

Bosons in Optical Lattices

Matthias Ohliger

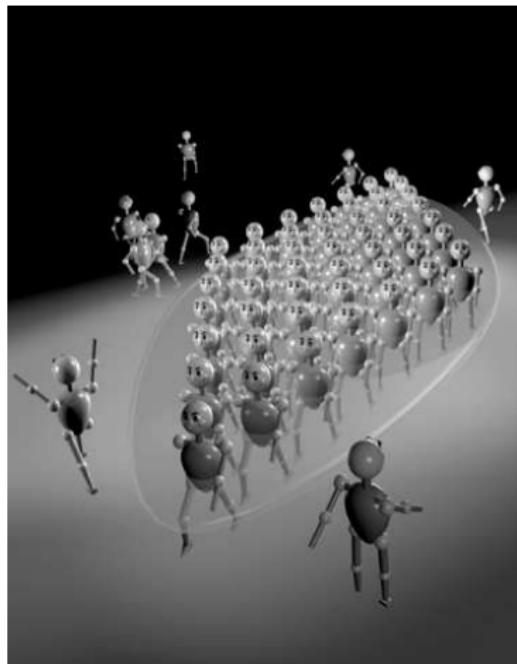
Institut für Theoretische Physik
Freie Universität Berlin



16th of April 2008
Theory Seminar - Universität Duisburg-Essen

Content

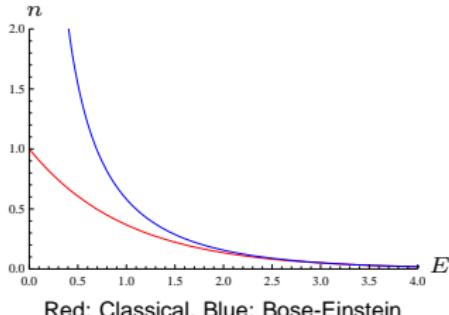
- Introduction
 - Bose-Einstein Condensates
 - Optical Lattices
- Green's Function Approach
W. Metzner, PRB (1993)
- Applications
 - Time-of-Flight/Visibility
 - Phase Diagram
 - Excitations
- Spin-1 Bosons
 - Optical Trapping
 - Phase Diagram
 - Time-of-Flight/Visibility
- Summary
- Outlook



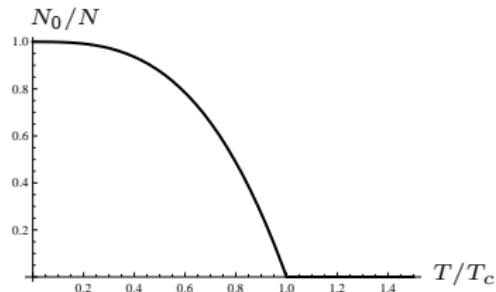
Science Cover, December 1995

Theoretical Prediction

- Predicted by Bose and Einstein for ideal gas of Bosons (1924)
- Macroscopic occupation of ground state
- Purely statistical effect, no interaction involved
- Connected to suprafluid Helium



Ground-state occupation:



$$\lambda_c = \sqrt{\frac{2\pi\hbar^2}{Mk_B T_c}} \approx n^{-1/3}$$

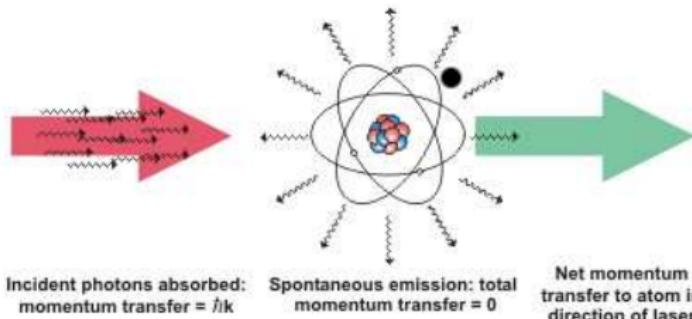
Critical temperature:

$$T_c \approx 0.08 \frac{\hbar^2}{Mk_B} n^{2/3}$$

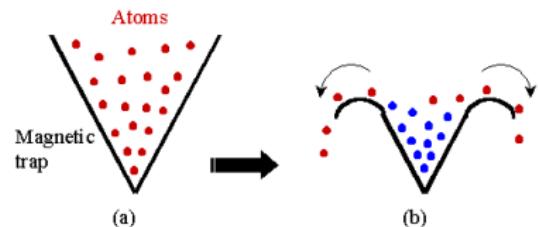
Cooling Techniques

- BEC only possible in very dilute gases to avoid “freezing”
- Nano-Kelvin temperatures necessary to reach BEC
- Various cooling methods applied successively

Laser cooling:



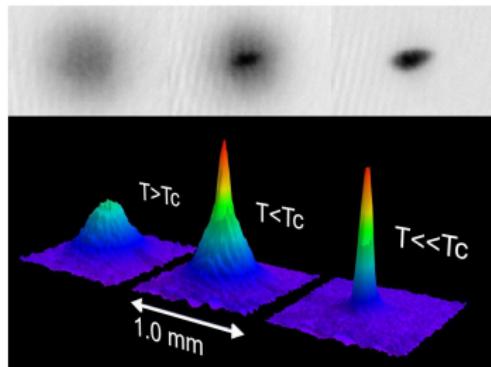
Evaporative cooling:



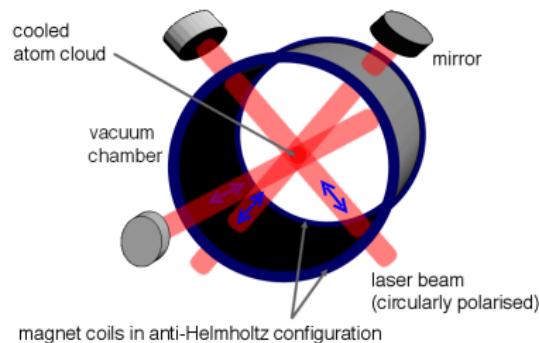
Experimental Observation

- First observed 1995 at JILA and MIT in Rubidium and Sodium
- $6 \cdot 10^5$ atoms, $T_c \approx 250 \text{ nK}$

Time-of-flight absorption image

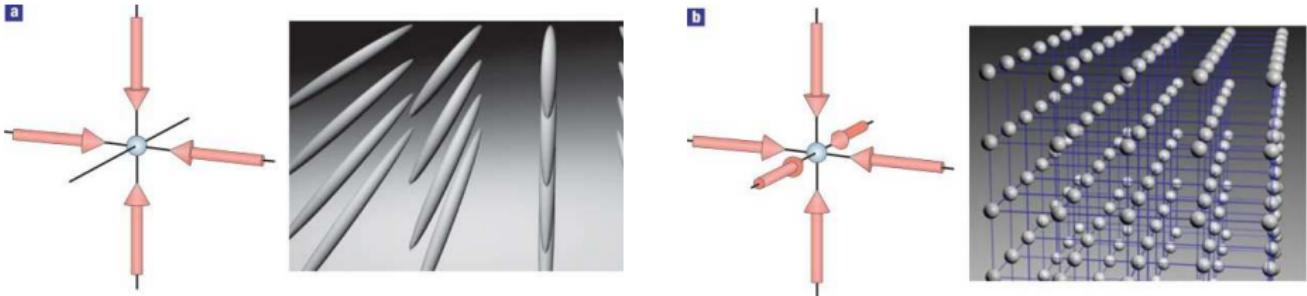


Magneto-optical trap (MOT)



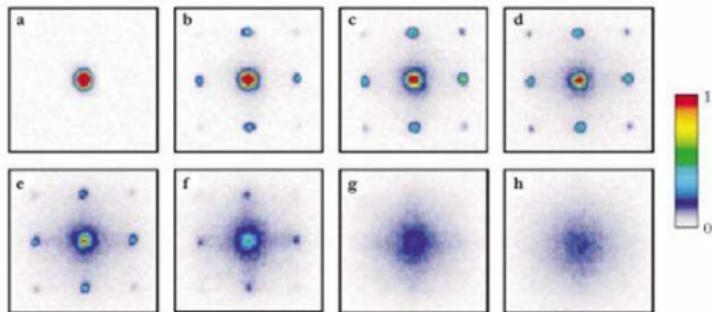
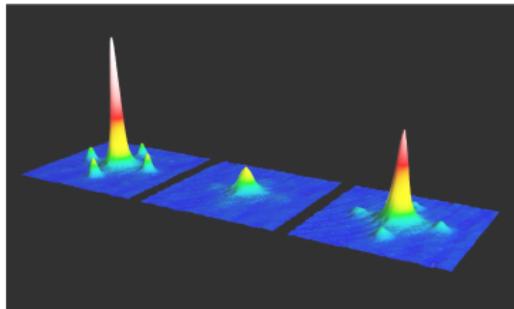
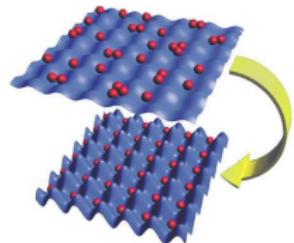
Principles of Optical Lattices

- Optical lattices produced by counter-propagating lasers
- $V = V_0 \sum_{i=1}^D \sin^2(2\pi x_i/\lambda)$
- Relative strength of hopping and interaction controllable
- (Quasi) one-, two-, and three-dimensional configurations possible
- Model system for condensed matter physics



Realization of Superfluid-Mott insulator transition

- Increasing the laser intensity drives transition from delocalized to localized state
- Experimentally detectable in time-of-flight pictures



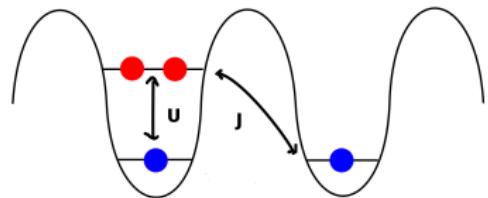
Bose-Hubbard Model

- Bose-Hubbard Hamiltonian:

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

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

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



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

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

Bose-Hubbard Model

- Bose-Hubbard Hamiltonian:

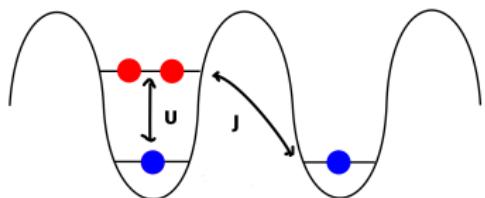
$$\hat{H}_{\text{BHM}} = \hat{H}_0 + \hat{H}_1$$

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

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

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

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



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

- Heisenberg operators in imaginary time ($\hbar = 1$):

$$\hat{X}_{\text{H}}(\tau) = e^{-\hat{H}\tau} \hat{X} e^{\hat{H}\tau}$$

Dirac Interaction Picture

- Time evolution of the operators determined only by \hat{H}_0 :

$$\hat{O}_D(\tau) = e^{\hat{H}_0\tau} \hat{O} e^{-\hat{H}_0\tau}$$

- Dirac time-evolution operator calculated by Dyson series:

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

Partition Function

- Full partition function:

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

Partition Function

- Full partition function:

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

- 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

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:

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

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*

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

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

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

Diagrammatic Rules for Green's Function

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

Diagrammatic Rules for Green's Function

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

- Diagrams have external lines with *fixed* time and site variables

Diagrammatic Rules for Green's Function

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

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

Diagrammatic Rules for Green's Function

$$G_1(\tau', i' | \tau, i) = \frac{1}{\mathcal{Z}} \text{Tr} \left\{ e^{-\beta \hat{H}_0} \hat{T} \hat{a}_{i'}^\dagger(\tau') \hat{a}_i(\tau) \hat{U}_D(\beta, 0) \right\}$$

$$\begin{aligned} G_1^{(n)}(\tau', i' | \tau, i) &= \frac{\mathcal{Z}^{(0)}}{\mathcal{Z}} \frac{1}{n!} \sum_{i_1, j_1, \dots, i_n, j_n} J_{i_1 j_1} \dots J_{i_n j_n} \int_0^\beta d\tau_1 \dots \int_0^\beta d\tau_n \\ &\quad \times G_{n+1}^{(0)}(\tau_1, j_1; \dots; \tau_n, j_n; \tau', i' | \tau_1, i_1; \dots; \tau_n, i_n, \tau, i) \end{aligned}$$

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

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

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

Calculations in Matsubara Space

- Translational invariance in time suggests Matsubara transform

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

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:

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

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

First-Order Resummation

- Improvement of perturbation theory by resummation

$$\tilde{G}_1(i, \omega_m | j) = \text{Diagram } 1 + \text{Diagram } 2 + \text{Diagram } 3 + \text{Diagram } 4 + \dots$$

First-Order Resummation

- Improvement of perturbation theory by resummation

$$\tilde{G}_1(i, \omega_m | j) = \text{Diagram } i \xrightarrow{\omega_m} + \text{Diagram } i \xrightarrow{\omega_m} j \xrightarrow{\omega_m} + \text{Diagram } i \xrightarrow{\omega_m} k \xrightarrow{\omega_m} j \xrightarrow{\omega_m} + \text{Diagram } i \xrightarrow{\omega_m} k \xrightarrow{\omega_m} h \xrightarrow{\omega_m} j \xrightarrow{\omega_m} + \dots$$

- Summed most easily in Fourier space:

$$\tilde{G}_1^{(1)}(\omega_m, \mathbf{k}) = \frac{C_1^{(0)}(\omega_m)}{1 - J(\mathbf{k}) C_1^{(0)}(\omega_m)}, \quad J(\mathbf{k}) = 2J \sum_{l=1}^D \cos(k_l a)$$

First-Order Resummation

- Improvement of perturbation theory by resummation

$$\tilde{G}_1(i, \omega_m | j) = \text{Diagram } i \xrightarrow{\omega_m} + \text{Diagram } i \xrightarrow{\omega_m} j \xrightarrow{\omega_m} + \text{Diagram } i \xrightarrow{\omega_m} k \xrightarrow{\omega_m} j \xrightarrow{\omega_m} + \text{Diagram } i \xrightarrow{\omega_m} k \xrightarrow{\omega_m} h \xrightarrow{\omega_m} j \xrightarrow{\omega_m} + \dots$$

- Summed most easily in Fourier space:

$$\tilde{G}_1^{(1)}(\omega_m, \mathbf{k}) = \frac{C_1^{(0)}(\omega_m)}{1 - J(\mathbf{k}) C_1^{(0)}(\omega_m)}, \quad J(\mathbf{k}) = 2J \sum_{l=1}^D \cos(k_l a)$$

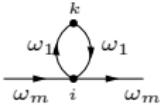
First-Order Resummation

- Improvement of perturbation theory by resummation

$$\tilde{G}_1(i, \omega_m | j) = \text{Diagram } i \xrightarrow{\omega_m} + \text{Diagram } i \xrightarrow{\omega_m} j \xrightarrow{\omega_m} + \text{Diagram } i \xrightarrow{\omega_m} k \xrightarrow{\omega_m} j \xrightarrow{\omega_m} + \text{Diagram } i \xrightarrow{\omega_m} k \xrightarrow{\omega_m} h \xrightarrow{\omega_m} j \xrightarrow{\omega_m} + \dots$$

- Summed most easily in Fourier space:

$$\tilde{G}_1^{(1)}(\omega_m, \mathbf{k}) = \frac{C_1^{(0)}(\omega_m)}{1 - J(\mathbf{k}) C_1^{(0)}(\omega_m)}, \quad J(\mathbf{k}) = 2J \sum_{l=1}^D \cos(k_l a)$$

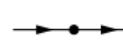
- Neglected contributions like  vanish at least as $1/D$
for $D \rightarrow \infty$

General Resummation Technique

- Replace  by sum over all one-particle irreducible diagrams:

$$\rightarrow \text{---} \otimes \text{---} = \rightarrow \cdot \text{---} \rightarrow + \rightarrow \text{---} \circlearrowleft \text{---} \rightarrow + \left(\frac{1}{2} \rightarrow \text{---} \circlearrowleft \text{---} \circlearrowright \text{---} \rightarrow + \dots \right)$$

General Resummation Technique

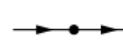
- Replace  by sum over all one-particle irreducible diagrams:

$$\rightarrow \otimes \rightarrow = \rightarrow \bullet \rightarrow + \rightarrow \circlearrowleft \rightarrow + \left(\frac{1}{2} \rightarrow \circlearrowleft \circlearrowright \rightarrow + \dots \right)$$

- Full Green's function obtained by

$$G_1(\omega_m, \mathbf{k}) = \sum_{l=0}^{\infty} (\rightarrow \otimes \rightarrow)^{l+1} J(\mathbf{k})^l$$

General Resummation Technique

- Replace  by sum over all one-particle irreducible diagrams:

$$\rightarrow \text{---} \text{---} = \rightarrow \bullet \rightarrow + \rightarrow \text{---} \text{---} \text{---} + \left(\frac{1}{2} \rightarrow \text{---} \text{---} \text{---} \text{---} \text{---} + \dots \right)$$

- Full Green's function obtained by

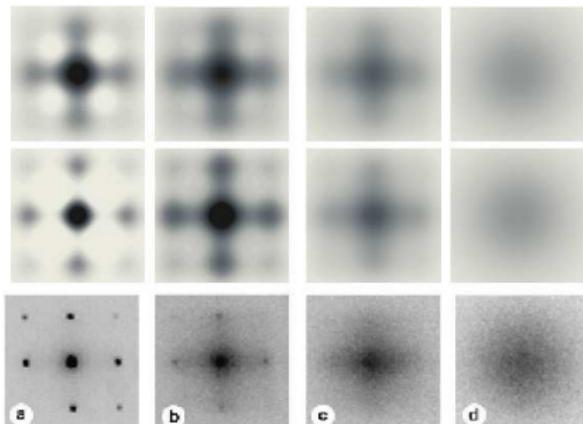
$$G_1(\omega_m, \mathbf{k}) = \sum_{l=0}^{\infty} (\rightarrow \text{---} \text{---} \text{---} \text{---} \text{---})^{l+1} J(\mathbf{k})^l$$

- One-loop approximation by considering only the first two terms in 

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

Momentum space density:

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

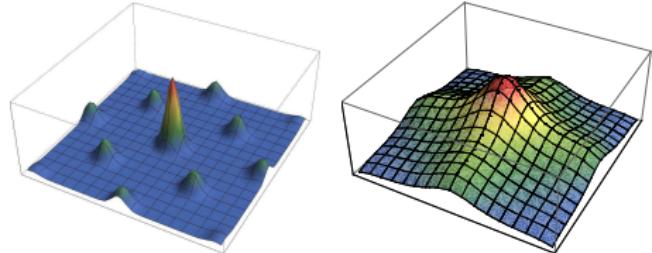


Top to bottom: 1st order, 2nd order, experiment

Left to right: $V_0 = 8 E_R$, $V_0 = 14 E_R$

$V_0 = 18 E_R$, $V_0 = 30 E_R$

Resummed Greens function yields sharp peaks in superfluid phase:



$V_0 = 8 E_R$

$V_0 = 18 E_R$

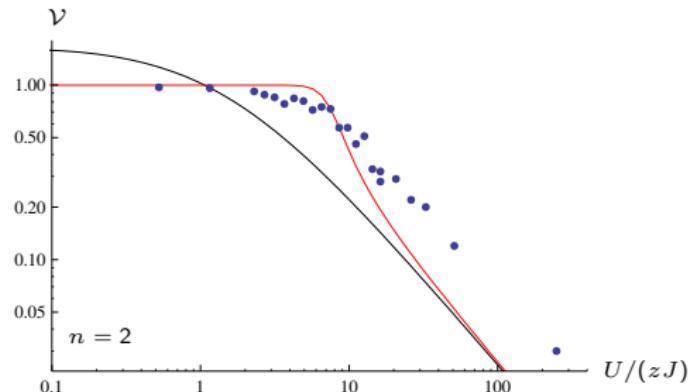
Recoil energy: $E_R = \frac{\hbar^2}{2m\lambda^2}$

Visibility

- Visibility allows quantitative discussion of TOF-Pictures

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

- Expected to converge to unity for $U = 0$ at $T = 0$
- Reduced by thermal fluctuations



Black: First-order perturbation theory.

Red: First-order resummed.

Dots: Experimental Data, Gerbier, et. al PRA **72**, 053606 (2005)

First-Order Phase Diagram

- Phase boundary given by $\tilde{G}_1^{(1)}(0, \mathbf{0}) \rightarrow \infty$

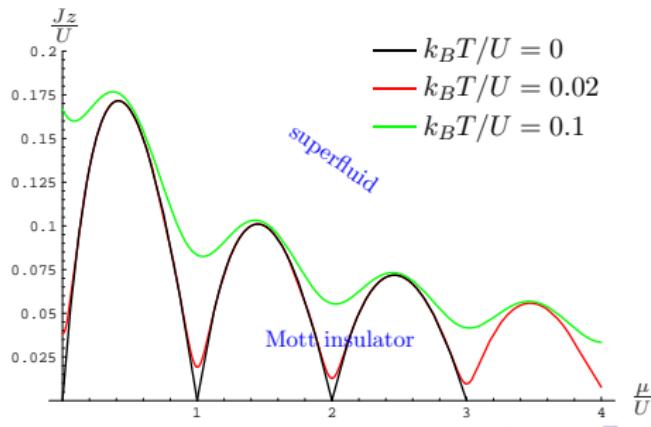
$$2D J_c = \frac{\sum_n e^{-\beta E_n}}{\sum_n e^{-\beta E_n} \left(\frac{n+1}{E_{n+1}-E_n} - \frac{n}{E_n-E_{n-1}} \right)} \xrightarrow{T \rightarrow 0} \frac{1}{\frac{n+1}{E_{n+1}-E_n} - \frac{n}{E_n-E_{n-1}}}$$

First-Order Phase Diagram

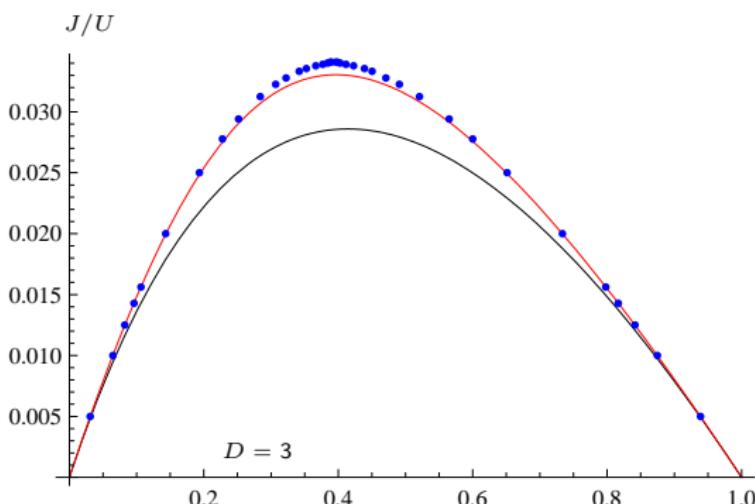
- Phase boundary given by $\tilde{G}_1^{(1)}(0, \mathbf{0}) \rightarrow \infty$

$$2D J_c = \frac{\sum_n e^{-\beta E_n}}{\sum_n e^{-\beta E_n} \left(\frac{n+1}{E_{n+1}-E_n} - \frac{n}{E_n-E_{n-1}} \right)} \xrightarrow{T \rightarrow 0} \frac{1}{\frac{n+1}{E_{n+1}-E_n} - \frac{n}{E_n-E_{n-1}}}$$

- Same result as obtained by mean-field theory ($z = 2D$)



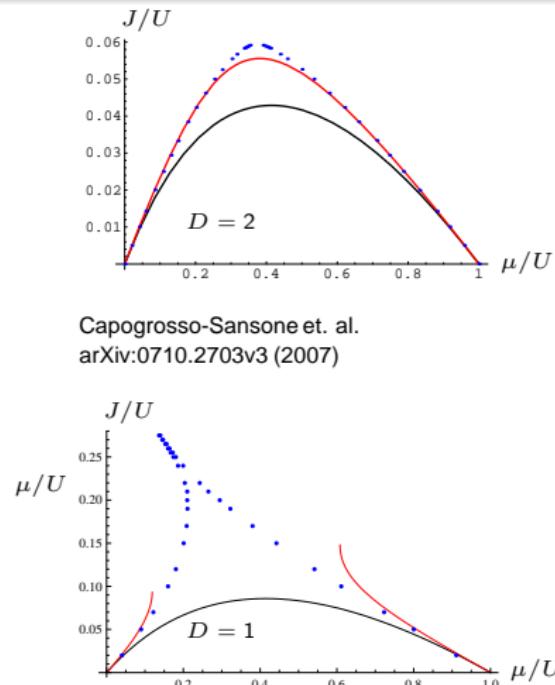
Comparison with Simulations for $T = 0$



Capogrosso-Sansone et. al. PRB 75, 134302 (2007)

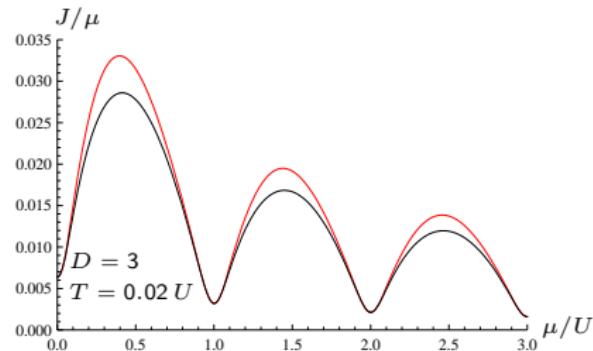
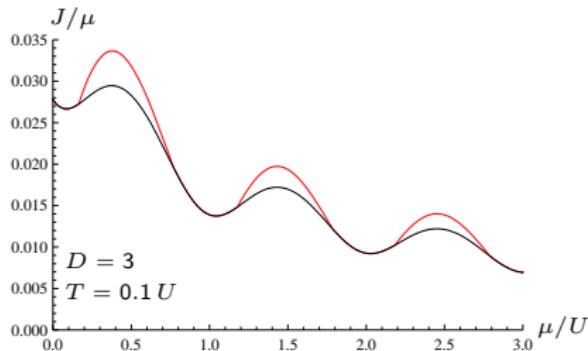
$n = 1$. Black: First order (Mean field)

Red: One-loop corrected



Kühner et al. PRB 58 R14741 (1998)

One-Loop Corrected Finite Temperature Phase Diagram



- Temperature effects small at tip of lobe
- One-loop correction largest at zero temperature

Real-Time Green's Function

- Dynamic properties determined by Green's function in real-time:

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

- Can be obtained by analytic continuation of imaginary-time result by replacing

$$\omega_m \longrightarrow -i\omega$$

- Zeroth order:

$$G_1^{(0)}(\omega; i, j) = \frac{-i\delta_{i,j}}{\mathcal{Z}^{(0)}} \sum_n \left[\frac{(n+1)}{E_{n+1} - E_n - \omega} - \frac{n}{E_n - E_{n-1} - \omega} \right] e^{-\beta E_n}$$

Excitation Spectrum

- Excitation spectrum given by poles of real-time Green's function

Excitation Spectrum

- Excitation spectrum given by poles of real-time Green's function
- For $T = 0$:

$$\tilde{G}_1^{(1)}(\omega, \mathbf{k}) \stackrel{!}{=} 0$$

$$\implies \omega_{1,2} = \frac{U}{2}(2n - 1) - \mu - J(\mathbf{k}) \pm \frac{1}{2}\sqrt{U - 2DJ(\mathbf{k})(4n + 2) + [2DJ(\mathbf{k})]^2}$$

- Different signs correspond to particle and hole excitations

Excitation Spectrum

- Excitation spectrum given by poles of real-time Green's function
- For $T = 0$:

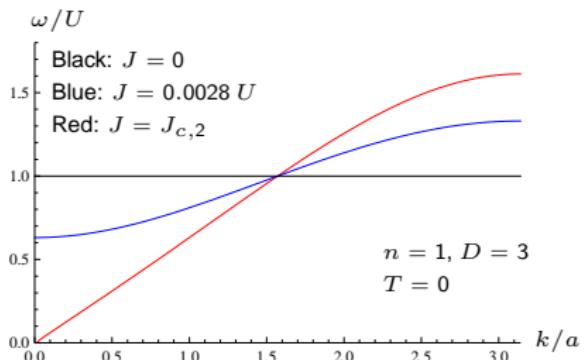
$$\tilde{G}_1^{(1)}(\omega, \mathbf{k}) \stackrel{!}{=} 0$$

$$\implies \omega_{1,2} = \frac{U}{2}(2n - 1) - \mu - J(\mathbf{k}) \pm \frac{1}{2}\sqrt{U - 2DJ(\mathbf{k})(4n + 2) + [2DJ(\mathbf{k})]^2}$$

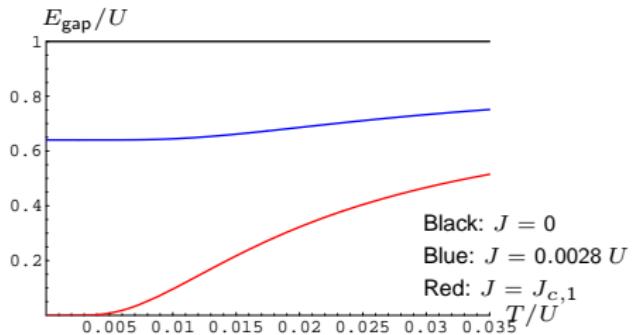
- Different signs correspond to particle and hole excitations
- Dispersion relation of pairs:

$$\omega_{\text{ph}}(\mathbf{k}) = \omega_1(\mathbf{k}) - \omega_2(\mathbf{k}) = \sqrt{U - 2DJ(\mathbf{k})(4n + 2) + [2DJ(\mathbf{k})]^2}$$

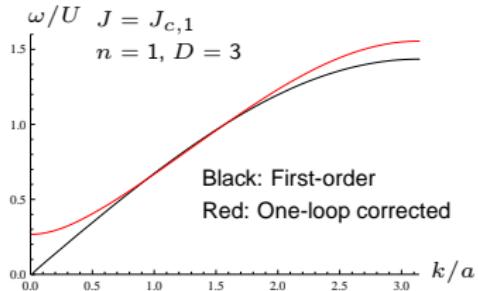
Dispersion Relation



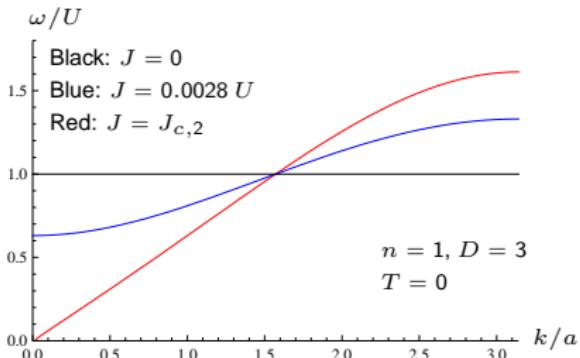
One-loop corrected pairs dispersion relation



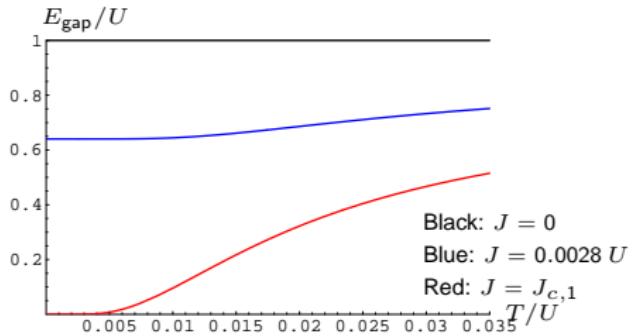
Dependence of gap on temperature (first-order)



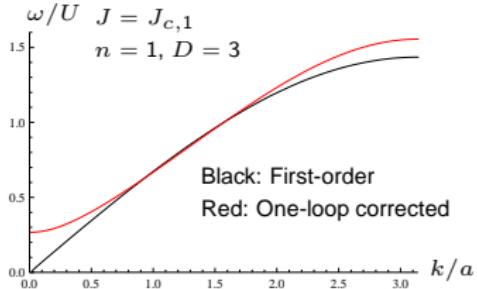
Dispersion Relation



One-loop corrected pairs dispersion relation



Dependence of gap on temperature (first-order)



- Gap vanishes at critical hopping J_c
- Gap experimentally measurable, could serve as thermometer

Effective Masses

- Defined by:

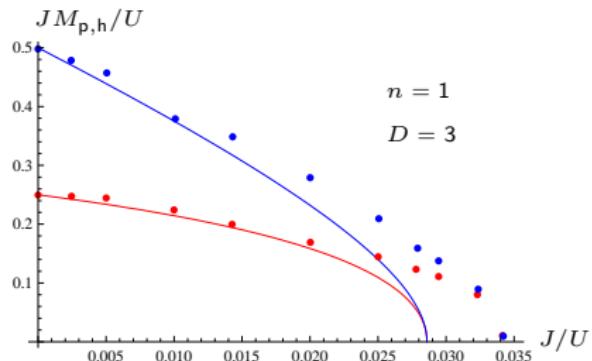
$$\omega_{p,h}(\mathbf{k}) = E_{\text{gap}} + \frac{\mathbf{k}^2}{2M_{p,h}} + \dots$$

$$\tilde{J}M_{p,h} = \frac{\sqrt{1 + 36\tilde{J}(\tilde{J} - 1)}}{3 - 6\tilde{J} \pm \sqrt{1 + 36\tilde{J}(\tilde{J} - 1)}}$$

- At critical J :
Excitations become massless

$$\omega_{p,h}(\mathbf{k}) \propto |\mathbf{k}|$$

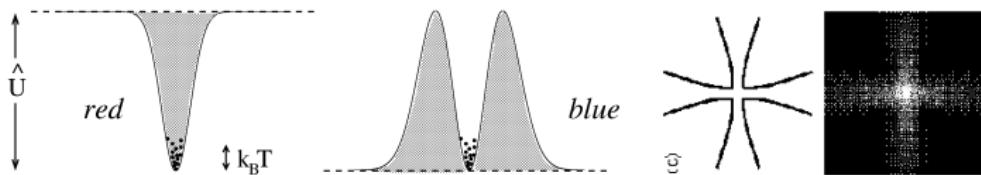
- Particle-hole symmetry at tip of Mott lobe



First-order effective masses of particles (red) and holes (blue).
Dots: QMC data. Capogrosso-Sansone et. al.
PRB **75**, 134302 (2007)

Optical Trap

- Far detuned lasers induce electric dipole moments
- Electric forces push atoms towards center of trap (Stark effect)
 - Red detuned light \Rightarrow Atoms are pushed to maximal intensity
 - Blue detuned light \Rightarrow Atoms are pushed to minimal intensity
- Very shallow, depth smaller than 1mK
- No forced evaporative cooling possible



Spin-1 Bose-Hubbard Hamiltonian

Decomposition of field operators into Wannier functions yields
Bose-Hubbard model:

$$\hat{H}_{\text{BH}} = \hat{H}^{(0)} + \hat{H}^{(1)}$$

$$\hat{H}^{(0)} = \sum_i \left[\frac{1}{2} U_0 \hat{n}_i (\hat{n}_i - 1) + \frac{1}{2} U_2 (\hat{\mathbf{S}}_i^2 - 2\hat{n}_i) - \mu \hat{n}_i - \eta \hat{S}_i^z \right]$$

$$\hat{H}^{(1)} = -J \sum_{\alpha} \sum_{} \hat{a}_{i\alpha}^\dagger \hat{a}_{j\alpha}$$

J : tunnel matrix element between nearest neighbors

$U_0 \propto a_0 + 2a_2$: spin independent interaction

$U_2 \propto a_0 - a_2$: spin dependent interaction

\hat{n}_i : particle number operator on site i

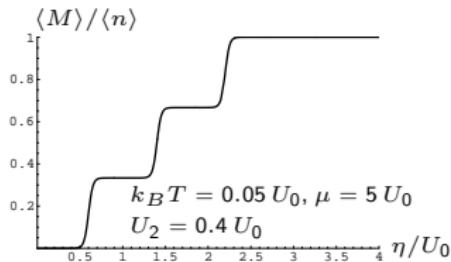
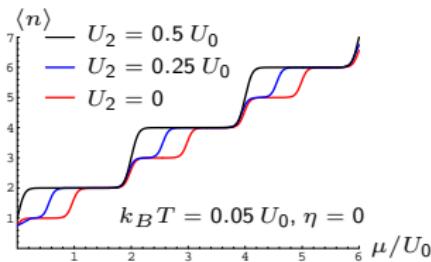
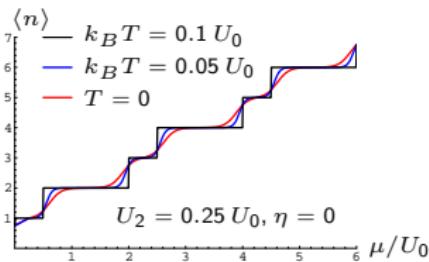
$\hat{\mathbf{S}}_i$: spin operators on site i with $[\hat{S}_j^\alpha, \hat{S}_k^\beta] = i\delta_{jk} \sum_\gamma \epsilon_{\alpha\beta\gamma} \hat{S}_j^\gamma$

Thermal Properties of $J = 0$ System

Hamiltonian site diagonal. Eigenstates characterized by particle number n , total spin S and z -component of spin m .

$$\hat{H}^{(0)}|S, m, n\rangle = N_S E_{S,m,n}^{(0)}|S, m, n\rangle$$

$$E_{S,m,n}^{(0)} = \frac{1}{2}U_0n(n-1) + \frac{1}{2}U_2[S(S+1) - 2n] - \mu n - \eta m$$



Mean-Field Approximation and Landau Expansion

- Decoupling the hopping term:

$$\hat{a}_{i\alpha}^\dagger \hat{a}_{j\alpha} \approx \Psi_\alpha \hat{a}_{i\alpha}^\dagger + \Psi_\alpha^* \hat{a}_{j\alpha} - \Psi_\alpha^* \Psi_\alpha, \quad \Psi_\alpha = \langle \hat{a}_{i\alpha} \rangle, \quad \Psi_\alpha^* = \langle \hat{a}_{i\alpha}^\dagger \rangle$$

$$\hat{H}_{\text{MF}}^{(1)} = -Jz \sum_i \sum_\alpha \left(\Psi_\alpha \hat{a}_{i\alpha}^\dagger + \Psi_\alpha^* \hat{a}_{i\alpha} - \Psi_\alpha^* \Psi_\alpha \right), \quad z = 2D$$

- Perturbative expansion in $\hat{H}_{\text{MF}}^{(1)}$ needs:

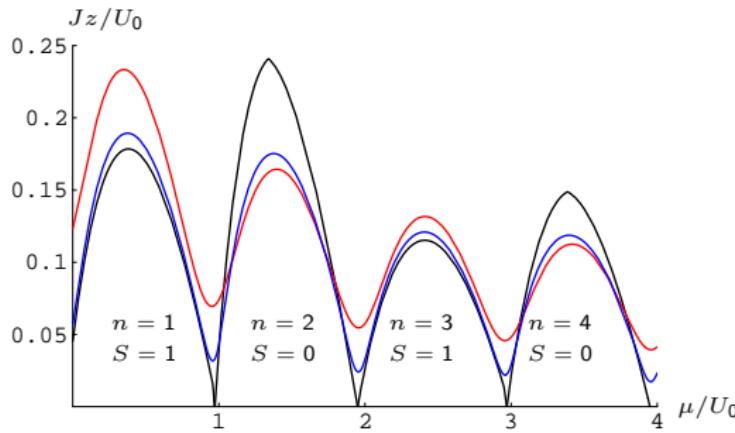
$$\hat{a}_\alpha^\dagger |S, m, n\rangle = M_{\alpha, S, m, n} |S+1, m+\alpha, n+1\rangle + N_{\alpha, S, m, n} |S-1, m+\alpha, n+1\rangle$$

$$\hat{a}_\alpha |S, m, n\rangle = O_{\alpha, S, m, n} |S+1, m-\alpha, n-1\rangle + P_{\alpha, S, m, n} |S-1, m-\alpha, n-1\rangle$$

- Matrix elements M, N, O, P calculated by recursion relation
- Expanding the grand-canonical free energy:

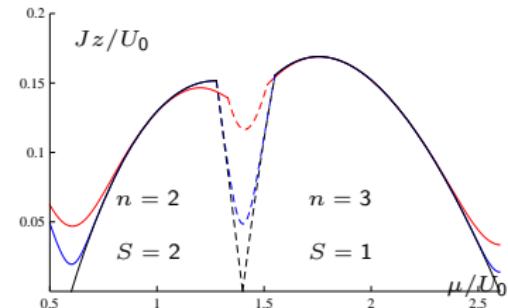
$$\begin{aligned} \mathcal{F}(\Psi^*, \Psi) &= -k_B T \log \text{Tr} \left\{ e^{-(\hat{H}^{(0)} + \hat{H}_{\text{MF}}^{(1)})/k_B T} \right\} \\ &= -k_B T \log \mathcal{Z}^{(0)} + \sum_\alpha A_\alpha^{(2)} |\Psi_\alpha|^2 + O(\Psi^4) \end{aligned}$$

Phase Diagram



$U_2 = 0.04 U_0$, $\eta = 0.05 U_0$, $k_B T = 0.05 U_0$ (red)

$k_B T = 0.09 U_0$ (blue), $k_B T = 0$ (black)



Solid: $\Psi_1 \neq 0$, Dashed: $\Psi_{-1} \neq 0$

$U_2 = 0.5 U_0$, $\eta = 0.09 U_0$,

$k_B T = 0.05 U_0$ (red), $k_B T = 0.02 U_0$ (blue),

$k_B T = 0$ (black)

- Strong asymmetry between even and odd fillings for $T = 0$
- Thermal fluctuations lead to melting of singlet pairs and vanishing of asymmetry

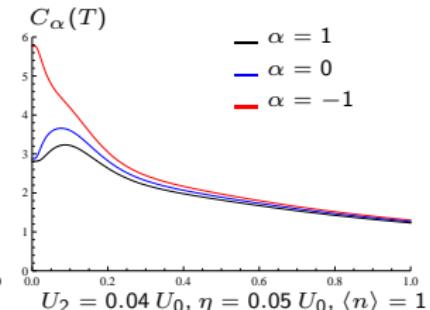
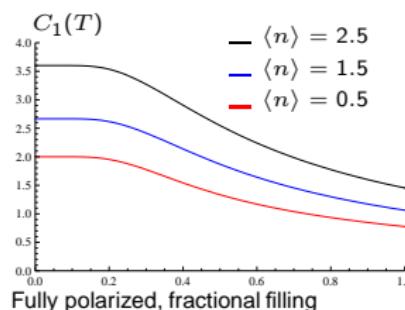
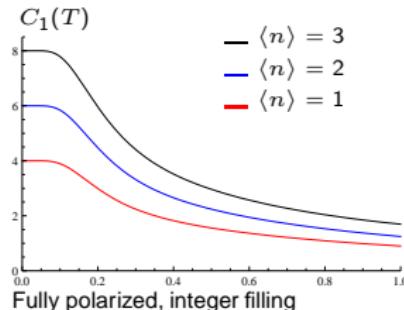
Visibility

- Extended definition for Spin-1 system

$$\mathcal{V}_\alpha = \frac{n_{\alpha\max} - n_{\alpha\min}}{n_{\alpha\max} + n_{\alpha\min}} \approx \frac{S_\alpha(\mathbf{k}_{\max}) - S_\alpha(\mathbf{k}_{\min})}{S_\alpha(\mathbf{k}_{\max}) + S_\alpha(\mathbf{k}_{\min})}$$

- First-order calculation for finite temperature:

$$\mathcal{V}_\alpha(T) = 4zJ \left[1 - \cos(\sqrt{2}\pi) \right] C_\alpha(T) + O(J^2)$$



Summary

- Atoms in optical lattices provide unique model system for condensed matter physics
- Green's functions provide access to various properties of Bosons in optical lattices
- Diagrammatic representation facilitates resummation
- Time-of-Flight pictures well explained especially in Mott phase
- One-loop corrected phase diagram in good agreement with Quantum Monte-Carlo data
- Effective masses of particle and hole excitations vanish for critical hopping parameter
- Spin-1 Bosons show richer phase diagram due to internal degrees of freedom

Outlook

- Scalar Model

- Critical exponents of quantum phase transition
- Green's function within superfluid phase: near phase boundary with Landau expansion, far away with Bogoliubov theory
- Dynamic properties – Collapse and Revival
- Four-point correlations – Hanbury-Brown-Twiss Effect

Outlook

- Scalar Model

- Critical exponents of quantum phase transition
- Green's function within superfluid phase: near phase boundary with Landau expansion, far away with Bogoliubov theory
- Dynamic properties – Collapse and Revival
- Four-point correlations – Hanbury-Brown-Twiss Effect

- Spinor Model

- Different phases within superfluid
- Quantum corrections
- Order of phase transition

Calculation of One-Loop Diagram

$$\begin{aligned}
 2D\delta_{i,j}J^2G_1^{(2B)}(\omega) &= \frac{\omega_1}{\omega_m - i} \cdot \frac{\omega_1}{\omega_m} = \frac{2D\delta_{i,j}}{\mathcal{Z}^{(0)2}} \left(\frac{1}{U^2} \sum_{n,k} e^{-\beta(E_n + E_k)} \right. \\
 &\times \left\{ \frac{(k+1)(n-1)n [k^2 + 2(n-1)^2 - \mu^2 + 2k(2-2n-\mu)]}{(k-n+1)^2(k-2n+\mu)(1-n+\mu)^2} \right. \\
 &\quad \left. + 7 \text{ more terms} \right\} - C_1^{(0)}(\omega)^3 \\
 &+ \beta \left\{ \sum_{n,k} \left[\frac{(n+1)k}{k-n+1} + \frac{n(k+1)}{n-k+1} \right] \left[\frac{n+1}{n-\mu-i\omega} - \frac{n}{n-1-\mu-i\omega} \right] e^{-\beta(E_n + E_k)} \right. \\
 &\quad \left. - C_1^{(0)}(\omega) \sum_{n,k} \left[\frac{(n+1)k}{k-n+1} + \frac{n(k+1)}{n-k+1} \right] e^{-\beta(E_n + E_k)} \right\}
 \end{aligned}$$

Calculation of Cumulants

- Generating functional:

$$C_0^{(0)}[j, j^*] = \log \left\langle \hat{T} \exp \left(\int_0^\beta d\tau j^*(\tau) \hat{a}(\tau) + j(\tau) \hat{a}^\dagger(\tau) \right) \right\rangle^{(0)}$$

- Cumulants calculated by functional derivatives:

$$C_n^{(0)}(\tau'_1, \dots, \tau'_n | \tau_1, \dots, \tau_n)$$

$$= \frac{\delta^{2n}}{\delta j(\tau'_1) \dots \delta j(\tau'_n) \delta j^*(\tau_1) \dots \delta j^*(\tau_n)} C_0^{(0)}[j, j^*] \Big|_{j=j^*=0}$$

$$\begin{aligned} C_1^{(0)}(\tau' | \tau) &= \frac{1}{Z^{(0)}} \sum_{n=0}^{\infty} \left[\Theta(\tau - \tau') (n+1) e^{(E_n - E_{n+1})(\tau - \tau')} \right. \\ &\quad \left. + \Theta(\tau' - \tau) n e^{(E_n - E_{n-1})(\tau' - \tau)} \right] \end{aligned}$$