



The Abdus Salam
International Centre for Theoretical Physics



SMR 1666 - 21

**SCHOOL ON QUANTUM PHASE TRANSITIONS
AND
NON-EQUILIBRIUM PHENOMENA IN COLD ATOMIC GASES**

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Bose-Fermi mixtures: Theory

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Bose-Fermi mixtures: Theory

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Outline:

- I. Fermi-Bose mixtures “in clouds”
- II. Fermi-Bose mixtures in optical lattices

I. Fermi-Bose mixtures “in clouds”

$$H = H_b + H_f + H_{bf}$$

where

$$H_b = \hat{\phi}^+ \left\{ -\frac{\hbar^2 \nabla^2}{2m_b} - \mu_b + V_{trap}^b(\vec{r}) + \frac{g_b}{2} \hat{n}_b \right\} \hat{\phi}, \quad \hat{n}_b = \hat{\phi}^+ \hat{\phi}$$

bosonic Hamiltonian,

$$g_b = 4\pi\hbar^2 a_b / m_b > 0$$

$$H_f = \hat{\psi}^+ \left\{ -\frac{\hbar^2 \nabla^2}{2m_f} - \mu_f + V_{trap}^f(\vec{r}) \right\} \hat{\psi}$$

fermionic Hamiltonian,

$$H_{bf} = g_{bf} \hat{n}_b \hat{\psi}^+ \hat{\psi} \quad g_{bf} = \frac{2\pi\hbar^2 a_{bf}}{m_{bf}}, \quad m_{bf} = \frac{m_b m_f}{m_b + m_f}$$

Fermi-Bose interaction

Physical examples:

1. ${}^3\text{He}-{}^4\text{He}$ solution

2. ${}^6\text{Li}-{}^7\text{Li}$

3. ${}^{40}\text{K}-{}^{87}\text{Rb}$

4. ${}^6\text{Li}-{}^{87}\text{Rb}$

Mean-field analysis

Assumption: $|\Psi\rangle = |\Psi_B\rangle \otimes |\Psi_F\rangle$

Decoupling of the Fermi-Bose interaction:

$$H_{bf} = g_{bf} \hat{n}_b \hat{\psi}^+ \hat{\psi} \rightarrow \frac{1}{2} g_{bf} (n_b \hat{\psi}^+ \hat{\psi} + n_f \hat{\phi}^+ \hat{\phi})$$

results in

$$V_{trap}^b \rightarrow V_{eff}^b = V_{trap}^b + g_{bf} n_f$$

and

$$V_{trap}^f \rightarrow V_{eff}^f = V_{trap}^f + g_{bf} n_b$$

effective (mean-field)
potentials

Fermionic part

$$H_f^{eff} = \hat{\psi}^+ \left\{ -\frac{\hbar^2 \nabla^2}{2m_f} - \mu_f + \underbrace{V_{trap}^f(\vec{r}) + g_{bf} n_b(\vec{r})}_{V_{eff}^f(\vec{r})} \right\} \hat{\psi}$$

For a large number of fermions N_F one can use the Thomas-Fermi approximation:

$$n_f(\vec{r}) = \frac{1}{6\pi^2 \hbar^3} \left[2m_f (\mu_f - V_{eff}^f(\vec{r})) \right]^{3/2}$$

For $g_{bf} = 0$ in a spherical harmonic trap

$$\mu_f = \varepsilon_F \equiv \frac{\hbar^2 k_F^2}{2m_f} = \hbar\omega(6N_F)^{1/3}$$

Bosonic part

$$H_b^{eff} = \hat{\phi}^+ \left\{ -\frac{\hbar^2 \nabla^2}{2m_b} - \mu_b + \underbrace{V_{trap}^b(\vec{r}) + g_{bf} n_f(\vec{r})}_{V_{eff}^b(\vec{r})} + \frac{g_b}{2} \hat{\phi}^+ \hat{\phi} \right\} \hat{\phi}$$

Mean-field: $\hat{\phi}(\vec{r}) \rightarrow \varphi_c(\vec{r})$ - classical field, $n_b(\vec{r}) = \varphi_c^2(\vec{r})$

Minimum energy \rightarrow Gross-Pitaevskii equation on $\varphi_c(\vec{r})$

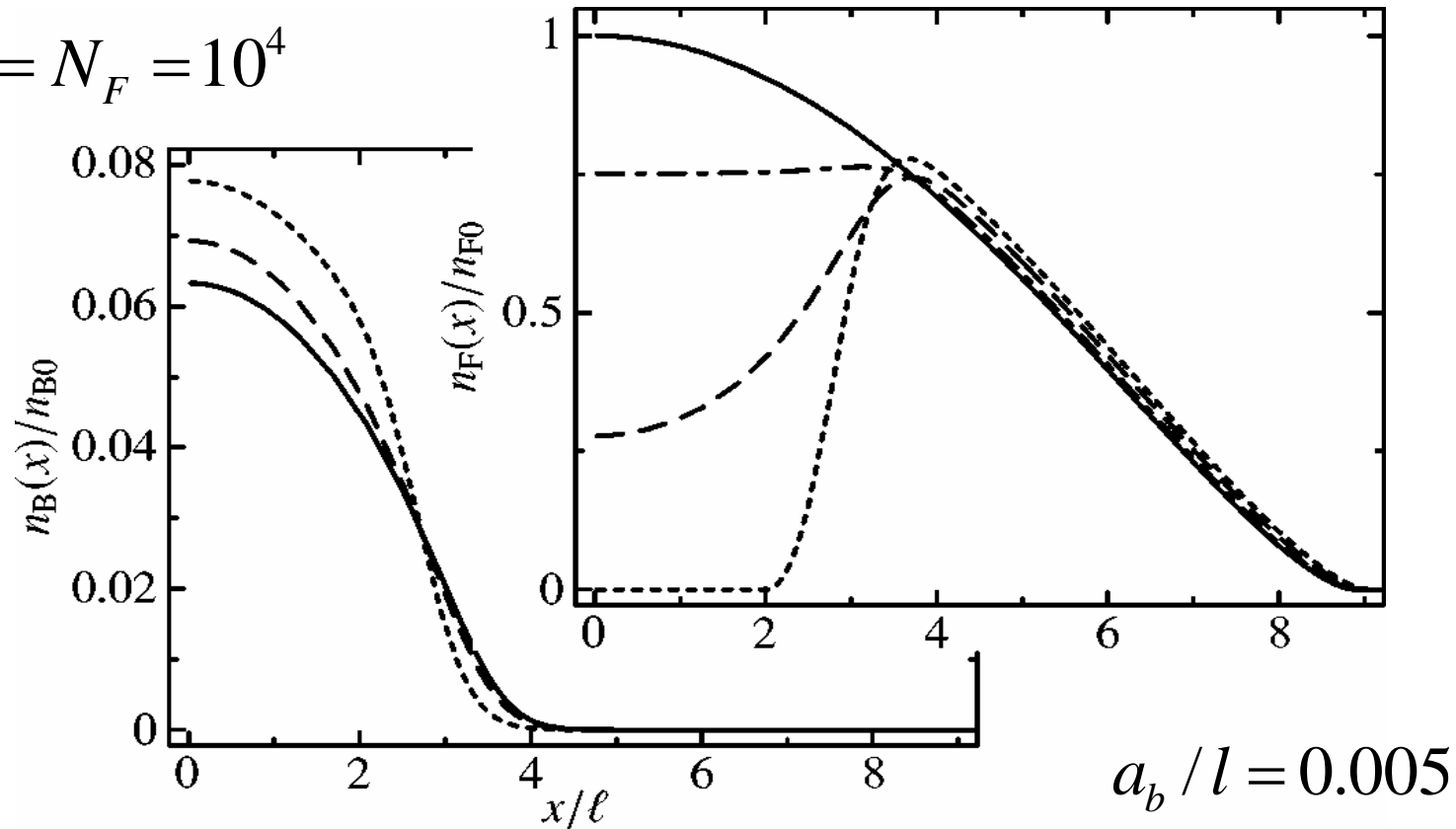
$$\left\{ -\frac{\hbar^2 \nabla^2}{2m_b} - \mu_b + V_{trap}^b(\vec{r}) + g_{bf} n_f(\vec{r}) + g_b \varphi_c^2 \right\} \varphi_c = 0$$

Should be combined with

$$n_f(\vec{r}) = \left[2m_f \left(\mu_f - V_{trap}^f(\vec{r}) - g_{bf} n_b(\vec{r}) \right) \right]^{3/2} / 6\pi^2 \hbar^3$$

Results for $g_{bf} > 0$: Mølmer 1999, Nygaard et al. 1999, Roth 2002*

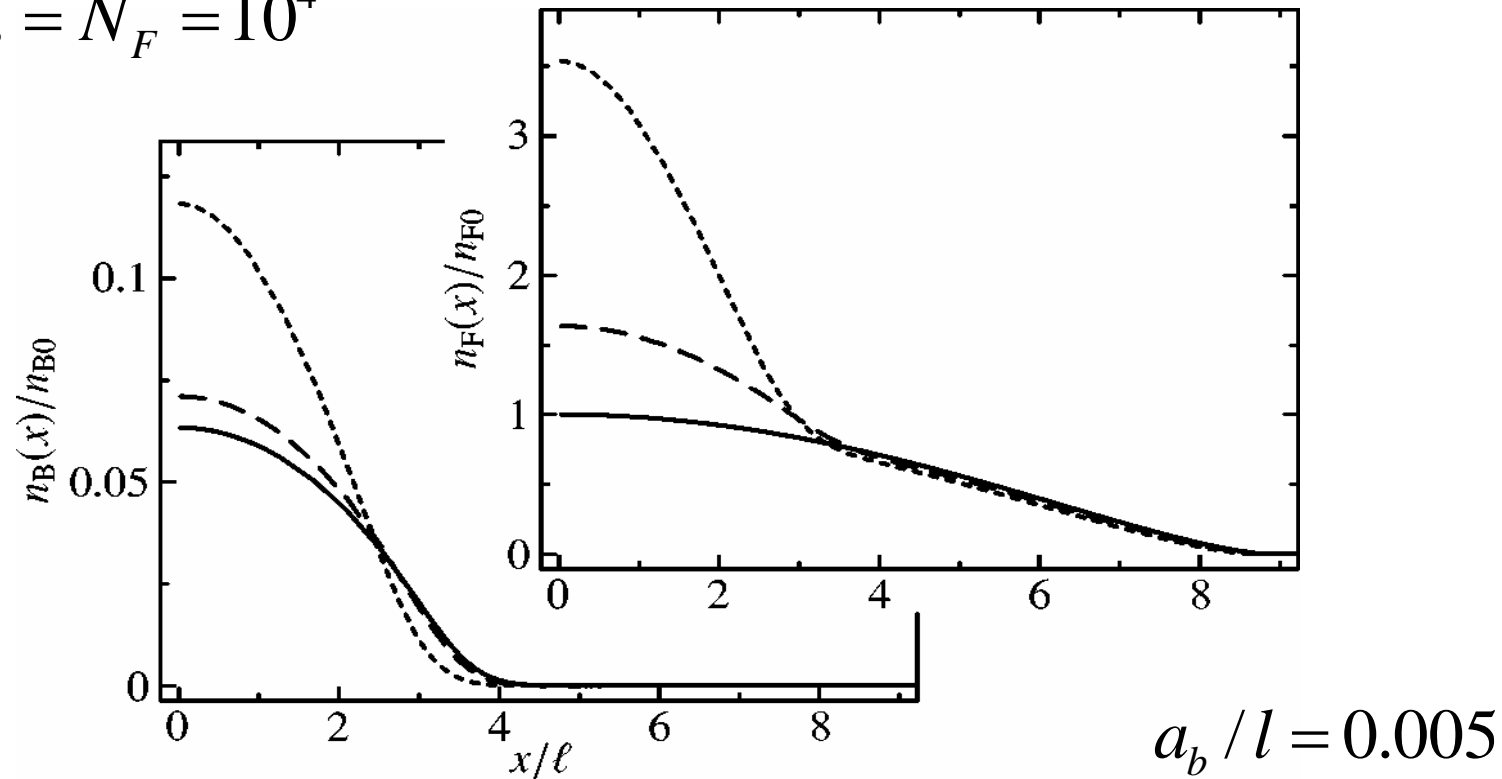
$$N_B = N_F = 10^4$$



- $a_{bf} / l = 0.0$ - solid
 $= 0.005$ - dash-dotted
 $= 0.015$ - dashed
 $= 0.03$ - dotted

Results for $g_{bf} < 0$: Roth 2002*, Roth et al. 2002, Modugno 2003

$$N_B = N_F = 10^4$$



- $a_{bf} / l = 0.0$ - solid
- $= -0.01$ - dashed
- $= -0.02$ - dotted

Stability of Fermi-Bose mixtures

(simple Thomas-Fermi analysis in the homogeneous case)

The energy

$$E(n_b, n_f) / V = \frac{3 \hbar^2}{5 m_f} \frac{n_f^{5/3}}{(6\pi^2)^{2/3}} - \mu_f n_f + \frac{2\pi\hbar^2 a_{bf}}{m_{bf}} n_b n_f \\ + \frac{2\pi\hbar^2 a_b}{m_b} n_b^2 - \mu_b n_b$$

Equilibrium densities: $\frac{\partial E}{\partial n_b} = \frac{\partial E}{\partial n_f} = 0$

Stability: $\delta^2 E = \sum_{\alpha, \beta=b, f} \frac{\partial^2 E}{\partial n_\alpha \partial n_\beta} \delta n_\alpha \delta n_\beta > 0$

Matrix $\frac{\partial^2 E}{\partial n_\alpha \partial n_\beta}$ must have **positive eigenvalues !**

Explicitly:

$$\frac{1}{V} \frac{\partial^2 E}{\partial n_\alpha \partial n_\beta} = \begin{pmatrix} 2\hbar^2 / 3(6\pi^2)^{2/3} m_f n_f^{1/3} & 4\pi\hbar^2 a_{bf} / m_{bf} \\ 4\pi\hbar^2 a_{bf} / m_{bf} & 4\pi\hbar^2 a_b / m_b \end{pmatrix}$$

Eigenvalues are positive if

$$a_b - (6\pi^2)^{5/3} \frac{m_b m_f}{m_{bf}^2} \frac{a_{bf}^2 n_f^{1/3}}{\pi} > 0$$

- stability condition

What happens in the region of instability?

1. For $a_{bf} > 0$

$\delta n_f \sim -\delta n_b$ for negative eigenvalue – phase separation

2. For $a_{bf} < 0$

$\delta n_f \sim \delta n_b$ for negative eigenvalue – mutual collapse

Note: in more rigorous approaches collapse corresponds to failure of the convergence during the iterative procedure

Consequence for the trap:

$$n_f \rightarrow n_f(0) \sim a_{bf}^{-6}$$

With $n_f(0) \sim N_f^{1/2}$ in a trap, it results in

$$N_{f,crit} \sim a_{bf}^{-12} \quad - \text{the critical number of fermions}$$

Experimental results will be given during next talk.
Stay in the audience!

Warning!

At the point of instability, interactions are not weak.
Therefore, higher order contributions (exchange)
have to be added (see Albus et al. 2003)

Beyond mean-field

$$\hat{\phi}(\vec{r}) \rightarrow \varphi_c(\vec{r}) + \hat{\phi}'(\vec{r})$$

excitations

$\varphi_c(\vec{r})$ obeys Gross-Pitaevskii equation.

The quadratic in $\hat{\phi}'$ part of H_b^{eff} can be diagonalized

$$H_b^{eff(2)} = E_0 + \sum_{\nu} \varepsilon_{\nu} \alpha_{\nu}^{+} \alpha_{\nu}$$

by using the Bogoliubov transformation

$$\hat{\phi}'(\vec{r}) = \sum_{\nu} \left\{ u_{\nu}(\vec{r}) \alpha_{\nu} + v_{\nu}(\vec{r}) \alpha_{\nu}^{+} \right\}$$

where $\alpha_{\nu}, \alpha_{\nu}^{+}$ bosonic creation/annihilation operators

and $\int_{\vec{r}} \left(|u_{\nu}|^2 - |v_{\nu}|^2 \right) = 1$

The amplitudes u_ν , v_ν and eigenvalues ϵ_ν (excitation eigenfrequencies) can be found from the

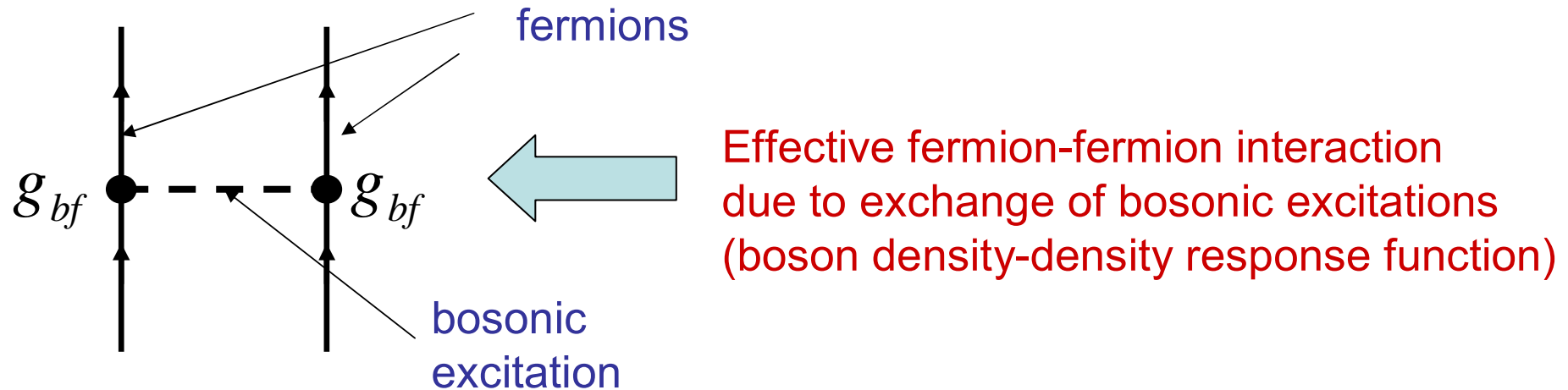
Bogoliubov – de Gennes equations

$$\left[-\frac{\hbar^2}{2m_b} \nabla^2 + V_b^{eff}(\vec{r}) - \mu_b + 2g_b n_{bc} \right] u_\nu + g_b n_{bc} v_\nu = \epsilon_\nu u_\nu$$
$$\left[-\frac{\hbar^2}{2m_b} \nabla^2 + V_b^{eff}(\vec{r}) - \mu_b + 2g_b n_{bc} \right] v_\nu + g_b n_{bc} u_\nu = -\epsilon_\nu v_\nu$$

Can be used, for example, for analysis of temperature effects
(Liu et al. 2003)

Consequences: induced fermion-fermion interaction

Bijlsma et al. 2000, Capuzzi et al. 2001, ...



$$V_{eff}(\omega, \vec{q}) = g_{bf}^2 \frac{n_b q^2}{m_b} \frac{1}{\omega^2 - \epsilon_q^0 (2n_b g_b + \epsilon_q^0)}$$

$$\epsilon_q^0 = \hbar^2 q^2 / 2m_b$$

BCS pairing (p-wave) Efremov et al. 2002

In a single component Fermi gas the s-wave scattering is forbidden. Therefore, the p-wave channel is dominant at low temperatures.

The p-wave harmonic of the effective interaction for two fermions on the Fermi surface is **negative !**

$$V_{eff}^{(l=1)} = -\frac{g_{bf}^2}{g_b} R_1\left(\frac{p_F}{m_b s}\right), \quad R_1(x) = \frac{2}{x^2} \left[\left(\frac{1}{x^2} + \frac{1}{2} \right) \ln(1+x^2) - 1 \right]$$

$$s = \sqrt{n_b g_b / m_b} \quad \text{the bosonic sound velocity}$$

Results in Cooper instability: formation of BCS-paired state (Cooper pairs)

The critical temperature

$$T_{c1} \sim \varepsilon_F \exp\left(-\frac{1}{\nu_F |V_{eff}^{(l=1)}(\omega=0)|}\right)$$

where

$$\nu_F = mp_F / 2\pi^2 \hbar^3 \quad \text{fermionic density of states at the Fermi energy}$$

For typical values of parameters

$$T_{c1} < 10^{-4} \varepsilon_F$$

The order parameter

$$\vec{\Delta} = -V_{eff}^{(l=1)} \langle \hat{\psi} \hat{\psi} \rangle = (\Delta_{-1}, \Delta_0, \Delta_1)$$

complex vector!

Is it possible to achieve the BCS transition?

Problem: required large values of a_{bf} could lead to instability of the mixture.

You will learn more about Fermi-Bose mixtures “in clouds” during next lecture!

II. Fermi-Bose mixtures in optical lattices:

M. Lewenstein et al. 2004

- Bose-Fermi mixture in an optical lattice
- Only the lowest band is occupied (fermionic filling factor $0 < \rho_F < 1$)
- Only short-range interactions

Bose-Fermi Hubbard Hamiltonian

$$H = - \sum_{\langle ij \rangle} J [f_i^+ f_j + b_i^+ b_j + h.c.] + \sum_i \left[\frac{U_{bb}}{2} n_i^{(b)} (n_i^{(b)} - 1) - \mu_b n_i^{(b)} \right] + U_{bf} \sum_i n_i^{(b)} n_i^{(f)}$$

H_1

Control parameters

H_0

$$0 < \rho_F < 1$$

$$J / U_{bb} \ll 1$$

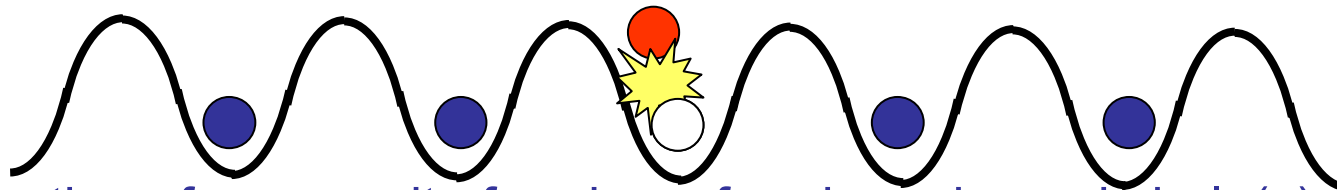
$$\alpha \equiv U_{bf} / U_{bb}$$

$$\bar{\mu} = \mu_b / U_{bb}$$

$J = 0$ limit

- If $U_{bf}=0$: MI state for the bosons with $n_0 = [\bar{\mu}] + 1$

- If $U_{bf} > 0$ and large enough the fermions push the bosons out



Formation of composite fermions: fermion + bosonic hole(s)

- If $U_{bf} < 0$ the fermions attract bosons to the sites they occupy and composites fermion + boson(s) are formed (Kuklov et al. 2003).

Pairing of a fermion with s bosonic holes (or $-s$ bosons) for

$$\bar{\mu} - n_0 + s < \frac{U_{bf}}{U_{bb}} < \bar{\mu} - n_0 + s + 1, \quad n_0 + s \geq 0$$

Composite fermion operators

$U_{bf} > 0, s > 0$ - pairing of a fermion with s bosonic holes

$$C_i = \sqrt{(n_0 - s)! / n_0!} (b_i^+)^s f_i$$

$U_{bf} < 0, s < 0$ - pairing of a fermion with $-s$ bosons

$$C_i = \sqrt{n_0! / (n_0 - s)!} (b_i)^{-s} f_i$$

Under the constraint (!): $n_i^b + s n_i^f = n_0$

the operators C_i and C_j^+ obey

$$C_i C_j^+ + C_j^+ C_i = \delta_{ij}$$

Limit of small tunneling $J \ll U_{bf}, U_{bb}$

can be analyzed by considering H_1 as a perturbation.

Effective Fermi-Hubbard Hamiltonian for composite fermions

$$H_{eff} = \sum_{\langle ij \rangle} \left(-J_{eff} [C_i^+ C_j + h.c.] + U_{eff} N_i N_j \right)$$

where J_{eff} is the nearest-neighbors tunneling and

U_{eff} the nearest-neighbors interaction

Interaction between composite fermions

$$U_{eff} = 2 \frac{J^2}{U_{bb}} \left[\frac{n_0(n_0 + 1 - s)}{1 + \alpha - s} + \frac{(n_0 + 1)(n_0 - s)}{1 - \alpha + s} + \frac{1}{\alpha s} - n_0(n_0 + 1) - (n_0 - s)(n_0 - s + 1) \right]$$

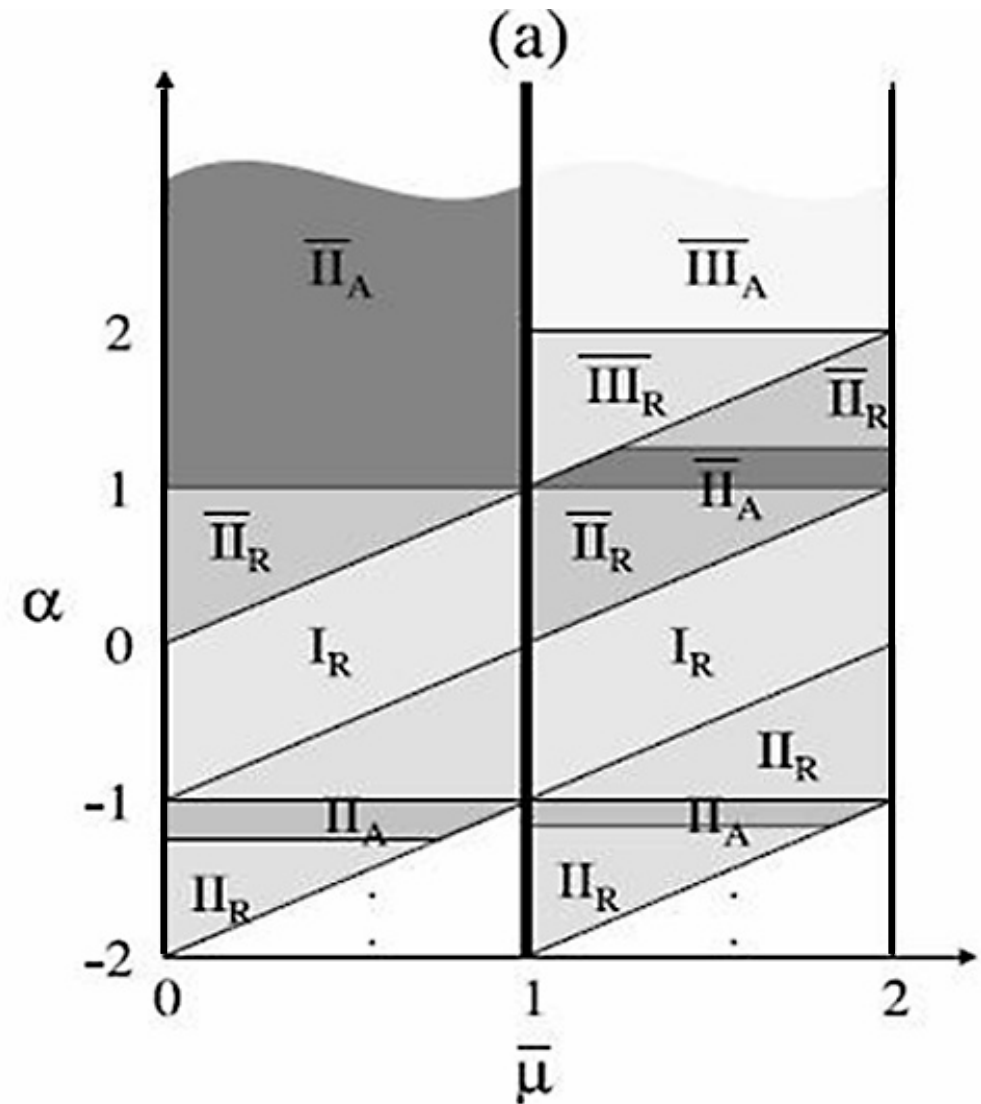
can be either attractive or repulsive!

How it looks?

R / A - repulsive/attractive interaction

Roman numbers I, II, etc
- number of particles that form composite fermion
(I - original fermion)

Bar over roman numbers, I, II, etc
- indicates composite fermion with bosonic holes



Tunneling of composite fermions

$$J_{eff} = J \quad \text{in I} \quad (0 < \bar{\mu} < 1)$$

$$J_{eff} = 4J^2 / |\alpha| U_{bb} \quad \text{in II}$$

$$J_{eff} = 2J^2 / \alpha U_{bb} \quad \text{in \overline{II}}$$

• • •

Phases of composite fermions

$$H_{eff} = \sum_{\langle ij \rangle} \left(-J_{eff} [C_i^+ C_j + h.c.] + U_{eff} N_i N_j \right)$$

Important parameter $\Delta = U_{eff} / 2J_{eff}$

I. Repulsive interaction

For $\rho_F \ll 1$ ($1 - \rho_F \ll 1$)

Fermi gas of composite fermions
(holes)

For $\rho_F \rightarrow 1/2$, $\Delta \sim 1$

Density wave – insulating phase
(for $\rho_F = 1/2$ - checkerboard state)

II. Attractive interaction

For $\rho_F \ll 1$ ($1 - \rho_F \ll 1$), $|\Delta| \ll 1$ BCS state with p-wave pairing

$$|\Psi\rangle = \prod_{\vec{k}} \left(u_{\vec{k}} |1_{\vec{k}}, 1_{-\vec{k}}\rangle + v_{\vec{k}} |0_{\vec{k}}, 0_{-\vec{k}}\rangle \right)$$

For $\Delta < -1$ Domains of composite fermions
("domain" isolator)

For ρ_F - arbitrary, $|\Delta| \rightarrow 1$ Strongly correlated state with
composite triples, quadruples, etc.

Phase diagram

$$\Delta = U_{eff} / 2J_{eff}$$

Attractive case: $U_{eff} < 0$

$|\Delta| \leq 1$ BCS (SF)

$|\Delta| > 1$ Fermionic domains (FD)

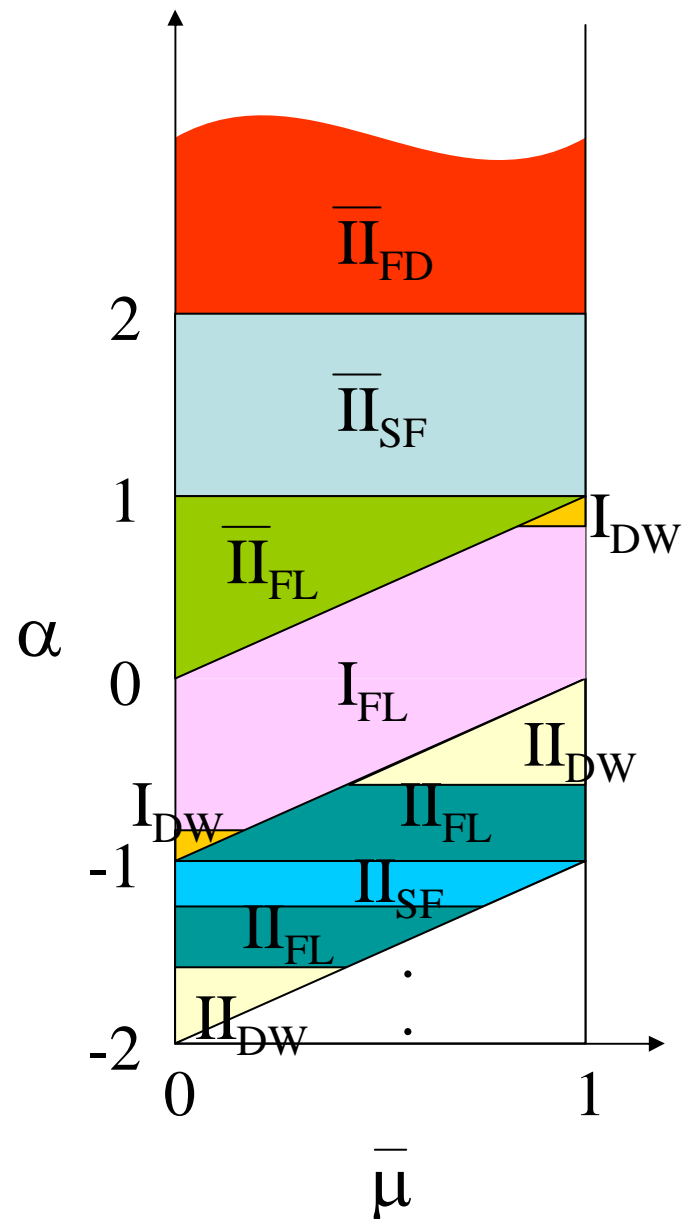
Repulsive case: $U_{eff} > 0$

$\Delta < \Delta_{crit}$ Fermi liquid (FL)

$\Delta > \Delta_{crit}$ Density wave (DW)

$$\Delta_{crit} \equiv (1 + m_z^2) / (1 - m_z^2)$$

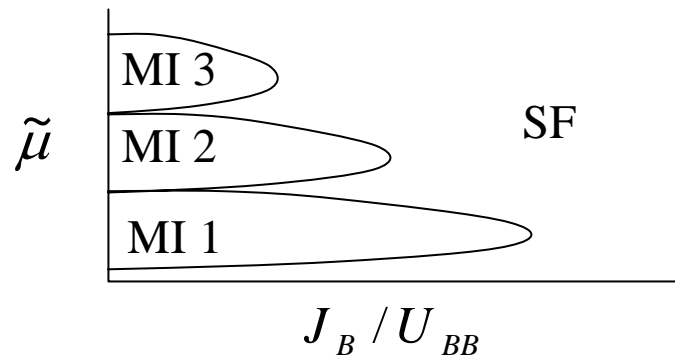
$$m_z = 2\rho_f - 1$$



Finite tunneling (Landau mean-field theory)

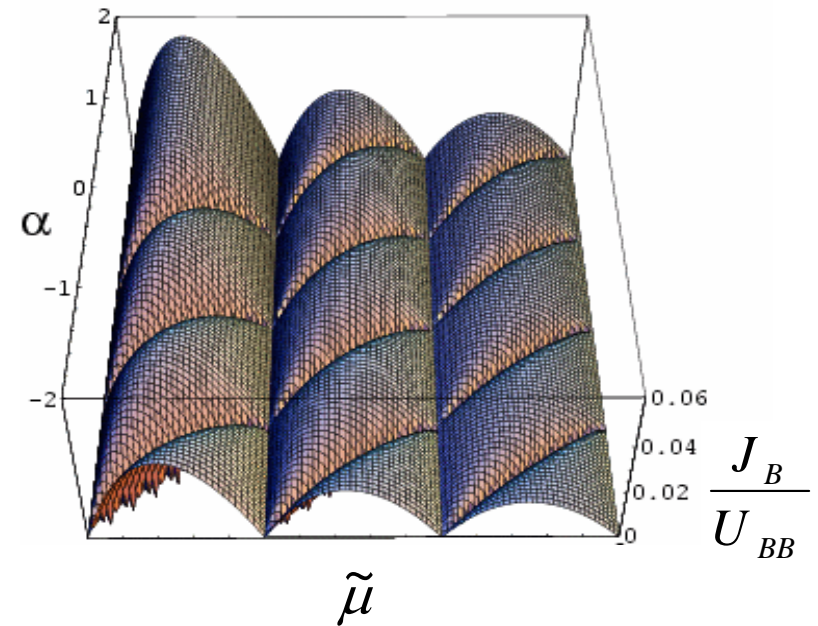
H. Fehrmann et al. 2005

Generalization of Fisher et al. 1989 for FB mixtures



$$\frac{J_B}{U_{BB}} = \frac{-1}{2d} \left\{ \left(\frac{n_0 + 1}{\varepsilon(n_0, 0)} - \frac{n_0}{\varepsilon(n_0 - 1, 0)} \right) (1 - \rho_F) + \left(\frac{n_0 - s + 1}{\varepsilon(n_0 - s, 1)} - \frac{n_0 - s}{\varepsilon(n_0 - s - 1, 1)} \right) \rho_F \right\}^{-1}$$

$$\varepsilon(n, m) = \tilde{\mu} - n + \alpha m$$



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Finite temperatures

Degenerated interacting gas in the I, II and <u>II</u> phases	Degenerated ideal gas In the I phase Ideal non-degenerated gas in the rest	Ideal non-degenerated gas of composites	No composites
$T < J^2 / U_{BB}$	$T < J$	$T < U_{BB}, U_{BF}$	

Conclusion:

Fermi-Bose mixtures show very rich physics
and definitely deserve attention!

Thank you for your attention !