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Universal properties of Bose-Fermi mixtures with a pairing interaction

Andrea Guidini and Pierbiagio Pieri

School of Science and Technology, Physics Division, University of Camerino, Italy

Gianluca Bertaina, Davide Galli

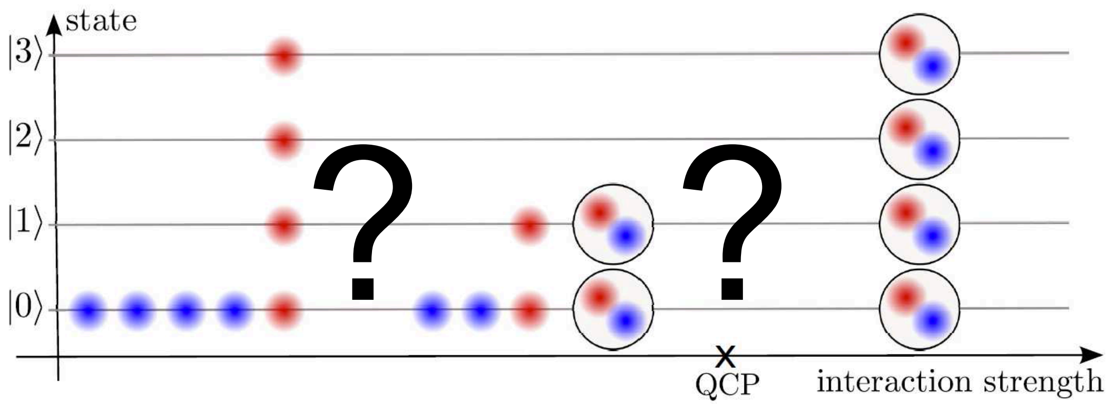
Physics Department, University of Milan, Italy

Bose-Fermi mixtures with a tunable BF attraction

• System of bosons of one species interacting with one-component fermions through a tunable boson-fermion attraction.

• For weak attraction, weakly interacting Bose-Fermi mixture: at sufficiently low temperature bosons condense, while fermions fill a Fermi sphere.

• For strong attraction bosons pair with fermions to form molecules. Condensation suppressed in favour of molecule formation. Fermi sphere of molecules coexisting with Fermi sphere of unpaired fermions for $n_F \geq n_B$.



• How does the system evolves from one limit to the other one?

• How to describe this evolution?

The model

• **Two-component Hamiltonian** with attractive contact interaction between bosons and fermions.

$$H_{\mathrm{BF}} = \sum_{s=\mathrm{B,F}} \int d\mathbf{r}\psi_s^\dagger(\mathbf{r}) \left(-\frac{\nabla^2}{2m_s} - \mu_s\right) \psi_s(\mathbf{r}) + v_0 \int d\mathbf{r}\psi_B^\dagger(\mathbf{r})\psi_F^\dagger(\mathbf{r})\psi_F(\mathbf{r})\psi_B(\mathbf{r})$$

• Bare contact-interaction strength between bosons and fermions expressed in terms of the **boson-fermion** scattering length a_{BF} .

$$\frac{1}{v_0} = \frac{m_r}{2\pi a_{\mathrm{BF}}} - \int \frac{d\mathbf{k}}{(2\pi)^3} \frac{2m_r}{\mathbf{k}^2} \qquad\qquad m_r = \frac{m_{\mathrm{B}} m_{\mathrm{F}}}{m_{\mathrm{B}} + m_{\mathrm{F}}}$$

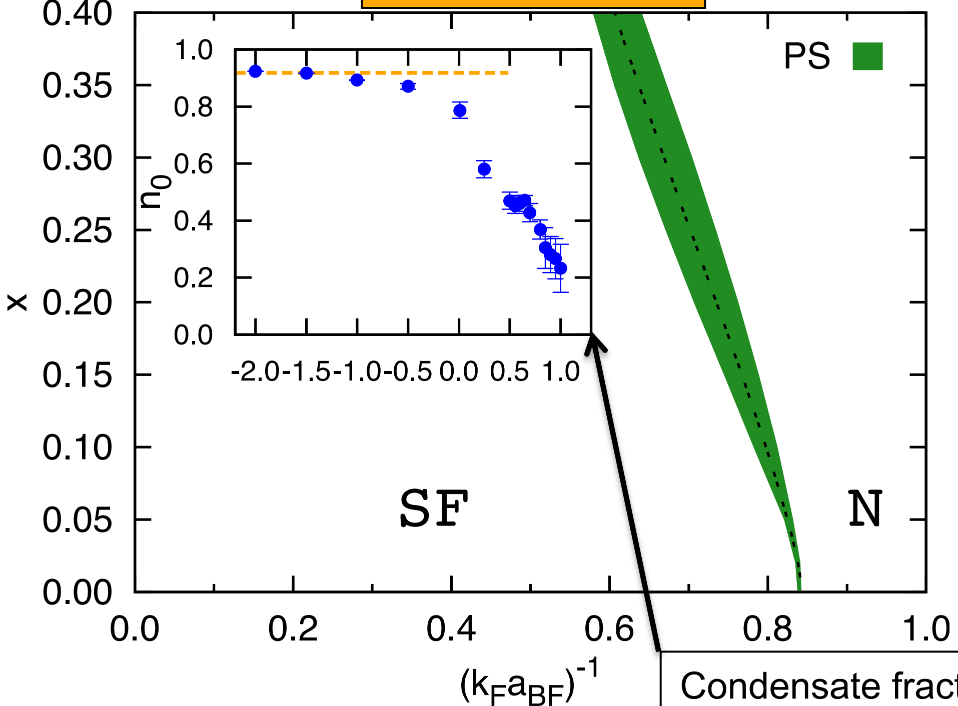
• No Fermi-Fermi interaction (fermions are identical: short-range interaction suppressed). Short-range **boson-boson interaction** is instead possible (and desired if repulsive). Add boson-boson short-range repulsion:

$$H = H_{\mathrm{BF}} + \frac{1}{2} \int d\mathbf{r} d\mathbf{r}' V_{\mathrm{BB}}(\mathbf{r} - \mathbf{r}')\psi_B^\dagger(\mathbf{r})\psi_B^\dagger(\mathbf{r}')\psi_B(\mathbf{r}')\psi_B(\mathbf{r})$$

• We focus on systems where $n_F \geq n_B$.

T=0 phase diagram concentration vs coupling obtained with FN-DMC

$k_F a_{BB} = 1; \; m_B = m_F$



Condensate fraction for $x=n_B/n_F=0.175$.

Boson concentration: $x = n_B / n_F$

Dimensionless coupling strength: $(k_F a_{BF})^{-1}$,

where: $k_F \equiv (6\pi^2 n_F)^{1/3}$.

Trial wavefunctions:

$$\Psi_{SF} = J_{BB} J_{BF} \Phi_F^{\text{Slater}}(N_F)$$

$$\Psi_N = J_{BB} \Phi_M^{\text{Slater}}(N_M = N_B, N_F - N_B)$$

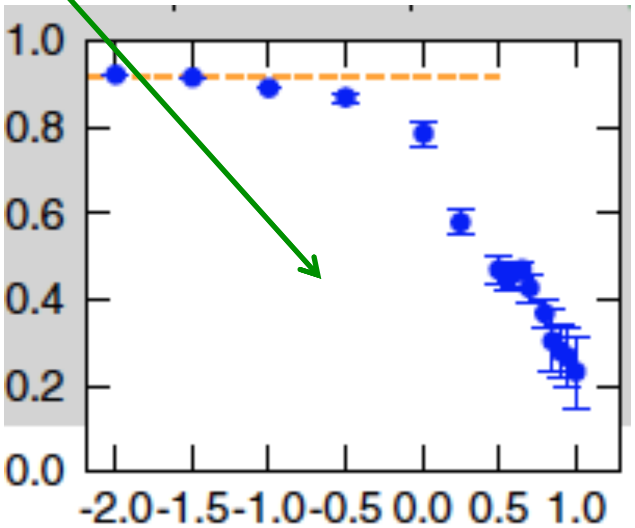
Molecular orbitals:

$$\varphi_{K_\alpha}(i,i') = \; f_{\text{B}}(|\mathbf{r}_i - \mathbf{r}_{i'}|) \exp\left[i\mathbf{K}_\alpha(\mathbf{r}_i + \mathbf{r}_{i'})/2\right]$$

G. Bertaina, E. Fratini, S. Giorgini, P. Pieri, PRL, **110**, 115303 (2013)

First order **quantum phase transition** between condensed phase and 'normal' phase, with a narrow phase separation region, which shrinks to zero for $x \to 0$.
Polaron-molecule transition point is recovered and unveiled in this limit.

Many-body diagrammatic approach for the **condensed** phase



Bosonic and fermionic self-energy diagrams for the **condensed** phase

Boson self-energy

$$\Sigma_{\rm B}^{11}(\bar{k}) = \frac{8\pi a_{\rm BB}}{m_B} n_0 + \Sigma_{\rm BF}(\bar{k})$$

$$\Sigma_{\rm B}^{12}(\bar{k}) = \frac{4\pi a_{\rm BB}}{m_B} n_0$$

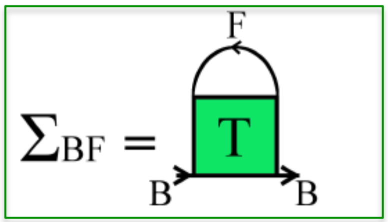
$$\Sigma_{\rm BF}(\bar{k}) = \int \frac{d\mathbf{P}}{(2\pi)^3} \int \frac{d\Omega}{2\pi} T(\bar{P}) G_{\rm F}^0(\bar{P} - \bar{k})$$

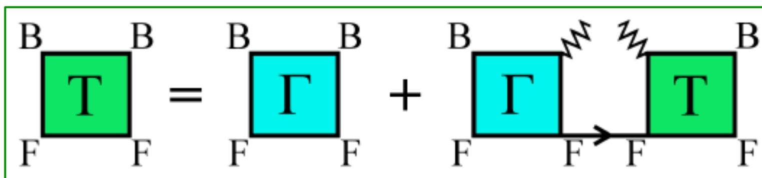
Boson-fermion T-matrix

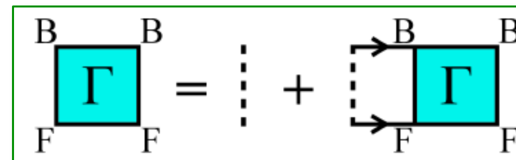
$$T(\bar{P})^{-1} = \Gamma(\bar{P})^{-1} - n_0 G_{\rm F}^0(\bar{P})$$

$$\Gamma(\bar{P})^{-1} = \frac{m_r}{2\pi a_{\rm BF}} - \frac{m_r^{3/2}}{\sqrt{2}\,\pi} \sqrt{\frac{P^2}{2M} - 2\mu - i\Omega - I_{\rm F}(\bar{P})}$$

$$I_{\rm F}(\bar{P}) \equiv \int \frac{d\mathbf{p}}{(2\pi)^3} \frac{\Theta(-\xi^{\rm F}_{\mathbf{P}-\mathbf{p}})}{\xi^{\rm F}_{\mathbf{P}-\mathbf{p}} + \xi^{\rm B}_{\mathbf{p}} - i\Omega}$$

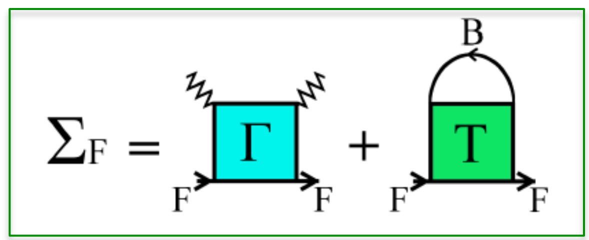






Fermion self-energy

$$\Sigma_{\rm F}(\bar{k}) = n_0 \Gamma(\bar{k}) - \int \frac{d\mathbf{P}}{(2\pi)^3} \int \frac{d\Omega}{2\pi} T(\bar{P}) G_{\rm B}^0(\bar{P} - \bar{k})$$



$$\bar{P} \equiv (\mathbf{P}, i\Omega),\ \bar{k} \equiv (\mathbf{k}, i\omega) \qquad \xi^s_{\mathbf{p}} = p^2/2m_s - \mu_s$$

$$\mu = (\mu_{\rm B} + \mu_{\rm F})/2 \qquad G^0_s(\bar{k})^{-1} = i\omega - \xi^s_{\mathbf{k}}$$

Coupled equations for chemical potentials and condensate density n_0

Green's functions obtained from the self-energies through Dyson's equations:

$$G_{\mathrm{F}}(\bar{k})^{-1} = G^{0}_{\mathrm{F}}(\bar{k})^{-1} - \Sigma_{\mathrm{F}}(\bar{k})$$

$$G'_{\mathrm{B}}(\bar{k}) = \frac{i\omega + \xi^{\mathrm{B}}_{\mathbf{k}} + \Sigma^{11}_{\mathrm{B}}(-\bar{k})}{[i\omega + \xi^{\mathrm{B}}_{\mathbf{k}} + \Sigma^{11}_{\mathrm{B}}(-\bar{k})][i\omega - \xi^{\mathrm{B}}_{\mathbf{k}} - \Sigma^{11}_{\mathrm{B}}(\bar{k})] + \Sigma^{12}_{\mathrm{B}}(\bar{k})^2}$$

momentum distributions obtained from the Green's functions:

$$n_{\mathrm{F}}(\mathbf{k}) = \int \frac{d\omega}{2\pi} G_{\mathrm{F}}(\bar{k})\, e^{i\omega 0^+} \qquad n_{\mathrm{B}}(\mathbf{k}) = -\int \frac{d\omega}{2\pi} G'_{\mathrm{B}}(\bar{k})\, e^{i\omega 0^+}$$

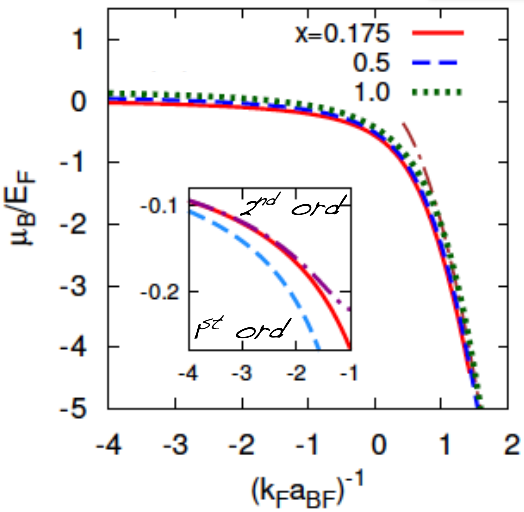
integration over **k** + Hugenholtz-Pines relation $\Rightarrow$ coupled eqs for μ_B, μ_F, n_0 :

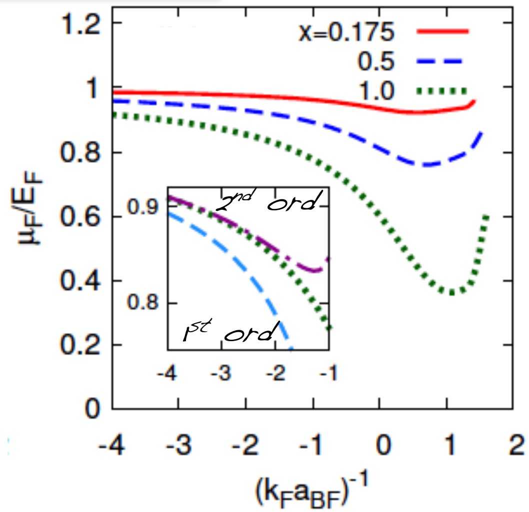
$$n_{\mathrm{F}} = \int \frac{d\mathbf{k}}{(2\pi)^3} n_{\mathrm{F}}(\mathbf{k}) \qquad n_{\mathrm{B}} = n_0 + \int \frac{d\mathbf{k}}{(2\pi)^3} n_{\mathrm{B}}(\mathbf{k})$$

$$\mu_{\mathrm{B}} = \Sigma^{11}_{\mathrm{B}}(0) - \Sigma^{12}_{\mathrm{B}}(0)$$

Results: chemical potentials and energy

$$n_B a_{BB}^3 = 3\times 10^{-3}$$



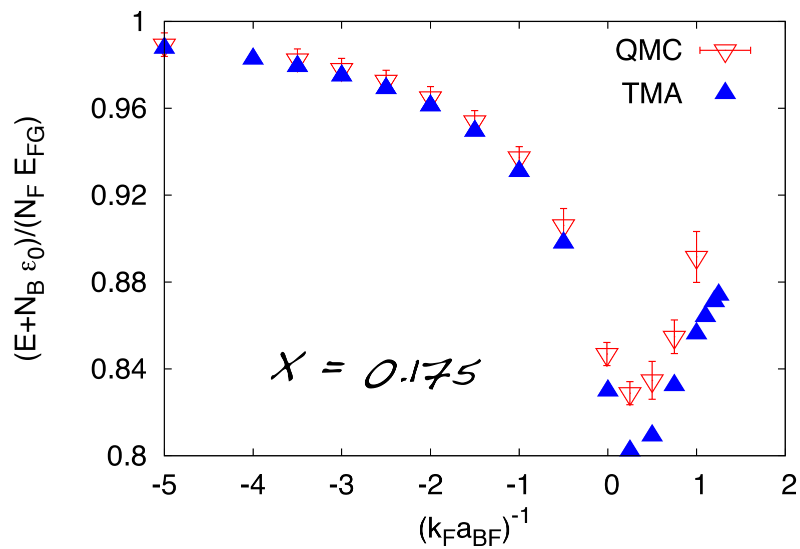


- ✓ 2nd order pert. results recovered for weak coupling [Albus et al.; Viverit & Giorgini (2002)]:

$$\mu_{\rm B} = 2\pi a_{\rm BF} n_{\rm F}/m_r(1 + 3\frac{k_{\rm F}a_{\rm BF}}{2\pi})$$

$$\mu_{\rm F} = E_{\rm F} + 2\pi a_{\rm BF} n_{\rm B}/m_r(1+2\frac{k_{\rm F}a_{\rm BF}}{\pi})$$

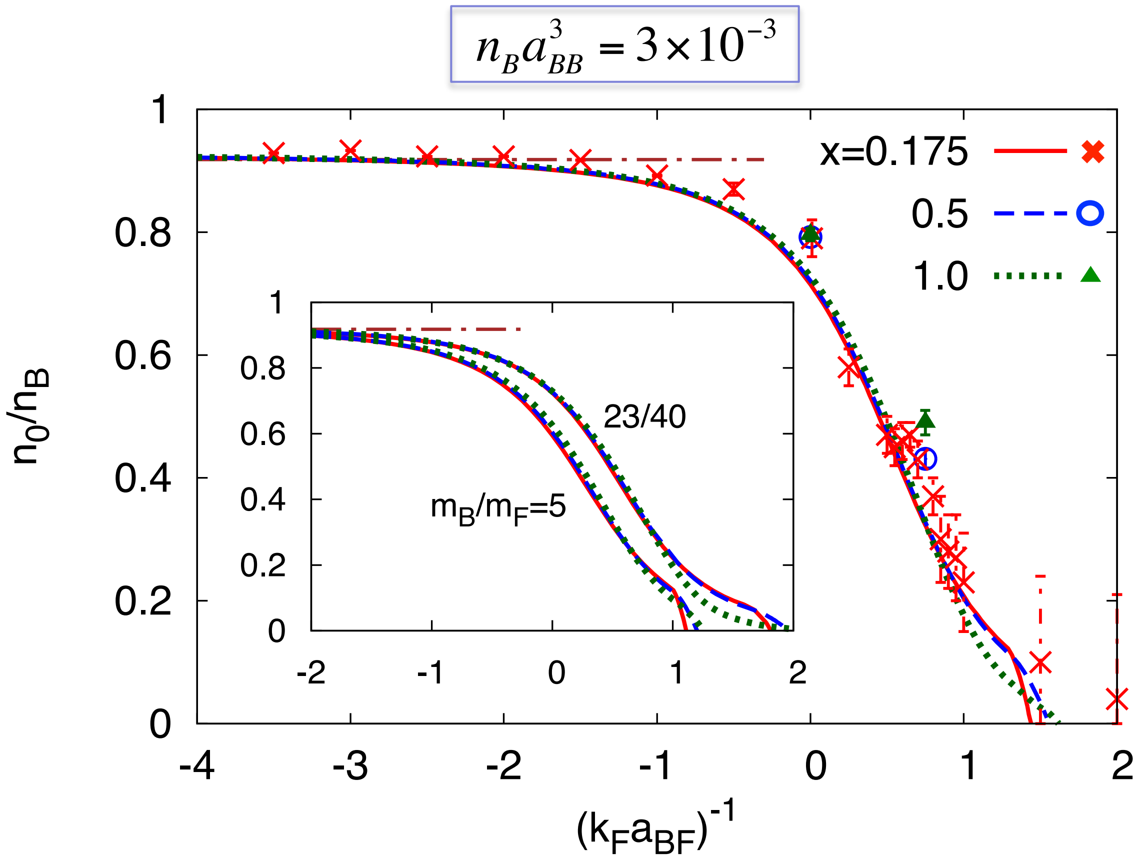
- ✓ molecular binding for strong coupling



- ✓ Good agreement with QMC results for the energy also in the nonperturbative region.

TMA: present work
QMC: G. Bertaina et al. PRL (2013).

Condensate fraction: universal behavior and comparison with QMC



Curves: present work.
Symbols: FN-DMC G. Bertaina et al. PRL (2013) at x=0.175 + new simulations at x=0.5 and 1.
Dashed-dotted line: Bogoliubov.

Condensate fraction **independent of the boson concentration** for most of the graph. Some dependence only in the transition region, when the condensate fraction approaches zero. Overall good agreement with FN-DQMC results.

Condensate fraction: connection with the polaron quasiparticle weight

$n_B / n_F \to 0$: **polaron problem**

- What is the analogous of the condensate fraction for the polaron?
- To which quantity does the condensate fraction of a Bose-Fermi mixture tend in the polaron limit?

Consider the quasiparticle weight Z at the Fermi level for the minority component of a **Fermi-Fermi** mixture. This weight yields the size of the Fermi step: $Z = n_\downarrow(k_{F\downarrow}^-) - n_\downarrow(k_{F\downarrow}^+)$.

For $n_\downarrow / n_\uparrow \to 0$ one has $k_{F\downarrow} \to 0$ and $n_\downarrow(k) \to n_{\text{pol}}(k)$, then yieding: $Z = n_{\text{pol}}(k=0) - n_{\text{pol}}(0^+)$.

But $n_{\text{pol}}(k \neq 0) \propto 1/V$ since its integral over k scales like $1/V$ (1 particle over the volume V).

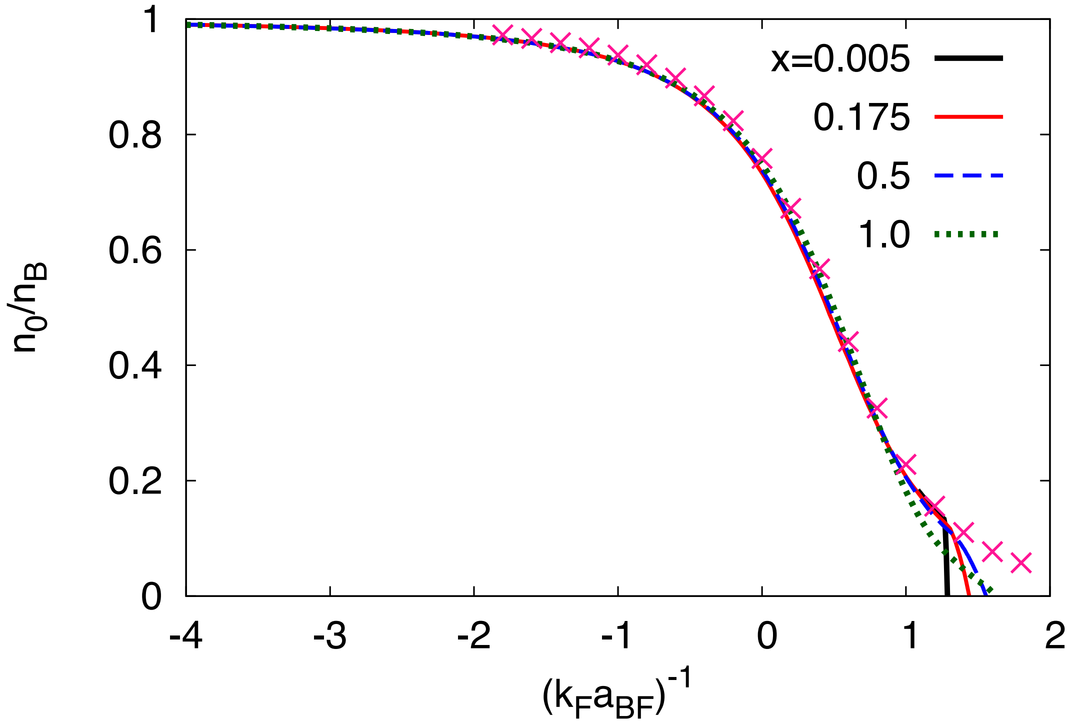
We have then $n_{\text{pol}}(0^+) \to 0$, in the thermodymamic limit. Thus: $Z_{\text{pol}} = n_{\text{pol}}(k=0)$.

But for a a **Bose-Fermi** mixture $n_{\text{pol}}(k=0)$ is the limit for $n_B / n_F \to 0$ of the condensate fraction:

$$\frac{n_0}{n_B} = \frac{n_B(k=0)}{N_B} = \frac{n_{\text{pol}}(k=0)}{1}$$

The condensate fraction tends to the quasiparticle weight Z in the polaron limit.

Condensate fraction: comparison with diag-MC for the polaron



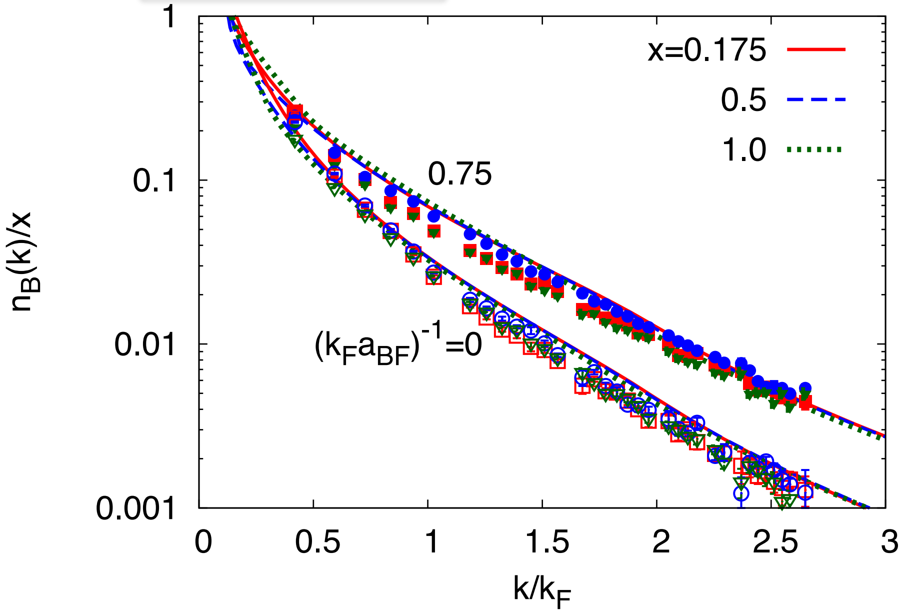
Curves: our calculations at three different concentrations for zero Bose repulsion.

Symbols: Diagrammatic MC results for Z_{pol} [J. Vlietinck, J. Ryckebusch & K. Van Houcke, PRB **87**, 115133 (2013)]

The 'universality' of the condensate fraction with respect to the boson concentration makes even the curve at concentration equal one to be 'ruled' by the polaron quasiparticle weight for most of its graph.

Momentum distribution functions

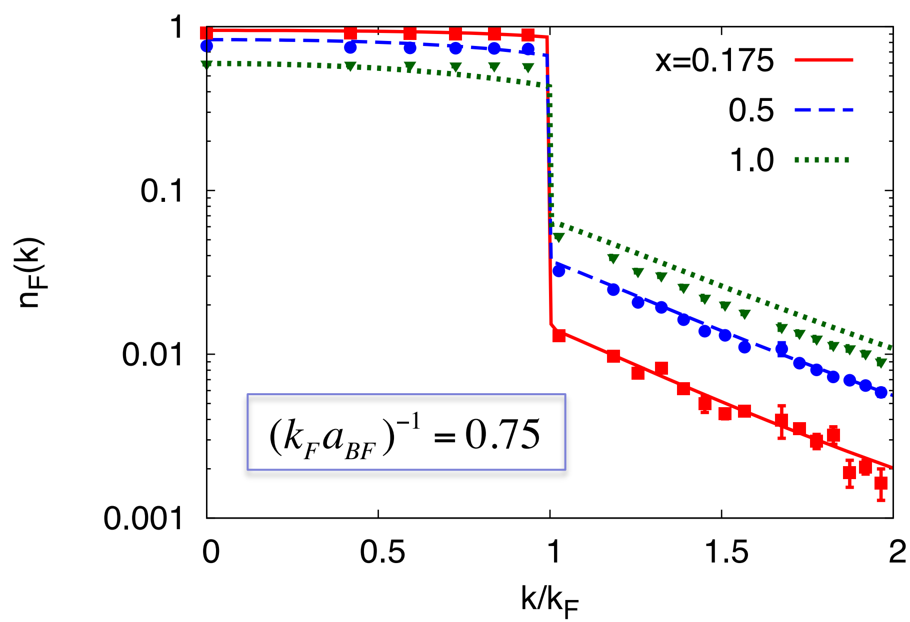
$n_B a_{BB}^3 = 3\times10^{-3}$



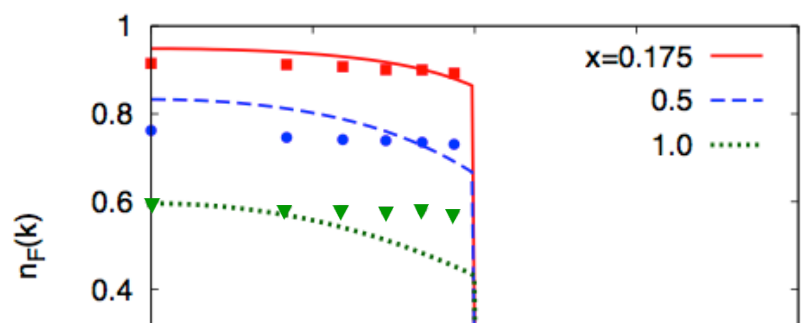
Universality of the bosonic momentum distribution. Very good agreement with FN-DQMC results (new calculations by G.Bertaina). Universality implies:

$$n_B(k) = n_B \times V n_{\rm pol}(k)$$
$$= N_B \times n_{\rm pol}(k)$$

as if the polarons were independent.



Good agreement with QMC data also for $n_F(k)$. For fermions, however, QMC is more affected by finite-size effects [Holzmann et al. PRL, **107**, 110402 (2011)]

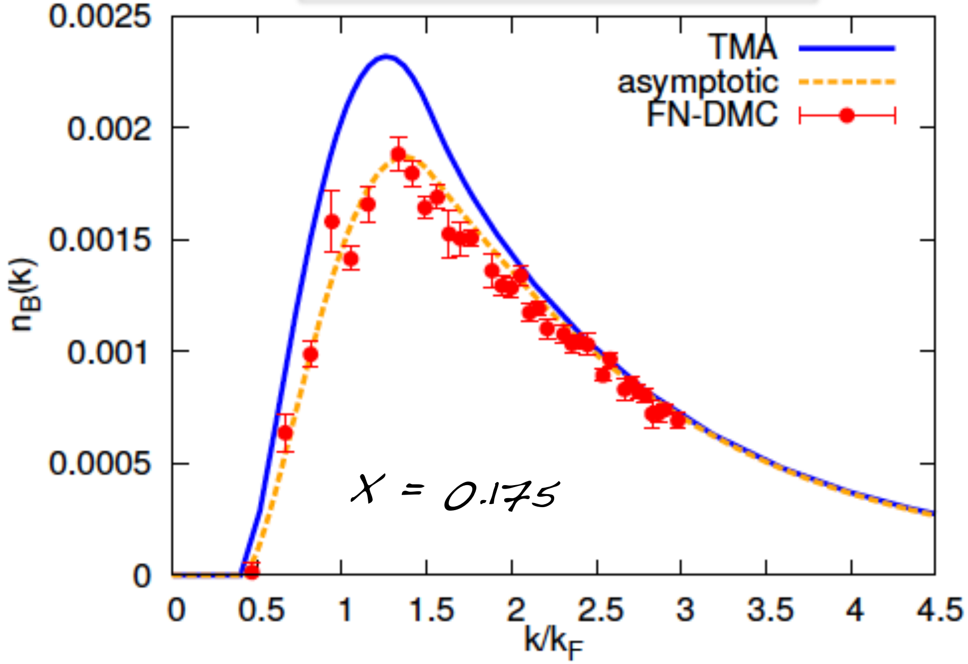


Results for the **normal** phase: indirect Pauli exclusion effect

A. Guidini, G. Bertaina, E. Fratini, P. Pieri, PRA, **89**, 023634 (2014)

Momentum distribution function at T=0: bosons

$m_F = m_B; \quad (k_F a_{BF})^{-1} = 3$



TMA: previous digrammatic theory for $n_0 = 0$.
FN-DMC: Calculation using molecular trial wave function.

Strong-coupling asymptotic expression for the momentum distribution function:

$$n_B(\mathbf{q}) \approx \frac{2\pi}{m_r^2 a_{BF}} \int \frac{d\mathbf{P}}{(2\pi)^3} \frac{\Theta(P_{CF} - P)\Theta(|\mathbf{q}-\mathbf{P}| - k_{UF})}{[\mathbf{q}^2/(2m_B) + (\mathbf{q}-\mathbf{P})^2/(2m_F) - \mathbf{P}^2/(2M) + \varepsilon_0]^2}$$

Effect of **Pauli exclusion on bosonic atoms**. States with $q < k_{UF} - P_{CF}$ are forbidden. Depleted region when $n_B < n_F/2$. Analogous of the Sarma phase in a BF mixture.

Experiments?

Several examples of quantum degenerate Bose-Fermi mixtures have been attained so far with ultracold atoms:

Mixture	Group
^{7}Li-^{6}Li	ENS(Paris), Rice
^{23}Na-^{6}Li	MIT
^{87}Rb-^{40}K	LENS,JILA,Hamburg
^{87}Rb-^{6}Li	Tübingen
^{85}Rb-^{6}Li	UBC (Vancouver)
^{174}Yb-^{173}Yb	Kyoto
^{84}Sr-^{87}Sr	Innsbruck
^{41}K-^{6}Li	MIT
^{41}K-^{40}K	MIT
^{174}Yb-^{6}Li	Kyoto, UW (Seattle)
^{23}Na-^{40}K	MIT

Tunability of the Bose-Fermi interaction via Fano-Feshbach resonance achieved in several mixtures. Weak Bose-Bose repulsion.
F-F interaction negligible.

Feshbach molecules created at JILA and Hamburg with a Rb-K mixture, and at MIT with Na-K (Zwierlein) and Na-Li (Ketterle).

But no exp. result so far in the intermermediate coupling region. Difficulties associated with three-atom recombination processes.

Loss-rate proportional to $n_B^2 n_F$. Working at low bosonic concentrations may reduce losses.

Summary and conclusions

- Presented many-body diagrammatic theory for Bose-Fermi mixtures at T=0 which interpolates smoothly from weak to strong Bose-Fermi attractions.

- Perturbative results recovered in weak coupling, good agreement with FN-DMC calculations even in the nonperturbative regime $|k_F a_{BF}| > 1$.

- "Universal" behavior found for the bosonic momentum distribution functions and condensate fraction: no dependence on the boson concentration from vanishing boson concentration up to concentration $n_B / n_F = 1.0$.

- Unexpected (?) connection between condensate fraction in a Bose-Fermi mixture and the polaron quasiparticle weight .

- Interesting "indirect Pauli exclusion effect" in the molecular regime.