Bose-Hubbard models: Phases & Excitations

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A tribute to Professor Satyendra Nath Bose on his 125th birth anniversary
International Workshop on Bose-Einstein Condensation and related phenomena (IWBECRP)
26-28th March, 2018

Goa University

Outline

Bose-Hubbard Models:

- Physical Realizations.
- Mean-field Theory : homogeneous
- Mean-field Theory : inhomogeneous
- Random Phase Approximation for Excitations.
- Finite Temperature:
- Bose Mixtures: Phases and Excitations
- Conclusions.

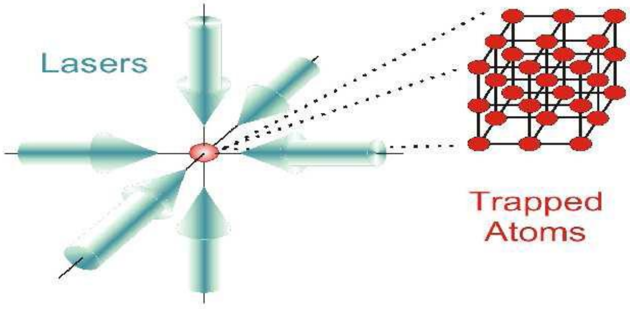
Physical Realizations

Interacting Bose Systems:

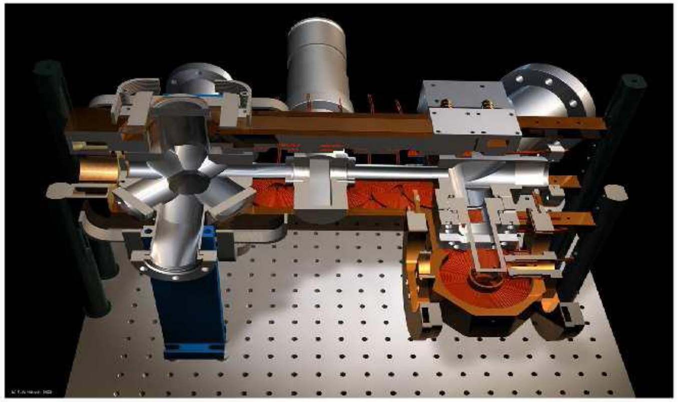
- ^{4}He in vycor or aerogel (disorder)
- Microfabricated Josephson junction arrays.
- Disorder-driven superconductor-insulator transition (e.g., thin films of bismuth).
- Type II superconductors with columnar defects.
- Ultra cold atoms in optical potentials.

Ultra Cold Atoms in Optical Lattices

Interference of standing wave laser beams is used to trap atoms in a periodic lattice potential:



Munich: I. Bloch, T. Haensch et al.



Cold Atoms in Optical Lattices

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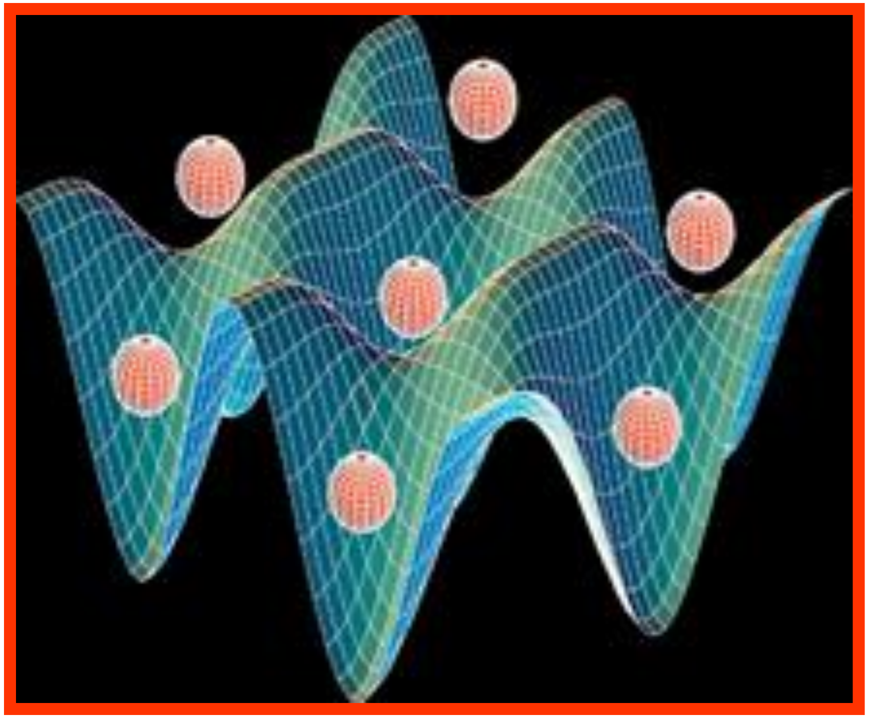
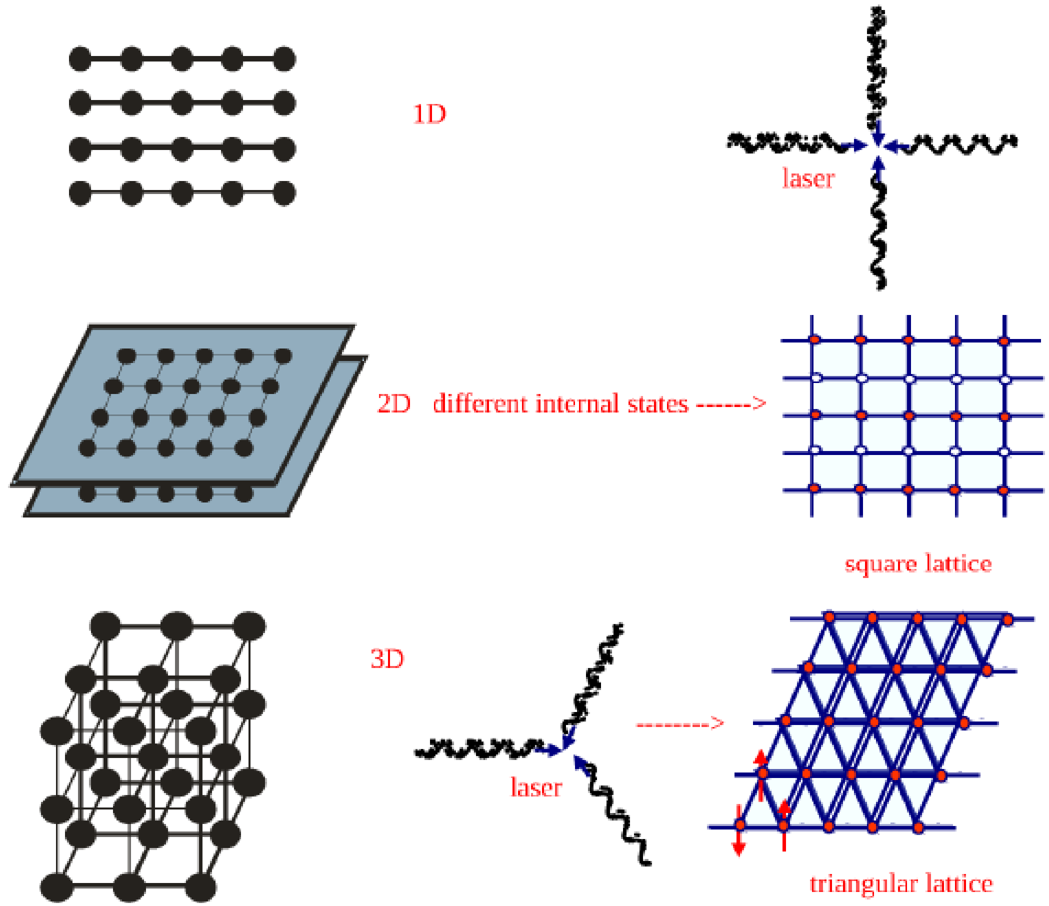
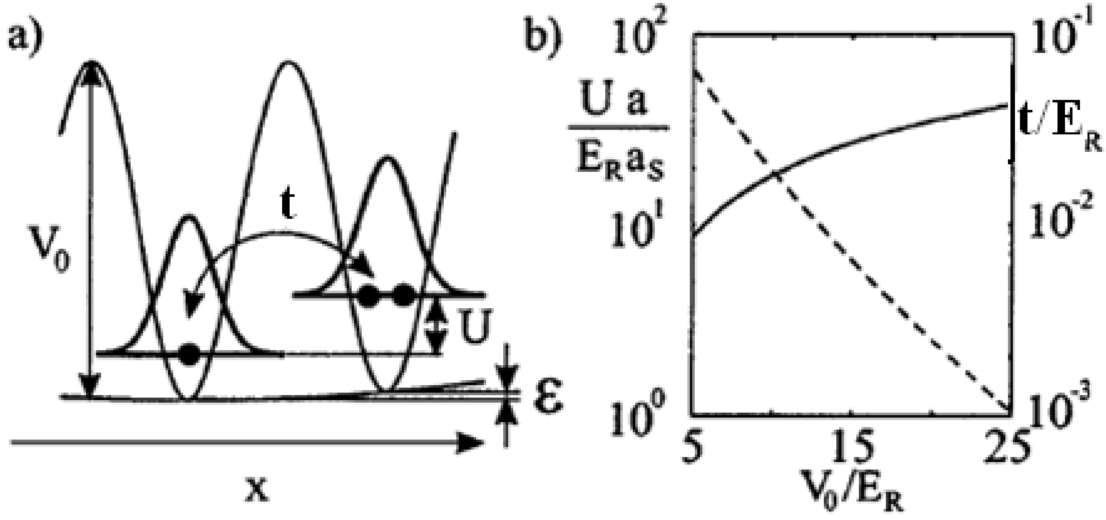


Lattice designs



Model



$$\frac{t}{E_r} = \frac{4}{\sqrt{\pi}}\left(\frac{V_0}{E_r}\right)^{3/4} e^{-2\sqrt{\frac{V_0}{E_r}}}$$

$$E_r = \frac{\hbar^2 k^2}{2m}$$ Recoil energy

$$\frac{U}{E_r} = \sqrt{8\pi}\,\frac{a_s}{a}\left(\frac{V_0}{E_r}\right)^{3/4}$$

a_s s-wave scattering length

$a = \lambda/2$ Lattice constant

Jaksch et. al. (1998) PRL **81**, 3108

Bose-Hubbard model

$$H = -t\sum_{<i,j>}(a_i^+ a_j + h.c) + \frac{U}{2}\sum_i n_i(n_i - 1)$$

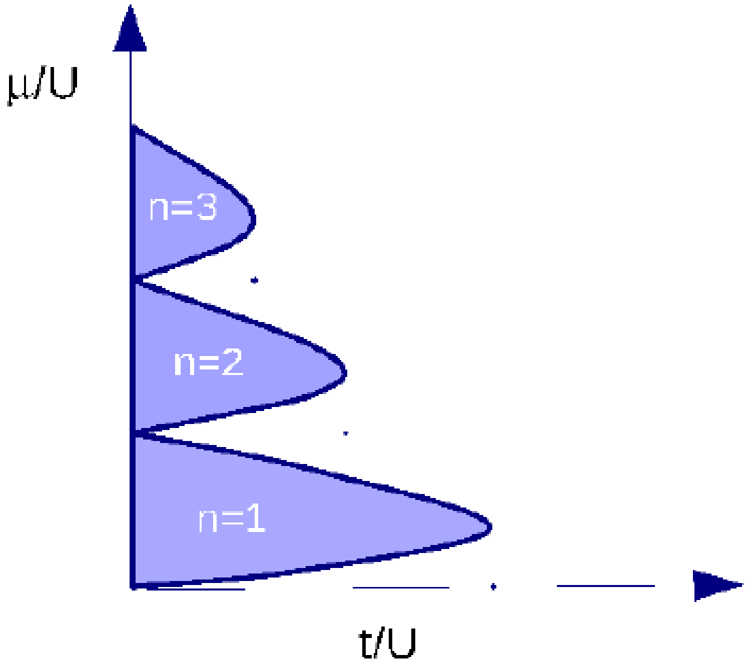
$$-\mu\sum_i n_i + V_T\sum_i n_i(\vec{r}_i - \vec{r}_0)^2$$

Where V_T is the strength of the trap potential and $\vec{r}_0$ is the center of the lattice

$$|\Psi_{SF}>_{\frac{U}{t}\approx 0} \propto \left(\sum_i a_i^+\right)^N |0>$$

$$|\Psi_{MI}>_{t\approx 0} \propto \Pi_i \left(a_i^+\right)^N |0>$$

Bose-Hubbard model: Phase Diagram



- M. Fisher el. al. Phys. Rev. B. **40**, 546 (1989)
- Sheshadri et. al. Europhys. Lett. **22** 257 (1993)
- Experiments: M. Greiner et. al. Nature **415**, 39 (2002).

Bose-Hubbard model: Mean-field theory

$$H = -t_a \sum_{<i,j>} (a_i^+ a_j + h.c) + \frac{U}{2} \sum_i n_i (n_i - 1) - \mu \sum_i n_i$$

$$a_i^+ a_j \approx < a_i^+ > a_j + a_i^+ < a_j > - < a_i^+ >< a_j >$$

Superfluid order parameter $\psi_i^a = < a_i >$

$$H = \sum_i H_i^{MF} - t \sum_{<i,j>} (\delta a_i^+ \delta a_j + h.c)$$

$$H_i^{MF} = \frac{U}{2} \hat{n}_i (\hat{n}_i - 1) - \mu n_i - (\psi_i^* a_i + \psi_i a_i^+) + |\psi_i|^2$$

Sheshadri et. al. Europhys. Lett. **22** 257 (1993)

Bose-Hubbard model
Mean-field theory

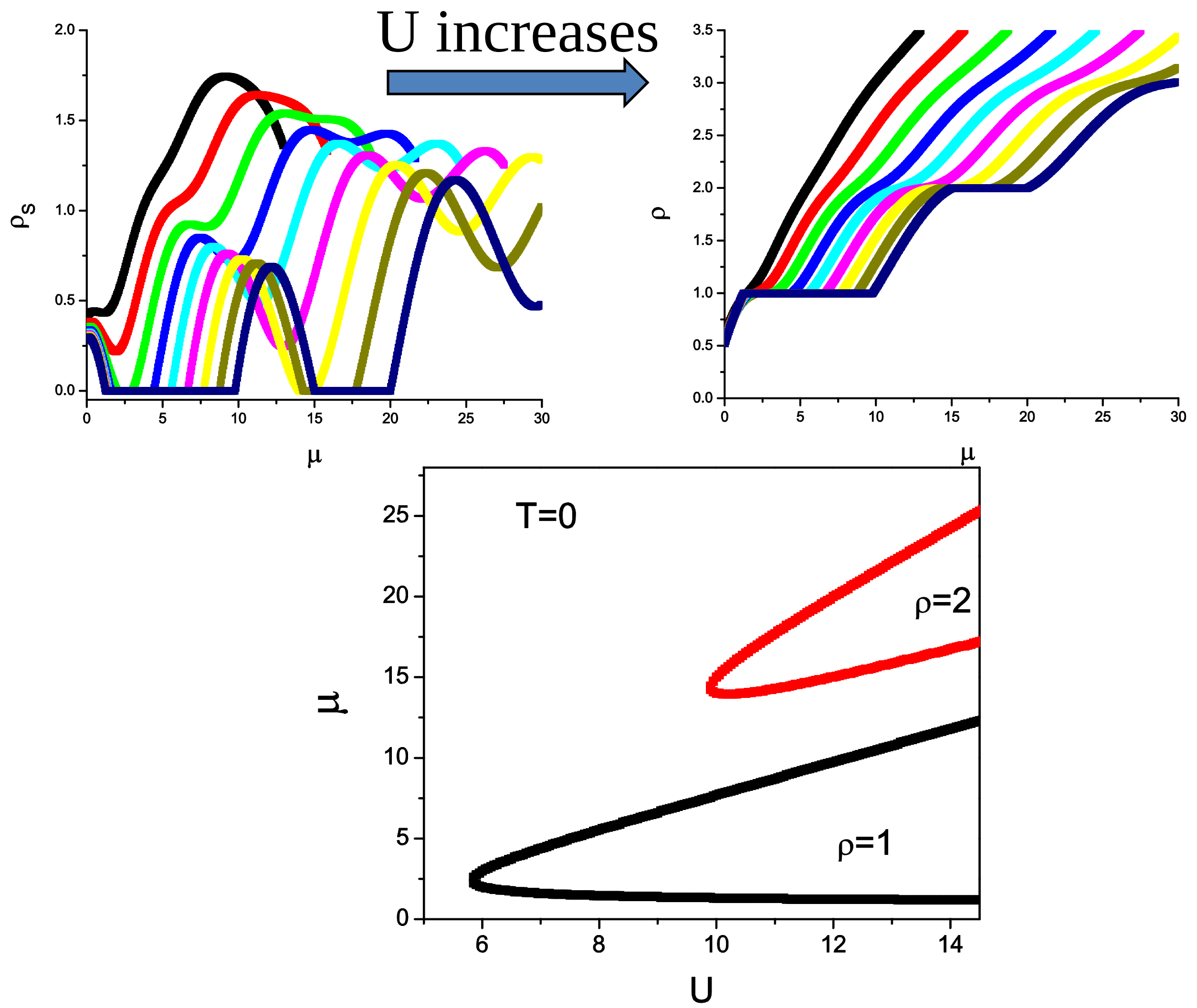
$$H_i^{MF} = \frac{U}{2}\hat{n}_i(\hat{n}_i - 1) - \mu n_i - (\psi_i^* a_i + \psi_i a_i^+) + |\psi_i|^2$$

- Superfluid density $(\rho_s)_i = |\psi_i|^2$
- Density $\rho_i = < \hat{n}_i >$
- Compressibility $\kappa_i = \frac{\partial \rho_i}{\partial \mu_i}$

$$\text{SF Phase}: \ \rho_S > 0 \quad \kappa > 0$$

$$\text{MI Phase}: \ \rho_S = 0 \quad \kappa = 0$$

Bose-Hubbard model: Phase Diagram



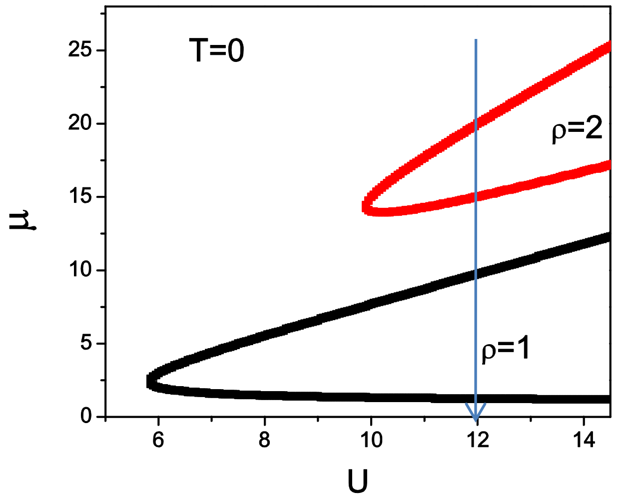
Bose-Hubbard model: Inhomogeneous MFT

$$H^{MF} = \sum_i H_i + \frac{1}{2z}\sum_{<ij>}(\psi_i^* \psi_j + \psi_i \psi_j^*)$$

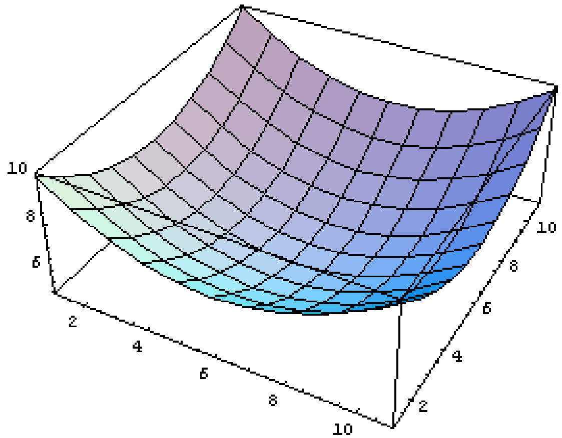
$$H_i = \frac{U}{2}\hat{n}_i(\hat{n}_i - 1) - \mu_i n_i - (\phi_i^* a_i + \phi_i a_i^+)$$

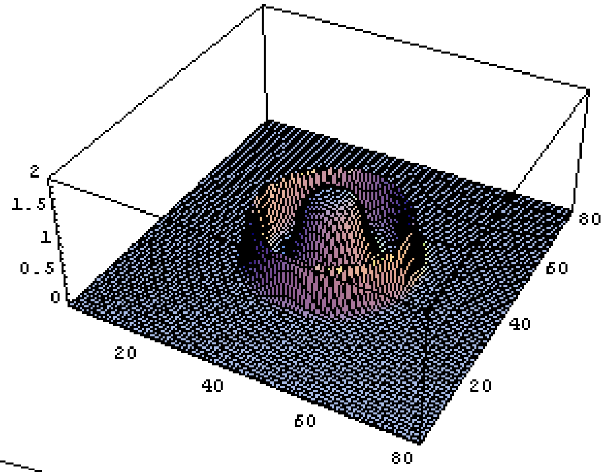
$$\phi_i = \frac{1}{z}\sum_\delta \psi_{i+\delta}$$

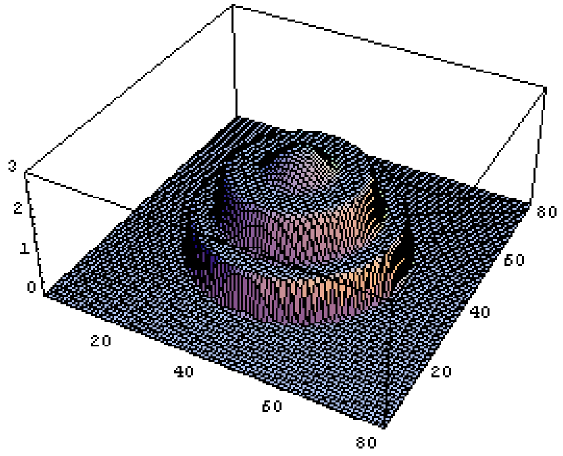
$$\mu_i = \mu - V_T(\vec{r}_i - \vec{r}_0)^2$$



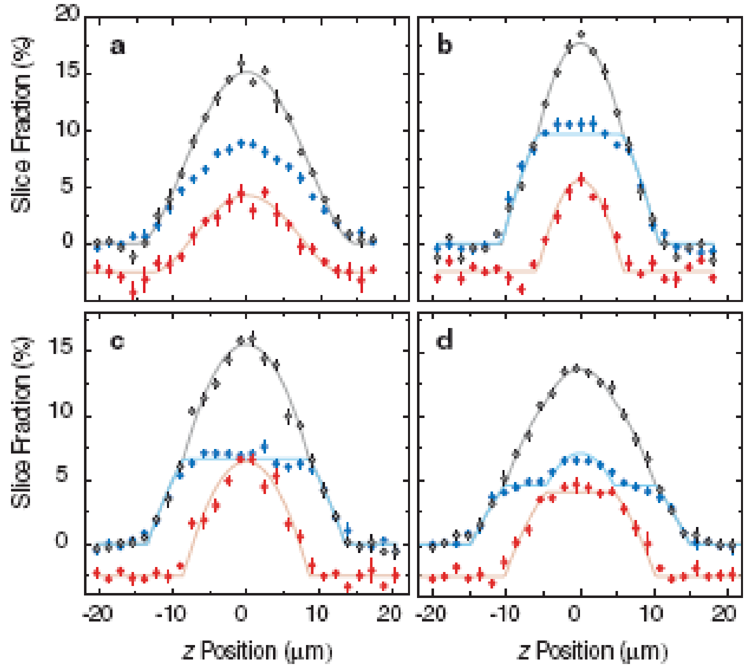
Bose-Hubbard model:
SF & MI shells







Bose-Hubbard model:
SF & MI shells



	Number of atoms	V_0 (E_r)
a	1.0×10^5	3
b	1.0×10^5	22
c	2.0×10^5	22
d	3.5×10^5	22

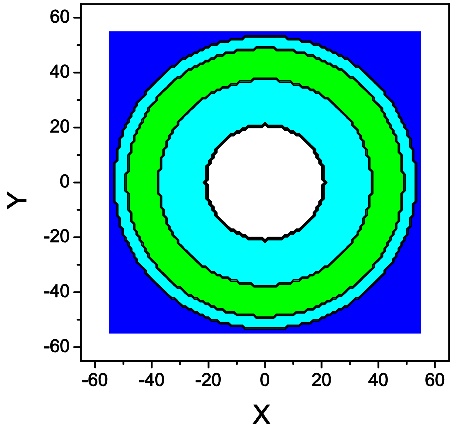
Gray: Total density distribution

Red: Density distribution with ρ=2

Blue: Gray - Red

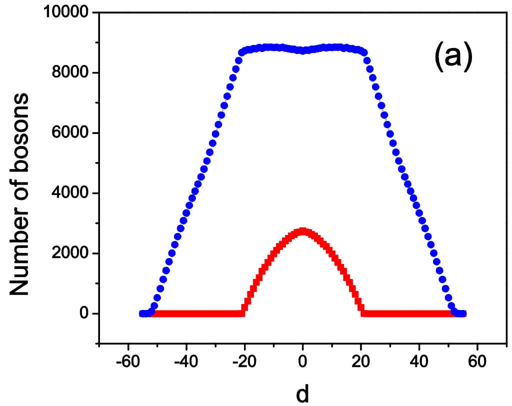
Folling et. al. PRL **97** 060403 (2006)

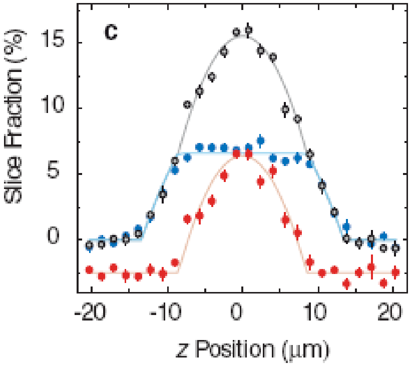
Bose-Hubbard model:
Density Distribution & Shells: Result



SF
MI (ρ=1)
MI (ρ=2)

	Number of atoms	V_0 (E_r)
a	7.1 X 10^5	15



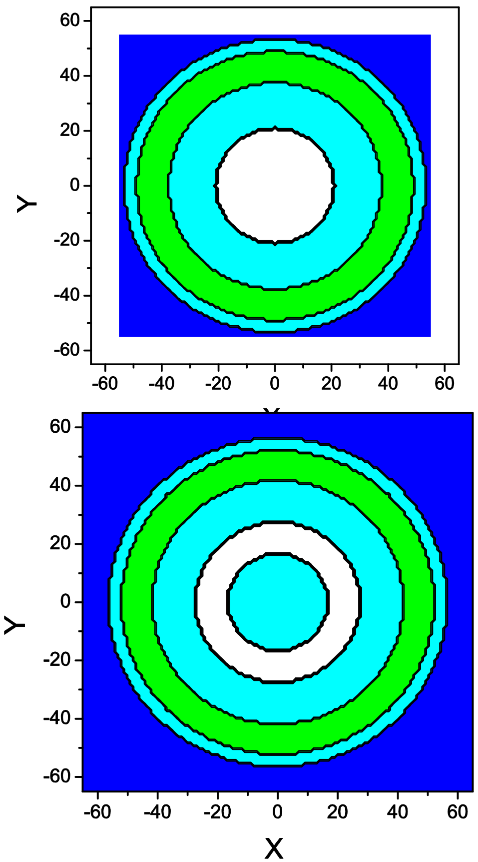


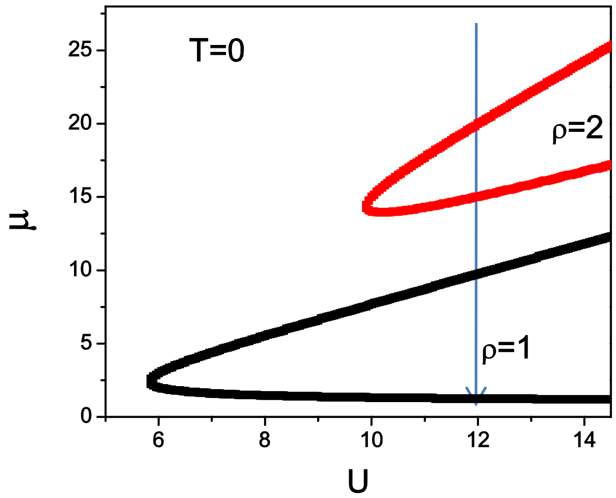
Red: Density distribution with ρ=2

Blue: Total Distribution - Red

Phys. Rev. B **85**, 214524 (2012)

Bose-Hubbard model: Density Distribution & Shells: Result

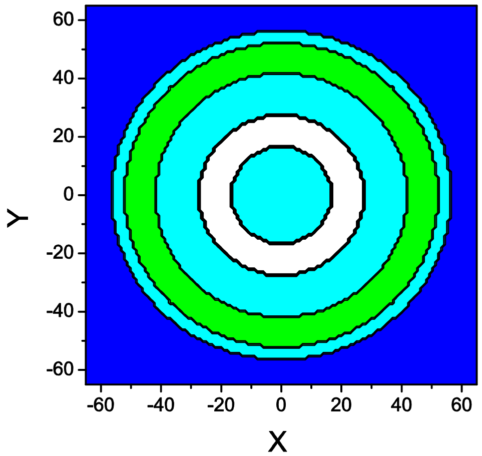




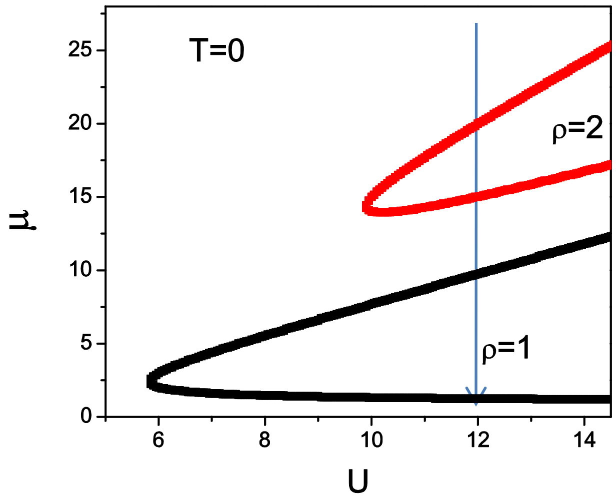
	Number of atoms	V_0 (E_r)
a	7.1×10^5	15
b	8.9×10^5	15

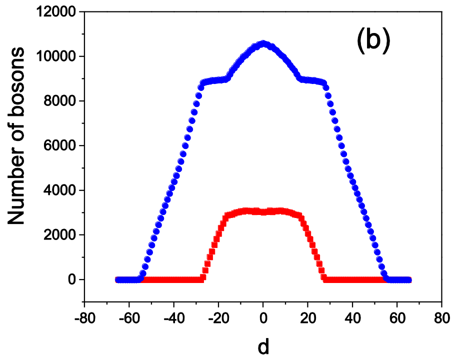
Phys. Rev. B **85**, 214524 (2012).

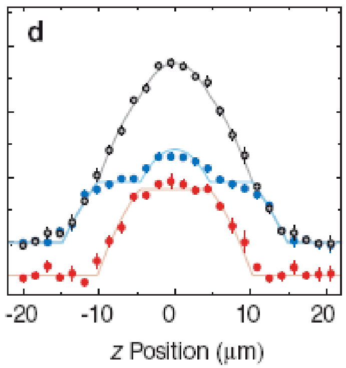
Bose-Hubbard model:
Density Distribution & Shells: Result



SF
MI (ρ=1)
MI (ρ=2)

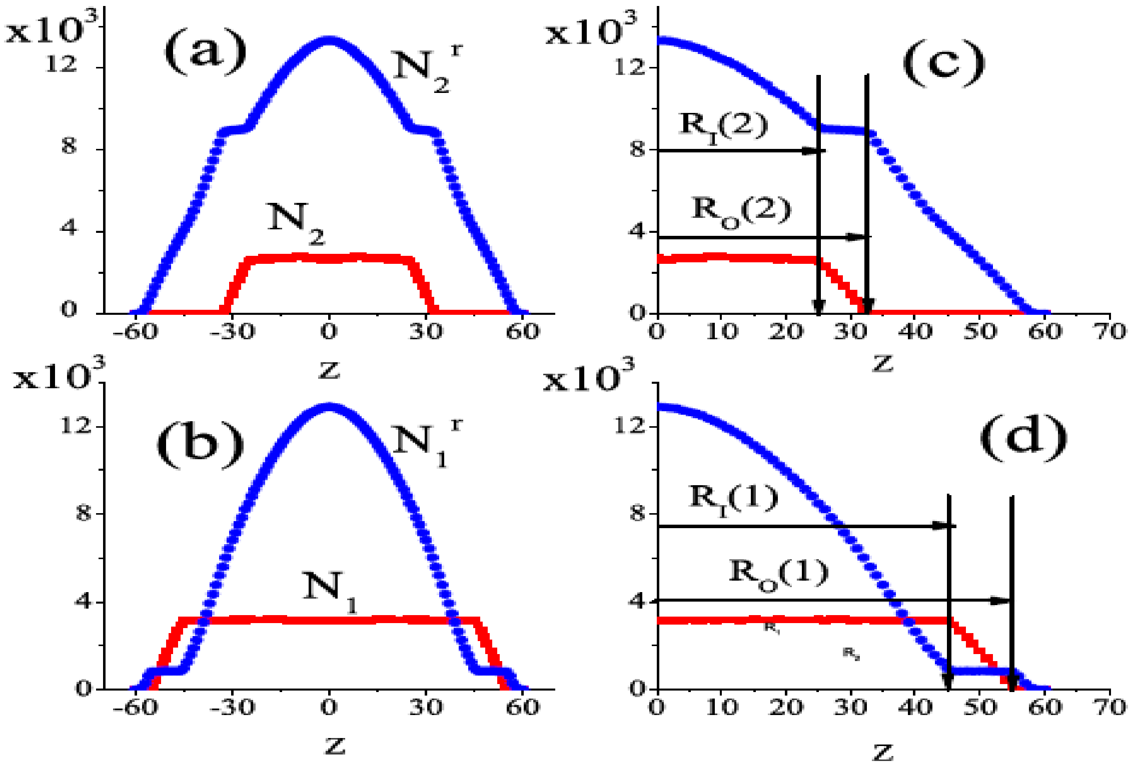


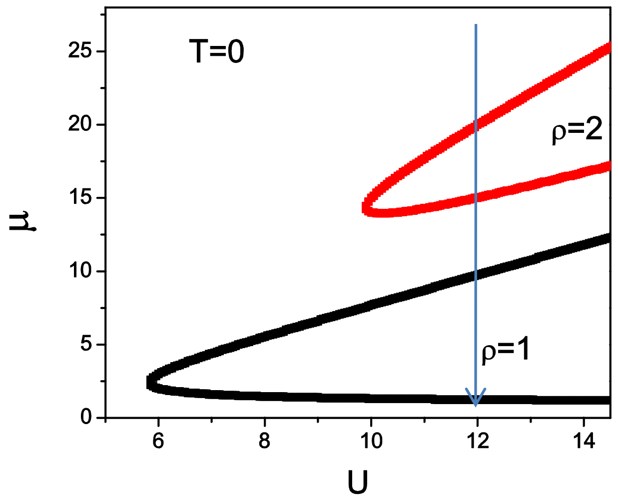




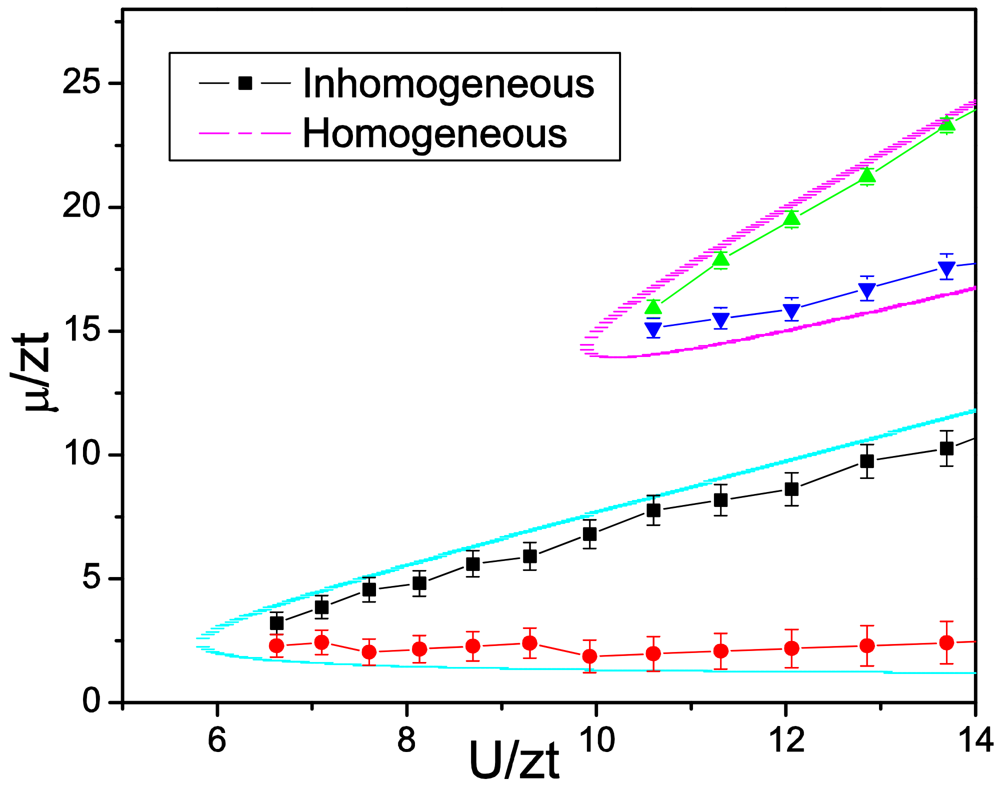
Phys. Rev. B **85**, 214524 (2012).

Bose-Hubbard model: Radii of MI shells





Bose-Hubbard model:
Radii to phase diagram



Bose-Hubbard model: Excitations

$$H = \sum_i H_i^{MF} - t \sum_{<i,j>} (\delta a_i^+ \delta a_j + h.c)$$

$$H_i^{MF} \,|\, i,\alpha > = E_\alpha \,|\, i,\alpha >$$

$$L^i_{\alpha\alpha'} = | \, i,\alpha >< i,\alpha' \, |$$ Define Projection Operator

$$\hat{O}_i = \sum_{\alpha\alpha'} < i,\alpha \,|\, \hat{O}_i \,|\, i,\alpha' > L^i_{\alpha\alpha'}$$ Single Site Operator :

$$H = \sum_{i\alpha} E_\alpha L^i_{\alpha\alpha} - \frac{t}{2} \sum_{<ij>\alpha\alpha'\beta\beta'} T^{ij}_{\alpha\alpha'\beta\beta'} L^i_{\alpha\alpha'} L^j_{\beta\beta'}$$

$$T^{ij}_{\alpha\alpha'\beta\beta'} = < i,\alpha \,|\, \delta a_i^+ \,|\, i,\alpha' >< j,\beta \,|\, \delta a_j \,|\, j,\beta' > + h.c.$$

Bose-Hubbard model: Green's Function

$$G^{ij}_{\alpha\alpha'\beta\beta'}(t) = -i\theta(t) < [L^{i}_{\alpha\alpha'}(t), L^{j}_{\beta\beta'}(0)] >$$

Equation of motion (RPA approximation):

$$\left(\omega - E_{\alpha} + E_{\alpha'}\right) G_{\alpha\alpha'\beta\beta'}(q,\omega) + P_{\alpha\alpha'} \sum_{\mu\nu} T_{\alpha\alpha'\nu\mu}(q) G_{\mu\nu\beta\beta'}(q,\omega) = \frac{1}{2\pi} P_{\alpha\alpha'} \delta_{\alpha\beta'} \delta_{\alpha'\beta}$$

where $$T_{\alpha\alpha'\beta\beta'}(q) = \varepsilon_{q}\left(T^{ij}_{\alpha\alpha'\beta\beta'} + T^{ji}_{\beta\beta'\alpha\alpha'}\right),$$

$$\varepsilon_{q} = -2t \sum_{j=x,y,z} \cos q_{j}$$

$$P_{\alpha\alpha'} = < L_{\alpha\alpha} > - < L_{\alpha'\alpha'} >$$

Bose-Hubbard model
Single Particle Green Functions

$$g_{i,j}(t) = -i\theta(t) < [a_i(t), a_j^+] >$$

$$g(q,\omega) = \sum_{\alpha\alpha'\beta\beta'} < \alpha | a | \alpha' >< \beta | a^+ | \beta' > G_{\alpha\alpha'\beta\beta'}(q,\omega)$$

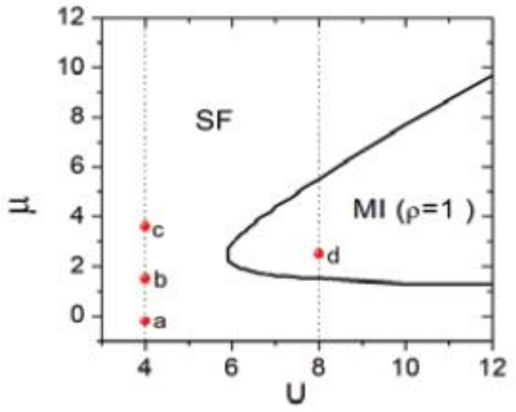
$$g(q,\omega) = \sum_r \frac{A(q)}{\omega - \omega_r(q)}$$

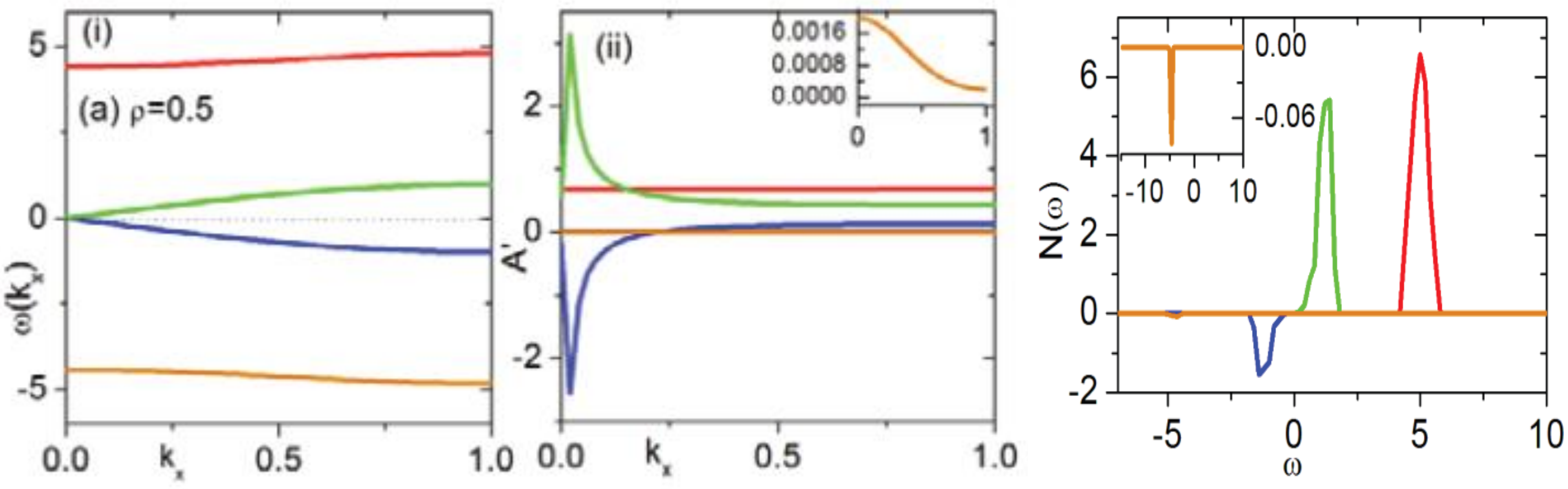
$$N(\omega) = -\frac{1}{\pi} \sum_q \mathrm{Im}\, g(q,\omega^+)$$

rf-tunnelling current I(ω) spectroscopy is a powerful method to observe these excitation spectra.

$$I(\omega) \propto N(\omega)$$

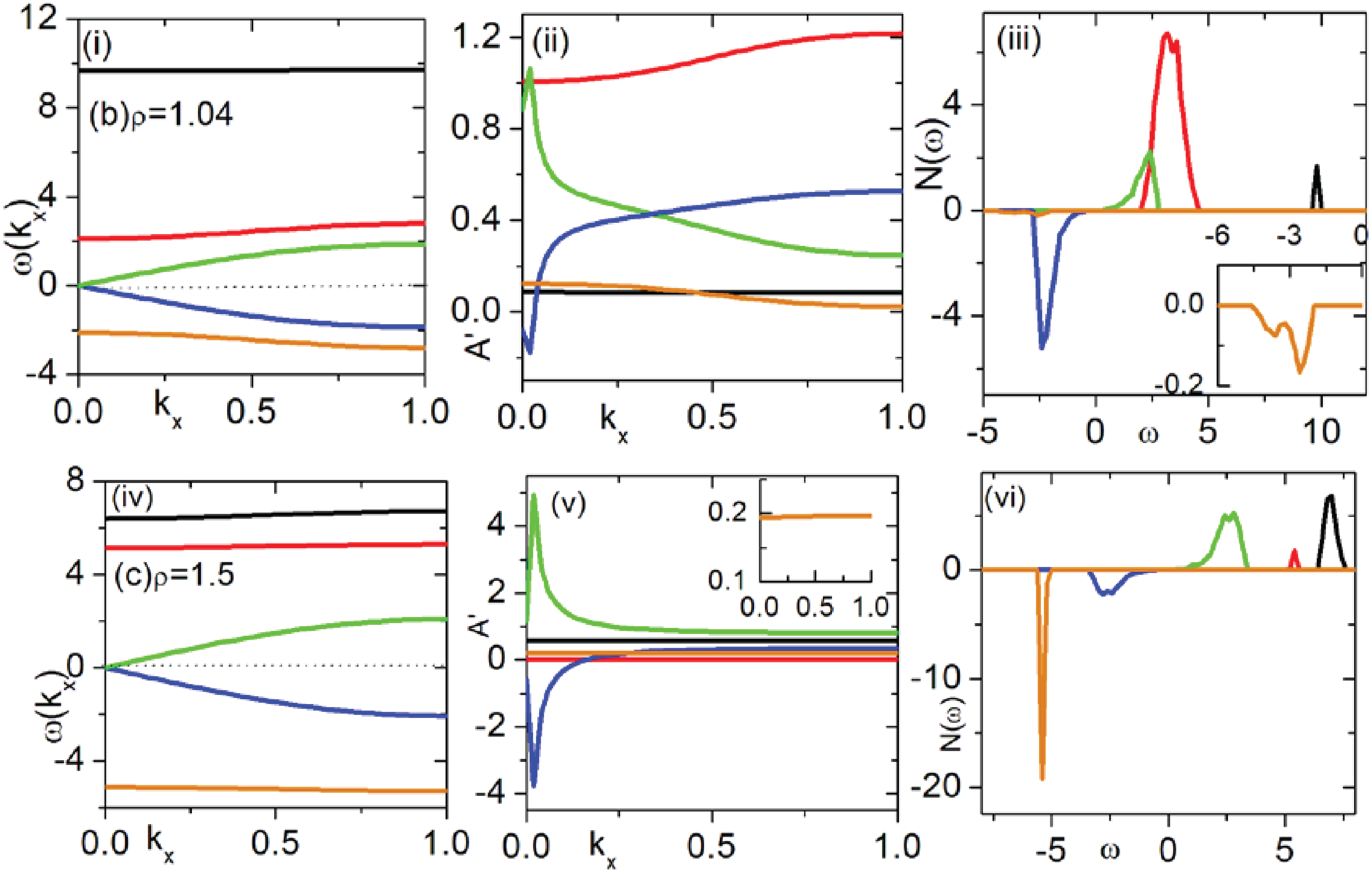
Bose-Hubbard model: Excitations – SF Phase





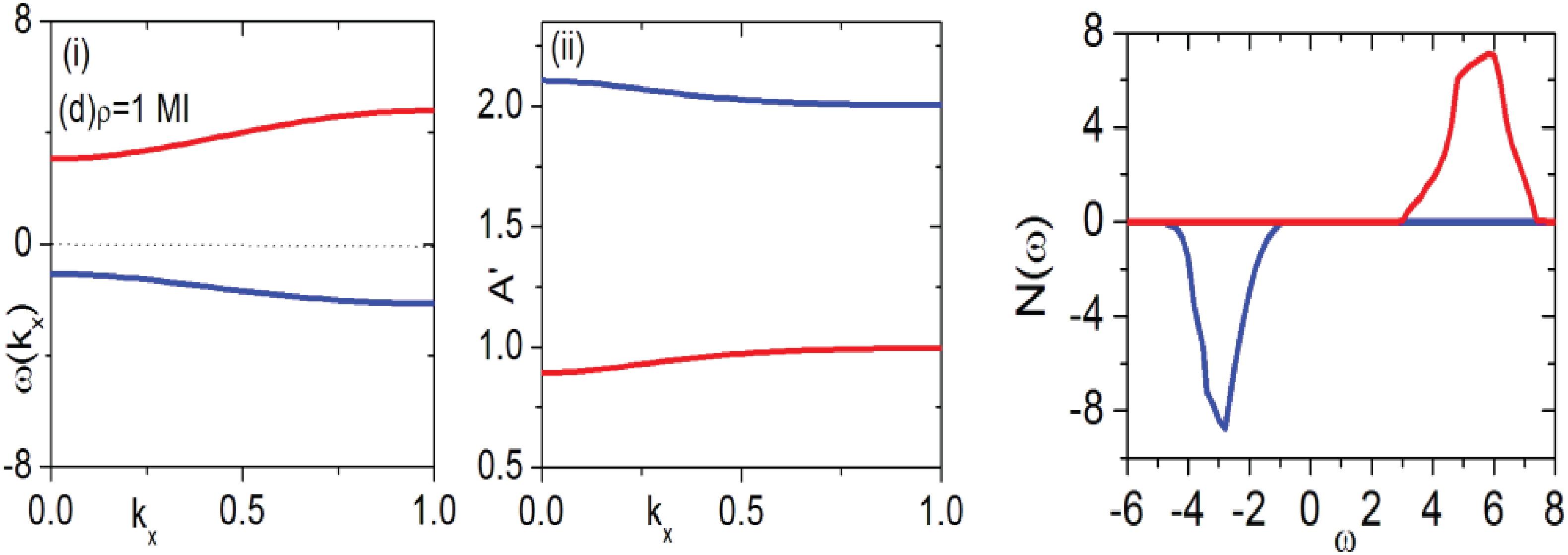
AIP Conference Proceedings **1832, 030009 (2017);**

Bose-Hubbard model: Excitations – SF Phase



AIP Conference Proceedings **1832, 030009 (2017);**

Bose-Hubbard model: Excitations - MI Phase



AIP Conference Proceedings **1832, 030009 (2017);**

Bose-Hubbard model: Finite Temperature MFT

$$H_i^{MF} = \frac{U}{2}\hat{n}_i(\hat{n}_i - 1) - \mu n_i - (\psi_i^* a_i + \psi_i a_i^+) + |\psi_i|^2$$

$$H_i^{MF} |i,\alpha> = E_\alpha |i,\alpha>$$

Partition Function

$$Z = \sum_\alpha e^{-\beta E_\alpha}$$

Superfluid Order parameter $\psi = \sum_\alpha P_\alpha < \alpha | \hat{a} | \alpha >$

Where $P_\alpha = \dfrac{e^{-\beta E_\alpha}}{Z}$

AIP Conference Proceedings **(2018);**

Bose-Hubbard model: Finite Temperature RPA

$$H = \sum_i H_i^{MF} - t \sum_{<i,j>} (\delta a_i^+ \delta a_j + h.c)$$

$$H_i^{MF} \, | i, \alpha >= E_\alpha \, | i, \alpha >$$

$$L^i_{\alpha\alpha'} = | i, \alpha >< i, \alpha' |$$ Define Projection Operator

$$\hat{O}_i = \sum_{\alpha\alpha'} < i, \alpha | \hat{O}_i | i, \alpha' > L^i_{\alpha\alpha'}$$ Single Site Operator :

$$H = \sum_{i\alpha} E_\alpha L^i_{\alpha\alpha} - \frac{t}{2} \sum_{<ij>\alpha\alpha'\beta\beta'} T^{ij}_{\alpha\alpha'\beta\beta'} L^i_{\alpha\alpha'} L^j_{\beta\beta'}$$

$$T^{ij}_{\alpha\alpha'\beta\beta'} = < i, \alpha | \delta a_i^+ | i, \alpha' >< j, \beta | \delta a_j | j, \beta' > + h.c.$$

Bose-Hubbard model: Finite Temperature RPA

$$G^{ij}_{\alpha\alpha'\beta\beta'}(t) = -i\theta(t) < [L^{i}_{\alpha\alpha'}(t), L^{j}_{\beta\beta'}(0)] >$$

Equation of motion (RPA approximation):

$$(\omega - E_{\alpha} + E_{\alpha'})G_{\alpha\alpha'\beta\beta'}(q,\omega) + P_{\alpha\alpha'}\sum_{\mu\nu} T_{\alpha\alpha'\nu\mu}(q)G_{\mu\nu\beta\beta'}(q,\omega) = \frac{1}{2\pi}P_{\alpha\alpha'}\delta_{\alpha\beta'}\delta_{\alpha'\beta}$$

where $$T_{\alpha\alpha'\beta\beta'}(q) = \varepsilon_{q}\left(T^{ij}_{\alpha\alpha'\beta\beta'} + T^{ji}_{\beta\beta'\alpha\alpha'}\right),$$

$$\varepsilon_{q} = -2t\sum_{j=x,y,z}\cos q_{j}$$

$$P_{\alpha\alpha'} = < L_{\alpha\alpha} > - < L_{\alpha'\alpha'} >$$

Bose-Hubbard model Finite Temperature RPA

$$G_{\alpha\alpha'\beta\beta'}(q,\omega) = \sum_r \frac{A(q)}{\omega - \omega_r(q)}$$

From this

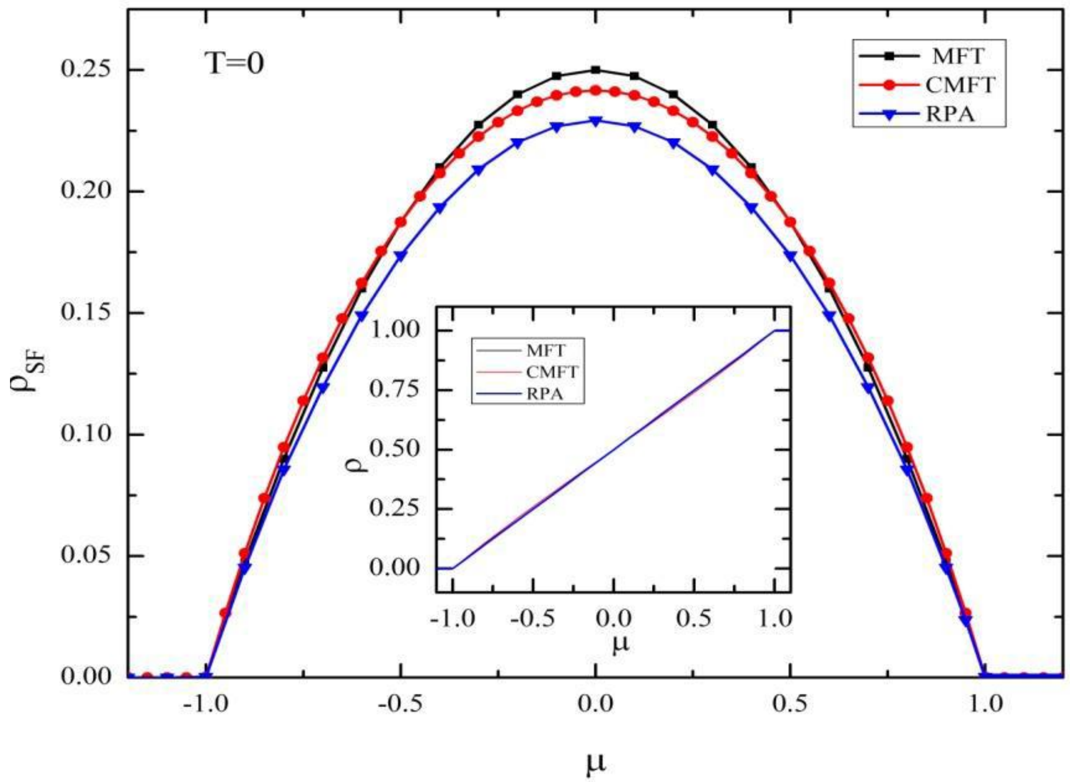
$$\psi = \sum_{\alpha} P_\alpha < \alpha | \hat{a} | \alpha > \qquad \text{where}$$

$$P_\alpha = \frac{1}{(2\pi)^3} \sum_{r,q} A(q) f(\omega_r(q)) \qquad \text{where}$$

$$f(\omega) = \left(e^{\beta\omega} - 1\right)^{-1}$$

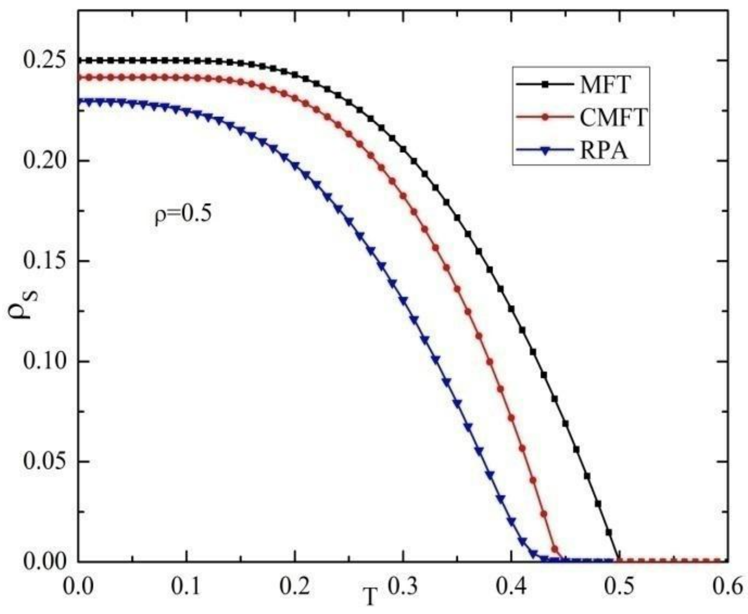
AIP Conference Proceedings **(2018);**

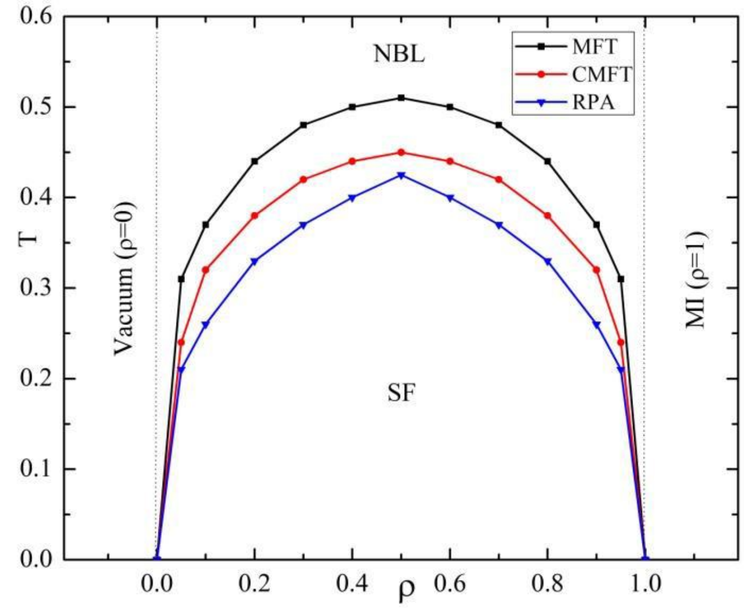
Hard Core Bose-Hubbard model: Finite Temperature Results



AIP Conference Proceedings **(2018);**

Hard Core Bose-Hubbard model:
Finite Temperature Results





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Bose-Hubbard model for two types of bosons

$$H = -t_a \sum_{<i,j>} (a_i^+ a_j + h.c) + \frac{U_a}{2} \sum_i n_i^a (n_i^a - 1)$$

$$- t_b \sum_{<i,j>} (b_i^+ b_j + h.c) + \frac{U_b}{2} \sum_i n_i^b (n_i^b - 1)$$

$$+ U_{ab} \sum_i n_i^a n_i^b - \mu_a \sum_i n_i^a - \mu_b \sum_i n_i^b$$

Bose-Hubbard model for two types of bosons
Mean field theory

$$a_i^+ a_j \approx \langle a_i^+ \rangle a_j + a_i^+ \langle a_j \rangle - \langle a_i^+ \rangle \langle a_j \rangle$$

$$b_i^+ b_j \approx \langle b_i^+ \rangle b_j + b_i^+ \langle b_j \rangle - \langle b_i^+ \rangle \langle b_j \rangle$$

Superfluid order parameters

$$\psi_i^a = \langle a_i \rangle \qquad \psi_i^b = \langle b_i \rangle$$

$$H = \sum_i H_i^{MF}$$

$$-t_a \sum_{\langle i,j \rangle} (\delta a_i^+ \delta a_j + h.c) - t_b \sum_{\langle i,j \rangle} (\delta b_i^+ \delta b_j + h.c)$$

Bose-Hubbard model for two types of bosons
Mean field theory

$$H_i^{MF} = \frac{U_a}{2}\hat{n}_i^a(\hat{n}_i^a - 1) - \mu_a n_i^a - (\psi_i^{a^*} a_i + \psi_i^a a_i^+) + |\psi_i^a|^2$$

$$+\frac{U_b}{2}\hat{n}_i^b(\hat{n}_i^b - 1) - \mu_b n_i^b - (\psi_i^{b^*} b_i + \psi_i^b b_i^+) + |\psi_i^b|^2$$

$$+U_{ab}\hat{n}_i^a\hat{n}_i^b$$

- Superfluid density $(\rho_s^a)_i = |\psi_i^a|^2$ $(\rho_s^b)_i = |\psi_i^b|^2$
- Density $\rho_i^a = <\hat{n}_i^a>$ $\rho_i^b = <\hat{n}_i^b>$

Bose-Hubbard model for two types of bosons
Mean field theory

$$H_i^{MF} = \frac{U_a}{2}\hat{n}_i^a(\hat{n}_i^a - 1) - \mu_a n_i^a - (\psi_i^{a^*} a_i + \psi_i^a a_i^+) + |\psi_i^a|^2$$

$$+\frac{U_b}{2}\hat{n}_i^b(\hat{n}_i^b - 1) - \mu_b n_i^b - (\psi_i^{b^*} b_i + \psi_i^b b_i^+) + |\psi_i^b|^2$$

$$+U_{ab}\hat{n}_i^a \hat{n}_i^b$$

- Superfluid density $(\rho_s^a)_i = |\psi_i^a|^2 \quad (\rho_s^b)_i = |\psi_i^b|^2$
- Density $\rho_i^a = <\hat{n}_i^a> \quad \rho_i^b = <\hat{n}_i^b>$

Bose-Hubbard model for two types of bosons
Mean field theory: Phases

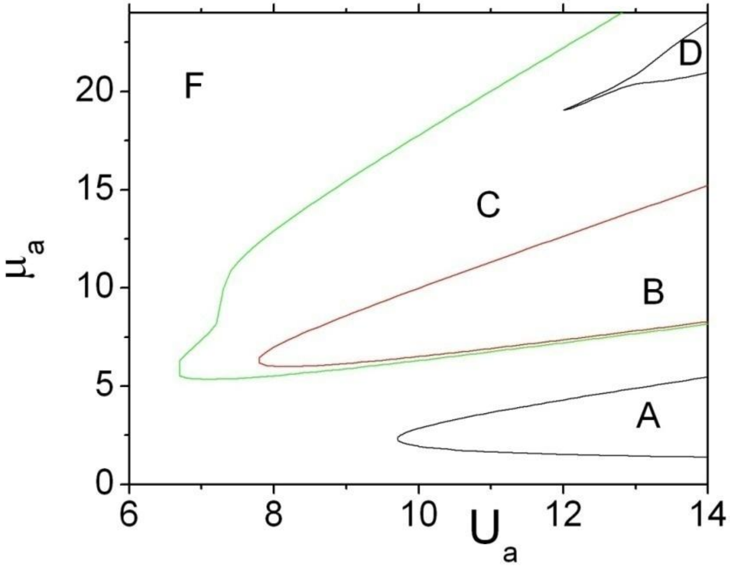
$$SF_A + SF_B \quad \rho_S^a > 0,\ \rho_S^b > 0$$

$$MI_A + MI_B \quad \rho_S^a = 0,\ \rho_S^b = 0$$

$$MI_A + SF_B \quad \rho_S^a = 0,\ \rho_S^b > 0$$

$$MI_B + SF_A \quad \rho_S^b = 0,\ \rho_S^a > 0$$

Bose-Hubbard model for two types of bosons
Mean field theory: Phases



A : MI-1 $\rho_A+\rho_B=1$

B : MI_A, MI_B $\rho_A=1$, $\rho_B=1$

C : MI_A, SF_B $\rho_A=1$, $\rho_B>1$

D : MI_A, MI_B $\rho_A=1$, $\rho_B=2$

F : SF_A, SF_B

Phase diagram, and plots versus μ of the for $U_{ab} = 0.5U_a$, $U_b = 0.75U_a$, $\mu_a = \mu_b = \mu$.

Bose-Hubbard model for two types of bosons
Excitations

$$H = \sum_i H_i^{MF} - t_a \sum_{<i,j>} (\delta a_i^+ \delta a_j + h.c) - t_b \sum_{<i,j>} (\delta b_i^+ \delta b_j + h.c)$$

$$H_i^{MF} \mid i,\alpha >= E_i \mid i,\alpha >$$

Define Projection Operator $L_{\alpha\alpha'}^i = \mid i,\alpha >< i,\alpha' \mid$

Single Site Operator : $\hat{O}_i = \sum_{\alpha\alpha'} < i,\alpha \mid \hat{O}_i \mid i,\alpha' > L_{\alpha\alpha'}^i$

Bose-Hubbard model for two types of bosons Excitations

$$H = \sum_{i\alpha} E_\alpha L^i_{\alpha\alpha} - \frac{1}{2} \sum_{<ij>\alpha\alpha'\beta\beta'} T^{ij}_{\alpha\alpha'\beta\beta'} L^i_{\alpha\alpha'} L^j_{\beta\beta'}$$

$$T^{ij}_{\alpha\alpha'\beta\beta'} = <i,\alpha|\delta a_i^+|i,\alpha'><j,\beta|\delta a_j|j,\beta'> + h.c.$$

$$+ <i,\alpha|\delta b_i^+|i,\alpha'><j,\beta|\delta b_j|j,\beta'> + h.c.$$

$$\delta a = a - <a>$$

$$\delta b = b - <b>$$

Bose-Hubbard model for two types of bosons Green Functions + RPA

$$G^{ij}_{\alpha\alpha'\beta\beta'}(t) = -i\theta(t) < [L^{i}_{\alpha\alpha'}(t), L^{j}_{\beta\beta'}(0)] >$$

Equation of motion (RPA approximation):

$$(\omega - E_{\alpha} + E_{\alpha'})G_{\alpha\alpha'\beta\beta'}(q,\omega) + P_{\alpha\alpha'}\sum_{\mu\nu} T_{\alpha\alpha'\nu\mu}(q) G_{\mu\nu\beta\beta'}(q,\omega) = \frac{1}{2\pi} P_{\alpha\alpha'}\delta_{\alpha\beta'}\delta_{\alpha'\beta}$$

where $T_{\alpha\alpha'\beta\beta'}(q) = \varepsilon_q \left(T^{ij}_{\alpha\alpha'\beta\beta'} + T^{ji}_{\beta\beta'\alpha\alpha'}\right),$

$$\varepsilon_q = -2t \sum_{j=x,y,z} \cos q_j$$

$$P_{\alpha\alpha'} = < L_{\alpha\alpha} > - < L_{\alpha'\alpha'} >$$

Bose-Hubbard model for two types of bosons
Single Particle Green Functions

$$g^{aa}_{i,j}(t) = -i\theta(t) < [a_i(t), a^+_j] >$$

$$g^{bb}_{i,j}(t) = -i\theta(t) < [b_i(t), b^+_j] >$$

$$g^{aa}(q,\omega) = \sum_{\alpha\alpha'\beta\beta'} < \alpha | a | \alpha' >< \beta | a^+ | \beta' > G_{\alpha\alpha'\beta\beta'}(q,\omega)$$

$$g^{bb}(q,\omega) = \sum_{\alpha\alpha'\beta\beta'} < \alpha | b | \alpha' >< \beta | b^+ | \beta' > G_{\alpha\alpha'\beta\beta'}(q,\omega)$$

Bose-Hubbard model for two types of bosons Excitations, Spectral Weights + DOS

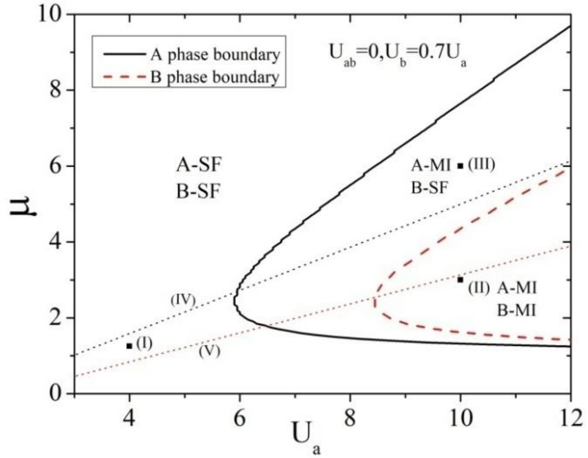
Solving the equation of motion for the Green function and writing it in the form

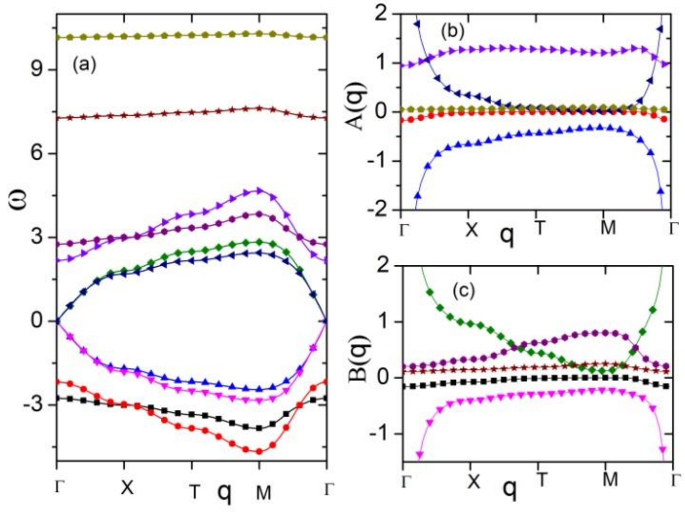
$$g^{aa}(q,\omega) = \sum_r \frac{A(q)}{\omega - \omega_r(q)}$$

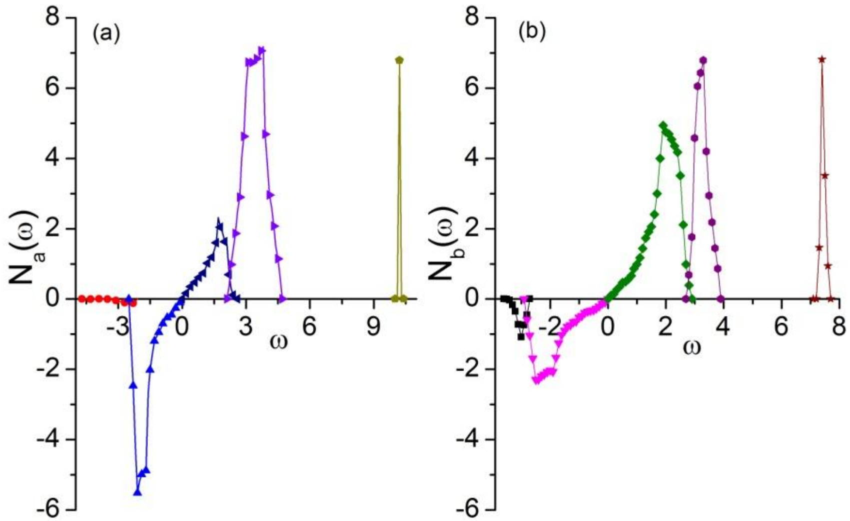
$$g^{bb}(q,\omega) = \sum_r \frac{B(q)}{\omega - \omega_r(q)}$$

$$N_a(\omega) = -\frac{1}{\pi} \sum_q \operatorname{Im} g^{aa}(q,\omega^+)$$

Bose-Hubbard model for two types of bosons
Excitations

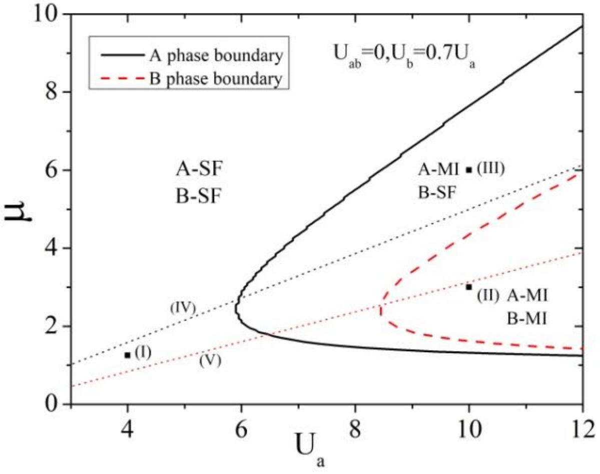


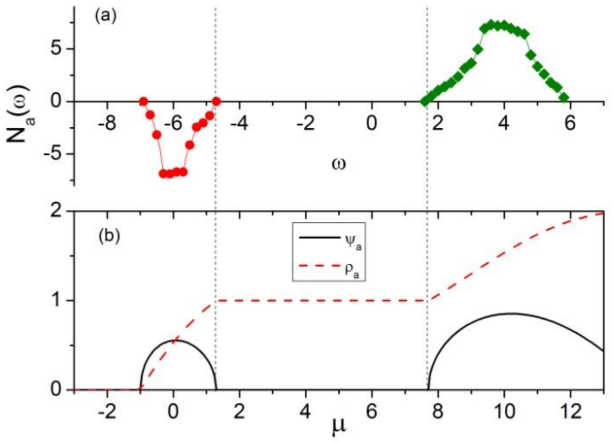


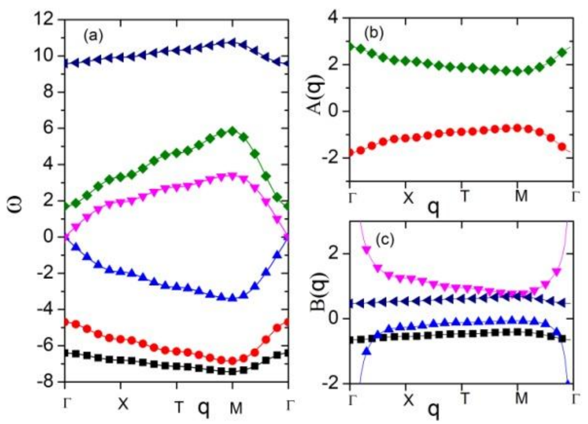


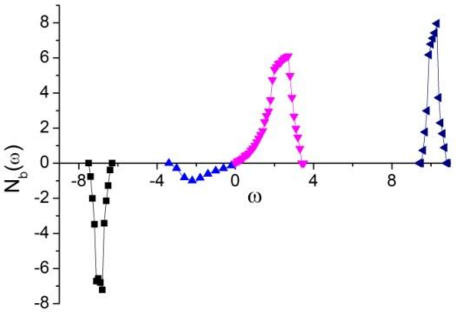
SF_A, SF_B

Bose-Hubbard model for two types of bosons
Excitations



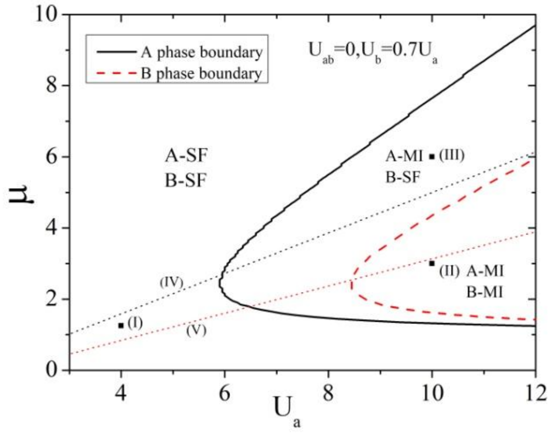


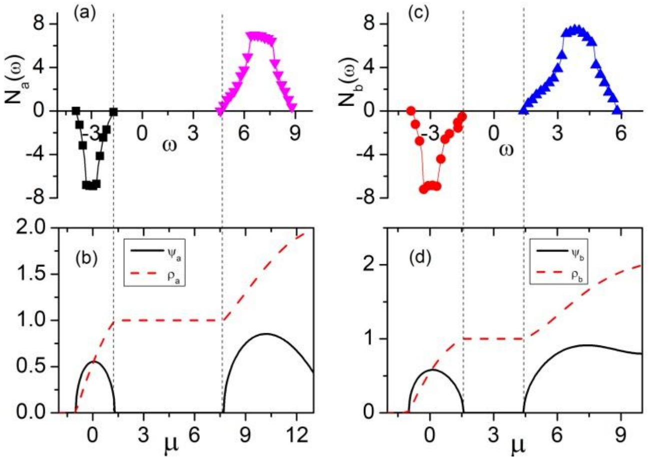


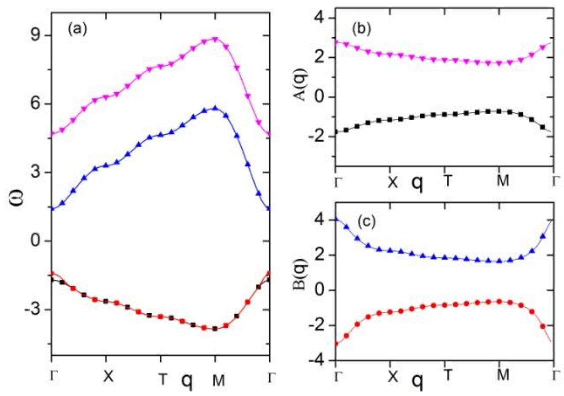


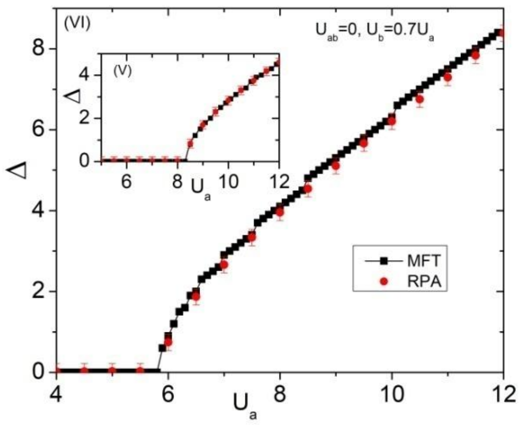
MI_A, SF_B

Bose-Hubbard model for two types of bosons
Excitations



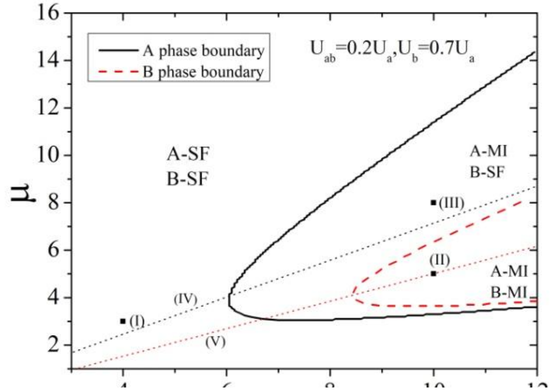


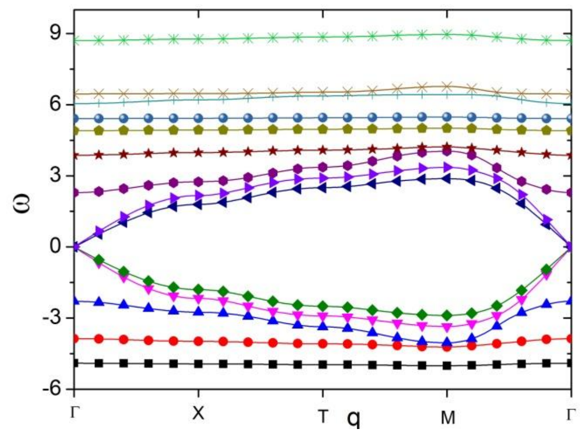


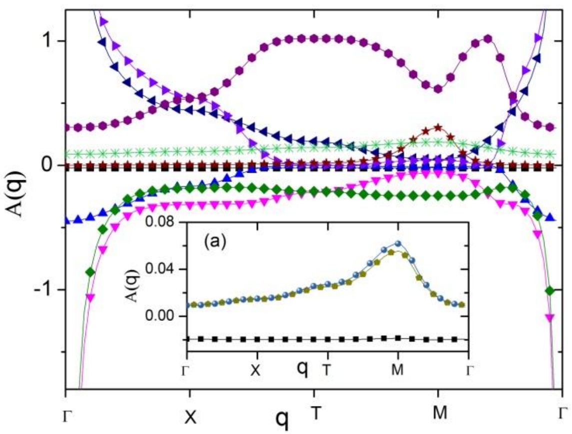


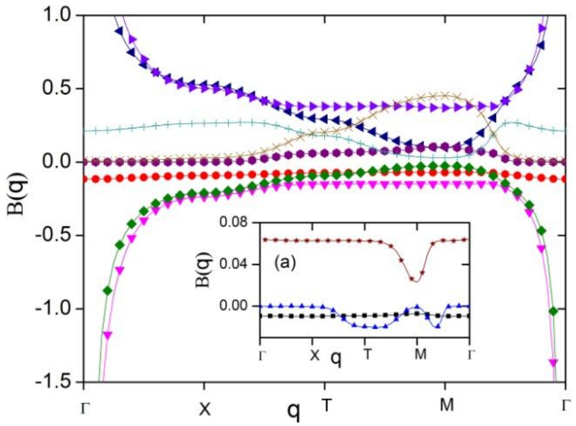
MI_A, MI_B

Bose-Hubbard model for two types of bosons
Excitations

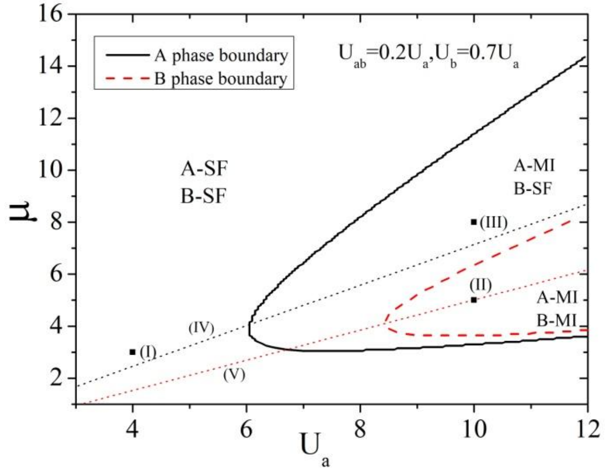


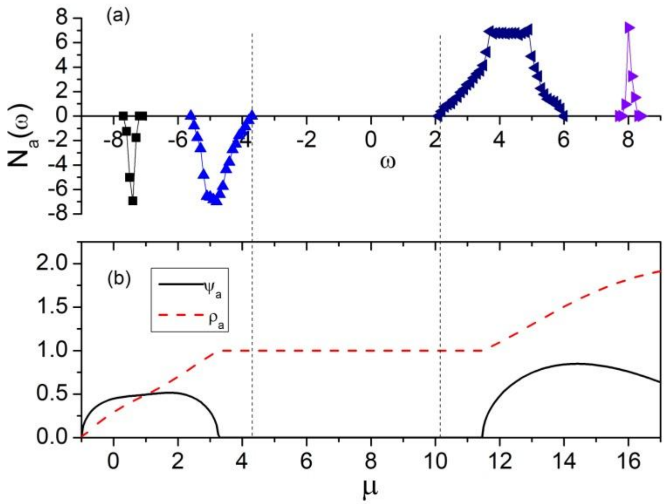


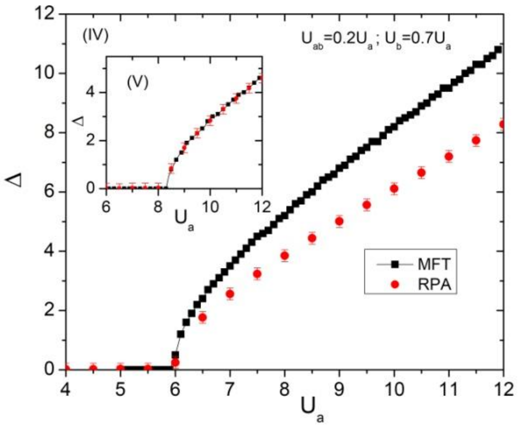




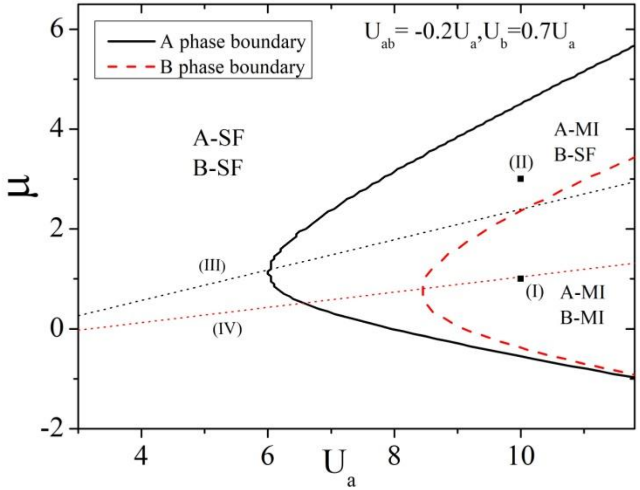
Bose-Hubbard model for two types of bosons
Excitations

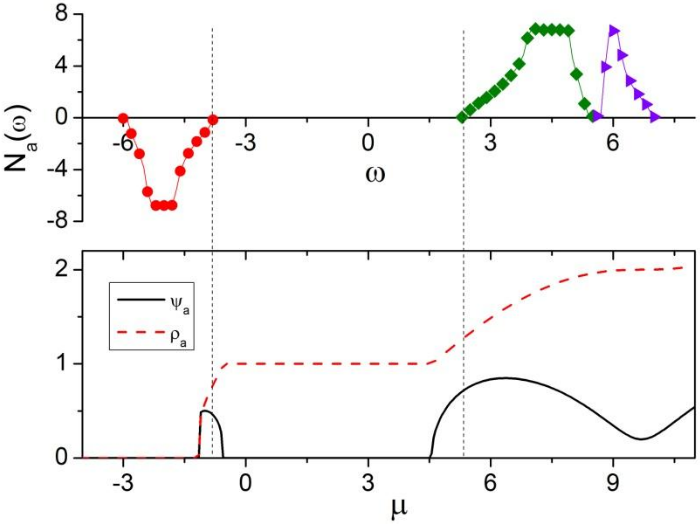


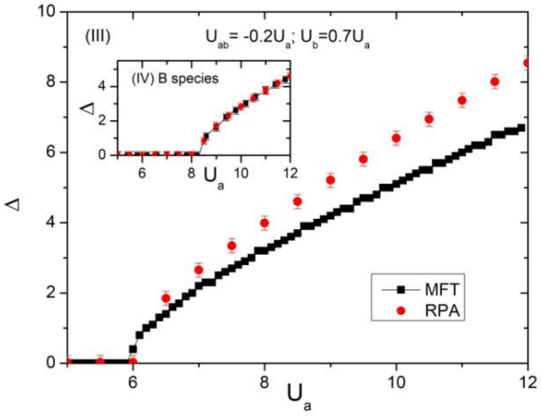




Bose-Hubbard model for two types of bosons
Excitations







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Thank You

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