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

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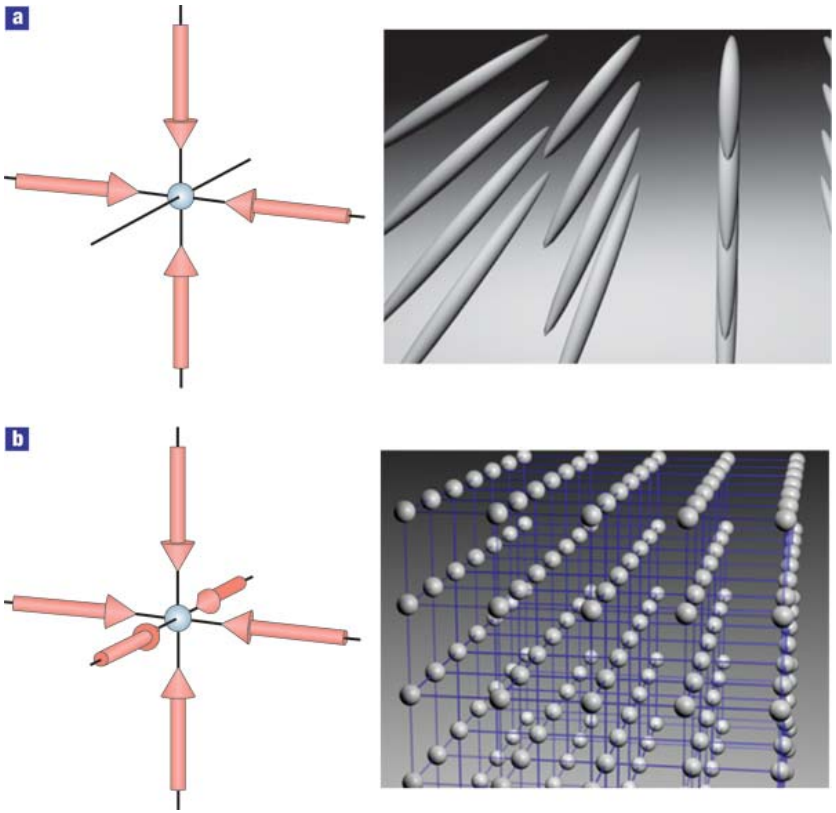
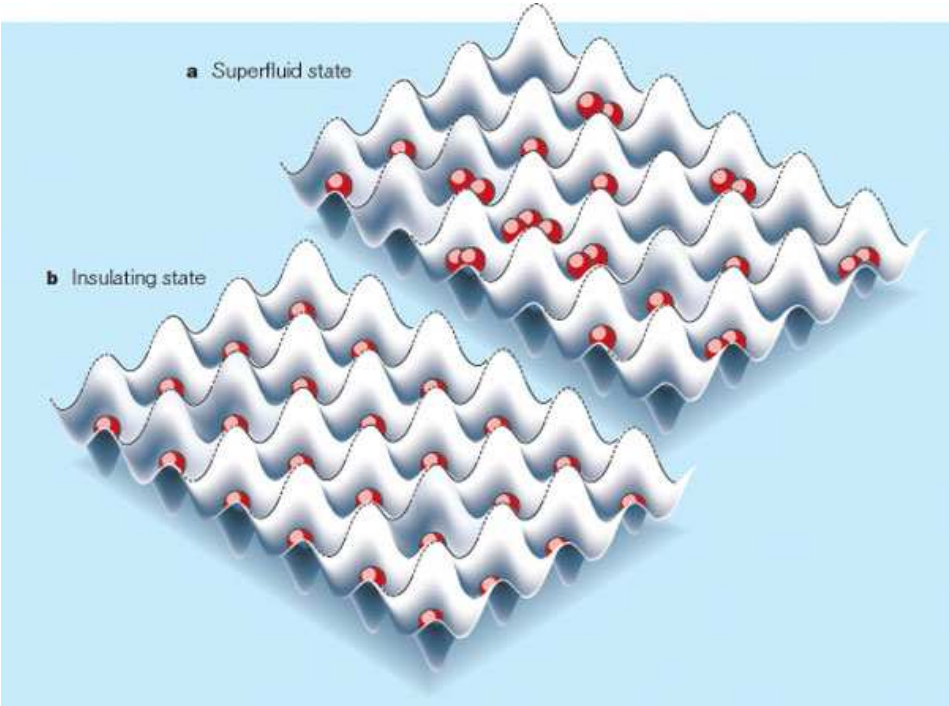
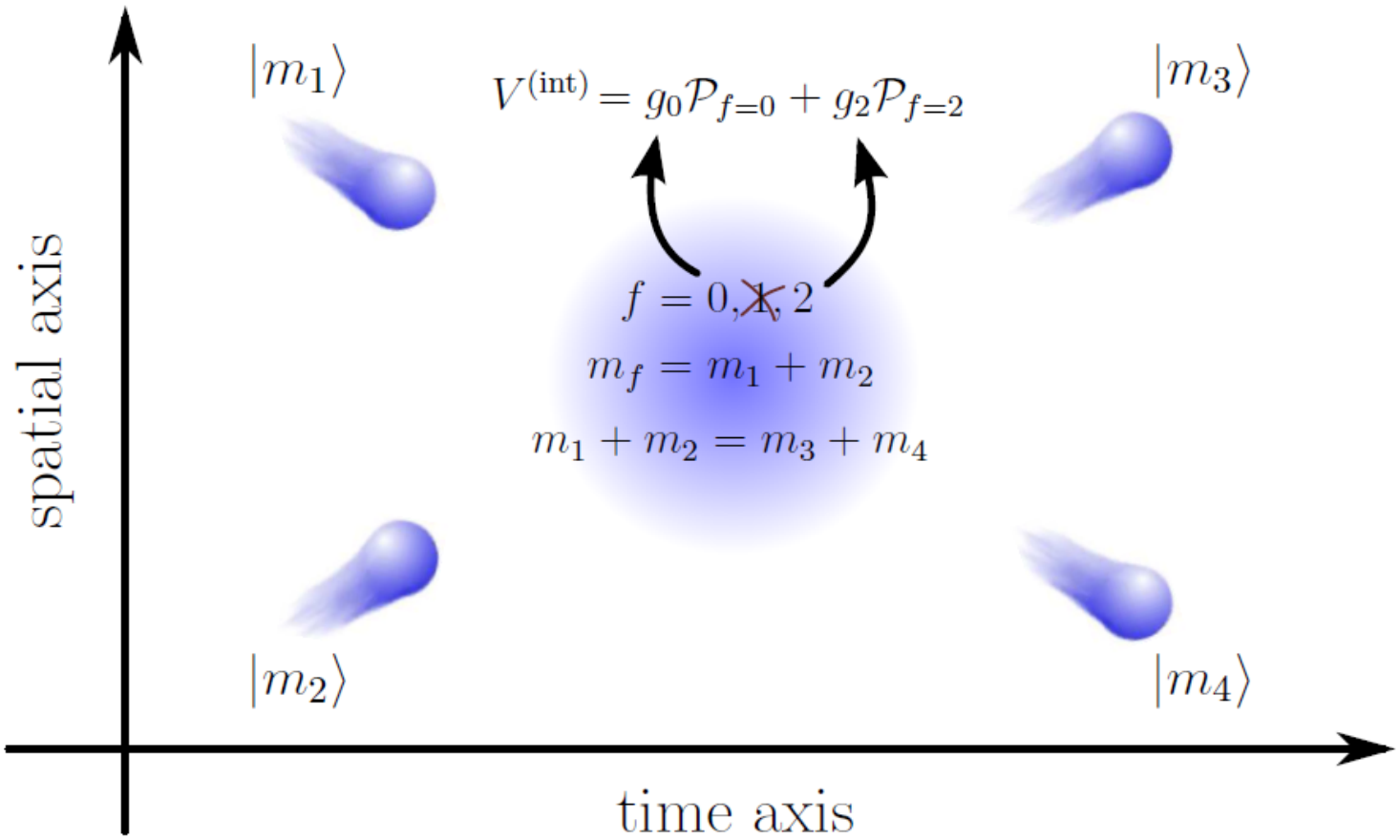
Introduction: Optical Lattice





I. Bloch et al., Nature **415**, 25 (2002)

Spinor Interaction



Bose-Hubbard Model for Spin-1

Second quantized Hamiltonian for spin-1 Bose gas

$$\hat{H} = \sum_{\alpha} \int d^3x \hat{\Psi}^{\dagger}_{\alpha}(\mathbf{x}) \left[-\frac{\hbar^2}{2M} \nabla^2 + V_0 \sum_{\nu=1}^{3} \sin^2\left(\frac{\pi}{a} x_\nu\right) - \mu \right] \hat{\Psi}_{\alpha}(\mathbf{x})$$
$$- \eta \sum_{\alpha,\beta} \int d^3x \hat{\Psi}^{\dagger}_{\alpha}(\mathbf{x}) F^z_{\alpha\beta} \hat{\Psi}_{\beta}(\mathbf{x})$$
$$+ \frac{c_0}{2} \sum_{\alpha,\beta} \int d^3x \hat{\Psi}^{\dagger}_{\alpha}(\mathbf{x}) \Psi^{\dagger}_{\beta}(\mathbf{x}) \hat{\Psi}_{\beta}(\mathbf{x}) \hat{\Psi}_{\alpha}(\mathbf{x})$$
$$+ \frac{c_2}{2} \sum_{\alpha,\beta,\gamma,\delta} \int d^3x \hat{\Psi}^{\dagger}_{\alpha}(\mathbf{x}) \Psi^{\dagger}_{\gamma}(\mathbf{x}) \mathbf{F}_{\alpha\beta} \cdot \mathbf{F}_{\gamma\delta} \hat{\Psi}_{\delta}(\mathbf{x}) \hat{\Psi}_{\beta}(\mathbf{x})$$

- η is magneto-chemical potential to keep magnetization fixed
- $\hat{\Psi}_{\alpha}(\mathbf{x})$ and $\hat{\Psi}^{\dagger}_{\alpha}(\mathbf{x})$ are field operators for an atom in hyperfine state $|F = 1, m_F = \alpha\rangle$ $(\alpha = 1,\ 0,\ -1)$

Scattering Properties

- Spin-independent interaction

$$c_0 = \frac{4\pi\hbar^2(a_0 + 2a_2)}{3M}$$

- Spin-dependent interaction

$$c_2 = \frac{4\pi\hbar^2(a_2 - a_0)}{3M}$$

-

	Anti-ferromagnetic example ^{23}Na	Ferromagnetic example ^{87}Rb
	$c_2 > 0$ i.e. $a_2 > a_0$	$c_2 < 0$ i.e. $a_2 < a_0$
a_0	$(46 \pm 5)a_B$	$(110 \pm 4)a_B$
a_2	$(52 \pm 5)a_B$	$(107 \pm 4)a_B$

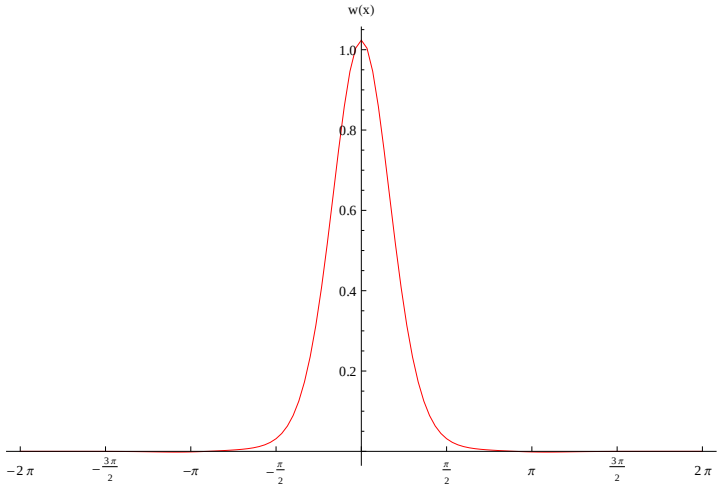
- a_B is Bohr radius

Wannier Decomposition

- Expanding field operator with respect to Wannier functions

$$\hat{\Psi}_\alpha(\mathbf{x}) = \sum_i \hat{a}_{i\alpha} w(\mathbf{x}-\mathbf{x}_i)$$

$$\hat{\Psi}^\dagger_\alpha(\mathbf{x}) = \sum_i \hat{a}^\dagger_{i\alpha} w^*(\mathbf{x}-\mathbf{x}_i)$$



- Hopping matrix element

$$J = J_{ij} = -\int d^3\mathbf{x} w_0^*(\mathbf{x}-\mathbf{x}_i)\left[-\frac{\hbar^2}{2M}\nabla^2 + V(\mathbf{x}) - \mu\right] w(\mathbf{x}-\mathbf{x}_j)$$

- On-site interaction ($F = 0, 2$)

$$U_F = c_F \int d^3\mathbf{x} \left|w(\mathbf{x}-\mathbf{x}_i)\right|^4$$

Bose-Hubbard Model for Spin-1 Boson

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

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

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

- $\hat{\mathbf{S}}_i = \sum_{\alpha,\beta} \hat{a}_{i\alpha}^{\dagger} \mathbf{F}_{\alpha\beta} \hat{a}_{i\beta}$: spin operator on site i

  with $\left[F_\alpha, F_\beta\right] = i \sum_\gamma \epsilon_{\alpha\beta\gamma} F_\gamma$ and $\left[\hat{S}_{i\nu}, \hat{S}_{i\rho}\right] = i \sum_k \epsilon_{\nu\rho k} \hat{S}_{ik}$
- $\hat{n}_i = \sum_\alpha \hat{n}_{i\alpha} = \sum_\alpha \hat{a}_{i\alpha}^{\dagger} \hat{a}_{i\alpha}$: total atom number operator on site i
- Hamiltonian $\hat{H}^{(0)} = \sum_i \hat{h}_i^{(0)}$ is site-diagonal:

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

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

Hamiltonian with inhomogeneous sources

$$\begin{aligned}\hat{H}(\tau)\,[j,j^*] &= \hat{H}_{\mathrm{BH}} + \sum_i \sum_\alpha \left[j^*_{i\alpha}(\tau)\hat{a}_{i\alpha} + j_{i\alpha}(\tau)\hat{a}^\dagger_{i\alpha} \right] \\ &= \hat{H}^{(0)} + \hat{H}^{(1)}\end{aligned}$$

where

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

Perturbative expansion needs

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

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

- where $M_{\alpha,S,m,n}$, $N_{\alpha,S,m,n}$, $O_{\alpha,S,m,n}$ and $P_{\alpha,S,m,n}$ are matrix elements

Matrix elements of creation

S	m	$M_{1,S,m,n}$	$M_{0,S,m,n}$	$M_{-1,S,m,n}$
0	0	$\sqrt{\frac{n+3}{3}}$	$\sqrt{\frac{n+3}{3}}$	$\sqrt{\frac{n+3}{3}}$
1	1	$\sqrt{\frac{2(n+4)}{5}}$	$\sqrt{\frac{n+4}{5}}$	$\sqrt{\frac{n+4}{15}}$
1	0	$\sqrt{\frac{n+4}{5}}$	$2\sqrt{\frac{n+4}{15}}$	$\sqrt{\frac{n+4}{5}}$
1	-1	$\sqrt{\frac{n+4}{15}}$	$\sqrt{\frac{n+4}{5}}$	$\sqrt{\frac{2(n+4)}{5}}$
2	2	$\sqrt{\frac{3(n+5)}{7}}$	$\sqrt{\frac{n+5}{7}}$	$\sqrt{\frac{3(n+5)}{105}}$
2	1	$\sqrt{\frac{2(n+5)}{7}}$	$2\sqrt{\frac{6(n+5)}{105}}$	$3\sqrt{\frac{n+5}{105}}$
2	0	$3\sqrt{\frac{2(n+5)}{105}}$	$3\sqrt{\frac{3(n+5)}{105}}$	$3\sqrt{\frac{2(n+5)}{105}}$
2	-1	$3\sqrt{\frac{n+5}{105}}$	$2\sqrt{\frac{6(n+5)}{105}}$	$\sqrt{\frac{2(n+5)}{7}}$
2	-2	$\sqrt{\frac{3(n+5)}{105}}$	$\sqrt{\frac{n+5}{7}}$	$\sqrt{\frac{3(n+5)}{7}}$

Partition Function

- Partition function in Dirac Interaction Picture ($\hbar = 1$):

$$\mathcal{Z}\left[j, j^*\right] = \mathrm{Tr}\left\{\hat{T} e^{-\int_0^\beta d\tau \hat{H}(\tau)[j,j^*]}\right\} = \mathrm{Tr}\left\{e^{-\beta \hat{H}^{(0)}} \hat{U}_D(\beta, 0)\right\}$$

Full partition function

$$\mathcal{Z} = \mathcal{Z}^{(0)} \left\langle \hat{U}_D(\beta, 0) \right\rangle^{(0)}, \qquad \langle \bullet \rangle^{(0)} = \frac{1}{\mathcal{Z}^{(0)}} \mathrm{Tr}\left[\bullet \exp\left\{-\beta \hat{H}^{(0)}\right\}\right]$$

- Perturbative calculation:

$$\begin{aligned}\mathcal{Z}\left[j, j^*\right] =& \mathcal{Z}^{(0)} \sum_{n=0}^{\infty} (-1)^n \frac{1}{n!} \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \cdots \int_0^\beta d\tau_n \\ & \times \left\langle \hat{T}\left[\hat{H}_D^{(1)}(\tau_1)\left[j, j^*\right] \cdots \hat{H}_D^{(1)}(\tau_n)\left[j, j^*\right]\right]\right\rangle^{(0)}\end{aligned}$$

averages correspond to n-particle Green functions

Cumulant Decomposition

Green function

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

- Decompose Green functions into simple parts
- $\hat{H}^{(0)}$ not harmonic $\Longrightarrow$ Wick's theorem not applicable
- Cumulants are local since $\hat{H}^{(0)}$ site-diagonal. For example:

$$G_2^{(0)}(i_1\alpha_1, \tau_1; i_2\alpha_2, \tau_2 | i_3\alpha_3, \tau_3; i_4\alpha_4, \tau_4) = \delta_{i_1,i_3}\delta_{i_2,i_4}\delta_{i_3,i_4}$$
$$\times {}_{i_1}C_1^{(0)}(\tau_1, \alpha_1; \tau_2, \alpha_2 | \tau_3, \alpha_3; \tau_4, \alpha_4) + \delta_{i_1,i_3}\delta_{i_2,i_4}\ {}_{i_1}C_1^{(0)}(\tau_1, \alpha_1 | \tau_3, \alpha_3)$$
$$\times {}_{i_1}C_1^{(0)}(\tau_2, \alpha_2 | \tau_4, \alpha_4) + \delta_{i_1,i_4}\delta_{i_2,i_3}\ {}_{i_1}C_1^{(0)}(\tau_1, \alpha_1 | \tau_4, \alpha_4)\ {}_{i_1}C_1^{(0)}(\tau_2, \alpha_2 | \tau_3, \alpha_3)$$

W. Metzner, *Phys. Rev. B* **43**, 8549 (1991)

Grand-Canonical Free Energy

Definition

$$\mathcal{F}[j,j^*] = -\frac{1}{\beta}\ln \mathcal{Z}[j,j^*]$$

$$\begin{aligned}
\mathcal{F}[j,j^*] =& \mathcal{F}_0 - \frac{1}{\beta}\sum_{i_1,i_2}\sum_{\alpha_1,\alpha_2}\int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \Bigg\{ j_{i_1\alpha_1}(\tau_1) j^*_{i_2\alpha_2}(\tau_2) \\
&\times \left[a_2^{(0)}(i_1\alpha_1,\tau_1|i_2\alpha_2,\tau_2) + J \sum_{<i_3,j_3>} a_2^{(1)}(i_1\alpha_1,\tau_1;i_3|i_2\alpha_2,\tau_2;j_3)\right] \\
&+ \frac{1}{4}\sum_{i_3,i_4}\sum_{\alpha_3,\alpha_4}\int_0^\beta d\tau_3 \int_0^\beta d\tau_4 j_{i_1\alpha_1}(\tau_1) j_{i_2\alpha_2}(\tau_2) j^*_{i_3\alpha_3}(\tau_3) j^*_{i_4\alpha_4}(\tau_4) \\
&\times \Bigg[a_4^{(0)}(i_1\alpha_1,\tau_1;i_2\alpha_2,\tau_2|i_3\alpha_3,\tau_3;i_4\alpha_4,\tau_4) \\
&+ J \sum_{<i_5,j_5>} a_4^{(1)}(i_1\alpha_1,\tau_1;i_2\alpha_2,\tau_2;i_5|i_3\alpha_3,\tau_3;i_4\alpha_4;j_5)\Bigg]\Bigg\} + \cdots
\end{aligned}$$

Ginzburg-Landau Theory

- Coupling Hamiltonian to currents introduces order parameter in Matsubara transformation

$$\psi_{i\alpha}(\omega_m) = \langle \hat{a}_{i\alpha}(\omega_m) \rangle = \beta \frac{\delta \mathcal{F}}{\delta j^*_{i\alpha}(\omega_m)}, \qquad \omega_m = \frac{2\pi m}{\beta}$$

- Motivates Legendre transformation

Effective action

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

- Conjugate fields: $j_{i\alpha}(\omega_m) = -\beta \frac{\delta \Gamma}{\delta \Psi^*_{i\alpha}(\omega_m)}, \qquad j^*_{i\alpha}(\omega_m) = -\beta \frac{\delta \Gamma}{\delta \Psi_{i\alpha}(\omega_m)}$

Equations of motion for vanishing currents

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

Ginzburg-Landau Expansion

$$\Gamma\left[\Psi_{i\alpha}(\omega_m), \Psi^*_{i\alpha}(\omega_m)\right] = \mathcal{F}_0 + \frac{1}{\beta}\sum_i \sum_{\alpha_1} \sum_{\omega_{m1}} \Bigg\{ \frac{|\Psi_{i\alpha_1}(\omega_{m1})|^2}{a_2^{(0)}(i\alpha_1, \omega_{m1})}$$

$$-J\sum_j \Psi_{i\alpha_1}(\omega_{m1})\Psi^*_{j\alpha_1}(\omega_{m1}) - \sum_{\alpha_2,\alpha_3,\alpha_4} \sum_{\omega_{m2},\omega_{m3},\omega_{m4}}$$

$$\frac{a_4^{(0)}(i\alpha_1, \omega_{m1}; i\alpha_2, \omega_{m2}|i\alpha_3, \omega_{m3}; i\alpha_4, \omega_{m4})\Psi_{i\alpha_1}(\omega_{m1})\Psi_{i\alpha_2}(\omega_{m2})\Psi^*_{i\alpha_3}(\omega_{m3})\Psi^*_{i\alpha_4}(\omega_{m4})}{4a_2^{(0)}(i\alpha_1, \omega_{m1})a_2^{(0)}(i\alpha_2, \omega_{m2})a_2^{(0)}(i\alpha_3, \omega_{m3})a_2^{(0)}(i\alpha_4, \omega_{m4})} \Bigg\}$$

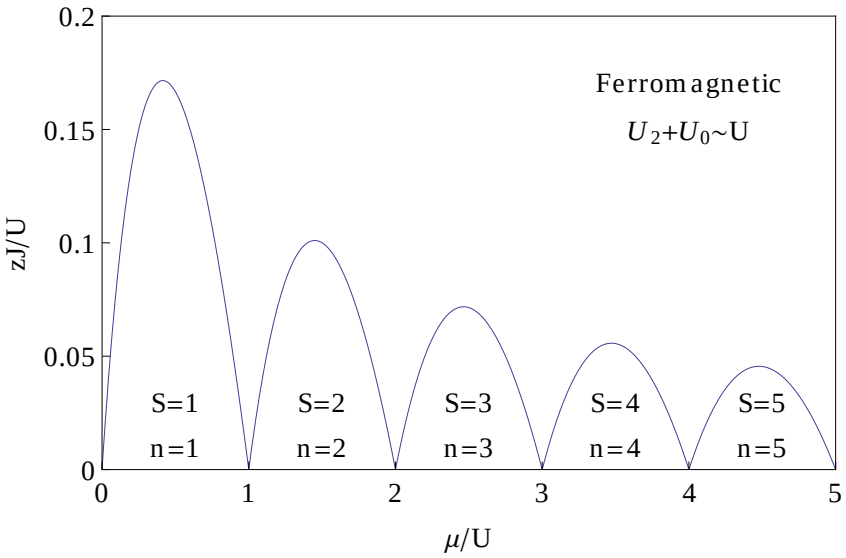
- Phase boundary condition with $\omega_m = 0$:

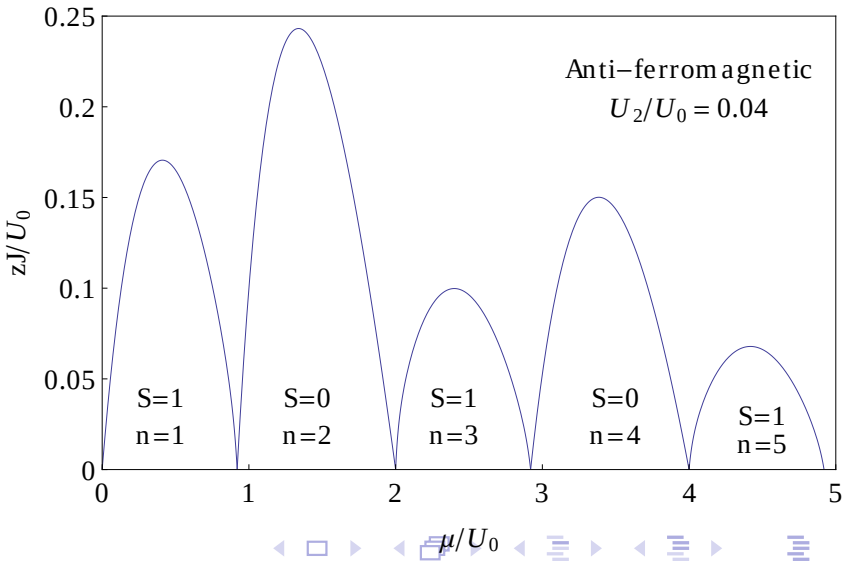
$$0 = \frac{1}{a_2^{(0)}(i\alpha, 0)} - zJ$$

Phase Boundary

$$zJ_{c,\alpha} = \left[\frac{M^2_{\alpha,S,m,n}}{E^{(0)}_{S+1,m+\alpha,n+1} - E^{(0)}_{S,m,n}} + \frac{N^2_{\alpha,S,m,n}}{E^{(0)}_{S-1,m+\alpha,n+1} - E^{(0)}_{S,m,n}} - \frac{O^2_{\alpha,S,m,n}}{E^{(0)}_{S,m,n} - E^{(0)}_{S+1,m-\alpha,n-1}} - \frac{P^2_{\alpha,S,m,n}}{E^{(0)}_{S,m,n} - E^{(0)}_{S-1,m-\alpha,n-1}} \right]^{-1}$$

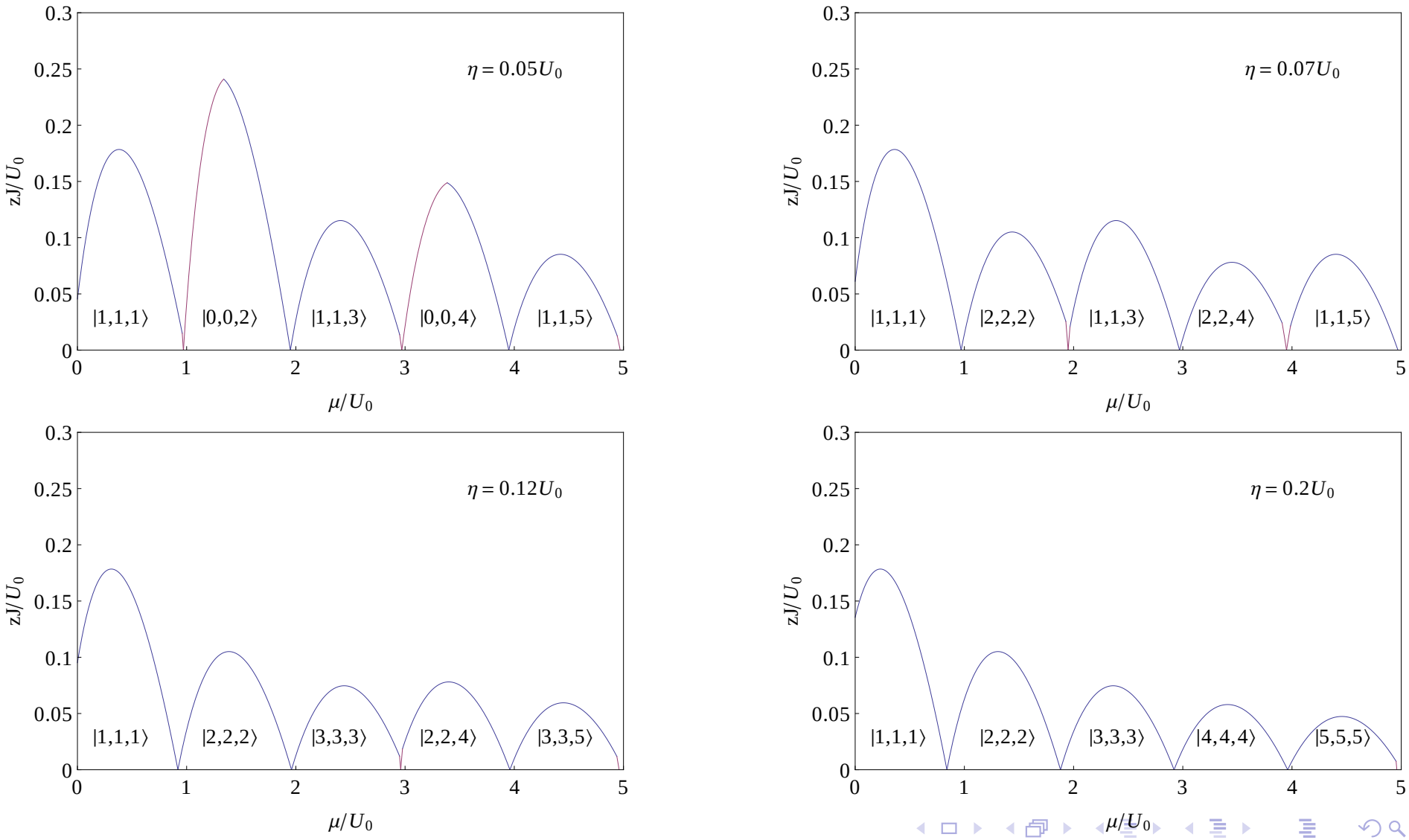
- Minimum of spin index: $J_c = \min_{\alpha} J_{c,\alpha}$
- No magnetization



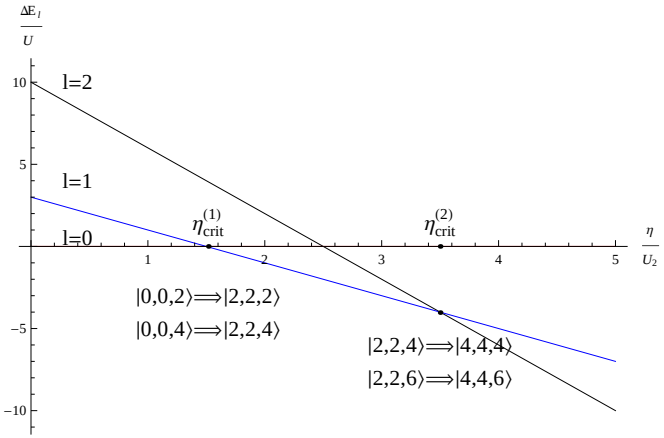
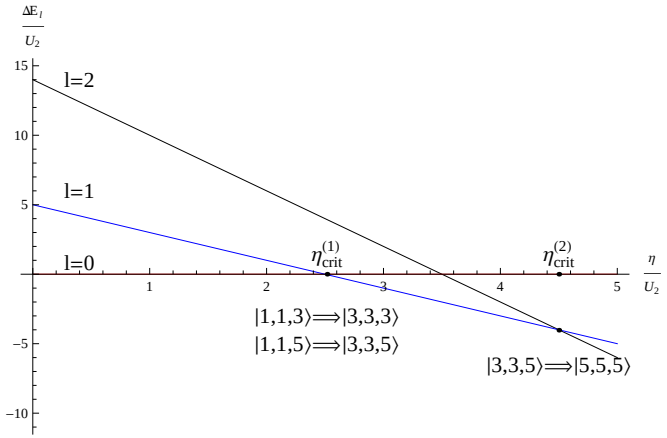


Phase Boundary with Magnetization

- $U_2 = 0.04U_0$ is fixed and η is changed



Important Results from Phase Boundary

Even Mott Lobe	Odd Mott Lobe
Particle number $n = 2k$	$n = 2k + 1$
Ground states $\lvert 2l, 2l, 2k\rangle$	$\lvert 2l+1, 2l+1, 2k1\rangle$
Energy difference $\triangle E(l) = -2l\eta + U_2 l\,(2l+1)$	$-2l\eta + U_2\left(2l^2 + 3l\right)$
$\eta_{crit}(l) = U_2\left(2l + \frac{3}{2}\right)$	$\eta_{crit}(l) = U_2\left(2l + \frac{5}{2}\right)$
	

Landau Theory

- On-site effective potential

$$\Gamma\left[\Psi_\alpha, \Psi_\alpha^*\right] = B_1 \left|\Psi_1\right|^2 + B_0 \left|\Psi_0\right|^2 + B_{-1} \left|\Psi_{-1}\right|^2 + A_{1111} \left|\Psi_1\right|^4$$
$$+A_{-1-1-1-1} \left|\Psi_{-1}\right|^4 + A_{0000} \left|\Psi_0\right|^4 + 4A_{1001} \left|\Psi_1\right|^2 \left|\Psi_0\right|^2 + 4A_{-100-1} \left|\Psi_{-1}\right|^2 \left|\Psi_0\right|^2$$
$$+4A_{1-11-1} \left|\Psi_{-1}\right|^2 \left|\Psi_1\right|^2 + 2A_{001-1}\Psi_0^*\Psi_0^*\Psi_1\Psi_{-1} + 2A_{1-100}\Psi_1^*\Psi_{-1}^*\Psi_0\Psi_0$$

- Landau coefficients

$$B_\alpha = \frac{1}{a_2^{(0)}(\alpha, 0)} - zJ$$

$$A_{\alpha_1\alpha_2\alpha_3\alpha_4} = -\frac{a_4^{(0)}(\alpha_1, 0; \alpha_2, 0|\alpha_3, 0; \alpha_4, 0)}{4a_2^{(0)}(\alpha_1, 0)a_2^{(0)}(\alpha_2, 0)a_2^{(0)}(\alpha_3, 0)a_2^{(0)}(\alpha_4, 0)}$$

Equations of Motion

$$\left(B_1 + 2A_{1111}\left|\Psi_1\right|^2 + 4A_{1001}\left|\Psi_0\right|^2 + 4A_{1-11-1}\left|\Psi_{-1}\right|^2\right)\Psi_1 + 2A_{1-100}\left|\Psi_0\right|^2\Psi_{-1}^* = 0$$

$$\left(B_{-1} + 2A_{-1-1-1-1}\left|\Psi_{-1}\right|^2 + 4A_{-100-1}\left|\Psi_0\right|^2 + 4A_{1-11-1}\left|\Psi_1\right|^2\right)\Psi_{-1} + 2A_{1-100}\left|\Psi_0\right|^2\Psi_1^* = 0$$

$$\left(B_0 + 2A_{0000}\left|\Psi_0\right|^2 + 4A_{1001}\left|\Psi_1\right|^2 + 4A_{-100-1}\left|\Psi_{-1}\right|^2\right)\Psi_0 + 2A_{001-1}\Psi_1\Psi_{-1}\Psi_0^* = 0$$

Superfluid Phases

- $\eta = 0.1U_0$ is fixed and U_2 is changed

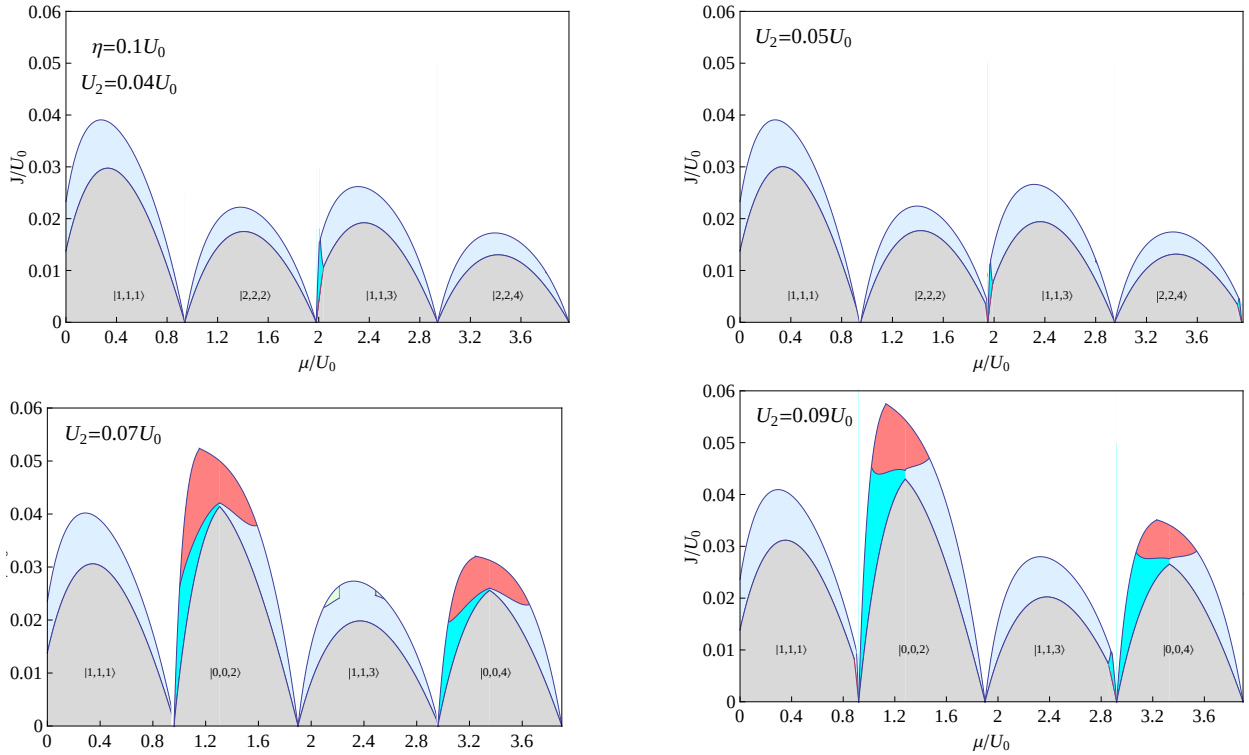


Figure : Superfluid phases which are calculated analytically with increasing anti-ferromagnetic interaction potential. $\Psi_1 \neq 0,\ \Psi_0 = \Psi_{-1} = 0$; $\Psi_{-1} \neq 0,\ \Psi_0 = \Psi_1 = 0$; $\Psi_1 \neq 0,\ \Psi_{-1} \neq 0,\ \Psi_0 = 0$; and $\Psi_1 \neq 0,\ \Psi_{-1} \neq 0,\ \Psi_0 \neq 0$

Superfluid Phases

- $\eta = 0.2U_0$ is fixed and U_2 is changed

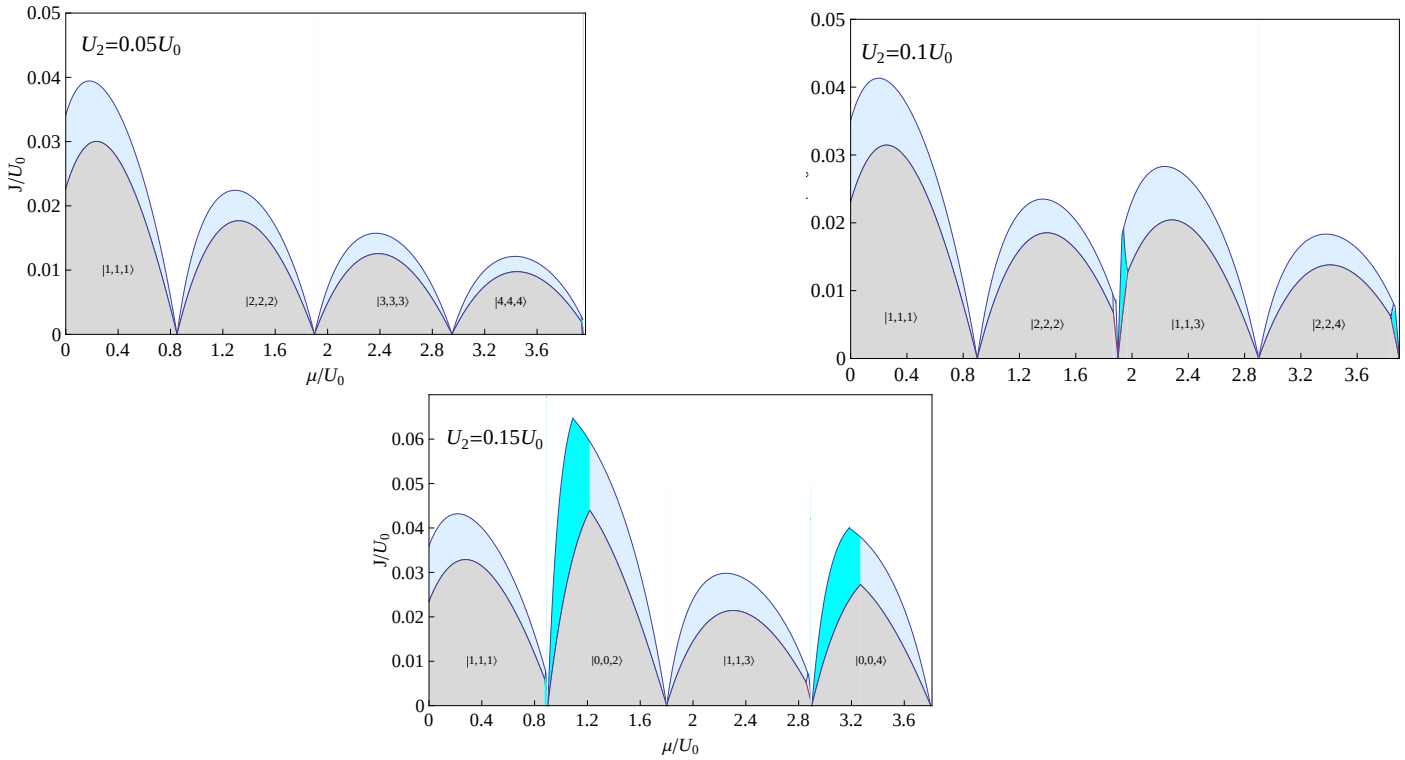


Figure : Superfluid phases which are calculated analytically with different spin dependent potential.$\Psi_1 \neq 0,\ \Psi_0 = \Psi_{-1} = 0$; and $\Psi_{-1} \neq 0,\ \Psi_0 = \Psi_1 = 0$

Summary

- At strong magnetic field phase boundary for an anti-ferromagnetic interaction becomes phase boundary for ferromagnetic interaction
- Various ferromagnetic and antiferromagnetic superfluid phases for an anti-ferromagnetic interaction and a non-vanishing magneto-chemical potential

Outlook

1-Different superfluid phases at non-zero temperature
2-Superfluid phases of spin-1 bosons in a triangular optical lattice
3-Study the frustration in a triangular optical lattice

Superfluid Phases

- $U_2 = 0.04U_0$ is fixed and η is changed

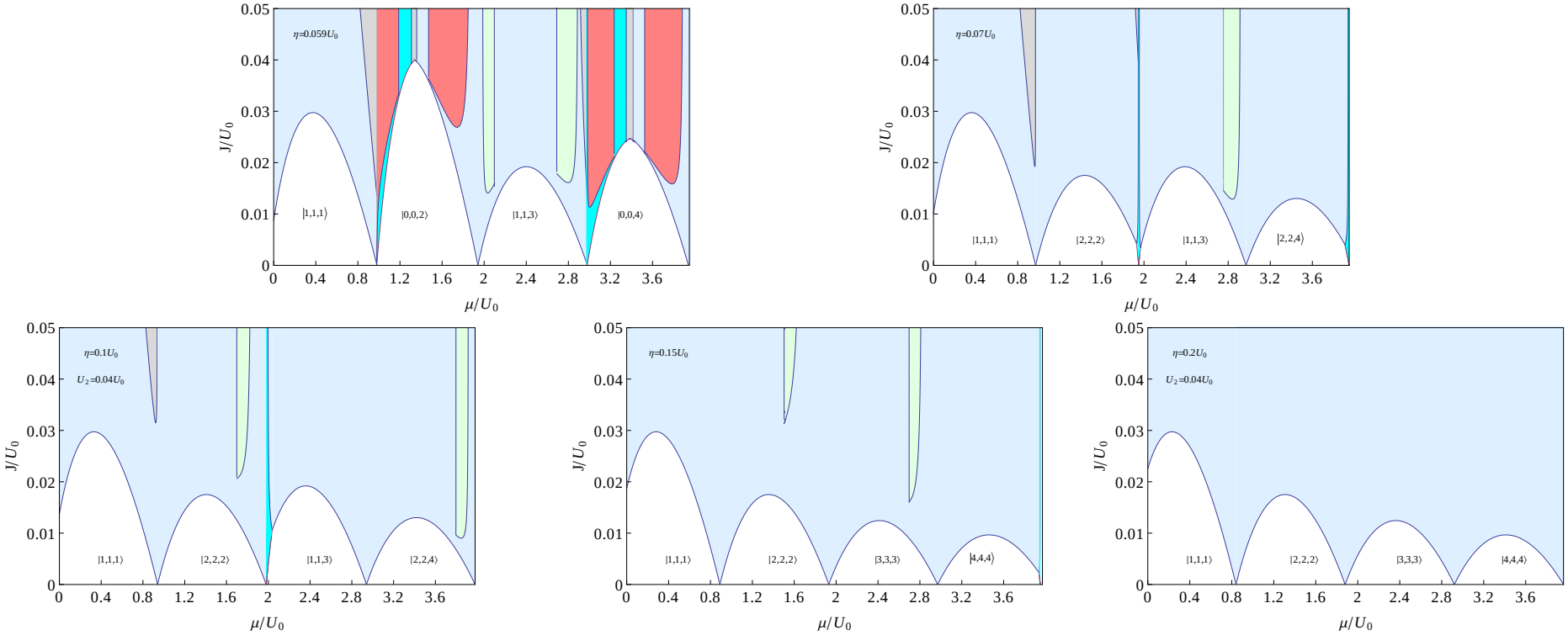


Figure : Superfluid phases which are calculated analytically with different mageno-chemical potential. $\Psi_1 \neq 0,\ \Psi_0 = \Psi_{-1} = 0$; $\Psi_{-1} \neq 0,\ \Psi_0 = \Psi_1 = 0$; $\Psi_1 \neq 0,\ \Psi_{-1} \neq 0,\ \Psi_0 = 0$; $\Psi_1 \neq 0,\ \Psi_{-1} \neq 0,\ \Psi_0 \neq 0$; and $\Psi_0 \neq 0,\ \Psi_1 = \Psi_{-1} = 0$

Superfluid Phases

- $\eta = 0.1U_0$ is fixed and U_2 is changed

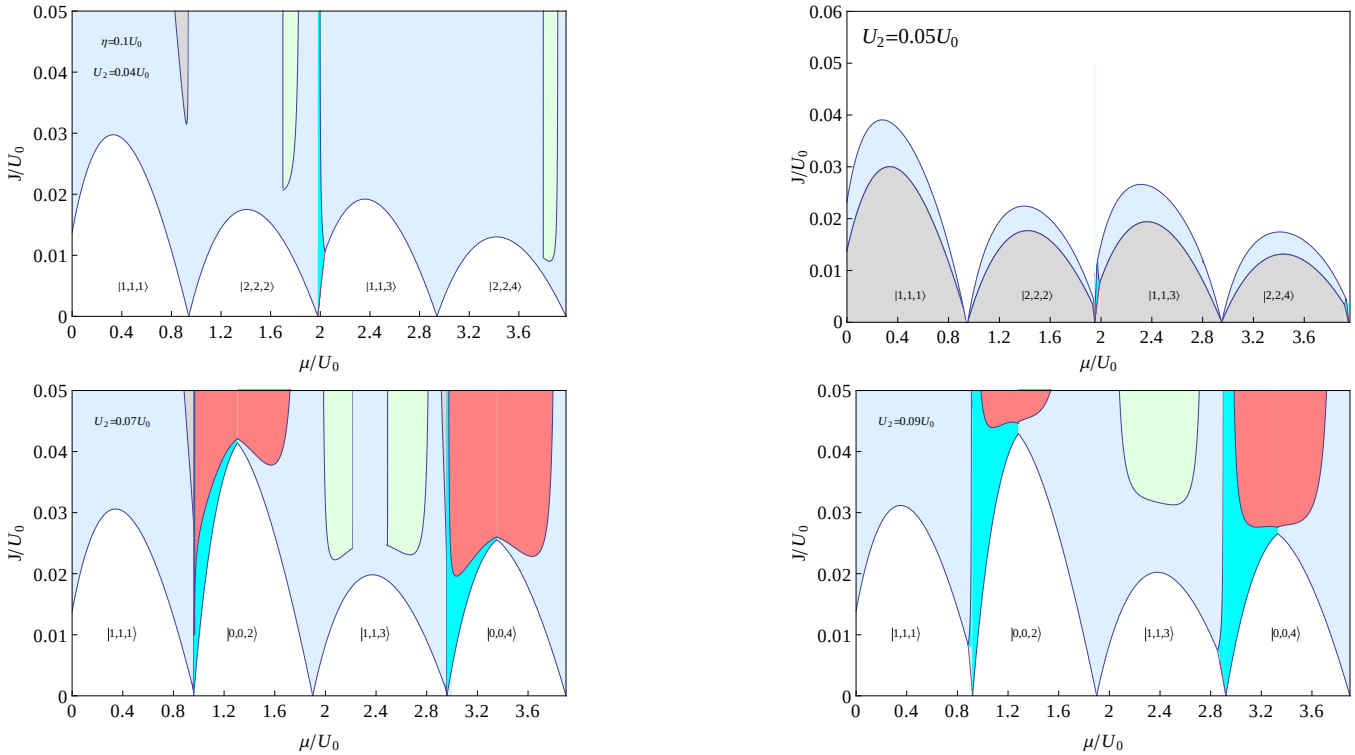


Figure : Superfluid phases which are calculated analytically with increasing anti-ferromagnetic interaction potential. $\Psi_1 \neq 0,\ \Psi_0 = \Psi_{-1} = 0$; $\Psi_{-1} \neq 0,\ \Psi_0 = \Psi_1 = 0$; $\Psi_1 \neq 0,\ \Psi_{-1} \neq 0,\ \Psi_0 = 0$; $\Psi_1 \neq 0,\ \Psi_{-1} \neq 0,\ \Psi_0 \neq 0$; and $\Psi_0 \neq 0,\ \Psi_1 = \Psi_{-1} = 0$

Diagrammatic rules

1. A vertex with n entering and n leaving with lines corresponds to a n-th order cumulant $C_n^{(0)}$
2. Each vertex is labelled with a site and each line with both an imaginary-time and a spin index
3. Each entering line is associated with a factor $j_{i\alpha}(\tau)$ and each leaving line is associated with a factor $j^*_{i\alpha}(\tau)$
4. Each internal line is associated with a factor of J
5. For a connected Green function of a given order draw all inequivalent connected diagrams
6. Integrate over all time variables and sum over all site and spin indices

Definitions

$$a_2^{(0)}(i_1\alpha_1,\tau_1|i_2\alpha_2,\tau_2) = G_1^{(0)}(i_1\alpha_1,\tau_1|i_2\alpha_2,\tau_2),$$

$$a_2^{(1)}(i_1\alpha_1,\tau_1;i_3|i_2\alpha_2,\tau_2;j_3) = \sum_{\alpha_3}\int_0^\beta d\tau_3\, G_2^{(0)}(i_1\alpha_1,\tau_1;i_3\alpha_3,\tau_3|i_2\alpha_2,\tau_2;i_3\alpha_3,\tau_3),$$

$$a_4^{(0)}(i_1\alpha_1,\tau_1;i_2\alpha_2,\tau_2|i_3\alpha_3,\tau_3;i_4\alpha_4,\tau_4) = G_2^{(0)}(i_1\alpha_1,\tau_1;i_2\alpha_2,\tau_2|i_3\alpha_3,\tau_3;i_4\alpha_4,\tau_4)$$
$$-2G_1^{(0)}(i_1\alpha_1,\tau_1|i_3\alpha_3,\tau_3)G_1^{(0)}(i_2\alpha_2,\tau_2|i_4\alpha_4,\tau_4),$$

$$a_4^{(1)}(i_1\alpha_1,\tau_1;i_2\alpha_2,\tau_2;i_5|i_3\alpha_3,\tau_3;i_4\alpha_4;j_5)$$
$$= \sum_{\alpha_5}\int_0^\beta d\tau_5\Big[G_3^{(0)}(i_1\alpha_1,\tau_1;i_2\alpha_2,\tau_2;i_5\alpha_5,\tau_5|i_3\alpha_3,\tau_3;i_4\alpha_4;j_5\alpha_5,\tau_5)$$
$$-2G_2^{(0)}(i_1\alpha_1,\tau_1;i_5\alpha_5,\tau_5|i_3\alpha_3,\tau_3;j_5\alpha_5,\tau_5)G_1^{(0)}(i_2\alpha_2,\tau_2|i_4\alpha_4,\tau_4)\Big]$$

Calculations in Matsubara Space

$$\mathcal{F}[j,j^*] = \mathcal{F}_0 - \frac{1}{\beta}\sum_{<i,j>}\sum_{\alpha_1,\alpha_2}\sum_{\omega_{m1},\omega_{m2}}\Bigg\{ M_{i\alpha_1,,j\alpha_2}(\omega_{m1}|\omega_{m2}) j_{i\alpha_1}(\omega_{m1}) j^*_{j\alpha_2}(\omega_{m2})$$

$$+\sum_{k,l}\sum_{\alpha_3,\alpha_4}\sum_{\omega_{m3},\omega_{m4}} N_{i\alpha_1,,j\alpha_2,k\alpha_3,l\alpha_4}(\omega_{m1};\omega_{m2}|\omega_{m3};\omega_{m4})$$

$$\times j_{i\alpha_1,}(\omega_{m1}) j_{j\alpha_2}(\omega_{m2}) j^*_{k\alpha_3}(\omega_{m3}) j^*_{l\alpha_4}(\omega_{m4})\Bigg\}, \qquad \omega_m = \frac{2\pi m}{\beta}$$

$$M_{i\alpha_1,,j\alpha_2}(\omega_{m1}|\omega_{m2}) = \Big[a_2^{(0)}(i\alpha_1,\omega_{m1})\delta_{i,j} + J a_2^{(0)}(i\alpha_1,\omega_{m1})$$

$$\times\ a_2^{(0)}(j\alpha_2,\omega_{m1})\Big]\,\delta_{\omega_{m1},\omega_{m2}}\delta_{\alpha_1,\alpha_2}$$

$$N_{i\alpha_1,,j\alpha_2,k\alpha_3,l\alpha_4}(\omega_{m1};\omega_{m2}|\omega_{m3};\omega_{m4})$$

$$= \frac{1}{4} a_4^{(0)}(i\alpha_1,\omega_{m1};i\alpha_2,\omega_{m2}|i\alpha_3,\omega_{m3};i\alpha_4,\omega_{m4})$$

$$[\delta_{i,j}\delta_{k,l}\delta_{i,k} + J a_2^{(0)}(j\alpha_2,\omega_{m2})\delta_{i,k}\delta_{k,l} + J a_2^{(0)}(k\alpha_3,\omega_{m3})\,\delta_{i,j}\delta_{j,l}]$$