Itinerant ferromagnetism in ultracold atomic gases
A path integral approach

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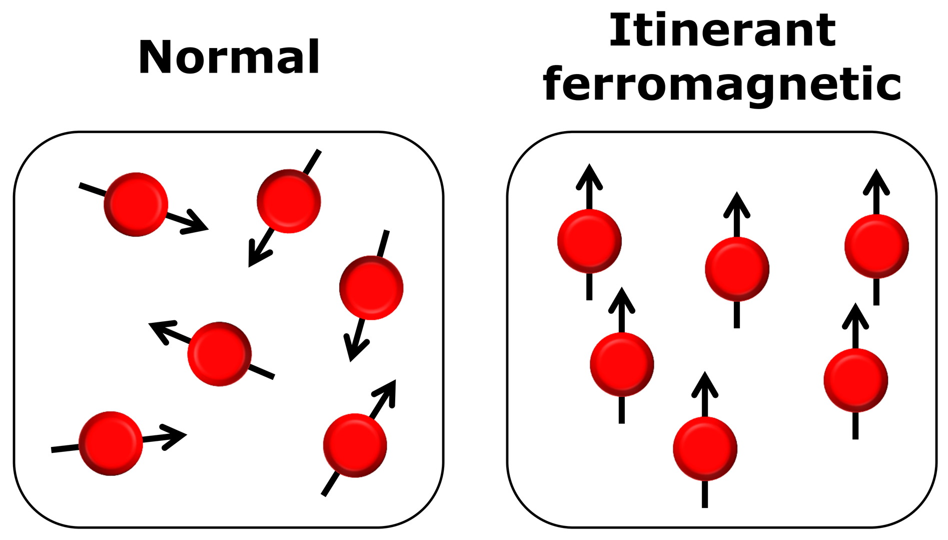
Introduction

Itinerant ferromagnetism in ultracold (fermionic) atomic gases

What is itinerant ferromagnetism?
- Ferromagnetism = spontaneous polarization
- Itinerant = "wandering" or non-localized
- Fermionic particles → Pauli principle

Where do we expect to observe it?
- Enegy cost: kinetic energy
- Energy gain: exchange energy
- → Expected for strong repulsive interactions



Brief history of itinerant ferromagnetism:
- 1933: Predicted by Stoner for elektrons [1].
- 2009: First experimental hints observed in ultracold atomic gases [2], but no magnetic domains were observed. The interpretation of the experiment remains unclear.
- → Was itinerant ferromagnetism observed?
- Today: An improved theoretical description is needed to understand the experiment.

Method

Path integral formalism and the Hubbard – Stratonovich transformation

Goal: Calculate the free energy per unit of volume $\Omega = -\frac{1}{\beta V}\ln Z$ by calculating the sum of states $Z = \prod_{\sigma=\uparrow,\downarrow}\left(\int \mathcal{D}\bar{\psi}_\sigma \int \mathcal{D}\psi_\sigma\right)\exp\left\{-S\left[\bar{\psi}_{\mathbf{x}\tau\sigma},\psi_{\mathbf{x}\tau\sigma}\right]\right\}$.

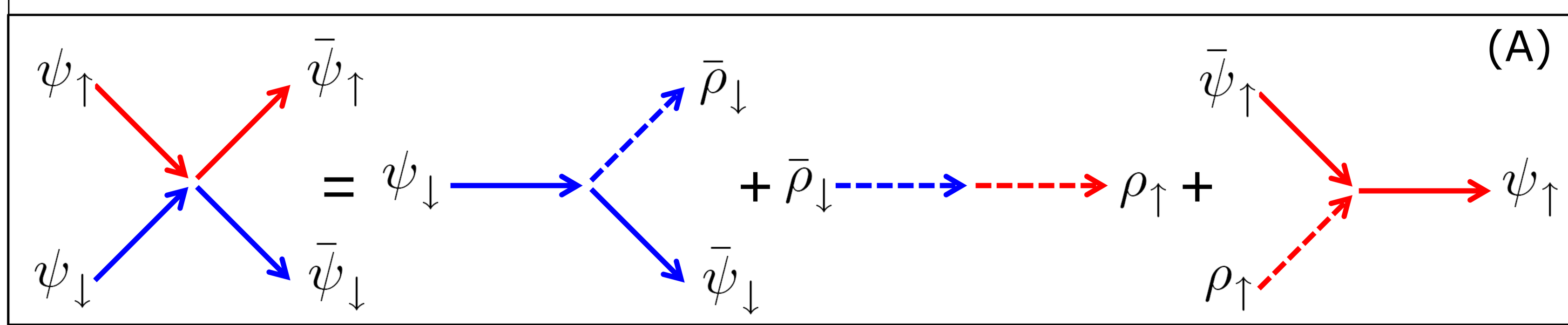
We use the standard expression for the action S for a gas of fermionic partices of spin ½ with contact interactions (without external potential).

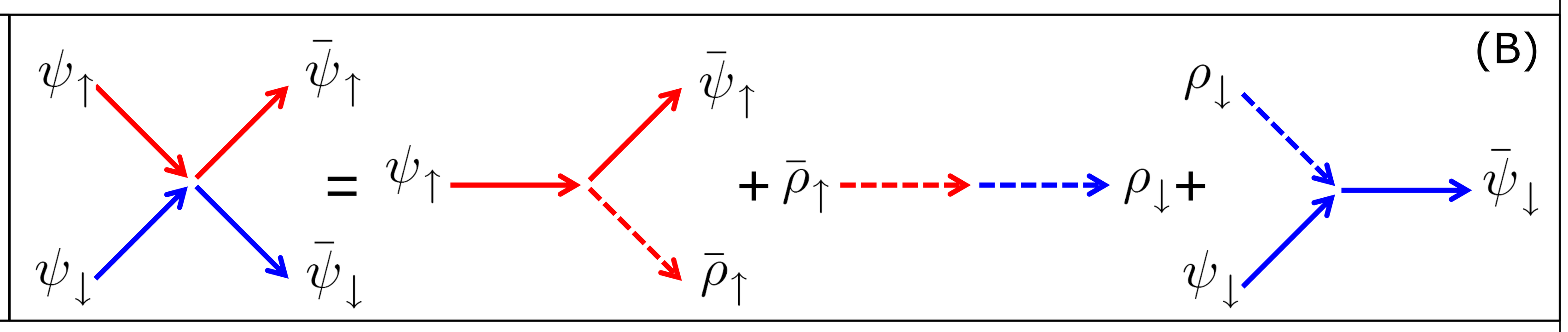
$$S\left[\bar{\psi}_{\mathbf{x}\tau\sigma},\psi_{\mathbf{x}\tau\sigma}\right] = \sum_{\sigma=\uparrow,\downarrow}\int_0^\beta d\tau \int d\mathbf{x}\bar{\psi}_{\mathbf{x}\tau\sigma}\left[\frac{\partial}{\partial\tau} - \nabla_{\mathbf{x}}^2 - \mu_\sigma\right]\psi_{\mathbf{x}\tau\sigma} + g\int_0^\beta d\tau\int d\mathbf{x}\bar{\psi}_{\mathbf{x}\tau\uparrow}\bar{\psi}_{\mathbf{x}\tau\downarrow}\psi_{\mathbf{x}\tau\downarrow}\psi_{\mathbf{x}\tau\uparrow}$$

Problem: This path integral can not be solved exactly, due to the presence of the interaction term (of 4th degree in the fermionic fields).
Solution: We transform the interaction term into terms of 2nd degree in the fermionic fields, at the cost of introducing an extra bosonic field (in this case two density fields and their conjugated counterparts). This transformation is called the Hubbard – Stratonovich transformation.

$$\exp\left\{-\frac{g}{2}\int_0^\beta d\tau\int d\mathbf{x}\bar{\psi}_{\mathbf{x}\tau\uparrow}\bar{\psi}_{\mathbf{x}\tau\downarrow}\psi_{\mathbf{x}\tau\downarrow}\psi_{\mathbf{x}\tau\uparrow}\right\} = \int\mathcal{D}\bar{\rho}_\downarrow\int\mathcal{D}\rho_\uparrow\exp\left\{\int_0^\beta d\tau\int d\mathbf{x}\left[-\bar{\rho}_{\mathbf{x}\tau\downarrow}\bar{\psi}_{\mathbf{x}\tau\downarrow}\psi_{\mathbf{x}\tau\downarrow} + \frac{\bar{\rho}_{\mathbf{x}\tau\downarrow}\rho_{\mathbf{x}\tau\uparrow}}{g} - \bar{\psi}_{\mathbf{x}\tau\uparrow}\psi_{\mathbf{x}\tau\uparrow}\rho_{\mathbf{x}\tau\uparrow}\right]\right\} \quad \text{(A)}$$

$$\exp\left\{-\frac{g}{2}\int_0^\beta d\tau\int d\mathbf{x}\bar{\psi}_{\mathbf{x}\tau\uparrow}\bar{\psi}_{\mathbf{x}\tau\downarrow}\psi_{\mathbf{x}\tau\downarrow}\psi_{\mathbf{x}\tau\uparrow}\right\} = \int\mathcal{D}\bar{\rho}_\uparrow\int\mathcal{D}\rho_\downarrow\exp\left\{\int_0^\beta d\tau\int d\mathbf{x}\left[-\bar{\rho}_{\mathbf{x}\tau\uparrow}\bar{\psi}_{\mathbf{x}\tau\uparrow}\psi_{\mathbf{x}\tau\uparrow} + \frac{\bar{\rho}_{\mathbf{x}\tau\uparrow}\rho_{\mathbf{x}\tau\downarrow}}{g} - \bar{\psi}_{\mathbf{x}\tau\downarrow}\psi_{\mathbf{x}\tau\downarrow}\rho_{\mathbf{x}\tau\downarrow}\right]\right\} \quad \text{(B)}$$





Next steps:
- Notation change $\begin{cases}\rho = \rho_\uparrow + \rho_\downarrow \\ \phi = \rho_\uparrow - \rho_\downarrow\end{cases}$ and $\begin{cases}\mu = \mu_\uparrow + \mu_\downarrow \\ \zeta = \zeta_\uparrow - \zeta_\downarrow\end{cases}$
- Fourier transform (removing the derivatives)
- Exact calculation of the fermionic path integral →

$$Z = \int\mathcal{D}\bar{\rho}\int\mathcal{D}\rho\int\mathcal{D}\bar{\phi}\int\mathcal{D}\phi\exp\left\{\sum_{\mathbf{k},n}\left(\frac{\bar{\rho}_{\mathbf{k}n}\rho_{\mathbf{k}n} - \bar{\phi}_{\mathbf{k}n}\phi_{\mathbf{k}n}}{g}\right) + \mathrm{Tr}\left(\ln\left[-\det_\sigma\left(-\mathbf{G}^{-1}_{\mathbf{k}n;\mathbf{k}'n'}\right)\right]\right)\right\}$$

$$-\mathbf{G}^{-1}_{k,k'} = \begin{pmatrix}-i\omega_n + \mathbf{k}^2 - \frac{\mu+\zeta}{2} & 0 \\ 0 & -i\omega_n - \mathbf{k}^2 + \frac{\mu_{-\zeta}}{2}\end{pmatrix}\delta(k-k')$$
$$+\frac{1}{2\sqrt{\beta V}}\begin{pmatrix}\left(\bar{\rho}_{-k+k'} + \rho_{k-k'}\right) - \left(\bar{\phi}_{-k+k'} + \phi_{k-k'}\right) & 0 \\ 0 & -\left(\bar{\rho}_{k-k'} + \rho_{-k+k'}\right) + \left(\bar{\phi}_{k-k'} + \phi_{-k+k'}\right)\end{pmatrix}$$

$$k = (\mathbf{k},\omega_n) \qquad \omega_n = \frac{(2n+1)\pi}{\beta}\ (n\in\mathbb{Z}) \qquad \Omega_m = \frac{2\pi m}{\beta}\ (m\in\mathbb{Z})$$

Saddle point approximation:
- Assume the bosonic fields have a constant value.
- Take into account only the most dominant contribution to the path integral (by minimizing free energy to this value).
- Only in this step the choice of the auxiliary bosonic fields becomes important.

Results

Free energy in saddle point approximation

Saddle point free energy:

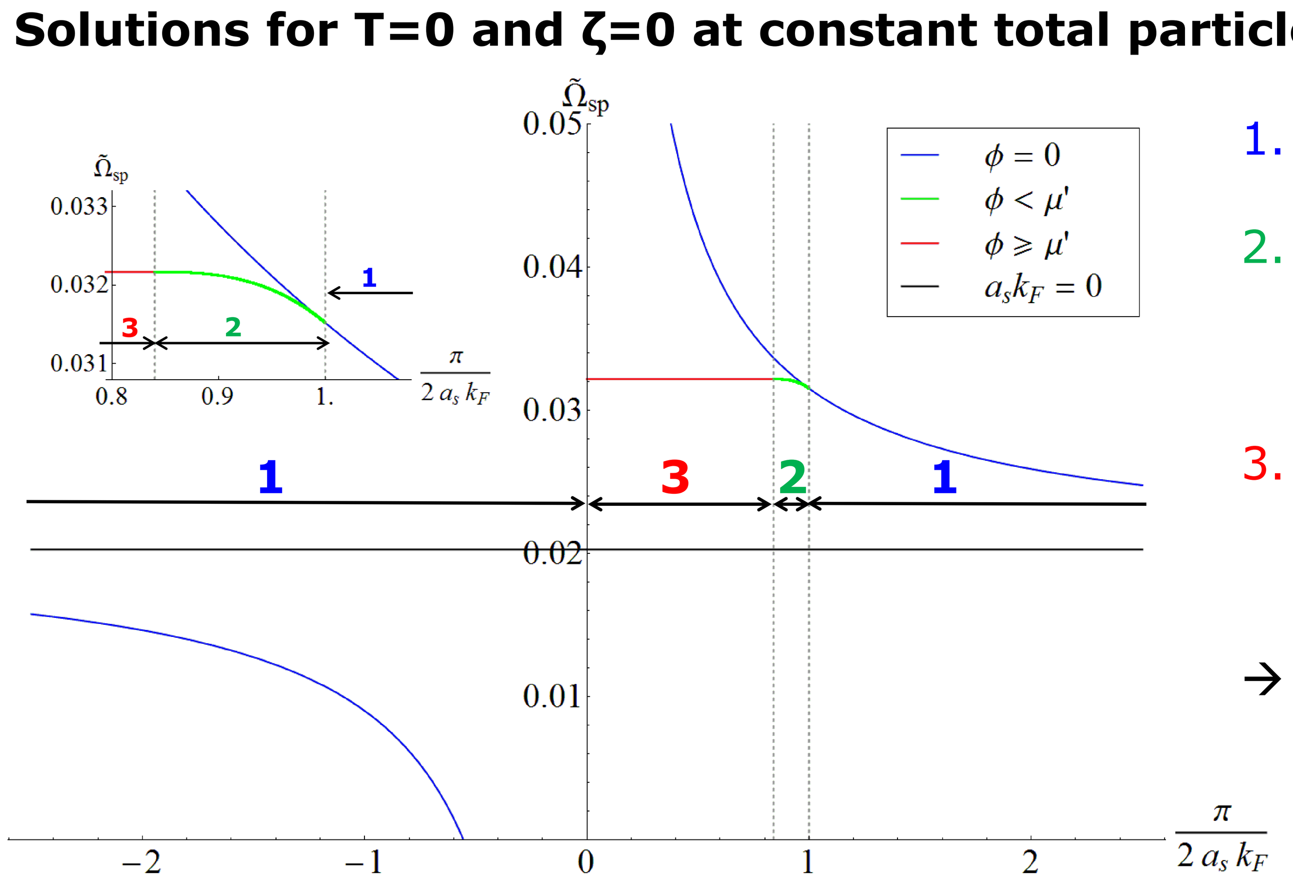
$$\Omega_{sp}(T,\mu,\zeta;\rho,\phi) = \underbrace{\frac{1}{g}\left(\phi_I^2 - \rho_I^2\right)}_{\text{A}} + \underbrace{\frac{1}{g}\left(\phi_R^2 - \rho_R^2\right)}_{\text{B}} \underbrace{-\frac{1}{\beta V}\sum_{\mathbf{k},n}\ln\left[-\left(-i\omega_n + E_{\mathbf{k}} - \zeta'\right)\left(-i\omega_n - E_{\mathbf{k}} - \zeta'\right)\right]}_{\text{C}}$$

$$\begin{cases}\rho_R = \mathrm{Re}[\rho] \\ \rho_I = \mathrm{Im}[\rho]\end{cases} \quad \begin{cases}\phi_R = \mathrm{Re}[\phi] \\ \phi_I = \mathrm{Im}[\phi]\end{cases} \quad \begin{cases}\mu' = \mu - \rho_R \\ \zeta' = \zeta + \phi_R\end{cases} \quad E_{\mathbf{k}} = k^2 - \mu'$$

A. The imaginary part of ρ and ϕ only appears in this term, changing the free energy with a constant, so we can ignore it.
B. Interaction energy
C. Kinetic energy, but with modified chemical potentials.
→ Saddle point equations to determine value of ρ_R and ϕ_R:

$$\left.\frac{\partial\Omega_{sp}(\beta,\mu,\zeta;\rho_R,\phi_R)}{\partial\phi_R}\right|_{\beta,\mu,\zeta;\rho_R} = 0 \qquad \left.\frac{\partial\Omega_{sp}(\beta,\mu,\zeta;\rho_R,\phi_R)}{\partial\rho_R}\right|_{\beta,\mu,\zeta;\phi_R} = 0$$

Solutions for T=0 and ζ=0 at constant total particle number (Φ≥0):



1. $a_S k_F \leq \frac{\pi}{2}$: Normal
2. $\frac{\pi}{2} < a_S k_F < \frac{3\pi}{2^{7/3}}$: Partial polarization
3. $\frac{3\pi}{2^{7/3}} \leq a_S k_F$: 100% polarization

→ Polarization for strong repulsive interactions

Conclusion

We find a qualitatively good description at the mean-field level. Using density fields in the Hubbard – Stratonovich transformation allows for a selection of the dominant correlations of the interactions for itinerant ferromagnetism.

Possible improvements:
1. Take into account fluctuations around the saddle point.
2. Take into account the effects of the competing pairing correlations.

[1] E. Stoner, Phil. Mag. 15, 1018 (1933).
[2] G.-B. Jo et al., Science 325, 1521 (2009).

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