Spin-1 Bosons in an Optical Lattice at Non-Zero Temperature

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1. Bose-Hubbard Model for Spin-1 Bosons

- Second-quantized Hamiltonian for magnetized hyperfine spin-1 bosons with spin dependent delta interaction in spin independent periodic potential [1–4]:

$$\hat{H} = \sum_\alpha \int d^3x \hat{\Psi}^\dagger_\alpha(\mathbf{x}) \left[-\frac{\hbar^2}{2M}\nabla^2 + V_0 \sum_{j=1}^{D} \sin^2(k_L x_j) - \mu \right] \hat{\Psi}_\alpha(\mathbf{x})$$
$$- \eta \sum_{\alpha,\beta} \int d^3x \hat{\Psi}^\dagger_\alpha(\mathbf{x}) F^z_{\alpha\beta} \hat{\Psi}_\beta(\mathbf{x}) + \frac{c_0}{2} \sum_{\alpha,\beta} \int d^3x \hat{\Psi}^\dagger_\alpha(\mathbf{x}) \hat{\Psi}^\dagger_\beta(\mathbf{x}) \hat{\Psi}_\beta(\mathbf{x}) \hat{\Psi}_\alpha(\mathbf{x})$$
$$+ \frac{c_2}{2} \sum_{\alpha,\beta,\gamma,\delta} \int d^3x \hat{\Psi}^\dagger_\alpha(\mathbf{x}) \hat{\Psi}^\dagger_\gamma(\mathbf{x}) \mathbf{F}_{\alpha\beta} \mathbf{F}_{\gamma\delta} \hat{\Psi}_\delta(\mathbf{x}) \hat{\Psi}_\beta(\mathbf{x})$$

$F^{x,y,z}$: spin-1 matrices.
Spin independent interaction: $c_0 = 4\pi\hbar^2(a_0 + 2a_2)/3M$
Spin dependent interaction: $c_2 = 4\pi\hbar^2(a_0 - a_2)/3M$
a_F: s-wave scattering length for total hyperfine spin F
η: magnetic chemical potential to keep magnetization fixed

	$c_2 < 0$ ferromagnetic example ^{87}Rb [5]	$c_2 > 0$ antiferromagnetic example ^{23}Na [6]
a_0	$50\, a_B$	$101.8\, a_B$
a_2	$55\, a_B$	$100.4\, a_B$

Can be tuned by using Feshbach resonances.

- Wannier decomposition yields Bose-Hubbard Model [4, 7–9]:

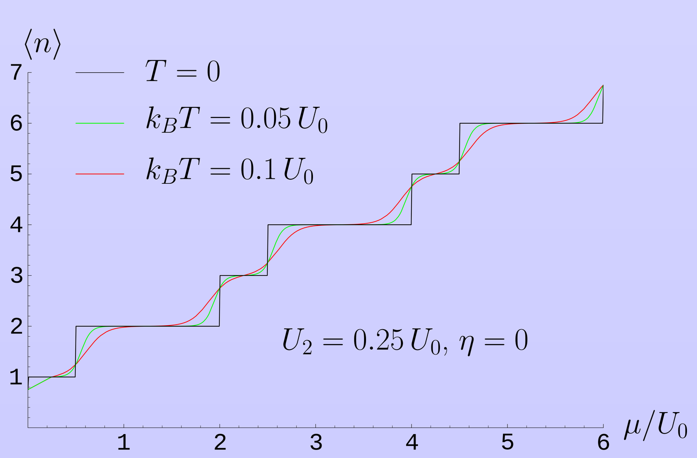
$$\hat{H}_{\rm BH} = \hat{H}^{(0)} + \hat{H}^{(1)}$$
$$\hat{H}^{(0)} = \sum_i \left[\frac{1}{2} U_0 \hat{n}_i(\hat{n}_i - 1) + \frac{1}{2} U_2(\hat{\mathbf{S}}_i^2 - 2\hat{n}_i) - \mu \hat{n}_i - \eta \hat{S}^z_i \right]$$
$$\hat{H}^{(1)} = -J \sum_\alpha \sum_{<i,j>} \hat{a}^\dagger_{i\alpha} \hat{a}_{j\alpha}$$

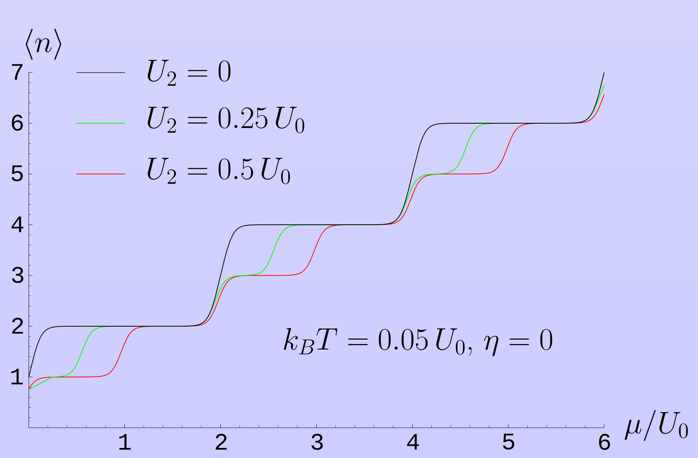
J: tunnel matrix element between nearest neighbors
$U_{0,2} \propto c_{0,2}$: the spin independ and dependent interaction.
$\hat{\mathbf{S}}_i$: spin operators on site i with $[\hat{S}^\alpha_j, \hat{S}^\beta_k] = i\delta_{jk} \sum_\gamma \epsilon_{\alpha\beta\gamma} \hat{S}^\gamma_j$

$$\hat{S}^{x,y}_i = \frac{1}{\sqrt{2}} (\hat{a}^\dagger_{i0}\hat{a}_{i1} \pm \hat{a}^\dagger_{i1}\hat{a}_{i0} + \hat{a}^\dagger_{i-1}\hat{a}_{i0} \pm \hat{a}^\dagger_{i0}\hat{a}_{i-1}) \quad , \quad \hat{S}^z_i = \hat{a}^\dagger_{i1}\hat{a}_{i1} - \hat{a}^\dagger_{i-1}\hat{a}_{i-1}$$

- No Hopping ($J = 0$): Hamiltonian site diagonal
Eigenstates characterized by particle number n, total spin S and z-component of spin m.
Note: $n + S$ even [10], especially n odd, $S = 0$ forbidden

$$\hat{H}^{(0)}|S, m, n\rangle = E^{(0)}_{S,m,n}|S, m, n\rangle$$
$$E^{(0)}_{S,m,n} = \frac{1}{2} U_0 n(n-1) + \frac{1}{2} U_2[S(S+1) - 2n] - \mu n - \eta m$$





2. Superfluid-Mott Insulator Transition

- Decoupling the hopping term by mean-field approximation [11]:

$$\hat{a}^\dagger_{i\alpha}\hat{a}_{j\alpha} \approx \Psi_\alpha \hat{a}^\dagger_{i\alpha} + \Psi^*_\alpha \hat{a}_{j\alpha} - \Psi^*_\alpha \Psi_\alpha \quad , \quad \Psi_\alpha = \langle \hat{a}_{i\alpha} \rangle \quad , \quad \Psi^*_\alpha = \langle \hat{a}^\dagger_{i\alpha} \rangle$$
$$\hat{H}^{(1)}_{\rm MF} = -Jz \sum_i \sum_\alpha \left(\Psi_\alpha \hat{a}^\dagger_{i\alpha} + \Psi^*_\alpha \hat{a}_{i\alpha} - \Psi^*_\alpha \Psi_\alpha \right)$$

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

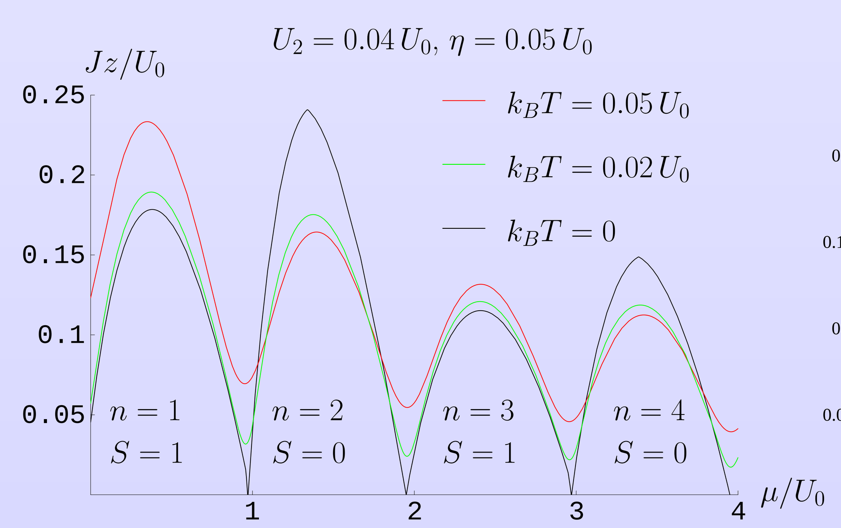
$$\hat{a}^\dagger_\alpha |S, m, n\rangle = M_{\alpha,S,m,n}|S+1, m+\alpha, n+1\rangle + N_{\alpha,S,m,n}|S-1, m+\alpha, n+1\rangle$$
$$\hat{a}_\alpha |S, m, n\rangle = O_{\alpha,S,m,n}|S+1, m-\alpha, n-1\rangle + P_{\alpha,S,m,n}|S-1, m-1, n-\alpha\rangle$$

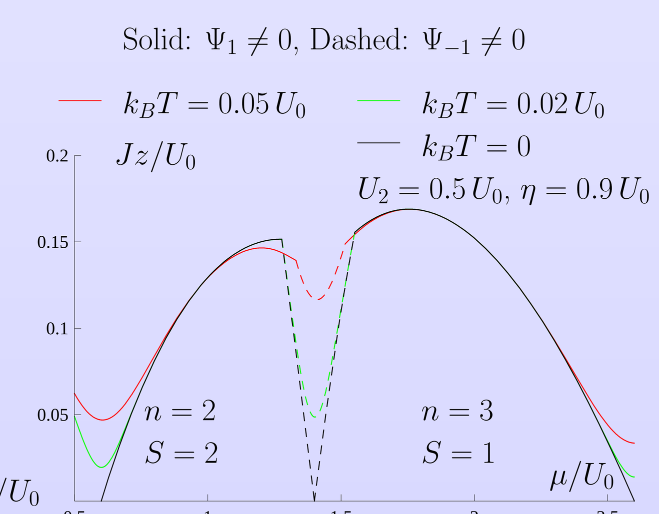
Matrix elements M, N, O, P calculated by recursion relation.

- Landau expansion of grand-canonical free energy [12]:

$$\mathcal{F}(\mathbf{\Psi}^*, \mathbf{\Psi}) = -k_BT \log {\rm Tr} \left\{ e^{-(\hat{H}^{(0)} + \hat{H}^{(1)}_{\rm MF})/k_BT} \right\}$$
$$= -k_BT \log \mathcal{Z}^{(0)} + \sum_\alpha A^{(2)}_\alpha |\Psi_\alpha|^2 + O(\mathbf{\Psi}^4)$$
$$A^{(2)}_\alpha = \frac{1}{\mathcal{Z}^{(0)}} \sum_{S,m,n} e^{-E^{(0)}_{S,m,n}/k_BT} \left[-Jz + J^2z^2 \left(\frac{M^2_{\alpha,S,m,n}}{E^{(0)}_{S+1,m+\alpha,n+1} - E^{(0)}_{S,m,n}} + \frac{N^2_{\alpha,S,m,n}}{E^{(0)}_{S-1,m+\alpha,n+1} - E^{(0)}_{S,m,n}} + \frac{O^2_{\alpha,S,m,n}}{E^{(0)}_{S+1,m-\alpha,n-1} - E^{(0)}_{S,m,n}} + \frac{P^2_{\alpha,S,m,n}}{E^{(0)}_{S-1,m-\alpha,n-1} - E^{(0)}_{S,m,n}} \right) \right] \quad , \quad \mathcal{Z}^{(0)} = \sum_{S,m,n} e^{-E^{(0)}_{S,m,n}/k_BT}$$

- Phase transition occurs when one of the coefficients $A^{(2)}_\alpha$ vanishes: different superfluid phases exist [13, 14]:
Magnetized gas ($\eta \neq 0$): $\Psi_1 \neq 0$ or $\Psi_{-1} \neq 0$
Unmagnetized gas ($\eta = 0$): $\Psi_0 \neq 0$





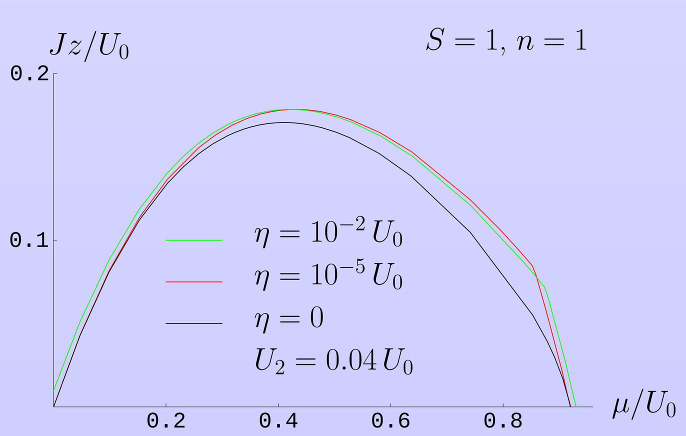
Fully polarized gas reproduces phase diagram of the scalar BHM [7, 15]

Zero temperature limit for non-magnetized ($\eta = 0$) antiferromagnetic bosons:

$\Phi^{(0)}_G = |0, 0, n\rangle$ if n even

$\Phi^{(0)}_G = |1, m, n\rangle$ $m = 0, \pm 1$ if n odd

Unperturbed ground state threefold degenerated, $\eta \to 0$ limit discontinuous.



3. Time-of-Flight

- Time-of-flight absorption pictures reveal momentum space density [16]. Different spin-components separable by inhomogeneous magnetic fields [17].

$$n(\mathbf{k}) = \sum_\alpha n_\alpha(\mathbf{k}) \,, \quad n_\alpha(\mathbf{k}) = |w(\mathbf{k})|^2 S_\alpha(\mathbf{k}) \,, \quad S_\alpha(\mathbf{k}) = \sum_{i,j} e^{i\mathbf{k}(\mathbf{r}_i - \mathbf{r}_j)} \langle \hat{a}^\dagger_{i\alpha} \hat{a}_{j\alpha} \rangle$$

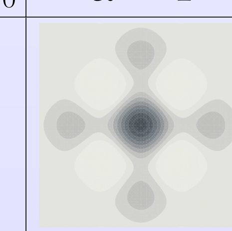
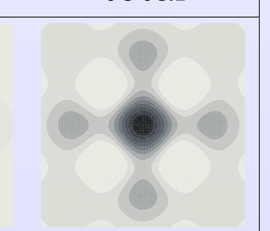
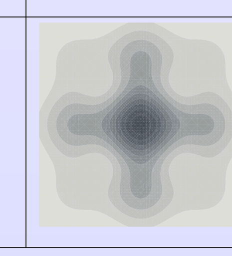
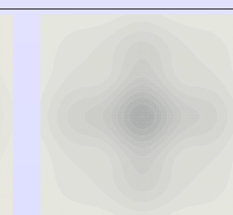
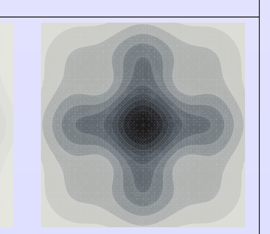
- First-order strong-coupling expansion at $T = 0$, $\Phi^{(0)}_G = |S, m, n\rangle$ [18]:

$$\langle \hat{a}^\dagger_{i\alpha} \hat{a}_{j\alpha} \rangle = \delta_{ij} n_\alpha + \delta_{d(i,j),1} 2JzC_\alpha + O(J^2)$$
$$C_\alpha = \frac{M^2_{\alpha,S,m,n} O^2_{\alpha,S,m,n}}{U_0 + (2S+2)U_2} + \frac{M^2_{\alpha,S,m,n} P^2_{\alpha,S,m,n}}{U_0 + U_2} + \frac{N^2_{\alpha,S,m,n} O^2_{\alpha,S,m,n}}{U_0 + U_2} + \frac{N^2_{\alpha,S,m,n} P^2_{\alpha,S,m,n}}{U_0 - 2SU_2} \,, \quad n_\alpha = O^2_{\alpha,S,m,n} + P^2_{\alpha,S,m,n}$$

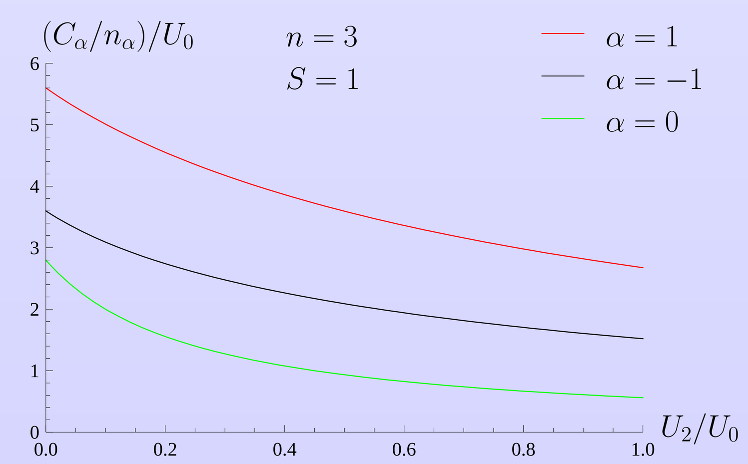
- Explicit result for ground state of magnetized gas $\Phi^{(0)}_G = |S, S, n\rangle$:

$$n_1 = \frac{n + (n+2)S + S^2}{3 + 2S}$$
$$C_1 = \frac{(n-S)(S+1)(n+S+3)}{(2S+1)(2S+3)^2[U_0 + (2S+2)U_2]} + \frac{(n+S+3)(n+S+1)(S+1)S}{[4(S+2)S+3](U_0 + U_2)}$$

Other two components completely analogous
Fully polarized gas $\Phi^{(0)}_G = |n, n, n\rangle$ yields $n_0(\mathbf{k}) = n_{-1}(\mathbf{k}) = 0$
$n_1(\mathbf{k})$ reproduces result of scalar BHM [15, 19]

$U_2 = 0.04\, U_0$	$\alpha = 1$	$\alpha = 0$	$\alpha = -1$	total
$n = 3$, $S = 1$, $V_0 = 8\, E_R$				
$n = 3$, $S = 1$, $V_0 = 14\, E_R$				

$\frac{C_\alpha}{n_\alpha}$ measures correlation
n even: all three spin components equal.
No direct dependence on η but important for determination of ground state.



4. Outlook

Phase Transition:

- Magnetic properties of superfluid phase and order of phase transition
- Quantum corrections to mean-field result
- Different phases within one Mott-lobe [20]

Time-of-flight:

- Further quantitative analysis: visibility
- Extension to the Hamburg triangular optical lattice to study frustration effects

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