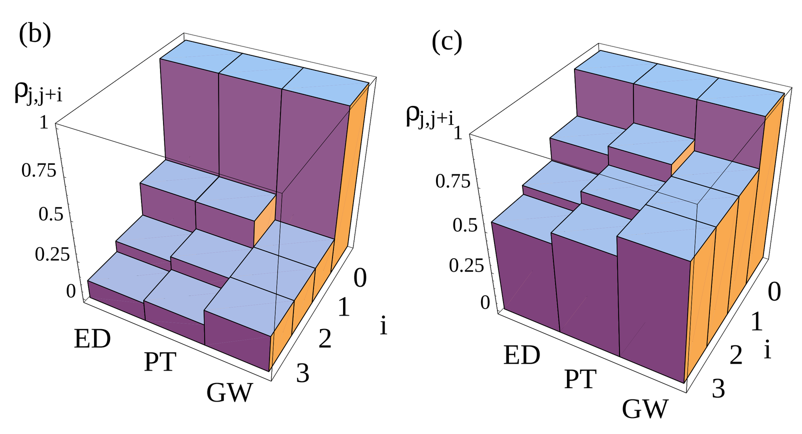
correlation function: $\rho_{kl} = \langle a_k^\dagger a_l \rangle$

Mott Insulator: 7 sites, $N = 7$, $J/U = 0.05$



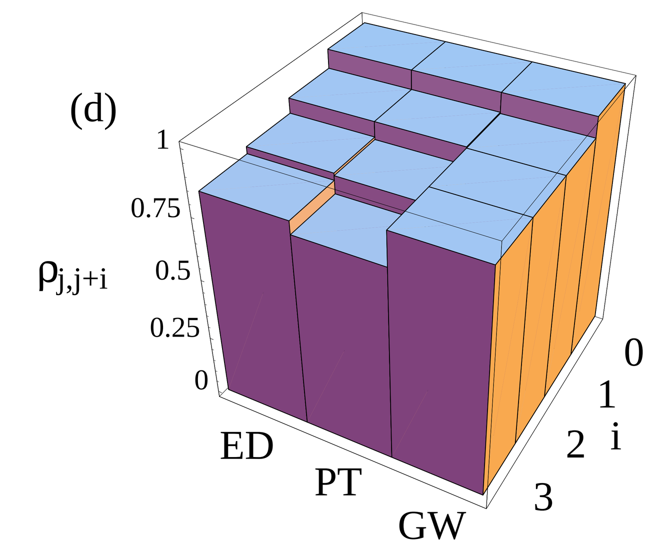
Intermediate: 7 sites, $N = 7$

Parameter (J/U) between $(J/U)_c^{\mathrm{MF}} = 0.086$ and $(J/U)_c \approx 0.2 \cdots 0.3$ from DMRG, ED, QMC.



$J/U = 0.1$ $J/U = 0.2$

Superfluid: 7 sites, $N = 7$, $J/U = 0.5$

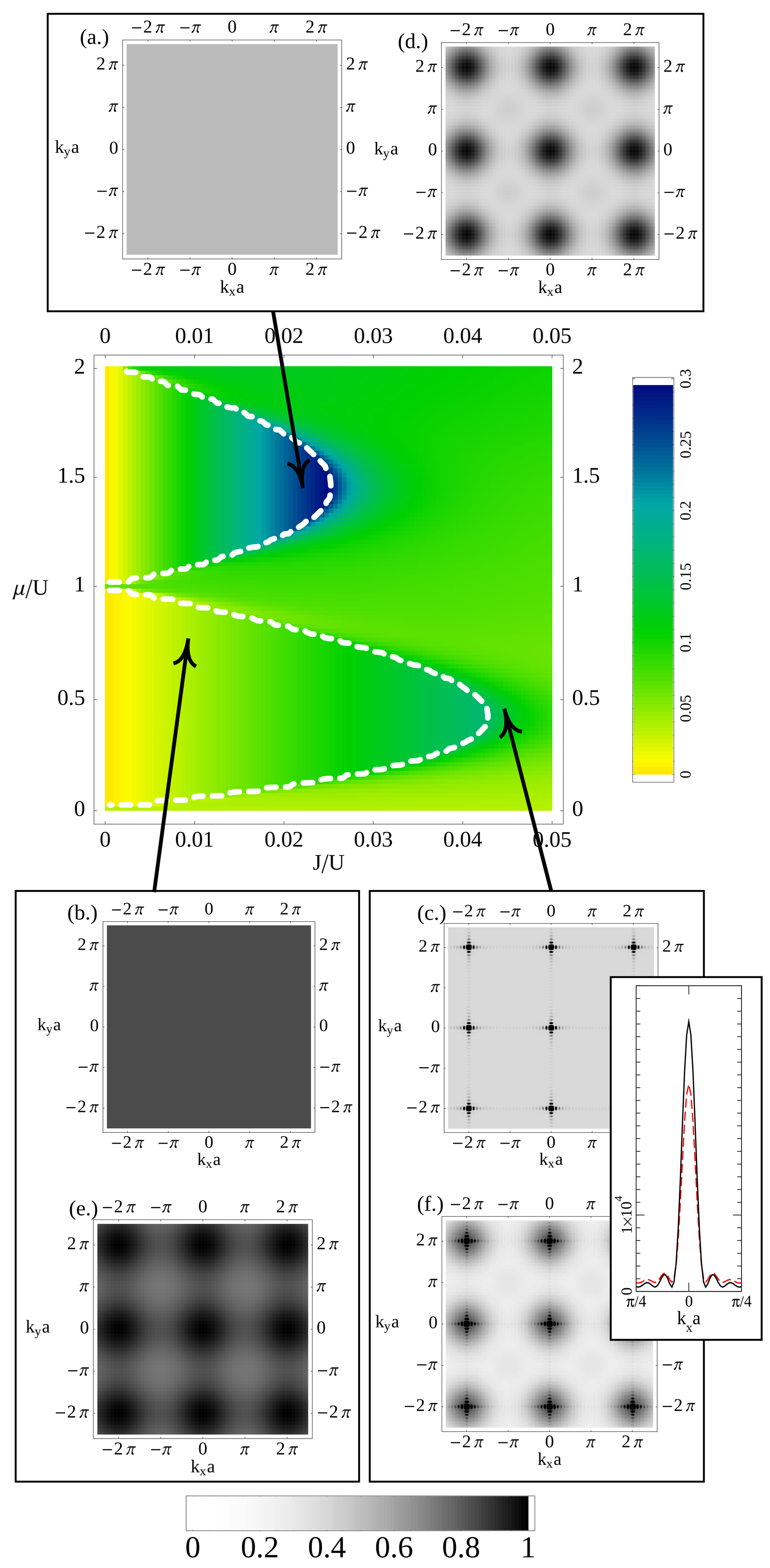


Expansion Patterns

Assuming a sufficiently dilute atomic cloud and long expansion times, the shape of the expanded cloud reflects the initial momentum distribution:

$$\rho(\mathbf{k}) = |w(\mathbf{k})|^2 \sum_{i,j=1}^{M} \rho_{ij} e^{i\mathbf{k}(\mathbf{r}_i - \mathbf{r}_j)}$$

Homogeneous 2D-lattice, $\epsilon = 0$:



- The central figure (color) shows the correction to $\rho_{i,i+1}$ in second order PT.
- Fig. (a)-(f): Expansion patterns for a 2D-lattice showing $\rho(\mathbf{k})/|w(\mathbf{k})|^2$.
  - Fig. (a)-(c): Expansion patterns obtained from the Gutzwiller (GW) ansatz
  - Fig. (d)-(f): Expansion patterns improved by perturbation theory (PT) up to 2[nd] order. (**Inset:** linecut along k_x for $k_y = 0$.)

Fig.	μ/U	J/U	normalized to:
a,d	0.75	0.01	peak max.
b,e	0.45	0.04	peak max.
c,f	1.5	0.0225	1/20× peak max

Consequences of PT:

- Broad peaks arise due to the inclusion of short range correlations.
- Considerable reduction of the SF-peak due to the correction of the mean field in PT.

Underlying HO-Potential

- Experiments: additional trapping potential in order to confine the condensate to a finite region of the optical lattice.
- the inhomogeneity caused by the trapping potential leads to slowly varying on-site energies ϵ_i,

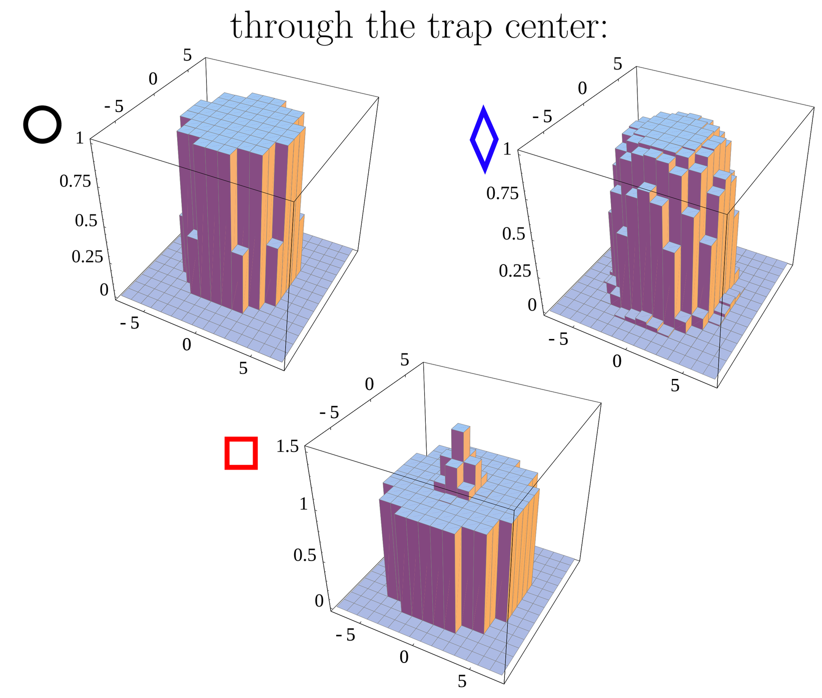
$$\epsilon_i = \alpha(i - i_c)^2$$

which can be interpreted as a spatially varying chemical potential $\mu - \epsilon_i$:

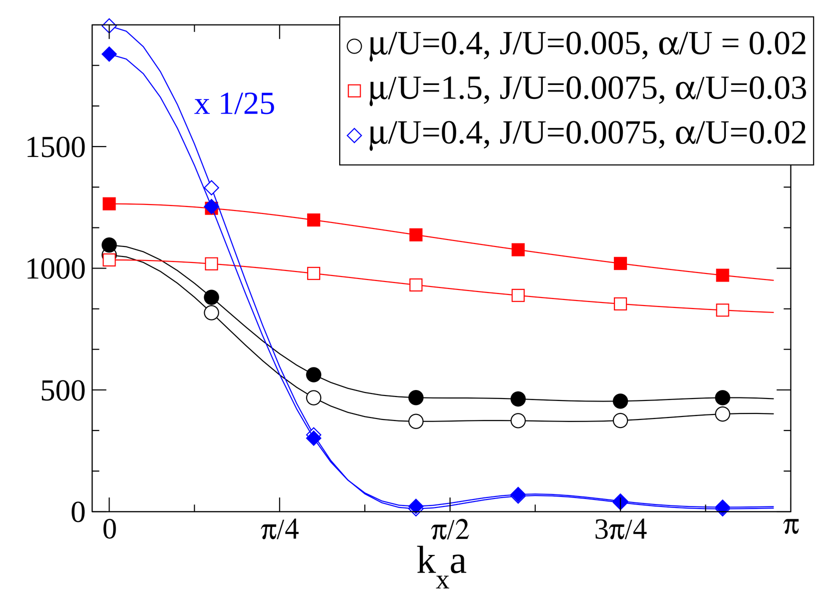
Expansions Patterns for a 3D-lattice:

3D-lattice: 15^3-sites

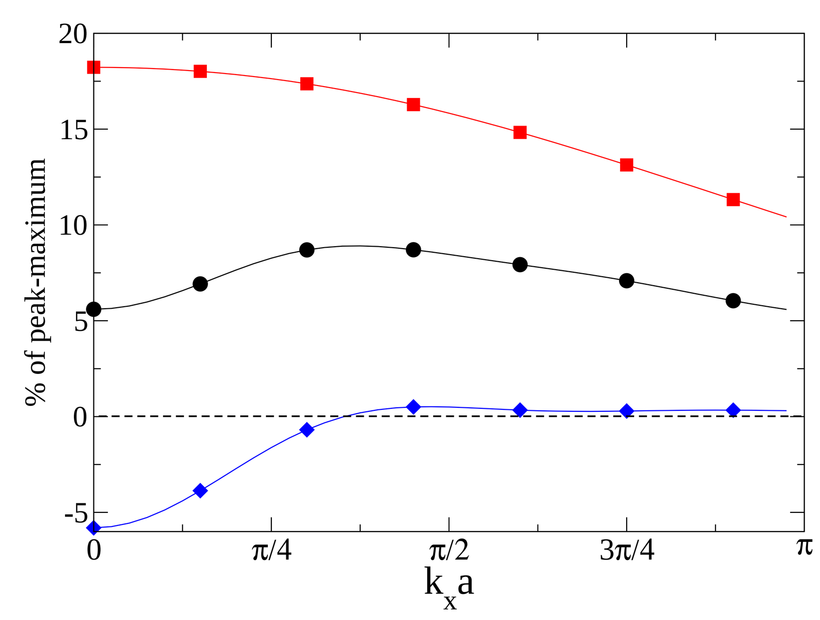
Lattice site occupation number along a cut through the trap center:



Expansion pattern: cut along the k_x-axis



Corrections in the expansion pattern in % of the peak maximum:



Conclusions:

The inclusion of short range correlations leads to:

- a modification of single lattice site observables:
  - number fluctuations σ_N in the MI-region
  - particularly strong corrections in 1D as GW is only a good approximation in higher dimensions.
- modifications in the expansion pattern:
  - homogeneous lattice $\Longrightarrow$ broad peaks are arising
  - HO-trap $\Longrightarrow$ modification of the peak structure e.g. peak broadening.

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