Mean Field Theory for Interacting Bosons on a Lattice

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Outline of the Presentation

Collaborations

- **Rahul Pandit, IISc, Bangalore**
- **K. Sheshadri,Bangalore**
- **Nandadeep Nasnolkar, Goa University, Goa**
- **B. P. Das, IIA, Bangalore**
- **Tapan Mishra, IIA, Bangalore**

Outline

- **History and experimental motivation.**
- **Models and phases.**
- **Theoretical Methods**
  - **Density Matrix Renormalization Group**
  - **Mean Field Theory**
- **Results Mean Field Theory**
  - **Spin-0 bosons**
  - **Spin-1 bosons**
- **Conclusions.**

History

SN Bose

Bose Distribution function

$$\boxed{f(\epsilon) = \frac{1}{e^{(\epsilon-\mu)/kT} - 1}}$$

For particles with integer spin $S = 0, 1, \ldots$

A Einstein

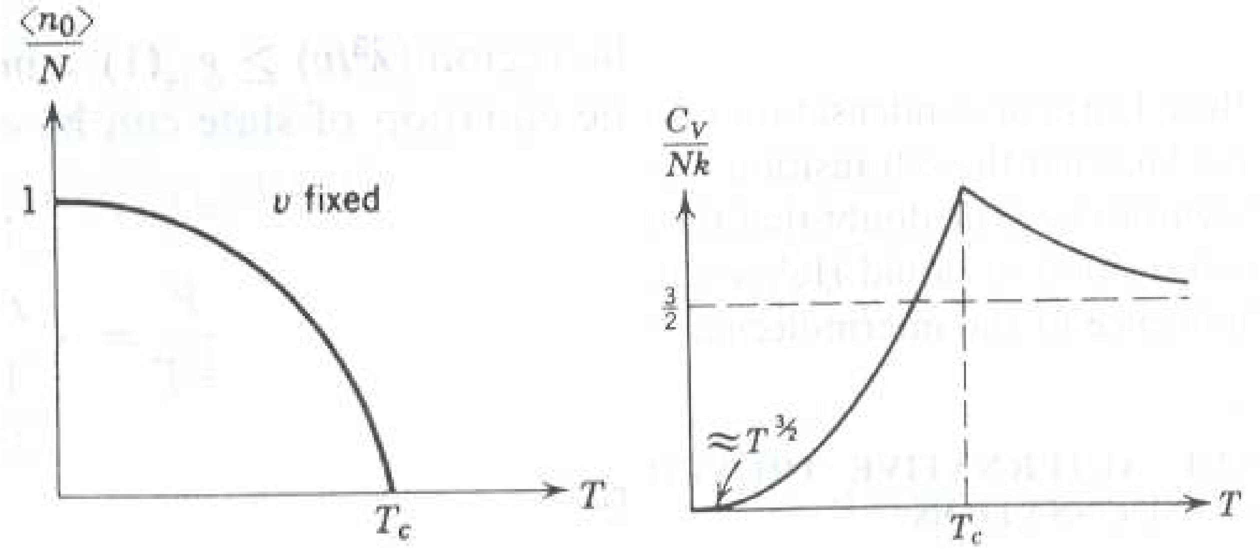
Bose-Einstein Condensation (BEC)

$T = T_c > 0$ for dimension $d > 2$

BEC for $d = 3$

$$\begin{aligned}
N_0/N &= 1 - [T/T_c]^{3/2} \\
k_B T_c &= [2\pi\hbar^2/m][N/(V\zeta(3/2))]^{2/3} \\
\Delta[\partial C_v/\partial T]_{T_c} &= \\
&- (27/4)[(\zeta(3/2)\Gamma(3/2))/\pi]^2 N k_B/T_c
\end{aligned}$$

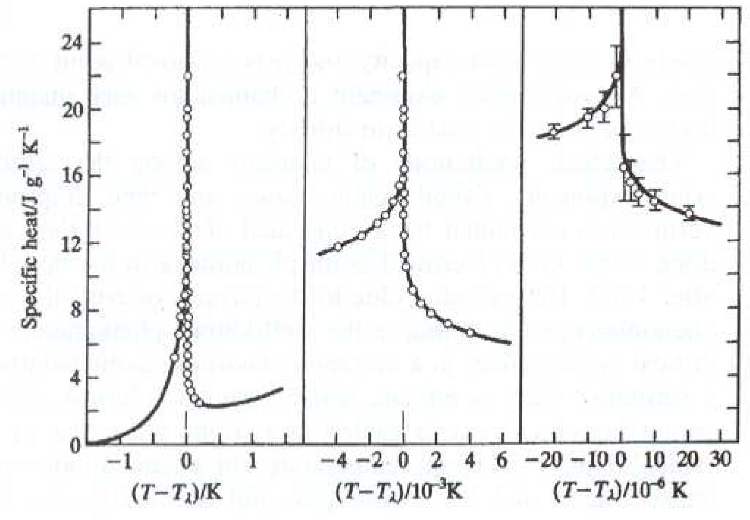
BEC for $d = 3$



K. Huang, *Statistical Mechanics*

Superfluidity of ^{4}He

The λ transition



M.J. Buckingham and W.M. Fairbank

Cusp sharper than in the ideal Bose gas

$$\alpha = -0.01285 \pm 0.00038$$

^{4}He is a strongly interacting Bose fluid.

Experimental Motivation

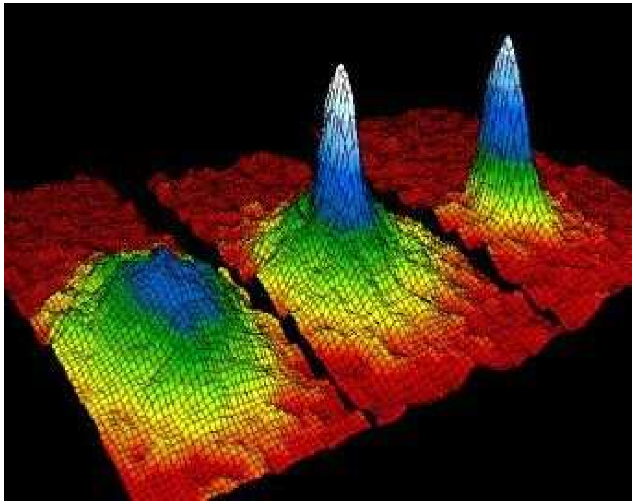
Weakly Interacting Bose Gases

- **^{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.**
- **Cold atoms (e.g., ^{87}Rb and ^{23}Na) in magnetic or optical traps (thermodynamics modified by confining potentials).**

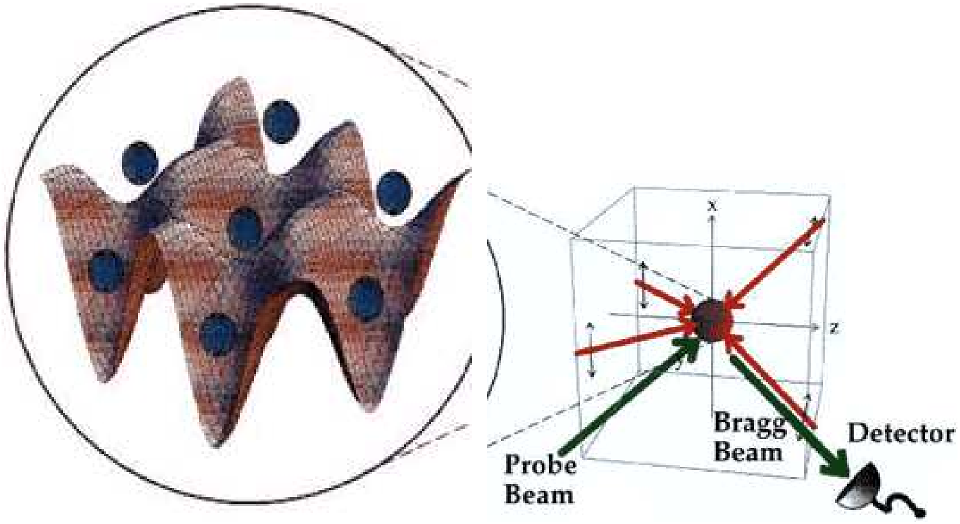
BEC in cold atoms

M.H. Anderson, J.R. Ensher, M.R. Matthews, C.E. Wiemann, and E.A. Cornell, 1995, Science **269**, 198.

Velocity distribution of ^{87} Rb
$T > T_c$; $T \simeq T_c$; $T < T_c$.



Optical Lattices



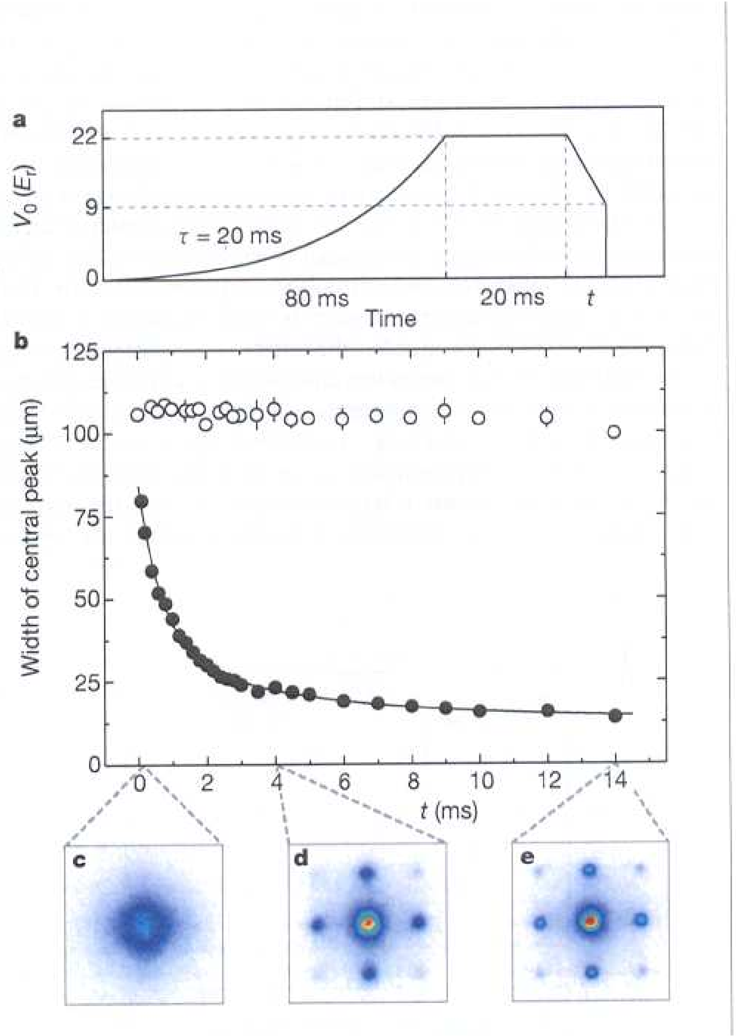
http://physics.nist.gov/Divisions/Div842/Gp4/lattices.html

Superfluid → Mott Insulator

- **Observation of this quantum phase transition in an ultracold gas of spin-polarised ^{87}Rb atoms in an optical lattice.**
- **M. Greiner, O. Mandel, T. Esslinger, T.W. Hänsch, and I. Bloch, Nature, 415, 39 (2002).**
- **Theory had preceded experiments!**
- **K. Sheshadri, H.R. Krishnamurthy, R. Pandit, and T.V. Ramakrishnan, Europhys. Lett., 22, 257 (1993) and refs. therein.**

Superfluid → Mott Insulator

Absorption images of interference patterns from a Mott Insulator after potential ramp-down times of (c) 0.1 ms (d) 4 ms and (e) 14 ms: Greiner, et al., op. cit.



Models and Phases

Bose-Hubbard Model (Spin-0)

$$\begin{aligned} \mathcal{H} &= -t\sum_{<i,j>}(a_i^\dagger a_j + hc) && \text{SuperFluid} \\ &+\frac{U}{2}\sum_i \hat{n}_i(\hat{n}_i - 1) && \text{Mott Insulator} \\ &+V\sum_{<i,j>}\hat{n}_i\hat{n}_j && \text{Mass Density Wave, SuperSolid} \\ &-\sum_i \mu_i\hat{n}_i && \text{Boss Glass, Trap} \end{aligned} \tag{1}$$

email: rvpai@unigoa.ac.in, September 3, 2006

Optical Lattice - Comments

Alkalis with nuclear spin $I = 3/2$ such as ^{23}Na, ^{39}K, ^{87}Rb have hyperfine spin $F = 1$.

In the conventional magnetic trap, the spins are frozen.

Alkalis can be treated as Bosons with Spin=0

However, in the optical trap, these spins are free and the Bose condensate can exhibit magnetic nature.

Alkalis should be treated as Bosons with Spin=1

Bose-Hubbard Model - (Spin 1)

$$\begin{aligned}\mathcal{H} &= -t\sum_{\langle i,j\rangle,\sigma}(a^{\dagger}_{i,\sigma}a_{j,\sigma}+h.c) \\ &+\frac{U_0}{2}\sum_i \hat{n}_i(\hat{n}_i-1) \\ &+\frac{U_2}{2}\sum_i(\vec{F}_i^2-2\hat{n}_i) \\ &-\sum_i \mu_i\hat{n}_i\end{aligned}$$

$$n_i=\sum_\sigma a^{\dagger}_{i,\sigma}a_{i,\sigma}$$

$$\vec{F}_i=\sum_{\sigma,\sigma'} a^{\dagger}_{i,\sigma}F_{\sigma,\sigma'}a_{i,\sigma'}$$

$F_{\sigma\sigma'}$ are components of the spin-1 operators:

Model: Comments

$$U_2/U_0 = (a_2 - a_0)/(a_0 + 2a_2)$$

a_0 scattering length in the channel S=0

a_2 scattering length in the channel S=2

Atom	a_0	a_2	U_2/U_0
^{23}Na	$49.4a_B$	$54.7a_B$	Positive
^{87}Rb	$(110 \pm 4)a_B$	$(107 \pm 4)a_B$	Negative.

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Outline of the Presentation

History

Experimental Motivation

Models and Phases
❖ Bose-Hubbard Model (Spin-0)
❖ Optical Lattice - Comments
❖ Bose-Hubbard Model - (Spin 1)
❖ Model: Comments
❖ Bose-Hubbard Model - (Two Species)
❖ Optical Lattice - Comments

Theoretical Methods

Bose-Hubbard Model - (Two Species)

$$\begin{aligned}
\mathcal{H} \quad = \quad & -t_a \sum_{\langle i,j \rangle} (a_i^\dagger a_j + h.c) \\
& -t_b \sum_{\langle i,j \rangle} (b_i^\dagger b_j + h.c) \\
& +\frac{U^a}{2} \sum_i \hat{n}_i^a (\hat{n}_i^a - 1) \\
& +\frac{U^b}{2} \sum_i \hat{n}_i^b (\hat{n}_i^b - 1) \\
& +U^{ab} \sum_i \hat{n}_i^a \hat{n}_i^b \\
& -\sum_i \mu_i^a \hat{n}_i^b - \sum_i \mu_i^b \hat{n}_i^b
\end{aligned}$$

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a and b stands for two different species of Bosons.

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- Bose-Hubbard Model (Spin-0)
- Optical Lattice - Comments
- Bose-Hubbard Model - (Spin 1)
- Model: Comments
- Bose-Hubbard Model - (Two Species)
- Optical Lattice - Comments

Theoretical Methods

Mean Field

Optical Lattice - Comments

Parameters in the Hamiltonian depends on

- Atomic Recoil Energy $E_R = \frac{\hbar^2 k^2}{2m}$,
- scattering between atoms a_s,
- depth of the optical potentails v,

$$t = \frac{\pi^2}{4} v \; exp[(\pi^2/4)(v/E_R)^{1/2}]$$

$$U = (\frac{8}{\pi})^{1/2} (k a_s)(E_R v^3)^{1/4}$$

which can be controlled to open a wide range of parameters to exploration.

Theoretical Methods

Theoretical Methods

- For One-Dimension: DMRG
  - ✦ R. V. Pai, R. Pandit, H. R. Krishnamurthy and S. Ramashesha. *One-Dimensional Boson Hubbard Model: A Density-Matrix Renormalisation Group Study*, Phys. Rev. Lett. **76** (1996) 2937.
  - ✦ R. V. Pai and R. Pandit *One Dimensional Extended Bose-Hubbard Model* Special issue of the Proceeding of the Indian Academy of Sciences (Chemical Sciences) in honour of the Professor CNR Rao on his 70th birthday, **115** (2003) 721-726.
  - ✦ R. V. Pai and R. Pandit *Superfluid, Mott Insulator, and Mass Density Wave Phases in the One-Dimensional Extended Bose-Hubbard Model.* Phys. Rev. B **71** (2005) 104508.
- For Higher Dimension: MFT

Theoretical Methods

- For One-Dimension: DMRG

- For Higher Dimension: MFT
  - ✦ K. Sheshadri, H. R. Krishnamurthy, R. Pandit, and T. V. Ramakrishnan Europhys. Lett. **22** 257 (1993); Phys. Rev. Lett. **75** 4075 (1995).
  - ✦ R.Pandit, K. Sheshadri, R. V. Pai, and H. R. Krishnamurthy *Interacting Bosons in Disordered Environments* Condensed Matter Theories, Vol **12** (Novo Science Publishers, Inc., 1997) pp 185-197.
  - ✦ R. V. Pai, K. Sheshadri and R. Pandit, *Meanfiled theory for interacting spin-1 bosons on a lattice* Proceeding of Topical Conference on Atomic, Molecular and Optical Physics (World Science, 2006) (in press).

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Mean Field Approximation

Mean Field Approximation

$$a^\dagger_{i,\sigma} a_{j,\sigma} = < a^\dagger_{i,\sigma} > a_{j,\sigma} + a^\dagger_{i,\sigma} < a_{j,\sigma} >$$
$$- < a^\dagger_{i,\sigma} >< a_{j,\sigma} >$$

Define superfluid order parameter in the spin component σ

$$\psi_\sigma = < a^\dagger_{i,\sigma} > = < a_{i,\sigma} >$$

$$\mathcal{H} = \sum_i \mathcal{H}_i^{MF}$$

$$\mathcal{H}_i^{MF} = \frac{U_0}{2}\hat{n}_i(\hat{n}_i - 1) + \frac{U_2}{2}(\vec{F}_i^2 - 2\hat{n}_i) - \mu\hat{n}_i$$
$$- \psi_\sigma(a^\dagger_{i,\sigma} + a_{i,\sigma}) + \sum_\sigma |\psi_\sigma|^2$$

Method: comments

- **If there is no disorder the mean-field Hamiltonian is the same at all sites.**
- **Hamiltonian Matrix in the occupation-number basis.**

$$\{|n>\}, n = 1, 2, 3, \cdots ;$$

truncate at n_{max}**.**

- $\frac{\partial F(\psi_\sigma)}{\partial \psi_\sigma} = 0$ **gives the** ψ_σ**.**
- $\rho_S = \sum_\sigma |\psi_\sigma|^2$**.**
- **Density** $\rho = -\frac{\partial F(\psi_\sigma)}{\partial \mu}$
- **Compressibility** $\kappa = \frac{\partial \rho}{\partial \mu}$
- $< \vec{F} >= \frac{\sum_{\sigma,\sigma'} \psi_\sigma \vec{F}_{\sigma,\sigma'} \psi_{\sigma'}}{\sum_\sigma |\psi_\sigma|^2}$,

Properties of Phases-spin 1

Phase	ρ_S	κ	$< \vec{F} >^2$
Polar SF	Non Zero	Non Zero	Zero
Ferro SF	Non Zero	Non Zero	One
Mott Insulator	Zero	Zero	Zero
Normal	Zero	Non Zero	

Since ψ_σ, assumed to be real

$$\begin{aligned} < \vec{F} > &= \sqrt{2}\frac{(\psi_1\psi_0 + \psi_{-1}\psi_0)}{\sum_\sigma |\psi_\sigma|^2}\hat{x} + \frac{(\psi_1^2 - \psi_{-1}^2)}{\sum_\sigma |\psi_\sigma|^2}\hat{z}; \\ < \vec{F} >^2 &= 2\frac{(\psi_1\psi_0 + \psi_{-1}\psi_0)^2}{\sum_\sigma |\psi_\sigma|^4} + \frac{(\psi_1^2 - \psi_{-1}^2)^2}{\sum_\sigma |\psi_\sigma|^4}. \end{aligned} \qquad (2)$$

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History

Experimental Motivation

Models and Phases

Theoretical Methods

Mean Field Approximation
- ❖ Mean Field Approximation
- ❖ Method: comments
- ❖ Properties of Phases-spin 1
- ❖ Properties of Phases-spin 1, Polar Superfluid
- ❖ Superfluid
- ❖ Polar Superfluid

Properties of Phases-spin 1, Polar Superfluid

Symmetry: $U(1) \times S^2$

$$\begin{pmatrix} \psi_1 \\ \psi_0 \\ \psi_{-1} \end{pmatrix} = \sqrt{\rho_s}\ e^{\imath\theta} \begin{pmatrix} -\frac{1}{\sqrt{2}} e^{-\imath\alpha} \sin\beta \\ \cos\beta \\ \frac{1}{\sqrt{2}} e^{\imath\alpha} \sin\beta \end{pmatrix}. \qquad (3)$$

θ=phase angle and (α, β, γ) are Euler angles.
Polar SF:

$\psi_1 = \psi_{-1} > 0$, $\psi_0 = 0$

or

$\psi_1 = \psi_{-1} = 0$, $\psi_0 > 0$

Superfluid

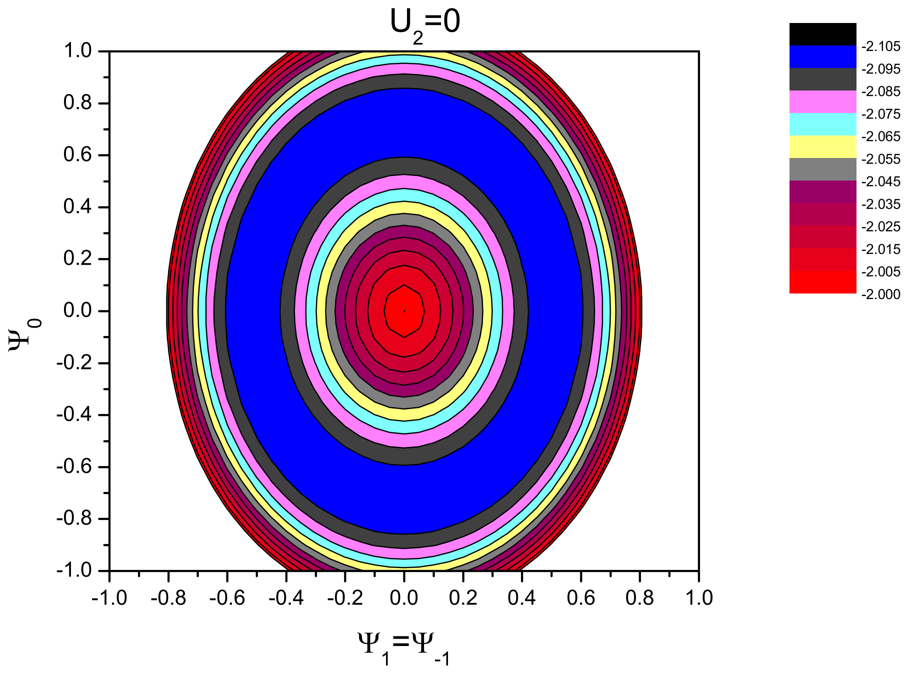

Figure 1: Free Energy

Polar Superfluid

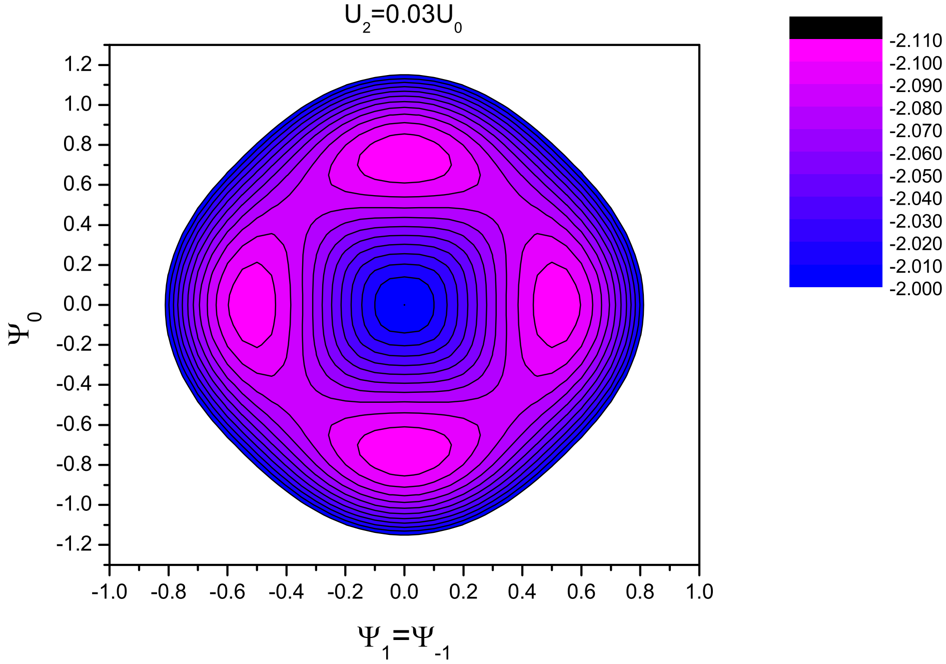

Figure 2: Free Energy

Properties of Phases-spin 1, Ferro Superfluid

Symmetry: $SO(3)$

$$\begin{pmatrix} \psi_1 \\ \psi_0 \\ \psi_{-1} \end{pmatrix} = \sqrt{\rho_s}\ e^{\imath(\theta-\gamma)} \begin{pmatrix} e^{-\imath\alpha}\cos^2\frac{\beta}{2} \\ \sqrt{2}\cos\frac{\beta}{2}\sin\frac{\beta}{2} \\ e^{\imath\alpha}\sin^2\frac{\beta}{2} \end{pmatrix}. \qquad (4)$$

Ferro SF: $\psi_1 = \psi_{-1} > 0$, $\psi_0 > 0$
but
$\psi_1 \neq \psi_0$

Ferro Superfluid

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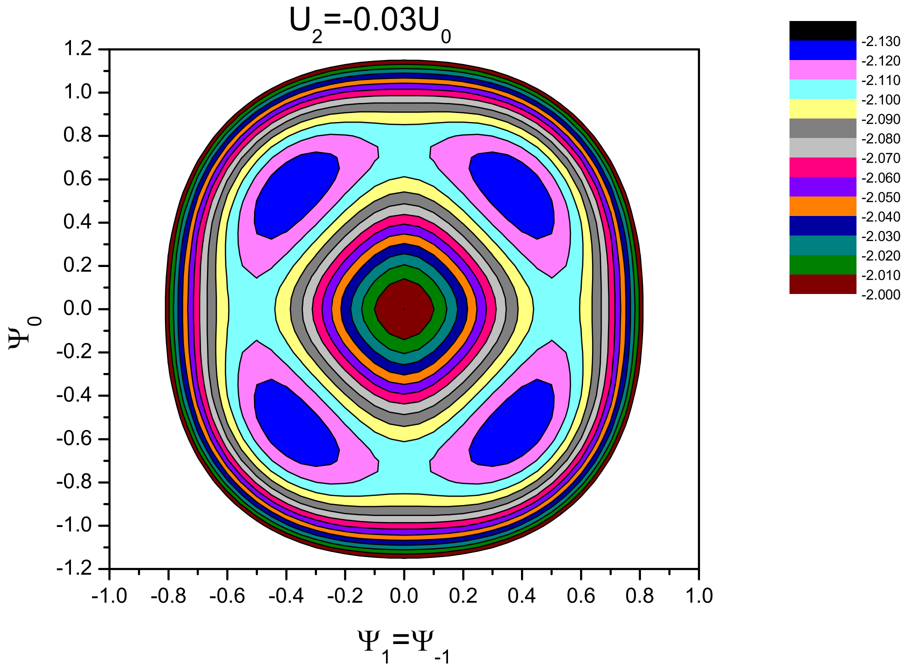

Figure 3: Free Energy

Results: $U_2 = 0$

Results $U_2 = 0$,T=0

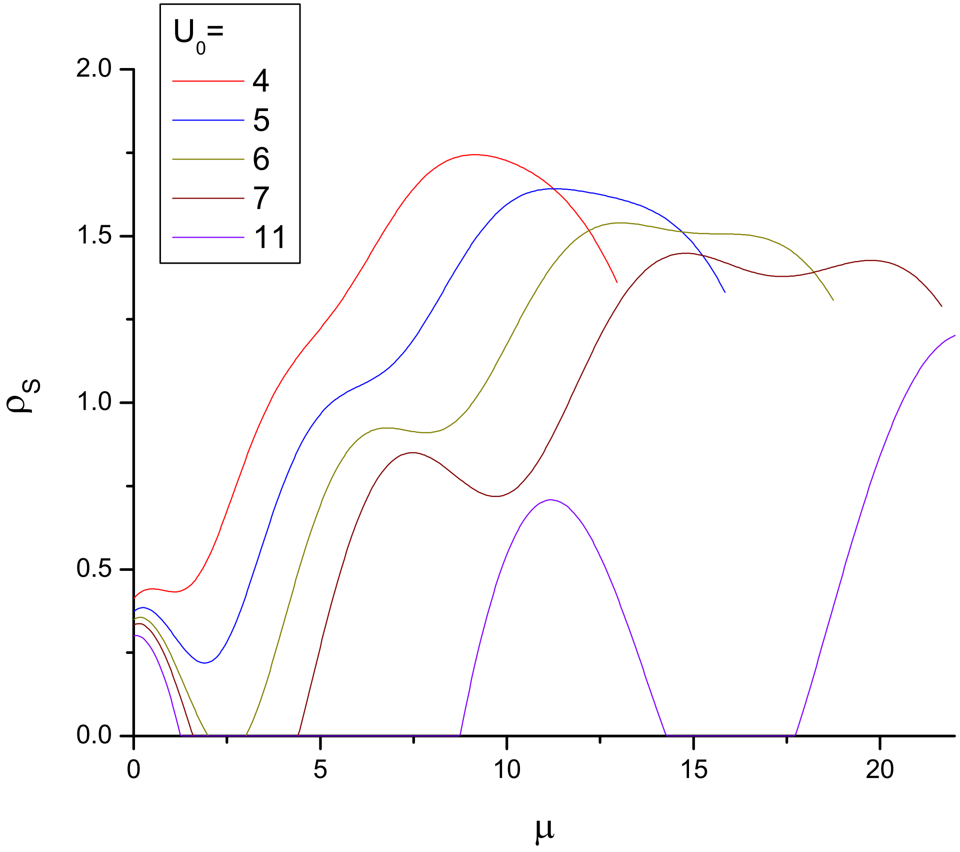

Figure 4: ρ_S versus μ. $\rho_S > 0 \rightarrow$ Superfluid Phase

Results $U_2 = 0$,T=0

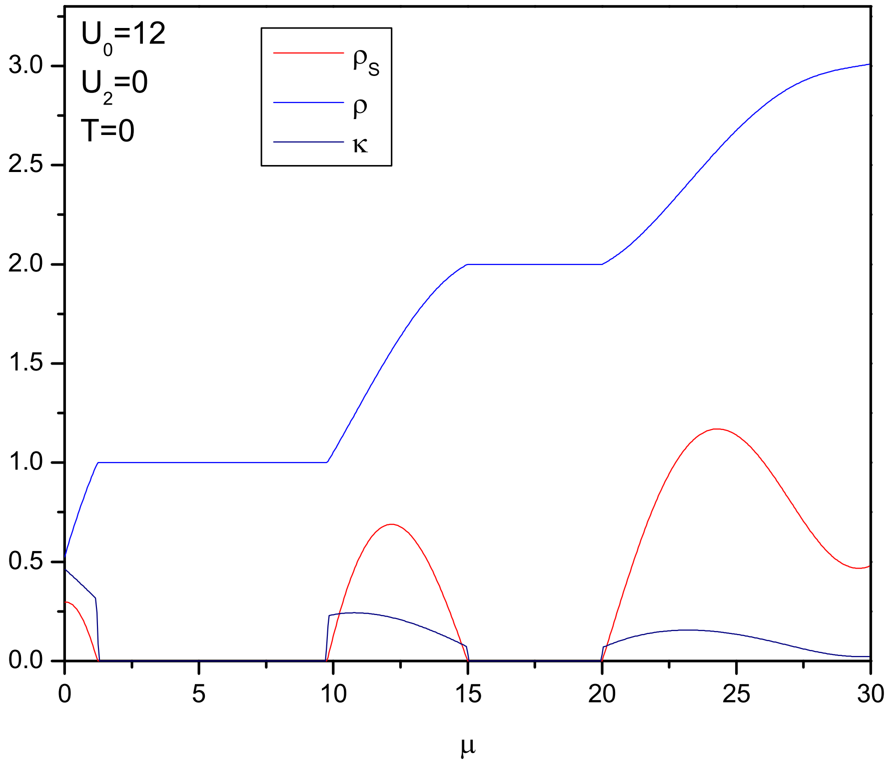

Figure 5: ρ_S, ρ, κ versus μ. Mott Insulator Phase has $\rho_S = 0$, $\rho = 1, 2, \cdots$ and $\kappa = 0$

Results $U_2 = 0$,T=0

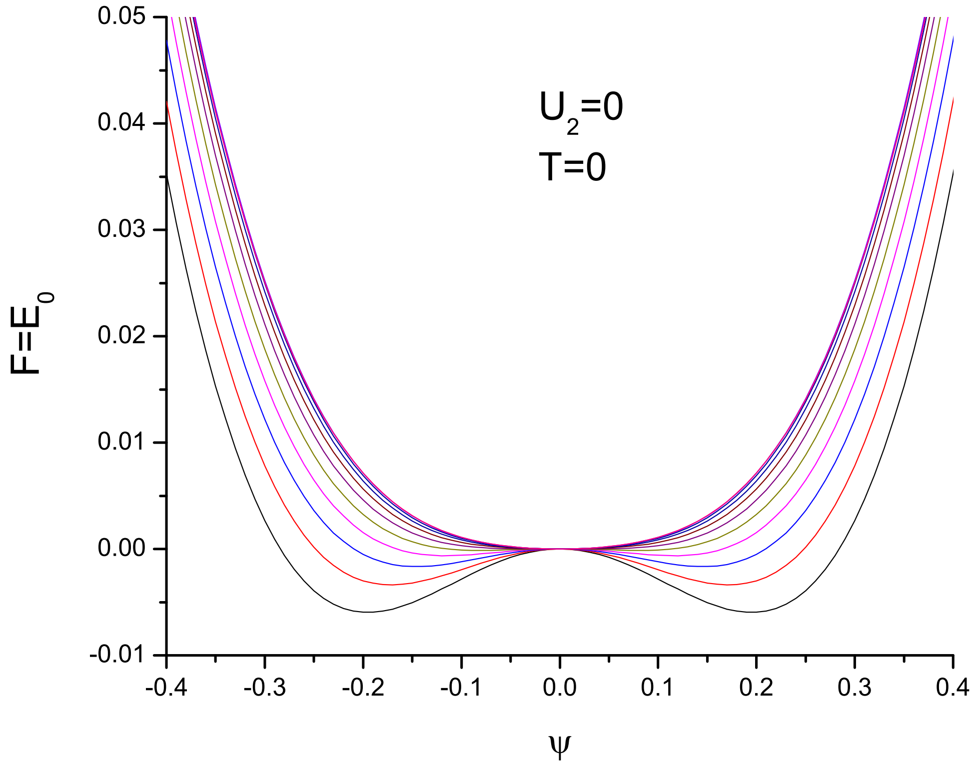

Figure 6: Ground State Energy E_0 versus Ψ. SF-MI transition is continuous.

Phase Diagram: $U_2 = 0$,T=0

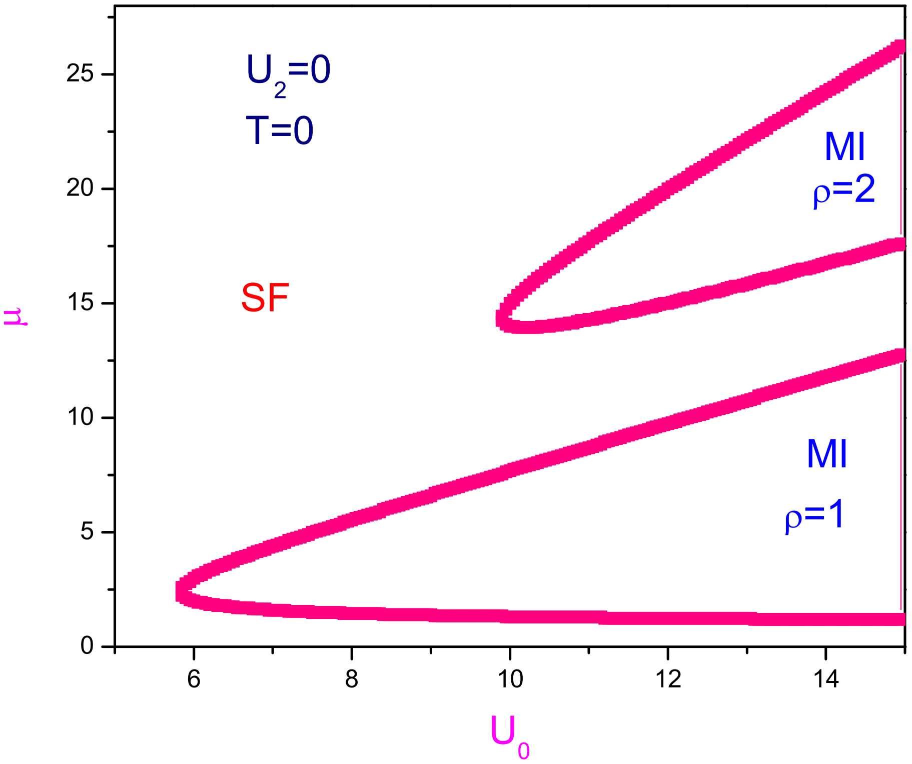

Figure 7: Phase Diagram showing SF and MI phases. SF-MI transition continuous.

Results $U_2 = 0$, Finite Temperature

Outline of the Presentation

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Mean Field Approximation

Results: $U_2 = 0$
- ❖ Results $U_2 = 0$,T=0
- ❖ Results $U_2 = 0$,T=0
- ❖ Results $U_2 = 0$,T=0
- ❖ Phase Diagram: $U_2 = 0$,T=0
- ❖ Results $U_2 = 0$,

For $T > 0$, $(k_B = 1)$.

$$F = E_0 - T \ln \sum_{i=\text{excited}} \left(1 + e^{-(E_i - E_0)/T}\right)$$

For commensurate densities and close to Mott insulator, the charge excitations are gapped, however, the spin excitations are gapless, which leads to many degenerate states i.e, $E_i = E_0$.

Results $U_2 = 0$,T=0.05

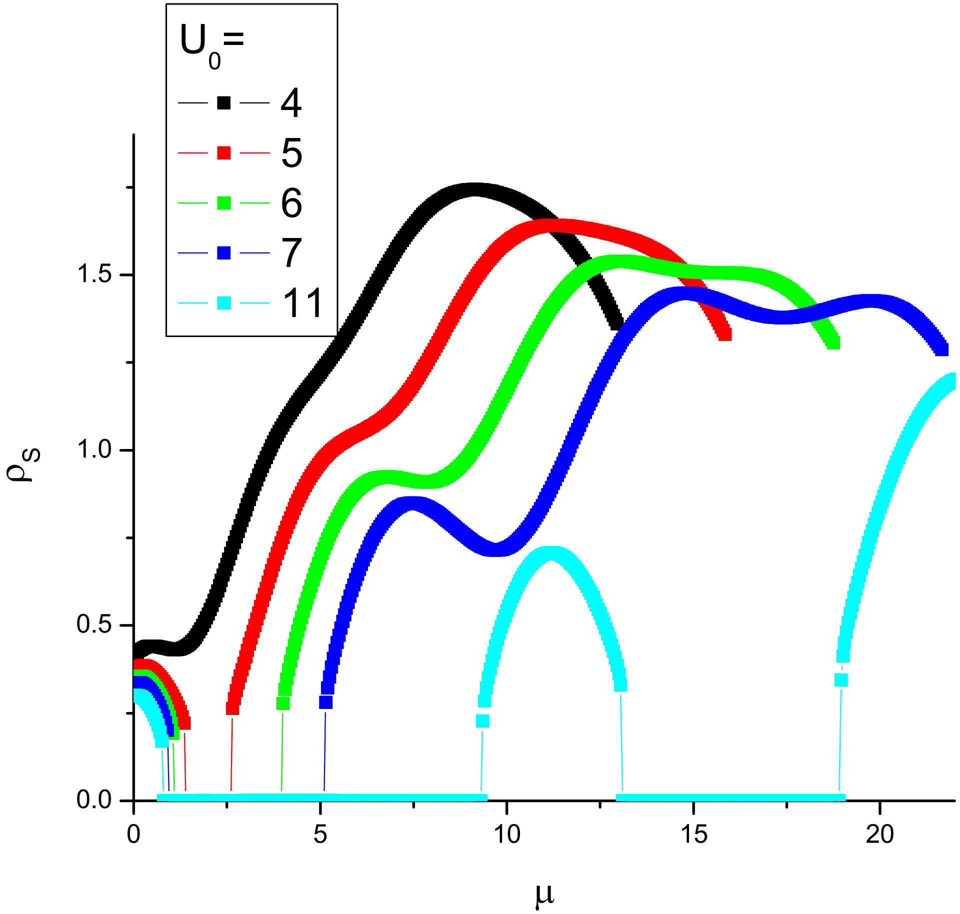

Figure 8: ρ_S versus μ. SF-MI transition become first order.

Results $U_2 = 0$,T=0.05

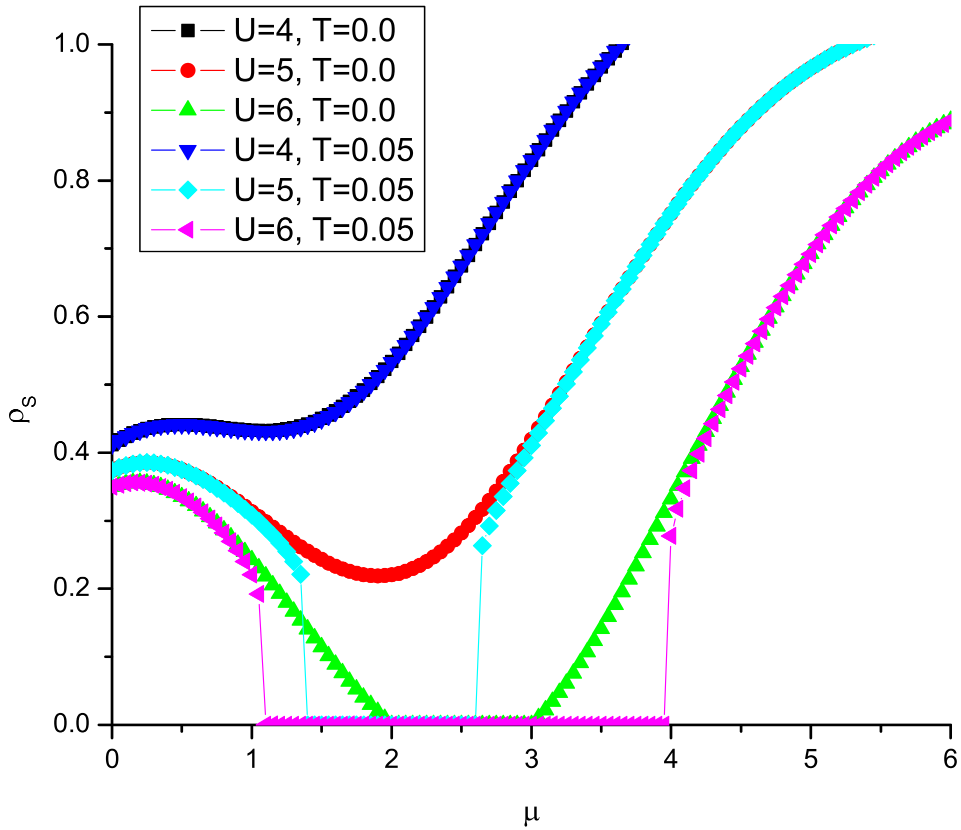

Figure 9: ρ_S versus μ. MI region enhances. First order SF-MI transition.

Results $U_2 = 0$,T=0.05

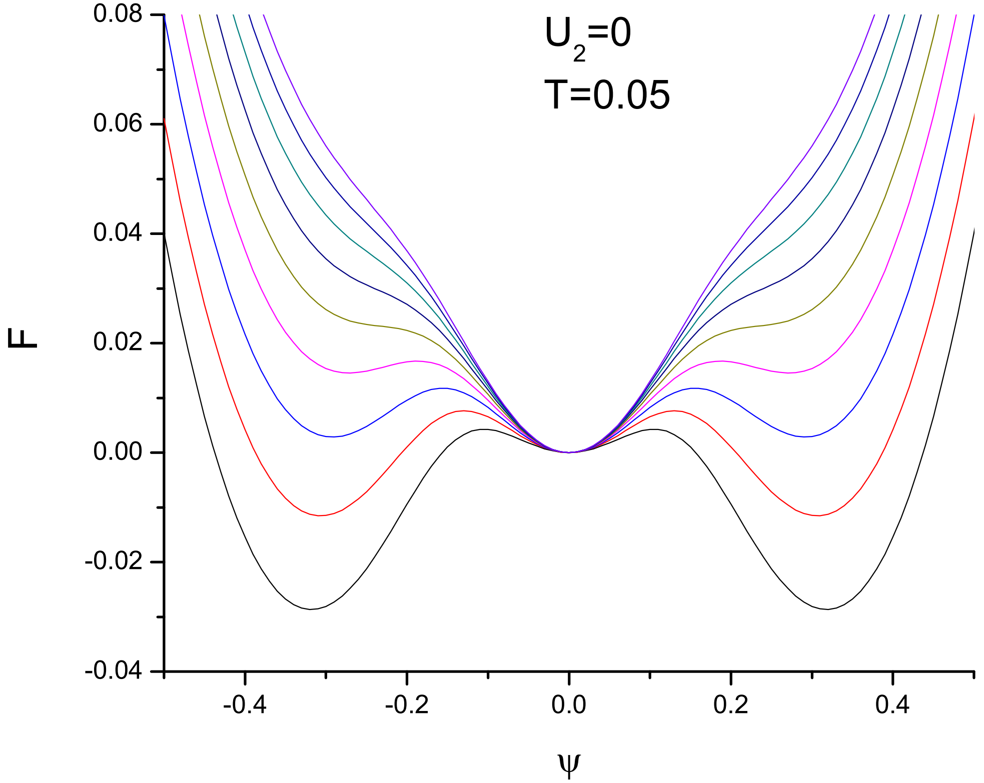

Figure 10: Free energy F versus Ψ. First order SF-MI transition.

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Phase Diagram: $U_2 = 0$,T=0.05

Outline of the Presentation
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Mean Field Approximation
Results: $U_2 = 0$
❖ Results $U_2 = 0$,T=0
❖ Results $U_2 = 0$,T=0
❖ Results $U_2 = 0$,T=0
❖ Phase Diagram: $U_2 = 0$,T=0
❖ Results $U_2 = 0$,

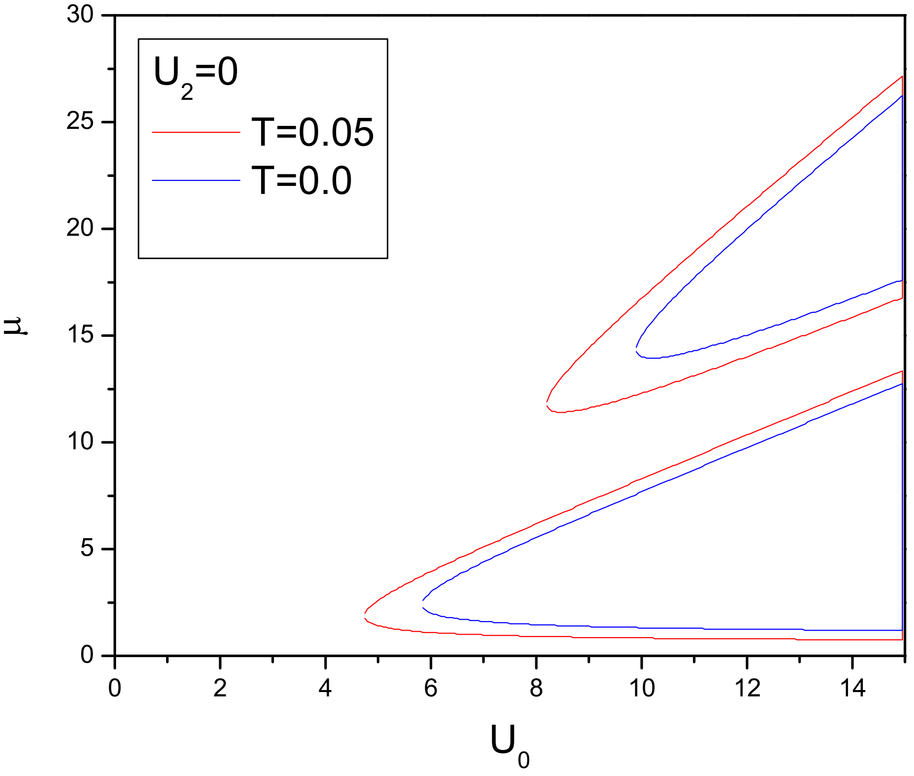

Figure 11: Phase Diagram showing SF and MI phases. $T = 0$ SF-MI transition continuous. Small T SF-MI transition first order

Phase Diagram: $U_2 = 0$

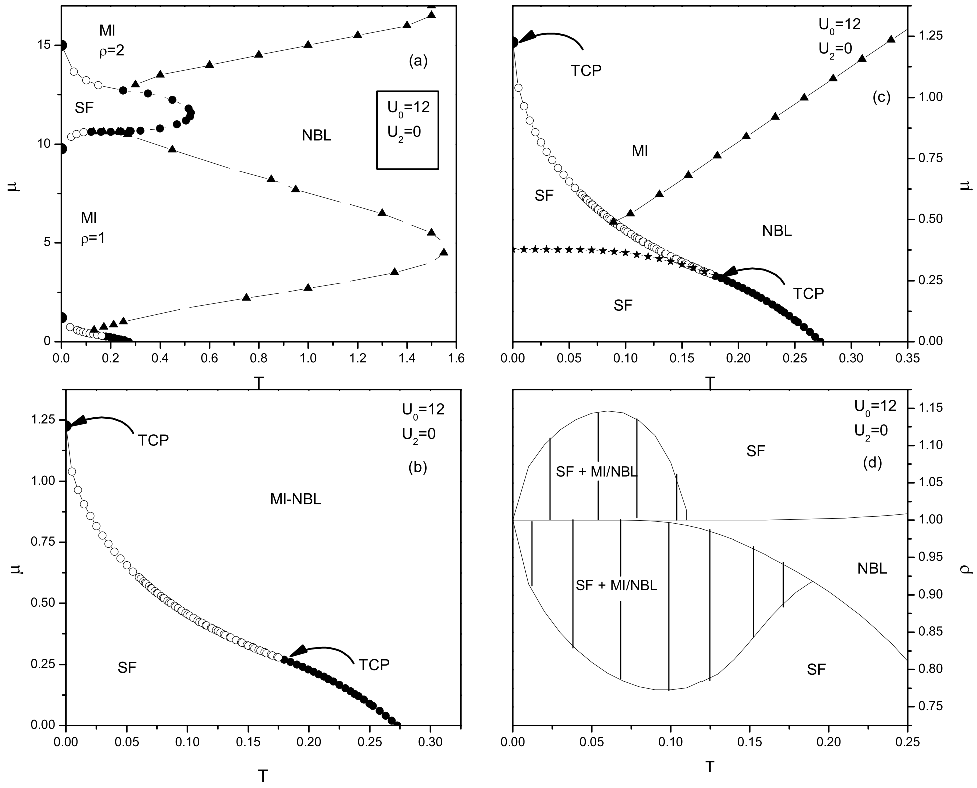

Figure 12: Phase Diagram

Results: $U_2 > 0$

Results $U_2 = 0.03U_0$, T=0.0

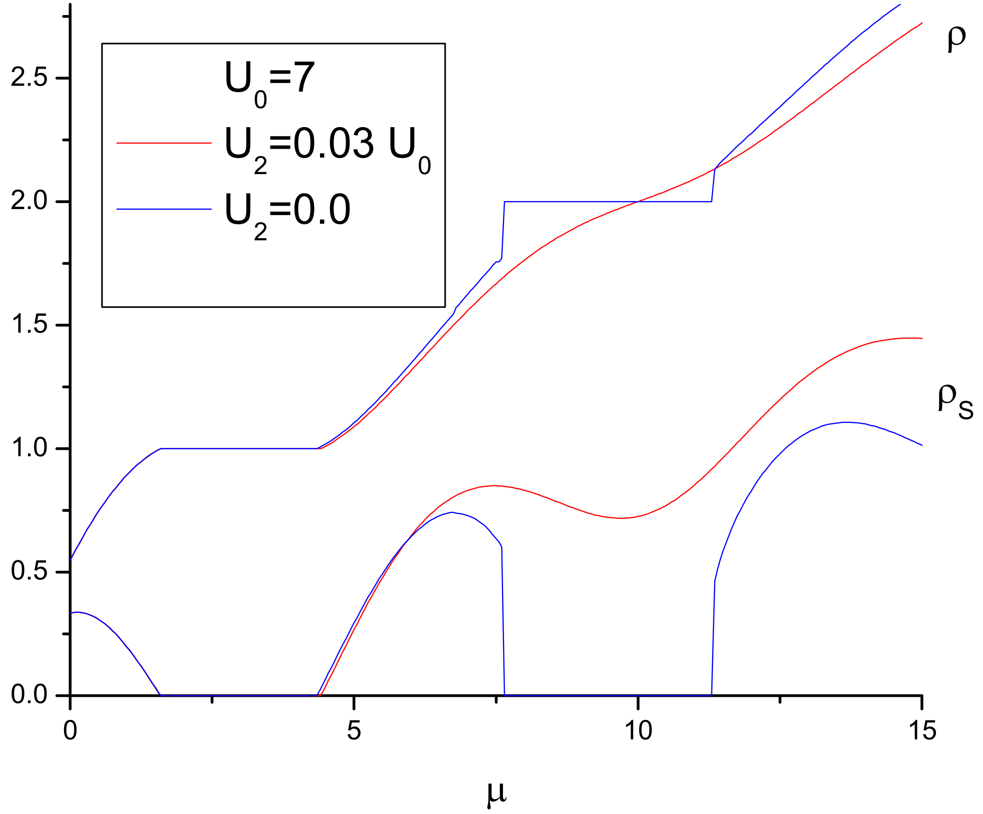

Figure 13: ρ_S versus μ. SF-MI transition for $\rho = 1$ is continuous. However, for $\rho = 2$, SF-MI transition is first order.

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Phase Diagram: $U_2 = 0.03\ U_0$,T=0

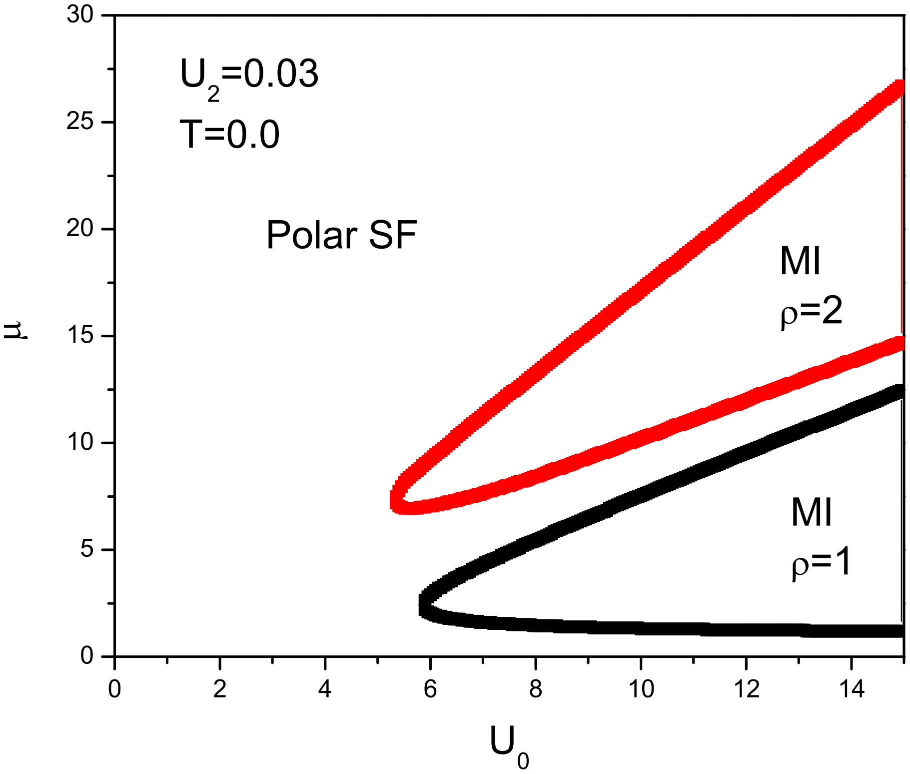

Figure 14: Phase Diagram showing SF and MI phases. $\rho = 1$ SF-MI transition continuous. $\rho = 2$ SF-MI transition is first order.

Phase Diagram: $U_2 = 0.03U_0$

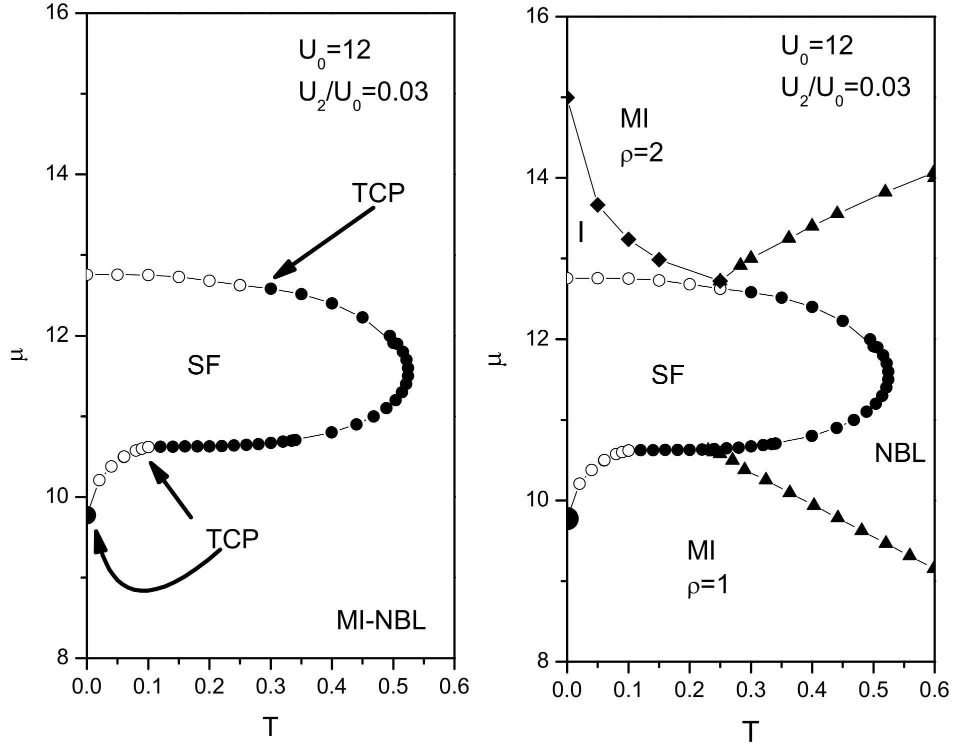

Figure 15: Phase Diagram in the T,μ plane

Conclusions

Conclusions

- Extensive studies of Bose-Hubbard model for spin 1 using Mean-Field Theory
- Elucidate phases, transitions
- These results can also be applied to Bose-Hubbard models for spin-2 and multiple types of Bosons.
- The phase diagram for spin-2 Bose-Hubbard model remain similar to spin-1 model.
- The phase diagram for two species Bose-Hubbard model consists of SF, MI and Phase separation.

Acknowledgments

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- INFLIBNET

Figure 16: Goa University Library

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Results: $U_2 = 0$
Results: $U_2 > 0$
Conclusions
Acknowledgments
❖ Acknowledgments
❖

Thank You
&
Wellcome to Goa
Land of Sea and Sand
&
Goa University

Goa University Link

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