

Field-Theoretic Description of Bosons in Optical Lattices

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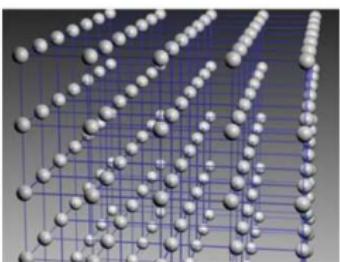
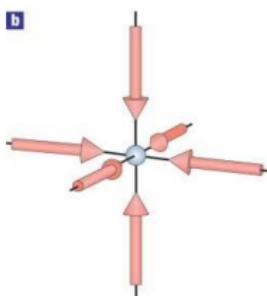
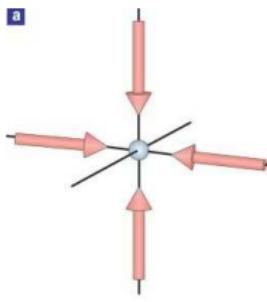
UNIVERSITÄT
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ESSEN

29th of October 2008
422 Wilhelm and Else Heraeus Seminar Quo Vadis BEC?
Bad Honnef, Germany

- Green's Function Approach

W. Metzner, PRB 43, 8549 (1993)

- Strong-Coupling Perturbation Theory
- Cumulant Decomposition
- Resummation
- Phase Diagram
- Excitations in Mott Phase
- Effective Action
 - Condensate Density
 - Excitations in Superfluid Phase
- Time-of-Flight/Visibility
- Summary/Outlook



Bose-Hubbard Model

- Bose-Hubbard Hamiltonian:

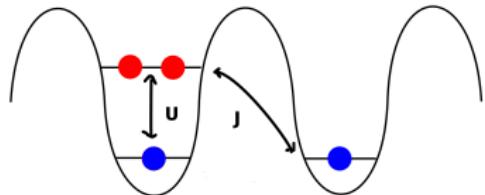
$$\hat{H}_{\text{BHM}} = \hat{H}_0 + \hat{H}_1$$

$$\hat{H}_0 = \sum_i \left[\frac{U}{2} \hat{n}_i (\hat{n}_i - 1) - \mu \hat{n}_i \right]$$

$$\hat{H}_1 = -J \sum_{\langle i,j \rangle} \hat{a}_i^\dagger \hat{a}_j = - \sum_{i,j} J_{i,j} \hat{a}_i^\dagger \hat{a}_j$$

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

$$J_{ij} = \begin{cases} J & \text{if } i, j \text{ nearest neighbors} \\ 0 & \text{otherwise} \end{cases}$$



- \hat{H}_0 site-diagonal

$$\hat{H}_0 |n\rangle = N_S E_n |n\rangle$$

$$E_n = \frac{U}{2} n(n-1) - \mu n$$

- Perturbative expansion in \hat{H}_1

Imaginary-Time Green's Function

- Definition:

$$G_1(\tau', j' | \tau, j) = \frac{1}{\mathcal{Z}} \text{Tr} \left\{ e^{-\beta \hat{H}} \hat{T} \left[\hat{a}_{j,\text{H}}(\tau) \hat{a}_{j',\text{H}}^\dagger(\tau') \right] \right\}$$

with $\mathcal{Z} = \text{Tr}\{e^{-\beta \hat{H}}\}$

- Time evolution of operators in *interaction picture* determined by \hat{H}_0 :

$$\hat{O}_{\text{D}}(\tau) = e^{\hat{H}_0 \tau} \hat{O} e^{-\hat{H}_0 \tau}$$

- Dirac time-evolution operator calculated by Dyson series:

$$\begin{aligned} \hat{U}_{\text{D}}(\tau, \tau_0) &= \sum_{n=0}^{\infty} (-1)^n \int_{\tau_0}^{\tau} d\tau_1 \dots \int_{\tau_0}^{\tau_{n-1}} d\tau_n \hat{H}_{1\text{D}}(\tau_1) \dots \hat{H}_{1\text{D}}(\tau_n) \\ &= \hat{T} \exp \left(- \int_{\tau_0}^{\tau} d\tau_1 \hat{H}_{1\text{D}}(\tau_1) \right) \end{aligned}$$

Partition Function

- Full partition function:

$$\mathcal{Z} = \text{Tr} \left\{ e^{-\beta \hat{H}_0} \hat{U}_{\text{D}}(\beta, 0) \right\}$$

- n th order contribution:

$$\begin{aligned} \mathcal{Z}^{(n)} = \frac{1}{n!} \mathcal{Z}^{(0)} \sum_{i_1, j_1, \dots, i_n, j_n} & J_{i_1 j_1} \dots J_{i_n j_n} \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \dots \int_0^\beta d\tau_n \\ & \times G_n^{(0)}(\tau_1, j_1; \dots; \tau_n, j_n | \tau_1, i_1; \dots; \tau_n, i_n) \end{aligned}$$

- Unperturbed n -particle Green's function:

$$G_n^{(0)}(\tau'_1, i'_1; \dots; \tau'_n, i'_n | \tau_1, i_1; \dots; \tau_n, i_n) = \left\langle \hat{T} \hat{a}_{i'_1}^\dagger(\tau'_1) \hat{a}_{i_1}(\tau_1) \dots \hat{a}_{i'_n}^\dagger(\tau'_n) \hat{a}_{i_n}(\tau_n) \right\rangle^{(0)}$$

Cumulant Decomposition

- Decompose $G_n^{(0)}(\tau'_1, i'_1; \dots; \tau'_n, i'_n | \tau_1, i_1; \dots; \tau_n, i_n)$ into “simple” parts
- \hat{H}_0 not harmonic \Rightarrow Wick’s theorem not applicable
- But: Decomposition into cumulants
- \hat{H}_0 site-diagonal \Rightarrow cumulants local. Example:

$$\begin{aligned} G_2^{(0)}(\tau'_1, i'_1; \tau'_2, i'_2 | \tau_1, i_1; \tau_2, i_2) &= \delta_{i_1, i_2} \delta_{i'_1, i'_2} \delta_{i_1, i'_1} C_2^{(0)}(\tau'_1, \tau'_2 | \tau_1, \tau_2) \\ &+ \delta_{i_1, i'_1} \delta_{i_2, i'_2} C_1^{(0)}(\tau'_1 | \tau_1) C_1^{(0)}(\tau'_2 | \tau_2) + \delta_{i_1, i'_2} \delta_{i_2, i'_1} C_1^{(0)}(\tau'_2 | \tau_1) C_1^{(0)}(\tau'_1 | \tau_2) \end{aligned}$$

- Denote contributions diagrammatically. Points for cumulants, lines for hopping matrix elements
- Perturbation theory in number of *lines*
- Cumulants obtained from generating functional

Diagrammatic Rules for $\mathcal{Z}^{(n)}$

- ① Draw all possible combinations of vertices with total n entering and leaving lines
- ② Connect them in all possible ways and assign time variables and hopping matrix elements onto the lines
- ③ Sum all site indices and integrate all time variables from 0 to β

$$\begin{array}{ccc} \text{---} \xrightarrow{\tau'} \bullet \xrightarrow{\tau} & = C_1^{(0)}(\tau'|\tau) & \begin{array}{c} \tau'_2 \\ \tau'_1 \end{array} \nearrow \bullet \xrightarrow{i} \nearrow \begin{array}{c} \tau_2 \\ \tau_1 \end{array} & = C_2^{(0)}(\tau'_1, \tau'_2 | \tau_1, \tau_2) & \text{---} \xrightarrow{\quad} & = J_{ij} \end{array}$$

$$\text{example : } \mathcal{Z}^{(2)} = \frac{1}{2} i \bullet \begin{array}{c} \nearrow \tau_1 \\ \searrow \tau_2 \end{array} j$$

Observe: Perturbation theory only valid in Mott phase

Thermodynamic Properties in Mott Phase

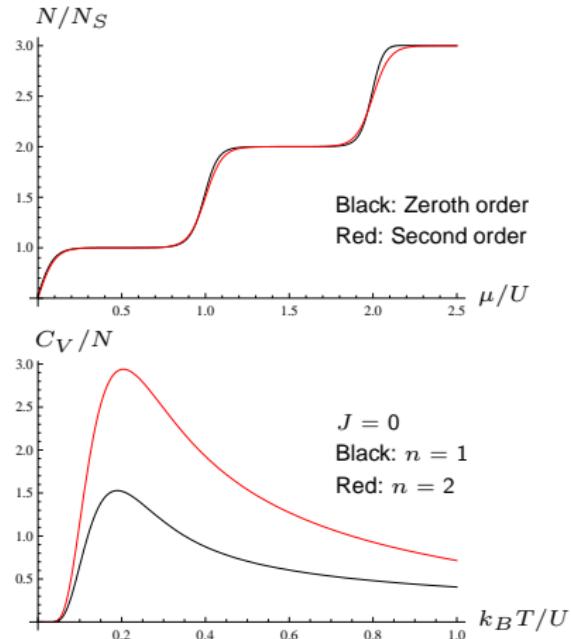
Thermodynamic properties obtained from free energy \mathcal{F}

- Particle number:

$$N = -\frac{\partial \mathcal{F}}{\partial \mu}$$

- Specific heat:

$$C_V = \left. \frac{\partial U_{in}}{\partial T} \right|_{V, N \text{ fixed}}$$



Diagrammatic Rules for Green's Function

$$G_1(\tau', i' | \tau, i) = \frac{1}{\mathcal{Z}} \text{Tr} \left\{ e^{-\beta \hat{H}_0} \hat{T} \hat{a}_{i'}^\dagger(\tau') \hat{a}_i(\tau) \hat{U}_D(\beta, 0) \right\}$$
$$G_1^{(n)}(\tau', i' | \tau, i) = \frac{\mathcal{Z}^{(0)}}{\mathcal{Z}} \frac{1}{n!} \sum_{i_1, j_1, \dots, i_n, j_n} J_{i_1 j_1} \dots J_{i_n j_n} \int_0^\beta d\tau_1 \dots \int_0^\beta d\tau_n$$
$$\times G_{n+1}^{(0)}(\tau_1, j_1; \dots; \tau_n, j_n; \tau', i' | \tau_1, i_1; \dots; \tau_n, i_n, \tau, i)$$

- Diagrams have external lines with *fixed* time and site variables
- Disconnected diagrams cancel $\mathcal{Z}^{(0)}/\mathcal{Z}$
- Zeroth and first order:

$$G_1^{(0)}(\tau', i | \tau, j) = \begin{array}{c} \xrightarrow{\tau'} \bullet \xrightarrow{\tau} \\ \quad \quad \quad \end{array}^i = \delta_{i,j} C_1^{(0)}(\tau' | \tau)$$

$$G_1^{(1)}(\tau', i | \tau, j) = \begin{array}{c} \xrightarrow{\tau'} \bullet \xrightarrow{\tau_1} \bullet \xrightarrow{\tau} \\ \quad \quad \quad \quad \quad \end{array}^i \quad ^j = J \delta_{d(i,j),1} \int_0^\beta d\tau_1 C_1^{(0)}(\tau' | \tau_1) C_1^{(0)}(\tau_1 | \tau)$$

Calculations in Matsubara Space

- Translational invariance in time suggests Matsubara transform

$$C_1^{(0)}(\omega_m) = \frac{1}{Z^{(0)}} \sum_n \left[\frac{n+1}{E_{n+1} - E_n - i\omega_m} - \frac{n}{E_n - E_{n-1} - i\omega_m} \right] e^{-\beta E_n}, \quad \omega_m = \frac{2\pi}{\beta} m$$

- In rule 3 integration over τ replaced by summation over ω_m under consideration of frequency conservation on vertices:

$$G_1^{(1)}(\omega_m; i, j) = \begin{array}{c} \xrightarrow{\hspace{1cm}} \\ \omega_m \end{array} \xrightarrow{\hspace{1cm}} \begin{array}{c} i \\ \bullet \\ \omega_m \end{array} \xrightarrow{\hspace{1cm}} \begin{array}{c} j \\ \bullet \\ \omega_m \end{array} \xrightarrow{\hspace{1cm}} \begin{array}{c} \omega_m \end{array} = J \delta_{d(i,j),1} C_1^{(0)}(\omega_m)^2$$

$$\begin{aligned} G_2^{(1)}(\omega_m; i, j) &= \begin{array}{c} \xrightarrow{\hspace{1cm}} \\ \omega_m \end{array} \xrightarrow{\hspace{1cm}} \begin{array}{c} i \\ \bullet \\ \omega_m \end{array} \xrightarrow{\hspace{1cm}} \begin{array}{c} k \\ \bullet \\ \omega_m \end{array} \xrightarrow{\hspace{1cm}} \begin{array}{c} j \\ \bullet \\ \omega_m \end{array} \xrightarrow{\hspace{1cm}} \begin{array}{c} \omega_m \end{array} + \begin{array}{c} \xrightarrow{\hspace{1cm}} \\ \omega_m \end{array} \xrightarrow{\hspace{1cm}} \begin{array}{c} k \\ \bullet \\ \omega_1 \end{array} \xrightarrow{\hspace{1cm}} \begin{array}{c} \omega_1 \\ \bullet \\ i \\ \omega_m \end{array} \xrightarrow{\hspace{1cm}} \begin{array}{c} \omega_m \end{array} \\ &= J^2 (\delta_{d(i,j),2} + 2\delta_{d(i,j),\sqrt{2}} + 2D\delta_{i,j}) C_1^{(0)}(\omega_m)^3 \\ &\quad + J^2 2D\delta_{i,j} \sum_{\omega_1} C_1^{(0)}(\omega_m) C_2^{(0)}(\omega_m, \omega_1 | \omega_m, \omega_1) \end{aligned}$$

Resummation Technique

- Non-perturbative results by summing infinite subsets of diagrams
- Self-energy $\Sigma = 1/G_1^{(0)} - 1/G_1$ given by sum over all one-particle irreducible diagrams

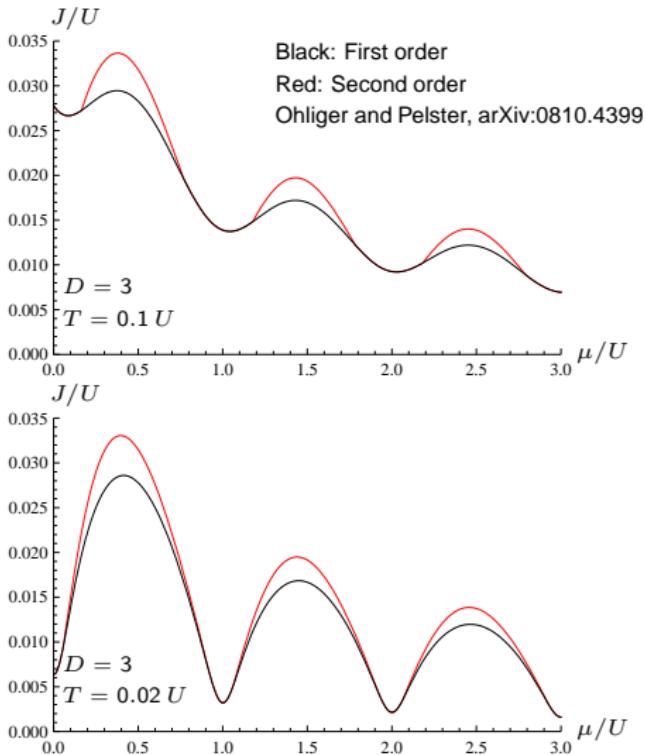
$$\Sigma(\omega_m, \mathbf{k}) = 1/G_1^{(0)}(\omega_m) - 1/\mathcal{C}_1(\omega_m, \mathbf{k}) + J(\mathbf{k}), \quad J(\mathbf{k}) = 2J \sum_{\nu=1}^D \cos(k_\nu a)$$

$$\mathcal{C}_1(\omega_m, \mathbf{k}) = \text{---} \bullet \text{---} + \text{---} \circlearrowleft \text{---} + \left(\frac{1}{2} \text{---} \bullet \text{---} \circlearrowleft \text{---} + \dots \right)$$

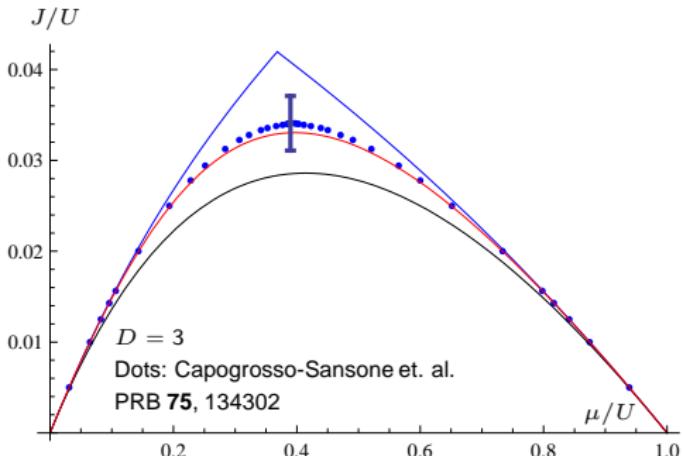
- Expanding Σ in powers of J
- $\Sigma^{(1)}$ corresponds to summation of all chain diagrams
- $\Sigma^{(2)}$ describes one-loop correction. Vanishes for $D \rightarrow \infty$

Quantum Phase Diagram for Finite Temperature

- Phase boundary given by $G_1^{(1)}(0, 0) \rightarrow \infty$
- First order reproduces mean-field result
- One-loop correction larger for lower dimension
- Temperature effects small at tip of lobe
- One-loop correction largest at zero temperature



Comparison with Simulations for $T = 0$

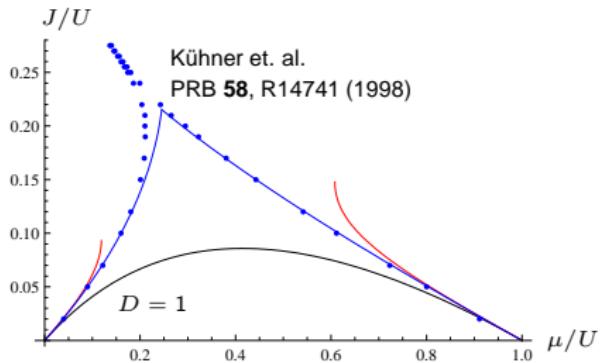
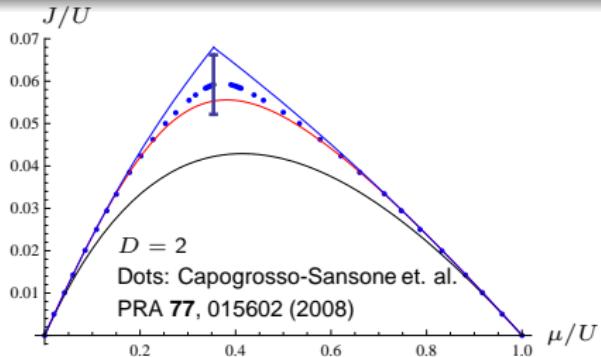


- Second-order coincides with effective potential method

Santos and Pelster, PRA (in press), arXiv: 0806.2812

- Numerically extendable to higher orders

Teichmann, Hinrichs, Holthaus, and Eckardt, et. al.
arXiv: 0810.0643



$n = 1$. Black: First order (Mean field)

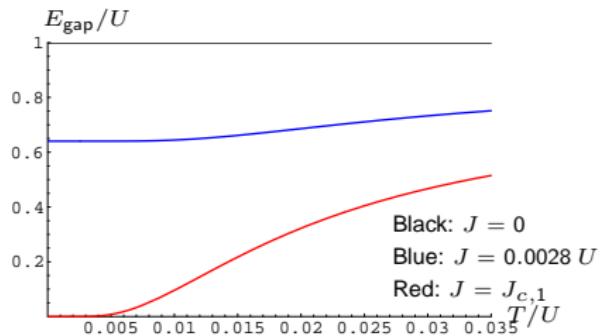
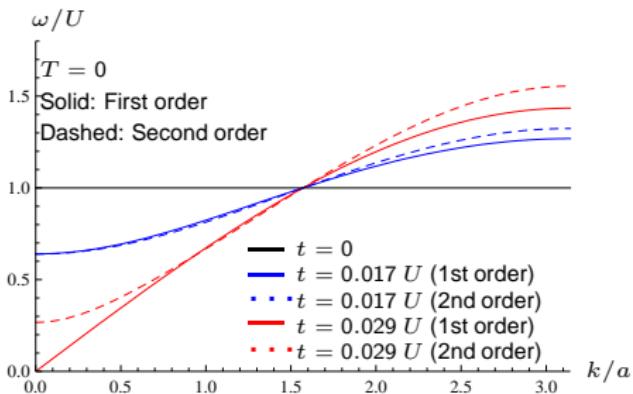
Red: One-loop corrected

Blue: Third order strong-coupling expansion

Freericks and Monien, PRB 53, 2691 (1996)

Excitation Spectrum in Mott Phase

- Dispersion relation given by poles of real-time Green's function
- One-loop correction most important for long wavelengths
- Characteristic gap larger at higher temperature due to thermal fluctuations



Ohliger and Pelster, arXiv:0810.4399

Effective Action Approach

- Coupling Hamiltonian to currents introduces order parameter

$$\psi_i(\omega_m) = \langle \hat{a}_i(\omega_m) \rangle = \beta \frac{\delta \mathcal{F}}{\delta j_i^*(\omega_m)}$$

- Perturbative Legendre transform to obtain effective action

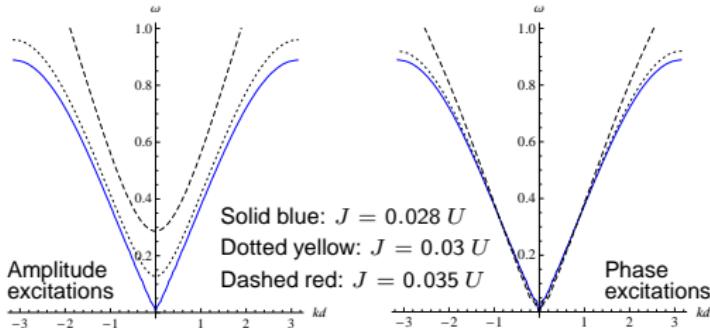
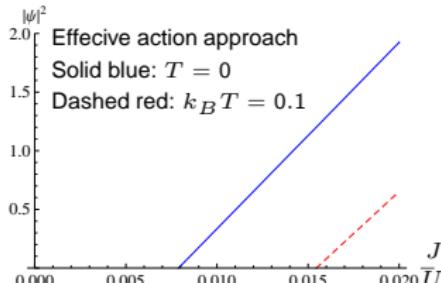
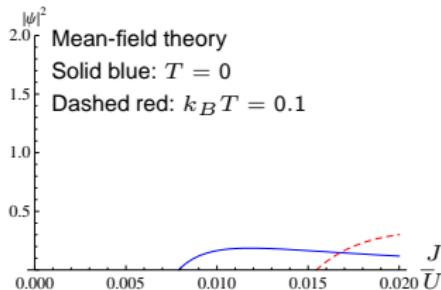
$$\Gamma[\psi_i(\omega_m), \psi_i^*(\omega_m)] = \mathcal{F} - \frac{1}{\beta} - \sum_i \sum_{\omega_m} [\psi_i(\omega_m) j_i^*(\omega_m) + \psi_i^*(\omega_m) j_i(\omega_m)]$$

- Extremalization yields value of order parameter

$$\left. \frac{\delta \Gamma}{\delta \psi_i^*(\omega_m)} \right|_{|\psi|^2 = |\psi|_{\text{eq}}^2} = \left. \frac{\delta \Gamma}{\delta \psi_i(\omega_m)} \right|_{|\psi|^2 = |\psi|_{\text{eq}}^2} = 0$$

- Suitable description both in superfluid and Mott phase

Properties of Superfluid Phase



- $|\Psi|^2$ identified with density of delocalized Bosons
- Phase boundary coincides with mean-field result, $|\Psi|^2$ differs
- Amplitude excitations gapless only at critical point
- Phase excitations always gapless

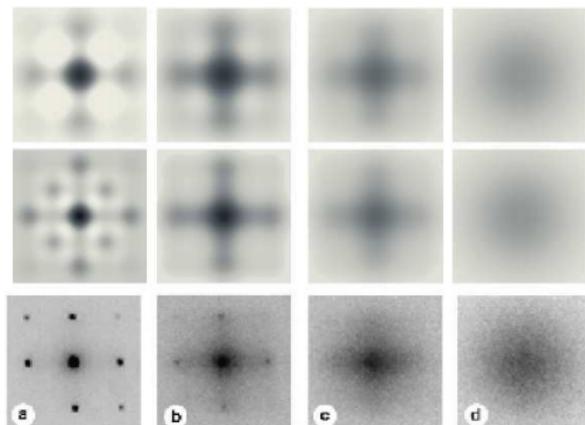
Bradlyn, Santos, and Pelster, PRA (in press), arXiv:0809:0706

Time-of-Flight Pictures for $T = 0$

Momentum-space density:

$$n_{\mathbf{k}} = \langle \hat{\psi}^\dagger(\mathbf{k}) \hat{\psi}(\mathbf{k}) \rangle = |w(\mathbf{k})|^2 S(\mathbf{k}), \quad S(\mathbf{k}) = \sum_{i,j} e^{i\mathbf{k}(\mathbf{r}_i - \mathbf{r}_j)} \lim_{\tau' \searrow 0} G_1(\tau', i|0, j)$$

$w(\mathbf{k})$: Fourier transform of Wannier function



Top to bottom: 1st order, 2nd order,
experiment Greiner et. al, Nature 415, 39 (2002)

Left to right: $V_0 = 8 E_R$, $V_0 = 14 E_R$
 $V_0 = 18 E_R$, $V_0 = 30 E_R$, $E_R = \hbar^2 k^2 / 2M$

- Free expansion maps momentum-space density to real space
- 2d-pictures obtained by integration along z -axis
- Good agreement for deep lattices
- Difference for shallow lattices due to neglecting the superfluid fraction

Visibility

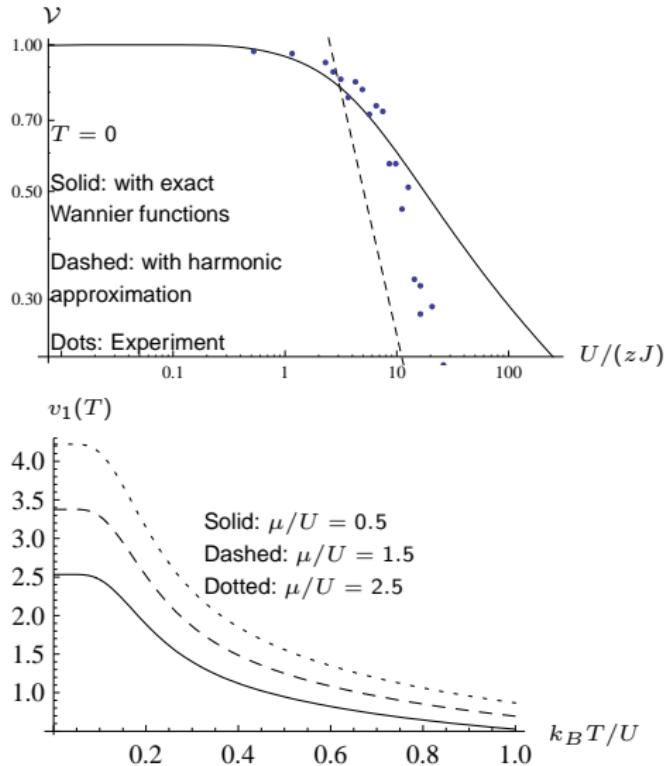
- Measure for interference patterns in TOF pictures

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

- Harmonic (Gaussian) approximation of Wannier functions yields considerable errors compared to exact numerical treatment
- Behavior for small J :

$$\mathcal{V} = v_1(T) \frac{zJ}{U} + v_2(T) \left(\frac{zJ}{U} \right)^2 + \dots$$

Hoffmann and Pelster, arXiv:0809.0771



Summary:

- Perturbative Green's function method allows for analytical calculation of various properties of Bose-Hubbard model
⇒ *Poster by M. Ohliger*
- Effective action approach provides description in whole parameter range ⇒ *Poster by F. E. A. Santos*
- Higher orders of effective potential ⇒ *Poster by N. Teichmann*
- Finite-temperature effects important when comparing with experiment

Outlook:

- Spinor Bosons ⇒ *Poster by M. Ohliger*
- Visibility from effective action approach
- Higher orders for effective action
- Bose-Fermi mixtures