Bosons in Optical Lattices

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  - 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
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:

\[ T_c \approx 0.08 \frac{\hbar^2}{Mk_B} n^{2/3} \]
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:

Incident photons absorbed: momentum transfer = ħk
Spontaneous emission: total momentum transfer = 0
Net momentum transfer to atom in direction of laser

Atoms
Magnetic trap
(a)  (b)
**Experimental Observation**

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

Time-of-flight absorption image

Magneto-optical trap (MOT)

- cooled atom cloud
- vacuum chamber
- laser beam (circularly polarised)
- magnet coils in anti-Helmholtz configuration
Principles of Optical Lattices

- Optical lattices produced by counter-propagating lasers
- \[ V = V_0 \sum_{i=1}^{D} \sin^2 \left( \frac{2\pi x_i}{\lambda} \right) \]
- 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:

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

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

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

\[ \hat{n}_i = \hat{a}_i^\dagger \hat{a}_i \]

\[ J_{i,j} = \begin{cases} J & \text{if } i, j \text{ nearest neighbors} \\ 0 & \text{otherwise} \end{cases} \]
Bose-Hubbard Model

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\[ \hat{n}_i = \hat{a}_i^\dagger \hat{a}_i \]

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

- \( \hat{H}_0 \) 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:

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

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

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

\[ \hat{X}_H(\tau) = e^{-\hat{H} \tau} \hat{X} e^{\hat{H} \tau} \]
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:

$$\hat{U}_D(\tau, \tau_0) = \sum_{n=0}^{\infty} (-1)^n \int_{\tau_0}^{\tau} d\tau_1 \ldots \int_{\tau_0}^{\tau_{n-1}} d\tau_n \hat{H}_{1D}(\tau_1) \ldots \hat{H}_{1D}(\tau_n)$$

$$= \hat{T} \exp \left( - \int_{\tau_0}^{\tau} d\tau_1 \hat{H}_{1D}(\tau_1) \right)$$
Partition Function

- Full partition function:

\[
Z = \text{Tr} \left\{ e^{-\beta \hat{H}_0} \hat{U}_D(\beta, 0) \right\}
\]
**Partition Function**

- Full partition function:

\[
Z = \text{Tr} \left\{ e^{-\beta \hat{H}_0} \hat{U}_D(\beta, 0) \right\}
\]

- \(n\)th order contribution:

\[
Z^{(n)} = \frac{1}{n!} Z^{(0)} \sum_{i_1, j_1, \ldots, i_n, j_n} J_{i_1 j_1} \cdots J_{i_n j_n} \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \cdots \int_0^\beta d\tau_n \\
\times G_n^{(0)}(\tau_1, j_1; \ldots; \tau_n, j_n | \tau_1, i_1; \ldots; \tau_n, i_n)
\]

- Unperturbed \(n\)-particle Green’s function:

\[
G_n^{(0)}(\tau_1', i_1'; \ldots; \tau_n', i_n' | \tau_1, i_1; \ldots; \tau_n, i_n) = \left\langle \hat{T} \hat{a}^\dagger_{i_1'}(\tau_1') \hat{a}_{i_1}(\tau_1) \cdots \hat{a}^\dagger_{i_n'}(\tau_n') \hat{a}_{i_n}(\tau_n) \right\rangle^{(0)}
\]
Cumulant Decomposition

- Decompose $G_n^{(0)}(τ_1', i_1'; \ldots ; τ_n', i_n'|τ_1, i_1; \ldots ; τ_n, i_n)$ into “simple” parts.
- $\hat{H}_0$ not harmonic $\Rightarrow$ Wick’s theorem not applicable.
Cumulant Decomposition

- Decompose $G_n^{(0)}(\tau'_1, i'_1; \ldots; \tau'_n, i'_n|\tau_1, i_1; \ldots; \tau_n, i_n)$ 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:

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

$$+ \delta_{i_1,i'_1} \delta_{i_2,i'_2} C_1^{(0)}(\tau'_1|\tau_1) C_1^{(0)}(\tau'_2|\tau_2) + \delta_{i_1,i'_2} \delta_{i_2,i'_1} C_1^{(0)}(\tau'_2|\tau_1) C_1^{(0)}(\tau'_1|\tau_2)$$
Cumulant Decomposition

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$$G_2^{(0)}(\tau_1', i_1'; \tau_2', i_2' | \tau_1, i_1; \tau_2, i_2) = \delta_{i_1, i_2} \delta_{i_1', i_2'} C_2^{(0)}(\tau_1', \tau_2' | \tau_1, \tau_2)$$

$$+ \delta_{i_1, i_1'} \delta_{i_2, i_2'} C_1^{(0)}(\tau_1' | \tau_1) C_1^{(0)}(\tau_2' | \tau_2) + \delta_{i_1, i_2} \delta_{i_1', i_2'} C_1^{(0)}(\tau_2' | \tau_1) C_1^{(0)}(\tau_1' | \tau_2)$$

- 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 $\beta$.

\[
\begin{align*}
   i \quad \tau' & \quad = \quad C_1^{(0)}(\tau' | \tau) \\
   \tau & \quad \tau & \quad = \quad C_2^{(0)}(\tau_1', \tau_2' | \tau_1, \tau_2) \\
   \tau_1 & \quad \tau_2 & \quad = \quad J_{ij}
\end{align*}
\]

Example: $\mathcal{Z}^{(2)} = \frac{1}{2} i \quad \tau_1 \quad \tau_2 \quad j$
Diagrammatic Rules for Green’s Function

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

\[ G_1^{(n)}(\tau', i' | \tau, i) = \frac{Z^{(0)}}{Z} \frac{1}{n!} \sum_{i_1, j_1, \ldots, i_n, j_n} J_{i_1 j_1} \cdots J_{i_n j_n} \int_0^\beta d\tau_1 \cdots \int_0^\beta d\tau_n \]

\[ \times G_1^{(0)}(\tau_1, j_1; \ldots; \tau_n, j_n; \tau', i' | \tau_1, i_1; \ldots; \tau_n, i_n, \tau, i) \]
Diagrammatic Rules for Green’s Function

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

$$G_1^{(n)}(\tau', i'|\tau, i) = \frac{Z^{(0)}}{Z} \frac{1}{n!} \sum_{i_1, j_1, \ldots, i_n, j_n} J_{i_1j_1} \cdots J_{i_nj_n} \int_0^\beta d\tau_1 \cdots \int_0^\beta d\tau_n$$

$$\times G_{n+1}^{(0)}(\tau_1, j_1; \ldots; \tau_n, j_n; \tau', i'|\tau_1, i_1; \ldots; \tau_n, i_n, \tau, i)$$

- Diagrams have external lines with fixed time and site variables
Diagrammatic Rules for Green’s Function

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\[ G_1^{(n)}(\tau', i'|\tau, i) = \frac{\mathcal{Z}^{(0)}}{\mathcal{Z}} \frac{1}{n!} \sum_{i_1, j_1, \ldots, i_n, j_n} J_{i_1 j_1} \cdots J_{i_n j_n} \int_0^\beta d\tau_1 \cdots \int_0^\beta d\tau_n \]

\[ \times G_{n+1}^{(0)}(\tau_1, j_1; \ldots; \tau_n, j_n; \tau', i'|\tau_1, i_1; \ldots; \tau_n, i_n, \tau, i) \]

- Diagrams have external lines with fixed time and site variables
- Disconnected diagrams cancel \( \mathcal{Z}^{(0)}/\mathcal{Z} \)
Diagrammatic Rules for Green’s Function

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\]

\[
G_1^{(n)}(\tau', i'| \tau, i) = \frac{\mathcal{Z}^{(0)}}{\mathcal{Z}} \frac{1}{n!} \sum_{i_1, j_1, \ldots, i_n, j_n} J_{i_1 j_1} \ldots J_{i_n j_n} \int_0^\beta d\tau_1 \ldots \int_0^\beta d\tau_n 
\times G_{n+1}^{(0)}(\tau_1, j_1; \ldots; \tau_n, j_n; \tau', i'| \tau_1, i_1; \ldots; \tau_n, i_n, \tau, i)
\]

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

\[
G_1^{(0)}(\tau', i| \tau, j) = \delta_{i,j} C_1^{(0)}(\tau'| \tau)
\]

\[
G_1^{(1)}(\tau', i| \tau, j) = J \delta_{d(i,j), 1} \int_0^\beta d\tau_1 C_1^{(0)}(\tau'| \tau_1) C_1^{(0)}(\tau_1 | \tau)
\]
Calculations in Matsubara Space

- Translational invariance in time suggests Matsubara transform

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

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- In rule 3 integration over \( \tau \) replaced by summation over \( \omega_m \) under consideration of frequency conservation on vertices:

\[ G_1^{(1)}(\omega_m; i, j) = \begin{array}{c}
\omega_m \quad \omega_m \quad \omega_m \\
\text{with} & \rightarrow \quad \rightarrow
\end{array} = J\delta_d(i,j)_1 C_1^{(0)}(\omega_m)^2 \]

\[ G_2^{(1)}(\omega_m; i, j) = \begin{array}{c}
\omega_m \quad \omega_m \quad \omega_m \quad \omega_m \\
\text{with} & \rightarrow \quad \rightarrow
\end{array} + \begin{array}{c}
\omega_1 \quad \omega_1 \\
\text{with} & \rightarrow \quad \rightarrow
\end{array} = J^2 (\delta_d(i,j)_2 + 2\delta_d(i,j)_2\sqrt{2} + 2D\delta_{i,j}) C_1^{(0)}(\omega_m)^3 \]

\[ + J^2 2D \delta_{i,j} \sum_{\omega_1} C_1^{(0)}(\omega_m) C_2^{(0)}(\omega_m, \omega_1 | \omega_m, \omega_1) \]
First-Order Resummation

- Improvement of perturbation theory by resummation

\[ \tilde{G}_1(i, \omega_m | j) = i \omega_m + i j \omega_m + i k j \omega_m + i k h j \omega_m + \ldots \]
First-Order Resummation

- Improvement of perturbation theory by resummation

\[ \tilde{G}_1(i, \omega_m | j) = \sum_{\text{terms}} \tilde{G}_1(i, \omega_m | j) \]

- Summed most easily in Fourier space:

\[ \tilde{G}_1^{(1)}(\omega_m, k) = \frac{C_1^{(0)}(\omega_m)}{1 - J(k) C_1^{(0)}(\omega_m)}, \quad J(k) = 2J \sum_{l=1}^{D} \cos(kl a) \]
First-Order Resummation

- Improvement of perturbation theory by resummation

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First-Order Resummation

- Improvement of perturbation theory by resummation

\[ \tilde{G}_1(i, \omega_m | j) = \sum_{\omega_m} i \omega_m i \omega_m j \omega_m + \sum_{\omega_m} i \omega_m k \omega_m j \omega_m + \sum_{\omega_m} i \omega_m k \omega_m h \omega_m j \omega_m + \ldots \]

- Summed most easily in Fourier space:

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

- Neglected contributions like \( i k \omega_1 \omega_1 \omega_m \) vanish at least as \( 1/D \) for \( D \to \infty \)
Replace $\rightarrow \rightarrow$ by sum over all one-particle irreducible diagrams:

$$\rightarrow \rightarrow = \rightarrow \rightarrow + \rightarrow \rightarrow + \left( \frac{1}{2} \rightarrow \rightarrow + \ldots \right)$$
General Resummation Technique

- Replace $\rightarrow \rightarrow$ by sum over all one-particle irreducible diagrams:

$$\rightarrow \rightarrow = \rightarrow \rightarrow + \rightarrow \rightarrow + \left( \frac{1}{2} \rightarrow \rightarrow + \ldots \right)$$

- Full Green’s function obtained by

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

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

\[ \rightarrow \rightarrow = \rightarrow \rightarrow + \bigcirc \rightarrow \rightarrow + \left( \frac{1}{2} \bigcirc \rightarrow \rightarrow + \ldots \right) \]

- Full Green’s function obtained by

\[ G_1(\omega_m, k) = \sum_{l=0}^{\infty} (\bigcirc \rightarrow \rightarrow)^{l+1} J(k)^l \]

- One-loop approximation by considering only the first two terms in \( \rightarrow \rightarrow \).
**Introduction**

**Green’s Function Approach**

**Applications**

**Spin-1 Bosons**

**Time-of-Flight/Visibility**

**Phase Boundary**

**Excitations**

---

**Time-of-Flight Pictures for \( T = 0 \)**

Momentum space density:

\[
n_{k} = \langle \hat{\psi}^\dagger(k)\hat{\psi}(k) \rangle = |w(k)|^2 S(k), \quad S(k) = \sum_{i,j} e^{ik(r_i-r_j)} \lim_{\tau' \to 0} G_1(\tau', i|0,j)\]

---

Resummed Greens function yields sharp peaks in superfluid phase:

---

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

Left to right: \( V_0 = 8 \, E_R \), \( V_0 = 14 \, E_R \)

\( V_0 = 18 \, E_R \), \( V_0 = 30 \, E_R \)

Recoil energy: \( E_R = \frac{h^2}{2m\lambda^2} \)
Visibility allows quantitative discussion of TOF-Pictures

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

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 $\tilde{G}_1^{(1)}(0,0) \to \infty$

\[
2DJ_c = \frac{\sum_n e^{-\beta E_n}}{\sum_n e^{-\beta E_n} \left( \frac{n+1}{E_{n+1} - E_n} - \frac{n}{E_n - E_{n-1}} \right)} \xrightarrow{T \to 0} \frac{1}{\frac{n+1}{E_{n+1} - E_n} - \frac{n}{E_n - E_{n-1}}}
\]
First-Order Phase Diagram

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

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

- Same result as obtained by mean-field theory ($z = 2D$)
Comparison with Simulations for $T = 0$

$n = 1$. Black: First order (Mean field)
Red: One-loop corrected
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:

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

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

\[
\omega_m \rightarrow -i\omega
\]

- Zeroth order:

\[
G_1^{(0)}(\omega; i, j) = \frac{-i\delta_{i,j}}{Z^{(0)}} \sum_n \left[ \frac{(n+1)}{E_{n+1} - E_n - \omega} - \frac{n}{E_n - E_{n-1} - \omega} \right] e^{-\beta E_n}
\]
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 $T = 0$:
  \[
  \tilde{G}_1^{(1)}(\omega, k) = 0
  \]
  \[
  \Rightarrow \omega_{1,2} = \frac{U}{2}(2n - 1) - \mu - J(k) \pm \frac{1}{2} \sqrt{U - 2DJ(k)(4n + 2) + [2DJ(k)]^2}
  \]
- Different signs correspond to particle and hole excitations
Excitation Spectrum

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

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

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

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

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

- Black: $J = 0$
- Blue: $J = 0.0028 \, U$
- Red: $J = J_{c,2}$

$n = 1, D = 3$
$T = 0$

- Black: First-order
- Red: One-loop corrected

- Black: $J = 0$
- Blue: $J = 0.0028 \, U$
- Red: $J = J_{c,1}$

$E_{\text{gap}} / U$

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Bosons in Optical Lattices
Dispersion Relation

\[ \omega / U \]

- Black: \( J = 0 \)
- Blue: \( J = 0.0028 \, U \)
- Red: \( J = J_{c,2} \)

\[ n = 1, \, D = 3 \]
\[ T = 0 \]

\[ k / a \]

One-loop corrected pairs dispersion relation

\[ E_{\text{gap}} / U \]

- Black: \( J = 0 \)
- Blue: \( J = 0.0028 \, U \)
- Red: \( J = J_{c,1} \)

\[ T / U \]

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:
  \[ \omega_{p,h}(k) = E_{\text{gap}} + \frac{k^2}{2M_{p,h}} + \ldots \]

- At critical \( J \):
  Excitations become massless
  \[ \omega_{p,h}(k) \propto |k| \]

- Particle-hole symmetry at tip of Mott lobe

![Graph showing first-order effective masses of particles (red) and holes (blue). Dots: QMC data. Capogrosso-Sansone et al. PRB 75, 134302 (2007).]

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 $1\text{mK}$
- No forced evaporative cooling possible
Spin-1 Bose-Hubbard Hamiltonian

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

\[ \hat{H}_{BH} = \hat{H}^{(0)} + \hat{H}^{(1)} \]

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

\[ \hat{H}^{(1)} = -J \sum_\alpha \sum_{<i,j>} \hat{a}_{i\alpha}^\dagger \hat{a}_{j\alpha} \]

\( J \): 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 \( i \)
\( \hat{S}_i \): 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 $m$.

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

$$E_{S,m,n}^{(0)} = \frac{1}{2}U_0 n(n - 1) + \frac{1}{2}U_2[S(S + 1) - 2n] - \mu n - \eta m$$
Mean-Field Approximation and Landau Expansion

- Decoupling the hopping term:
  \[
  \hat{a}_{i\alpha}^\dagger \hat{a}_{j\alpha} \approx \psi_{\alpha} \hat{a}_{i\alpha}^\dagger + \psi_{\alpha}^* \hat{a}_{j\alpha} - \psi_{\alpha}^* \psi_{\alpha}, \quad \psi_{\alpha} = \langle \hat{a}_{i\alpha} \rangle, \quad \psi_{\alpha}^* = \langle \hat{a}_{i\alpha}^\dagger \rangle
  \]
  \[
  \hat{H}^{(1)}_{\text{MF}} = -Jz \sum_i \sum_{\alpha} \left( \psi_{\alpha} \hat{a}_{i\alpha}^\dagger + \psi_{\alpha}^* \hat{a}_{i\alpha} - \psi_{\alpha}^* \psi_{\alpha} \right), \quad z = 2D
  \]

- Perturbative expansion in \( \hat{H}^{(1)}_{\text{MF}} \) 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:
  \[
  F(\Psi^*, \Psi) = -k_B T \log \text{Tr} \left\{ e^{-\left(\hat{H}^{(0)} + \hat{H}^{(1)}_{\text{MF}}\right)/k_B T} \right\}
  \]
  \[
  = -k_B T \log Z^{(0)} + \sum_{\alpha} A^{(2)}_{\alpha} |\psi_{\alpha}|^2 + O(\Psi^4)
  \]
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

\[ V_\alpha = \frac{n_{\alpha \text{max}} - n_{\alpha \text{min}}}{n_{\alpha \text{max}} + n_{\alpha \text{min}}} \approx \frac{S_\alpha(k_{\text{max}}) - S_\alpha(k_{\text{min}})}{S_\alpha(k_{\text{max}}) + S_\alpha(k_{\text{min}})} \]

- First-order calculation for finite temperature:

\[ V_\alpha(T) = 4zJ \left[ 1 - \cos(\sqrt{2}\pi) \right] C_\alpha(T) + O(J^2) \]
**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
- Diagramatic 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
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- **Spinor Model**
  - Different phases within superfluid
  - Quantum corrections
  - Order of phase transition
Calculation of One-Loop Diagram

\[
2D\delta_{i,j} J^2 G^{(2B)}_1(\omega) = \frac{2D\delta_{i,j}}{Z(0)^2} \left( \frac{1}{U^2} \sum_{n,k} e^{-\beta(E_n + E_k)} \right) \\
\times \left\{ \frac{(k+1)(n-1)n [k^2 + 2(n-1)^2 - \mu^2 + 2k(2 - 2n - \mu)]}{(k-n+1)^2(k-2n+\mu)(1-n+\mu)^2} \right\} \\
+ 7 \text{ more terms} \right\} - C_1^{(0)}(\omega)^3 \\
+ \beta \left\{ \sum_{n,k} \left[ \frac{(n+1)k}{k-n+1} + \frac{n(k+1)}{n-k+1} \right] \frac{n+1}{n-\mu-i\omega} - \frac{n}{n-1-\mu-i\omega} \right\} e^{-\beta(E_n + E_k)} \\
- C_1^{(0)}(\omega) \sum_{n,k} \left[ \frac{(n+1)k}{k-n+1} + \frac{n(k+1)}{n-k+1} \right] e^{-\beta(E_n + E_k)} \right\} 
\]
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:

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

\[
C_1^{(0)}(\tau' | \tau) = \frac{1}{\mathcal{Z}^{(0)}} \sum_{n=0}^\infty \left[ \Theta(\tau - \tau') (n + 1) e^{(E_n - E_{n+1})(\tau - \tau')} + \Theta(\tau' - \tau) n e^{(E_n - E_{n-1})(\tau' - \tau)} \right]
\]