Quantum Monte Carlo study of a resonant dilute Bose-Fermi mixture

Bertaina G, Fratini E, Giorgini S, Pieri P, Phys Rev Lett. 110, 115303 (2013)

Gianluca Bertaina

Physics Department, University of Milan (Italy)

email: gianluca.bertaina@zoho.com

in collaboration with

Elisa Fratini (University of Camerino and CNISM)

Stefano Giorgini (INO-BEC and University of Trento)

Pierbiagio Pieri (University of Camerino and CNISM)

Vincenzo Savona (ITP-EPFL, Lausanne)

Bose Einstein Condensation 2013, Sant Feliu de Guixols (SPAIN), September 7-13 2013

Bose-Fermi mixtures in ultracold dilute gases

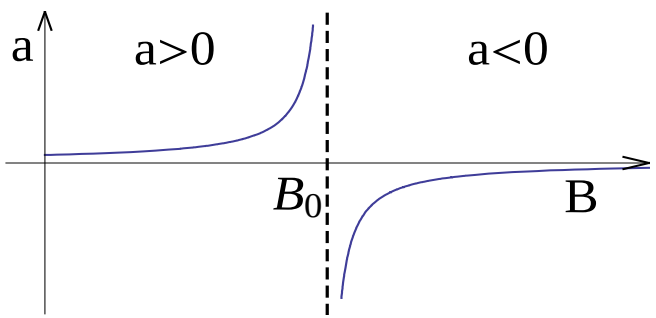
Rich phase diagram: role of statistics

- ➔ Bosonic / fermionic polarons
- ➔ Bosonic condensate depletion due to interspecies interaction
- ➔ Polar molecules, p-wave interactions

- ✗ (Three-body effects, Efimov states)
- ✗ (Boson mediated fermion pairing)
- ✗ (Mass imbalance)

Experiments

Issues: Finding good Feshbach resonances



3-body recombination

Feshbach molecules lifetime

Molecular chemical reactions

Quest of the rovibrational ground-state

^{40}K-^{87}Rb repulsive mixture: Ospelkaus et al. (PRL 2006)

Zaccanti et al. (PRA 2006)

^{40}K-^{87}Rb molecules: Ni et al. (Science 2008)

^{40}K-^{41}K-^{6}Li degenerate mixture: Wu et al. (PRA 2012)

^{23}Na-^{6}Li: Wu et al. (PRL 2012)

^{23}Na-^{40}K: Heo et al. (PRA 2012)

Theory

- Mean-field (Marchetti et al. PRB 2008)
- T-matrix (Fratini, Pieri PRA 2010, 2012, 2013, Schuck et al, PRA 2005, 2008, 2013)
- Functional approaches (Powell et al. PRB 2005, Ludwig et al. PRA 2011)
- Variational (Yu et al. PRA 2011)
- A lot of literature concerning lattice models, but we consider a continuous system

Our model

- $n_F = \frac{k_F^3}{6\pi^2}$ fermions (**single spin component**)

  n_B bosons (**no spin**)

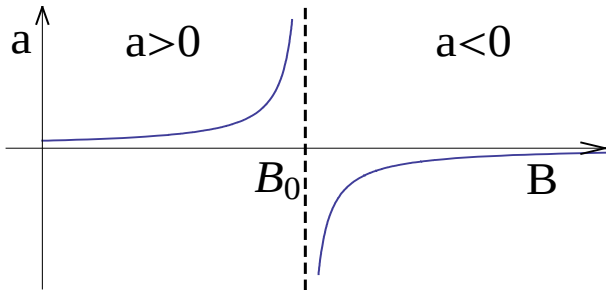
  $x = n_B / n_F$ concentration of bosons

  $m_B = m_F$ ~ isotopic mixture

- Hamiltonian (3D continuous system): $\hat{H} = \hat{K}_B + \hat{K}_F + \hat{V}_{BF} + \hat{V}_{BB}$
- Bose-Fermi (BF) attractive resonant interaction
- Bose-Bose (BB) repulsive interaction (for stability)

- Model BF: Square Well $g = 1/k_F a_{BF}$

  BB: Soft Sphere $\zeta = k_F a_{BB}$



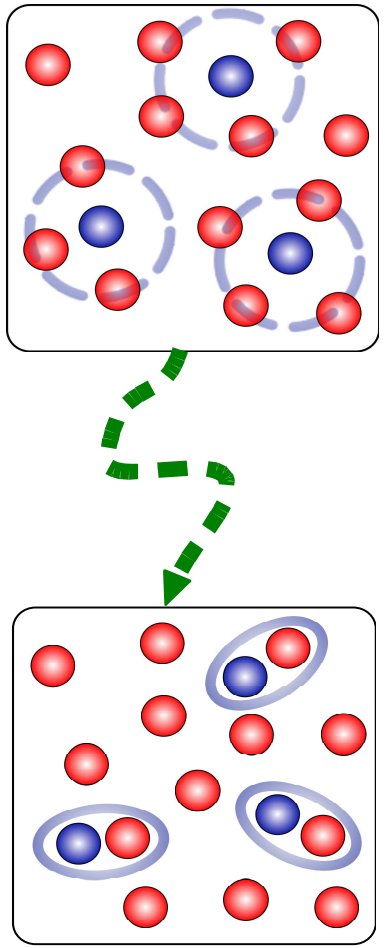
NOTE: we ignore deeper molecular channels

Heuristic Picture for small concentration of bosons

- Weak coupling:

  expected mixture of free bosons and fermions

  → Condensate of bosons



- Strong coupling:

  expected mixture of Feshbach

  molecular fermions and free remaining fermions

  → Complete depletion of the condensate

- Intermediate interaction: **quantum phase transition** (T=0)

Method: Diffusion Monte Carlo (DMC)

Schroedinger equation in imaginary time
(Fixed number of particles)

$$-\frac{\partial}{\partial\tau}\Psi(\tau) = \hat{H}\Psi(\tau)$$

Evolution

$$\Psi(\tau) = e^{-\hat{H}\tau}\Psi(0) = e^{-\hat{H}\tau}\Psi_T \xrightarrow{\tau\to\infty} \Psi_0(\tau)$$

Importance sampling

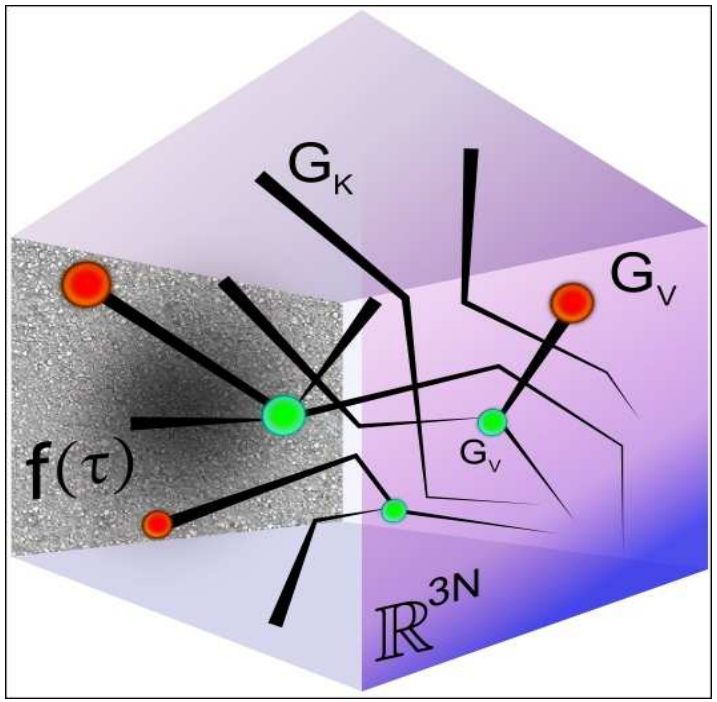
$$f(\tau) = \Psi(\tau)\Psi_T = e^{-\tilde{H}\tau}\Psi_T^2 \xrightarrow{\tau\to\infty} \Psi_0^{FN}(\tau)\Psi_T$$

Small time-step expansion

Ψ_T *Trial (guide) wavefunction: fixes nodal surface*

$$f(X,\tau) = \Psi(X,\tau)\Psi_T(X) \geq 0$$

Bosons : *exact (ground state)*
Fermions : *Fixed Node approximation.*
(*variational principle*)



Weak coupling nodal surface

- Condensate nodal surface: $\Psi_{JS} = J_{BB} J_{BF} \Phi_A^S(N_F)$

  Jastrow correlation factors $J_{SS'}(\mathbf{R}) = \prod_{\substack{i \in S \\ i' \in S'}} f_{SS'}(\mathbf{r}_i - \mathbf{r}_{i'})$

- Single Fermi sphere with all the fermions

- Stability issue: a repulsive interaction between bosons is introduced to prevent collapse of the bosonic component

  We choose $\zeta = k_F a_{BB} = 1 \rightarrow n_B a_{BB}^3 \approx 10^{-3}$

- Universality of BB potential: x < 0.2

Energy functional for condensate phase

Fermi sea

Binding energy of bosonic polarons (T-matrix)

$$\frac{E_{pol}}{N_F} = \frac{3}{5}\varepsilon_F \left(1 - A(g)x + \frac{10}{9\pi}\zeta x^2 \left(1 + D(g,\zeta)\right)\right)$$

Mean-field BB interaction

g	D
0.00	0.99(1)
0.25	1.33(5)
0.50	1.75(5)
0.75	1.95(5)
1.00	1.25(1)

Beyond Mean Field: Fit to JS-DMC data (fixed a_{BB})

Strong coupling nodal surface

- Molecular nodal surface: $\Psi_{JMS} = J_{BB}\Phi_A^{MS}(N_M = N_B, N_F)$

$$\Phi_A^{MS}(\mathbf{R}) = \det \begin{pmatrix} \varphi_{K_1}(1,1') & \cdots & \varphi_{K_1}(N_F,1') \\ \vdots & \ddots & \vdots \\ \varphi_{K_{N_M}}(1,N_M') & \cdots & \varphi_{K_{N_M}}(N_F,N_M') \\ \psi_{k_1}(1) & \cdots & \psi_{k_1}(N_F) \\ \vdots & \ddots & \vdots \\ \psi_{k_{N_R}}(1) & \cdots & \psi_{k_{N_R}}(N_F) \end{pmatrix}$$

- Center-of-mass motion of molecules is relevant (two Fermi spheres)

$$\varphi_{K_\alpha}(i,i') = f_b(|\mathbf{r}_i - \mathbf{r}_{i'}|)\exp\left(i\mathbf{K}_\alpha(\mathbf{r}_i + \mathbf{r}_{i'})/2\right)$$

- Complete antisymmetrization of fermions (molecular and free orbitals)
- Each boson in a molecular orbital
- No symmetrization of bosons (→ problems with one-body density matrix)

Energy functional for normal molecular phase

Bare binding energy contribution

Fermi-Fermi mixture

$$\frac{E_{mol}}{N_F} = \frac{3}{5}\varepsilon_F\Big(\varepsilon_b(g)x + \mathcal{E}_{FF}(x,g,\zeta)\Big)$$

Fermi sea of molecules

Fermi sea of remaining free fermions

$$\mathcal{E}_{FF} = \frac{m}{M^*(g)}x^{5/3}\Big(1 + xC(g,\zeta)\Big) + (1-x)^{5/3} + x(1-x)\frac{5\alpha(g)}{3\pi g}$$

Effective mass of molecules (Combescot et al EPL 2009)

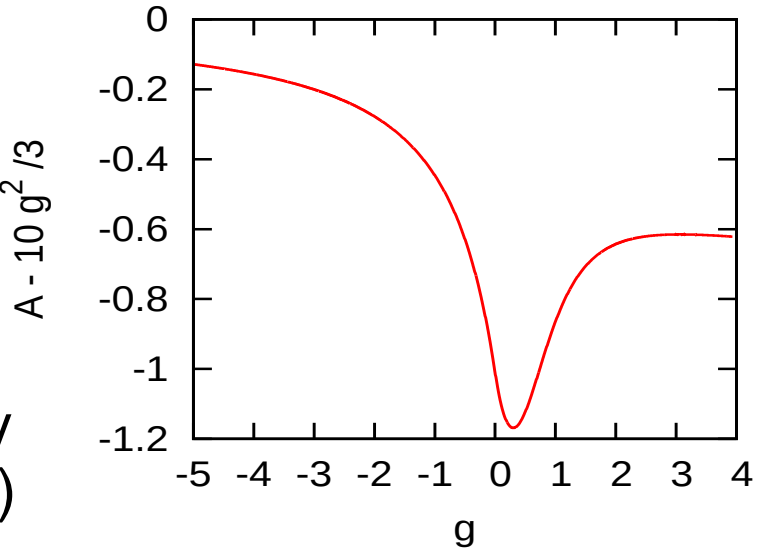
Effective Molecule - free fermions Interaction. (Combescot et al EPL 2009)

g	C
0.60	12.39(10)
0.75	3.37(2)
1.00	1.54(2)
5.00	0.60(1)

Correction to effective mass or p-wave energy contribution between fermionic molecules. Fit to JMS-DMC data (fixed a_{BB})

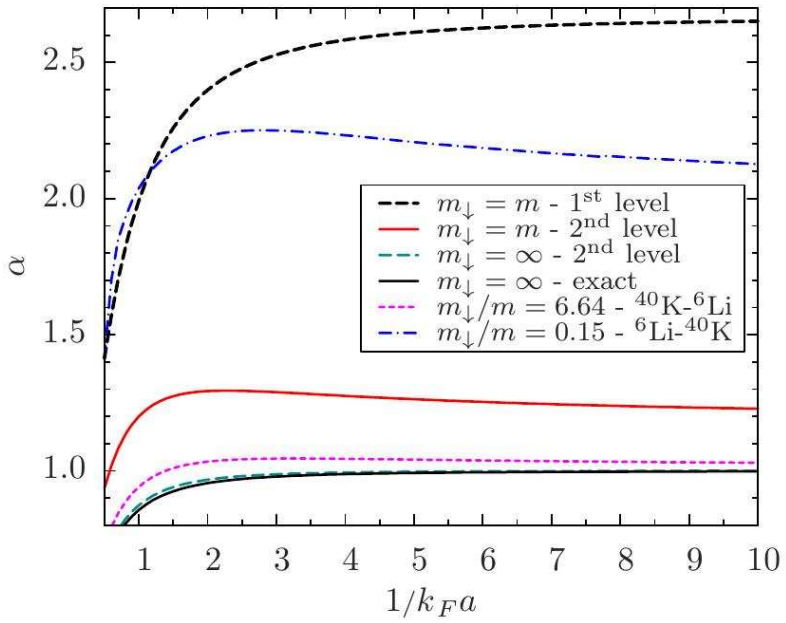
Polarons and molecules in 3D

Diagrammatic and QMC calculations agree
Transition at g~0.9
In Fermi-Fermi mixtures the transition is masked at finite concentration by phase separation



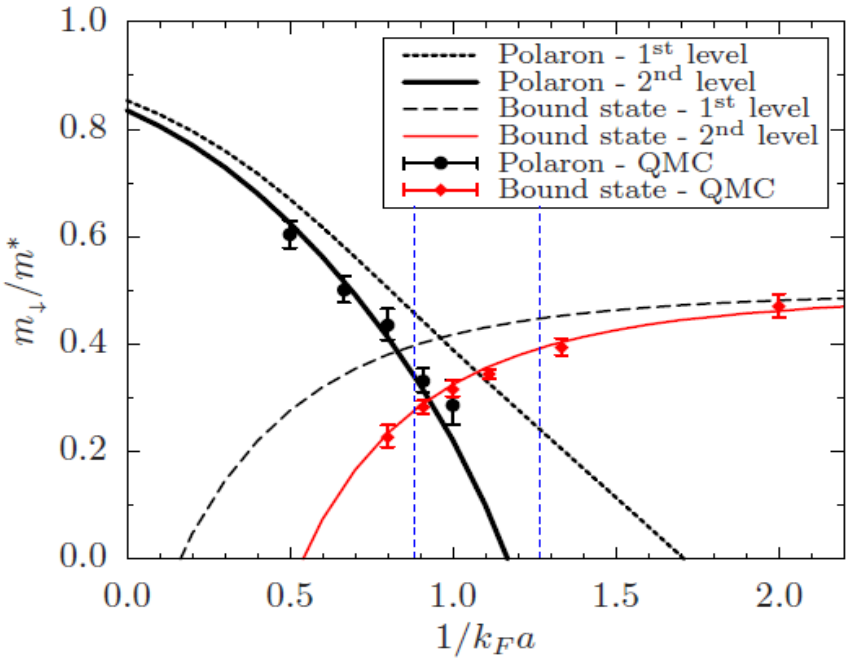
Polaron binding energy
(P. Pieri)

Atom - Molecule scattering

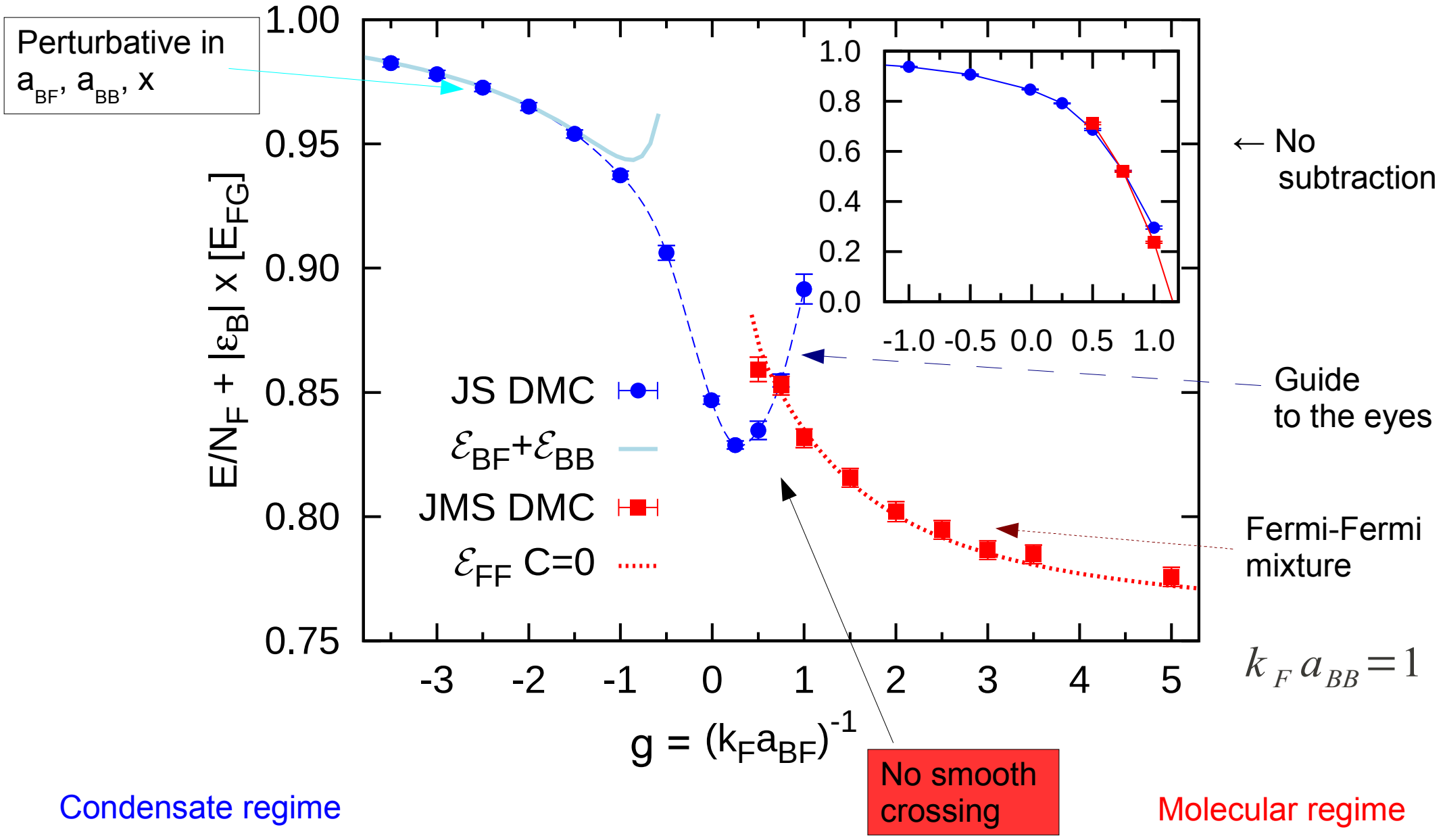


(from Combescot et al. EPL 2009)

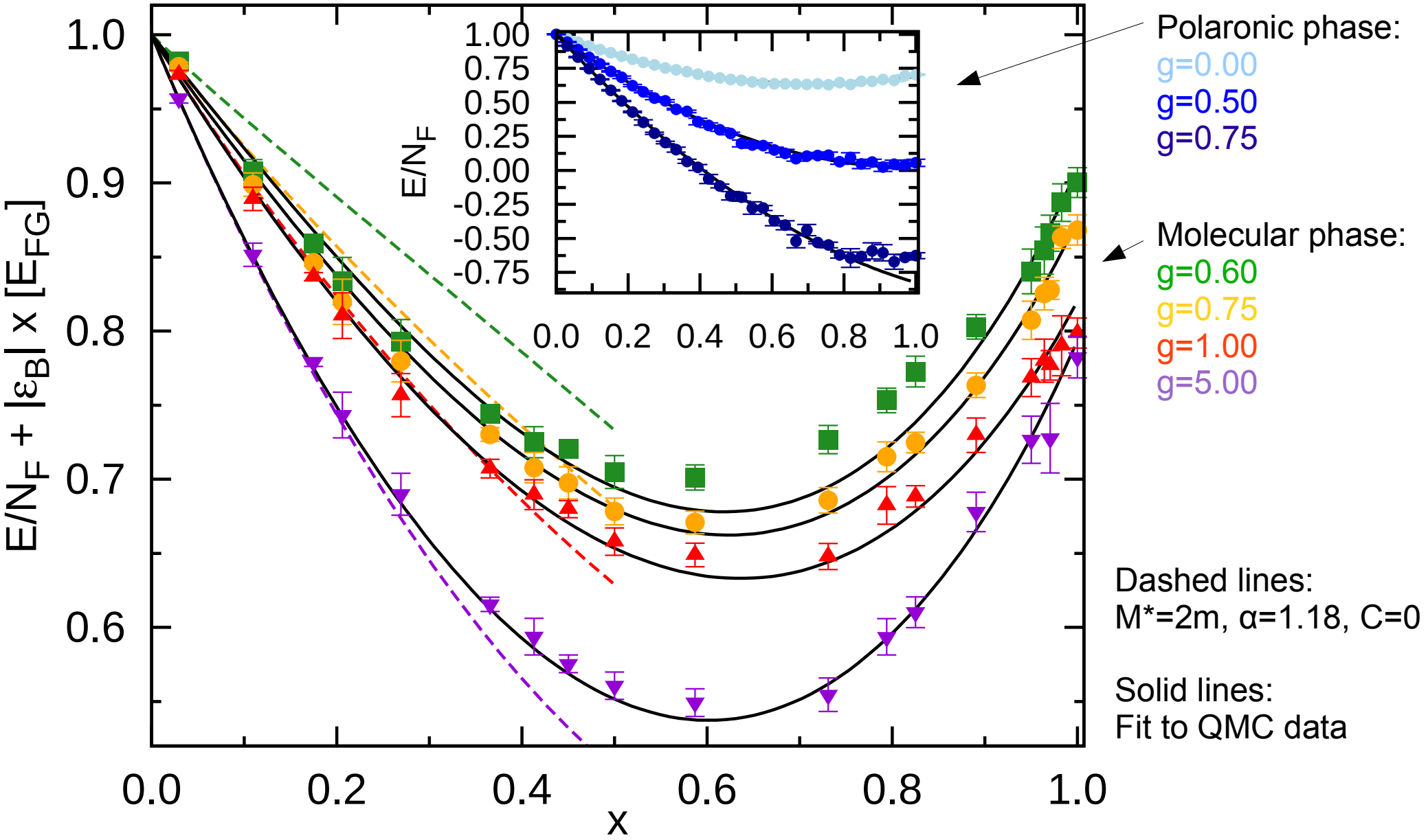
Molecule effective mass



Example: Energy per particle at x=0.175 with binding energy of molecules subtracted



Energy versus concentration of bosons, for various BF couplings



QMC Finite size correction ~ E(infinite)-E(N) for ideal Fermi gas

Phase Diagram at small concentration

$k_F a_{BB} = 1$

$$n_0 = \lim_{r \to \infty} g_B^{(1)}(r)$$

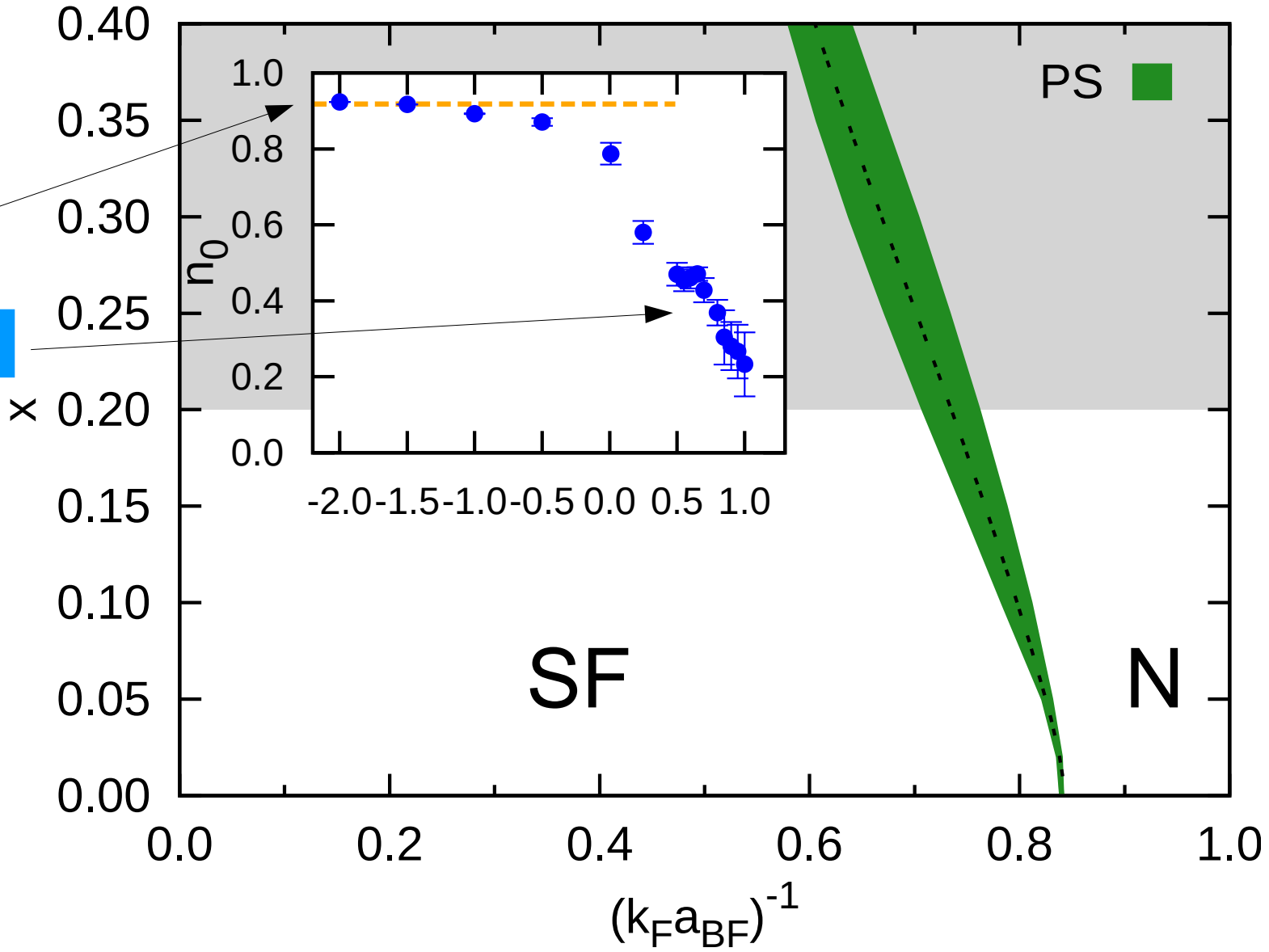
at x=0.175

BB depletion

Role of BF interaction

We assume
$n_0 = 0$
on molecular side

Local Density Approximation



Caveat: for $g^{(1)}$ dependence on the wavefunction in DMC calculations

First order transition (Note: predictions of second order transition exist)

Narrow phase separation at finite x, disappearing at x = 0.
Polaron - molecule transition not masked!

Each energy functional contains only a single fitting parameter

Outlook

- Role of BB repulsion for the stability of the bosonic component
- Mass imbalanced case
- Finite range effects
- Calculation of momentum distributions via unbiased path integral methods
- Investigation of a possible phase in which molecules and polarons coexist