Superfluid Phases of Spin-1 Bosons in a Cubic Optical Lattice at Zero Temperature

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Motivation Over the last years the exciting experimental progress in the field of ultracold atoms confined in optical lattices has led to numerous theoretical proposals which are devoted to the quantum simulation of condensed matter physics problems [1]. Here we analyze theoretically a spinor Bose gas loaded into a three-dimensional cubic optical lattice. In order to account for the different superfluid phases of spin-1 bosons, we generalize the recently developed Ginzburg-Landau theory for the Bose-Hubbard model [2,3]. In particular at zero temperature, our theory can distinguish between various ferromagnetic and antiferromagnetic superfluid phases for an anti-ferromagnetic interaction and a non-vanishing magneto-chemical potential. Furthermore, we show for a vanishing magneto-chemical potential that the superfluid phase is a polar state, where all the atoms condense in the spin-0 state [4].

Bose-Hubbard Model for spin-1 Bosons

- We start from the second quantized Hamiltonian for a spin-1 Bose gas in the grand-canonical ensemble [5–8] which is given by

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

$F^{x,y,z}$: 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: magneto-chemical potential to keep magnetization fixed

Periodic potential of a D-dimensional cubic optical lattice $V(\mathbf{x}) = V_0 \sum_{\nu=1}^{D} \sin^2(k_L x_\nu)$ with a lattice period $a = \pi/k_L$ where $k_L = 2\pi/\lambda$.

- Wannier decomposition yields Bose-Hubbard Model [4,7,10,11]

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

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

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

$$\hat{S}_{iz} = \hat{a}^\dagger_{i1}\hat{a}_{i1} - \hat{a}^\dagger_{i-1}\hat{a}_{i-1}, \quad \hat{S}_{ix} = \frac{1}{\sqrt{2}}(\hat{a}^\dagger_{i1}\hat{a}_{i0} + \hat{a}^\dagger_{i0}\hat{a}_{i1} + \hat{a}^\dagger_{i0}\hat{a}_{i-1} + \hat{a}^\dagger_{i-1}\hat{a}_{i0}),$$

$$\hat{S}_{iy} = \frac{i}{\sqrt{2}}(-\hat{a}^\dagger_{i1}\hat{a}_{i0} + \hat{a}^\dagger_{i0}\hat{a}_{i1} - \hat{a}^\dagger_{i0}\hat{a}_{i-1} + \hat{a}^\dagger_{i-1}\hat{a}_{i0}),$$

$$\hat{\mathbf{S}}_i^2 = 2\hat{n}_{i1}\hat{n}_{i0} + 2\hat{n}_{i0}\hat{n}_{i-1} + \hat{n}_{i1} + 2\hat{n}_{i0} + \hat{n}_{i-1} + \hat{n}_{i1}^2 - 2\hat{n}_{i1}\hat{n}_{i-1} + \hat{n}_{i-1}^2 + 2\hat{a}^\dagger_{i1}\hat{a}^\dagger_{i-1}\hat{a}^2_{i0} + 2\hat{a}^\dagger_{i0}\hat{a}^\dagger_{i0}\hat{a}_{i1}\hat{a}_{i-1}$$

Total atom number operator $\hat{n}_i = \sum_\alpha \hat{n}_{i\alpha}$ where $\hat{n}_{i\alpha} = \hat{a}^\dagger_{i\alpha}\hat{a}_{i\alpha}$

- Zero hopping ($J = 0$): Hamiltonian is site-diagonal
Eigenstates characterized by particle number n, total spin S and z component of spin m.

$$\hat{H}^{(0)} \mid S, m, n \rangle = E^{(0)}_{S,m,n} \mid S, m, n \rangle,$$

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

Note that $S + n =$ even [12].

Ginzburg-Landau Theory

- Coupling to local sources [2,3,13–15]

$$\hat{H}\left[j_{i\alpha}(\tau), j^*_{i\alpha}(\tau)\right] = \hat{H}_{BH} + \sum_i \sum_\alpha \left[j^*_{i\alpha}(\tau)\hat{a}_{i\alpha} + j_{i\alpha}(\tau)\hat{a}^\dagger_{i\alpha} \right]$$

$$\hat{H}^{(1)}_{\mathrm{GL}} = -J \sum_{\langle i,j \rangle} \sum_\alpha \hat{a}^\dagger_{i\alpha}\hat{a}_{j\alpha} + \sum_i \sum_\alpha \left[j^*_{i\alpha}(\tau)\hat{a}_{i\alpha} + j_{i\alpha}(\tau)\hat{a}^\dagger_{i\alpha} \right]$$

- Perturbative expansion in $\hat{H}^{(1)}_{\mathrm{GL}}$ needs [16,18]:

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

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

- Unperturbed n-particle Green function:

$$G^{(0)}_n(\tau'_1, i'_1\alpha'_1; \ldots; \tau'_n, i'_n\alpha'_n | \tau_1, i_1\alpha_1; \ldots; \tau_n, i_n\alpha_n) = \left\langle \hat{T}\left[\hat{a}^\dagger_{i'_1\alpha'_1}(\tau'_1)\hat{a}_{i_1\alpha_1}(\tau_1) \ldots \hat{a}^\dagger_{i'_n\alpha'_n}(\tau'_n)\hat{a}_{i_n\alpha_n}(\tau_n) \right] \right\rangle^{(0)}$$

- Grand-canconical free functional ($\hbar = 1$) in Matsubara space with $\omega_m = 2\pi m/\beta$:

$$\mathcal{F}\left[j_{i\alpha}(\omega_m), j^*_{i\alpha}(\omega_m)\right] = \mathcal{F}_0 - \frac{1}{\beta} \sum_{i_1,i_2} \sum_{\alpha_1,\alpha_2} \sum_{m1,m2} \Big\{ G^{(0)}_2(i_1\alpha_1, \omega_{m1} | i_2\alpha_2, \omega_{m2}) \times j_{i_1\alpha_1}(\omega_{m1}) j^*_{i_2\alpha_2}(\omega_{m2}) + \sum_{i_3,i_4} \sum_{\alpha_3,\alpha_4} \sum_{m3,m4} G^{(0)}_4(i_1\alpha_1\omega_{m1}; i_2\alpha_2, \omega_{m2} | i_3\alpha_3, \omega_{m3}; i_4\alpha_4, \omega_{m4}) \times j_{i_1\alpha_1}(\omega_{m1}) j_{i_2\alpha_2}(\omega_{m2}) j^*_{i_3\alpha_3}(\omega_{m3}) j^*_{i_4\alpha_4}(\omega_{m4}) + \ldots \Big\}$$

- Wick rule not applicable, use instead cumulant expansion [2,3,15,17,18]
- Order parameter field:

$$\psi_{i\alpha}(\omega_m) = \langle \hat{a}_{i\alpha}(\omega_m) \rangle = \beta \frac{\delta\mathcal{F}}{\delta j^*_{i\alpha}(\omega_m)}, \quad \psi^*_{i\alpha}(\omega_m) = \left\langle \hat{a}^\dagger_{i\alpha}(\omega_m) \right\rangle = \beta \frac{\delta\mathcal{F}}{\delta j_{i\alpha}(\omega_m)}$$

- Legendre transformation

$$\Gamma\left[\Psi_{i\alpha}(\omega_m), \Psi^*_{i\alpha}(\omega_m)\right] = \mathcal{F}\left[j_{i\alpha}(\omega_m), j^*_{i\alpha}(\omega_m)\right] - \frac{1}{\beta} \sum_i \sum_m \sum_\alpha \left[\Psi_{i\alpha}(\omega_m) j^*_{i\alpha}(\omega_m) + \Psi^*_{i\alpha}(\omega_m) j_{i\alpha}(\omega_m) \right]$$

- Resulting effective action

$$\Gamma\left[\Psi_{i\alpha}(\omega_m), \Psi^*_{i\alpha}(\omega_m)\right] = \mathcal{F}_0 + \frac{1}{\beta} \sum_i \sum_{\alpha_1} \sum_{\omega_{m1}} A^{(0)}_2(i\alpha_1, \omega_{m1}) \left|\Psi_{i\alpha_1}(\omega_{m1})\right|^2 - J \sum_{\langle i,j \rangle} \sum_i \sum_{\alpha_1} \sum_{\omega_{m1}} \Psi_{i\alpha_1}(\omega_{m1}) \Psi^*_{j\alpha_1}(\omega_{m1}) - \sum_i \sum_{\alpha_1,\alpha_2,\alpha_3,\alpha_4} \sum_{\omega_{m1},\omega_{m2},\omega_{m3},\omega_{m4}} A^{(0)}_4(i\alpha_1, \omega_{m1}; i\alpha_2, \omega_{m2} | i\alpha_3, \omega_{m3}; i\alpha_4, \omega_{m4}) \Psi_{i\alpha_1}(\omega_{m1}) \Psi_{i\alpha_2}(\omega_{m2}) \Psi^*_{i\alpha_3}(\omega_{m3}) \Psi^*_{i\alpha_4}(\omega_{m4})$$

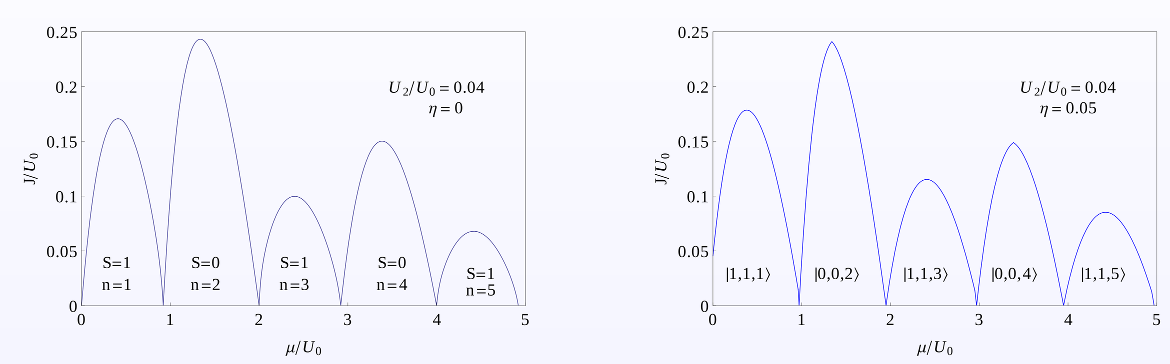
where $A^{(0)}_2(i\alpha_1, \omega_{m1})$ and $A^{(0)}_4(i\alpha_1, \omega_{m1}; i\alpha_2, \omega_{m2} | i\alpha_3, \omega_{m3}; i\alpha_4, \omega_{m4})$ are coefficients related to cumulants

- Equations of motion:

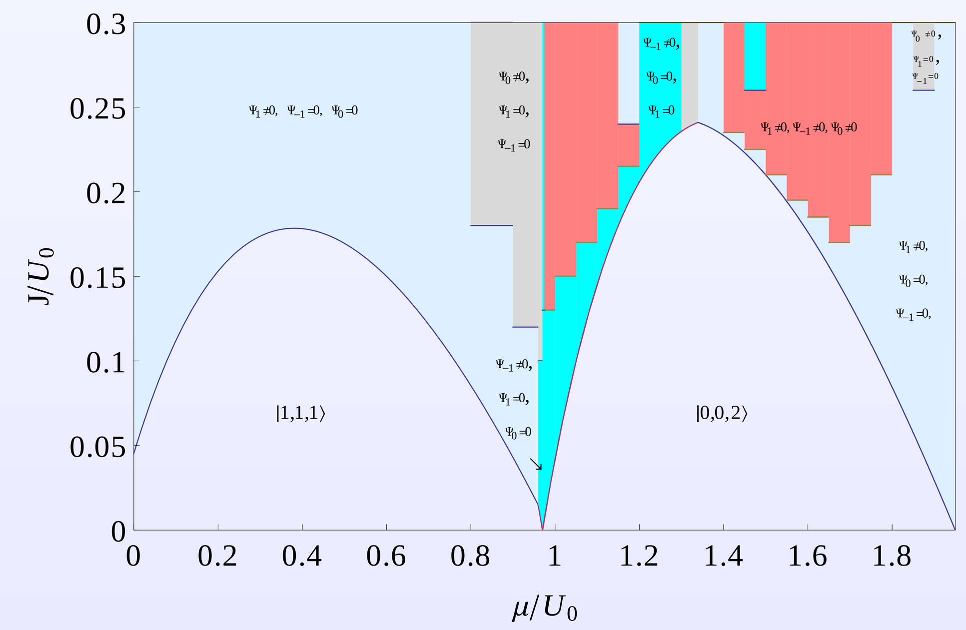
$$\left.\frac{\delta\Gamma}{\delta\Psi^*_{i\alpha}(\omega_m)}\right|_{\Psi=\Psi_{eq}} = 0, \quad \left.\frac{\delta\Gamma}{\delta\Psi_{i\alpha}(\omega_m)}\right|_{\Psi=\Psi_{eq}} = 0$$

Results

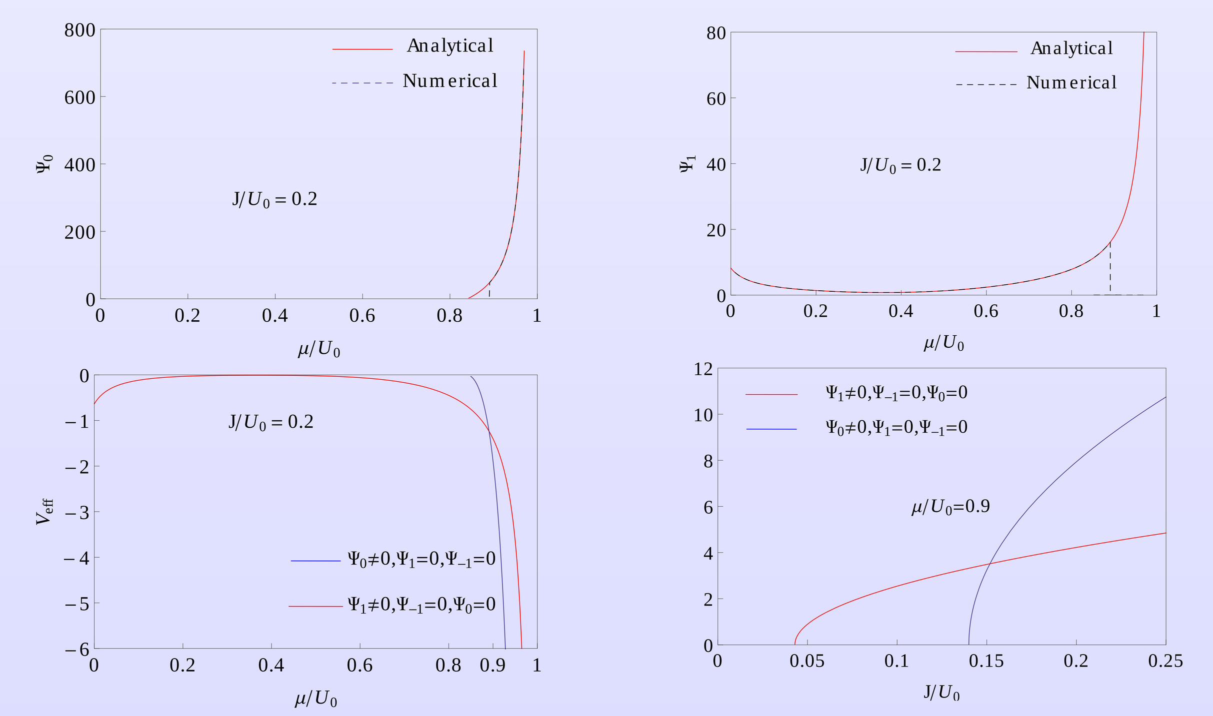
- Superfluid-Mott insulator transition: second order



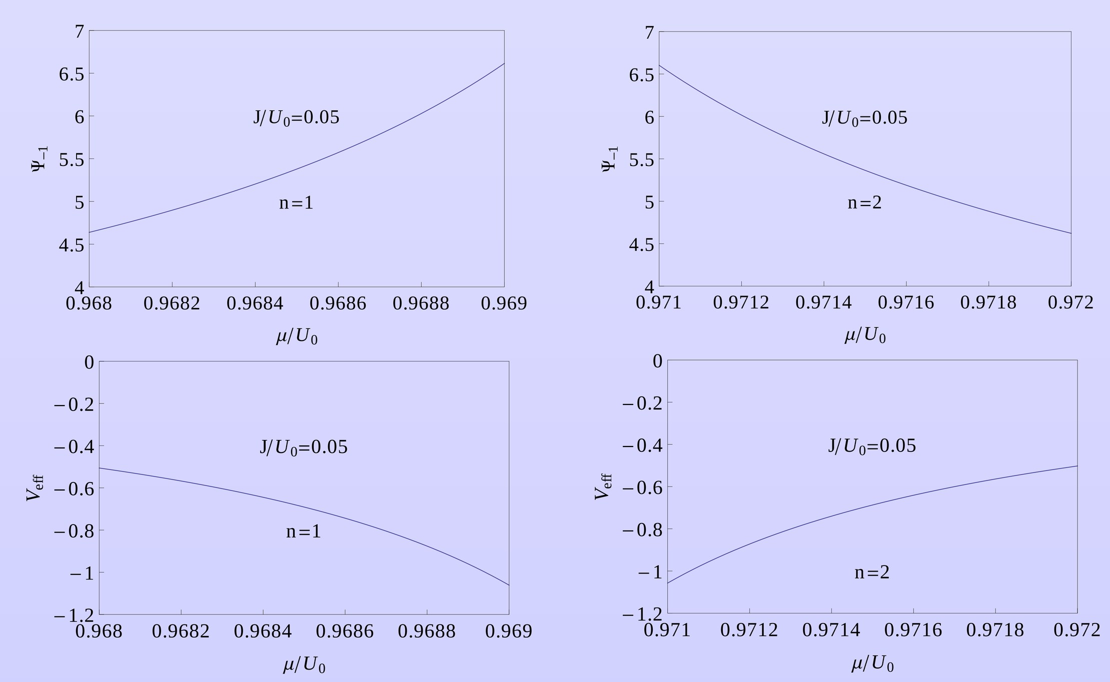
- Superfluid phase transitions: first order ($\eta = 0.05U_0$ and $U_2 = 0.04U_0$)



- First Mott lobe



- First - second Mott lobes transition



- Outlook
1-Different superfluid phases for the third and fourth lobes with $\eta \neq 0$ at zero-temperature. 2- Superfluid phases of spin-1 bosons in a triangular optical lattice at zero temperature. 3-Different superfluid phases at different temperature.

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