Quantum Monte Carlo study of a resonant Bose-Fermi mixture

ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE

G. Bertaina[1], E. Fratini[2], S. Giorgini[3], P. Pieri[2], V. Savona[1]

[1] *Institute of Theoretical Physics, Ecole polytechnique fédérale de Lausanne EPFL, CH-1015 Lausanne, Switzerland*
[2] *Sezione di Fisica, Scuola di Scienze e Tecnologie, Università di Camerino and CNISM, I-62032 Camerino, Italy*
[3] *INO-CNR BEC Center and Dipartimento di Fisica, Università di Trento, 38123 Povo, Italy*
[1] gianluca.bertaina@epfl.ch

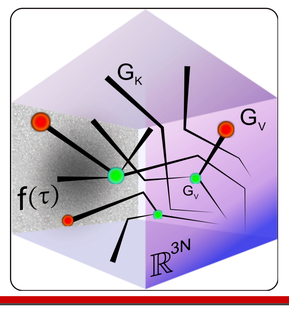
We study resonant Bose-Fermi mixtures at zero temperature, with different relative concentrations of the bosons. We use for the first time a Quantum Monte Carlo method with Fixed-Node approximation, to explore the system from the weak to the strong coupling limit. A repulsive interaction among bosons is introduced to provide stability to the bosonic component. Beyond the unitarity limit, the resonant attractive interaction supports a bound fermionic dimer. At the many-body level, increasing the boson-fermion coupling the system undergoes a quantum phase transition from a state with condensed bosons immersed in a Fermi sea, to a normal Fermi-Fermi mixture of the composite fermions and the bare fermions in excess. We obtain the equation of state and we characterize the momentum distributions both in the weakly and in the strongly interacting limits. We compare Quantum Monte Carlo results to T-matrix calculations, finding interesting signatures of the different many-body ground states.

Ultracold Gases and Diffusion Monte Carlo Method (DMC)

Heteronuclear atoms (B, F)
Low T $k_B T \ll \varepsilon_F$
Diluteness $k_F R \ll 1$

$\frac{E}{N} = E_{FG} e(x, \mu, \eta, \zeta)$

$E_{FG} = \frac{3}{5}\varepsilon_F = \frac{3}{5}\frac{\hbar^2 k_F^2}{2m_F}$, $n_F = \frac{k_F^3}{6\pi^2}$
$x = \frac{n_B}{n_F}$ $\mu = \frac{m_B}{m_F}$ $\eta = \frac{1}{k_F a_{BF}}$ $\zeta = k_F a_{BB}$
We set $m_B = m_F$ ($\simeq$ isotopic atoms)



Effective hamiltonian $H = K + V$: kinetic energy + 2-body single channel effective interactions
(We can only consider Feshbach molecules)
Observables: $\frac{\langle\Psi|\hat{\mathcal{O}}|\Psi\rangle}{\langle\Psi|\Psi\rangle}$ Variational MC (VMC): sampling from trial function $p(X) = |\Psi_T(X)|^2$ (Metropolis algorithm).
Diffusion MC (DMC): sampling from $f(X,\tau) = |\Psi_0^{FN}(X,\tau)\Psi_T(X)|$
DMC: Schroedinger equation in imaginary time $-\frac{\partial}{\partial\tau}\Psi(\tau) = \hat{H}\Psi(\tau)$ ($\rightarrow$ Fixed N_F,N_B)
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 with Trial (guide) wavefunction: fixed nodal surface $f(X,\tau) = \Psi^{FN}(X,\tau)\Psi_T(X) \geq 0$
Exact for bosons. For fermions, Fixed Node approximation: $\Psi_0^{FN}(X)$ not exact ground state, but same nodes as $\Psi_T(X)$

Bose-Fermi mixtures

Interesting phenomena:

- ♢ Role of statistics and mass imbalance
- ♢ Three-body effects (bosons), Efimov states
- ♢ p-wave boson mediated fermion pairing
- ♢ Dipolar molecules
- ♢ Interaction between Feshbach Fermi molecules
- ♢ Bosonic/fermionic polarons
- ♢ Condensate depletion due to BF interaction
- ♢ Presence of an optical lattice

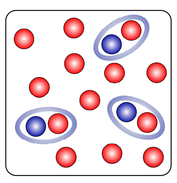
Theory:

- Mean-field Marchetti et al. PRB 2008
- T-matrix Fratini, Pieri PRA 2010,2012
- Functional approach Powell et al. PRB 2005, Ludwig et al. PRA 2011
- Variational Yu et al. PRA 2011

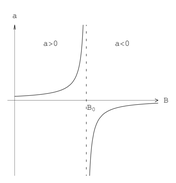
Experiments:

- Finding good Feshbach resonances
- Role of 3-body recombination
- Molecular chemical reactions
- Going to rovibrational ground-state

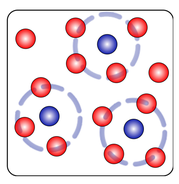
^{40}K-^{87}Rb Feshbach molecules in lattice, repulsive mixture, lifetimes ($\tau = 100ms$):
Ospelkaus et al. PRL 2006, Zaccanti et al. PRA 2006, Zirbel et al. PRL 2008
^{40}K-^{87}Rb ground state molecules:
Ni et al. Science 2008
^{40}K-^{41}K-^{6}Li degenerate mixture:
Wu et al. PRA 2012
^{23}Na-^{40}K: Feshbach molecules ($\tau = 8ms$)
Wu et al. arxiv 2012
^{23}Na-^{6}Li: Feshbach molecules ($\tau = 1.2ms$)
Heo et al. arxiv 2012



Strong coupling:
molecular fermions + free fermions
Complete depletion of the condensate



Resonant interaction
(Feshbach)
Tune a_{BF}



Weak coupling:
free bosons + free fermions
Condensate of bosons

Intermediate interaction: **Quantum phase transition (T=0)**

— Types of nodal surfaces —

Condensate nodal surface: $\Psi_{JS} = J_{BB}J_{BF}\Phi_A^S(N_F) \quad J_{SS'}(\mathbf{R}) = \prod_{\substack{i\in S\\ i'\in S'}} f_{SS'}(\mathbf{r}_i - \mathbf{r}_{i'})$

Single Fermi sphere: $\Phi_A^S(N_F)$ Slater determinant (PBC)
Stability: repulsive Bose-Bose interaction $\zeta = k_F a_{BB} = 1 \rightarrow n_B a_{BB}^3 \approx 10^{-3}$
Model potential: (not so-)Soft Sphere (Non-universality)

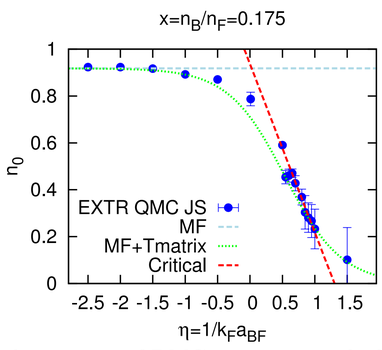
Molecular nodal surface: $\Psi_{JMS} = J_{BB}\Phi_A^{MS}(N_M = N_B, N_F)$

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

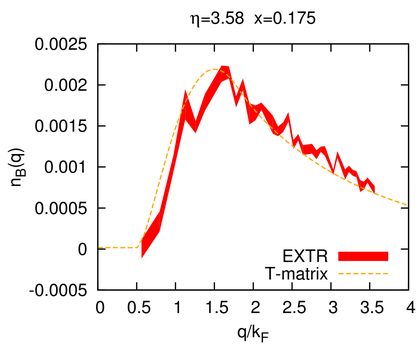
CM motion is relevant (two Fermi spheres)
$\varphi_{K_\alpha}(i,i') = f_b(|\mathbf{r}_i - \mathbf{r}_{i'}|)\exp(i\mathbf{K}_\alpha(\mathbf{r}_i + \mathbf{r}_{i'})/2)$
Each boson in a different molecular orbital
Symmetrization not necessary for energy
(but problems with OBDM)

— Momentum distributions of Bosons —

"Condensate" branch



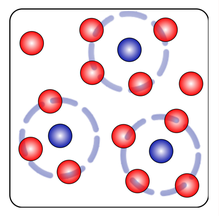
"Molecular" branch



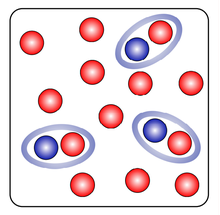
Due to limitations of DMC, we cannot calculate n_0 for JMS near unitarity:
assume $n_0 = 0$ (this implies a 1^{st} order transition)

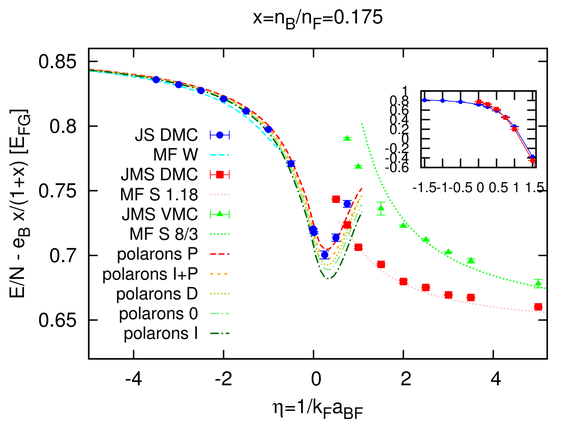
— Energy functionals —

Bosonic Polarons
$\frac{E^{pol}(x,\eta,\zeta)}{N_F E_{FG}} = 1 - A(\eta)x + \frac{10}{9\pi}\zeta x^2\left(1 + \sqrt{x}\zeta^{3/2}\frac{128}{15\pi\sqrt{6\pi}}\right) + F(\eta,\zeta)x^2$
$A(\eta)$ binding energy of polaron
$F(\eta,\zeta)$: role of induced interactions, depletion
(Yu, Pethick PRA 2012, Yu et al. PRA 2011, Mora, Chevy PRL 2011)



Fermi-Fermi mixture
$\frac{E^{mol}(x,\eta,\zeta)}{N_F E_{FG}} = -\frac{10}{3}\eta^2 x + \frac{m}{M^*(\eta)}x^{5/3} + (1-x)^{5/3} + \frac{5\alpha}{3\pi\eta}x(1-x) + I_2(x)\left(\frac{\alpha}{\eta}\right)^2 + E_d(x,\eta,\zeta)$
$\alpha = 1.18$ (8/3 Born approx.)
$\frac{m}{M^*(\eta)}$ effective mass of fermionic molecules
I_2 second order Fermi-Fermi interaction term
$E_d(x,\eta,\zeta)$ molecule-molecule interaction (see below)

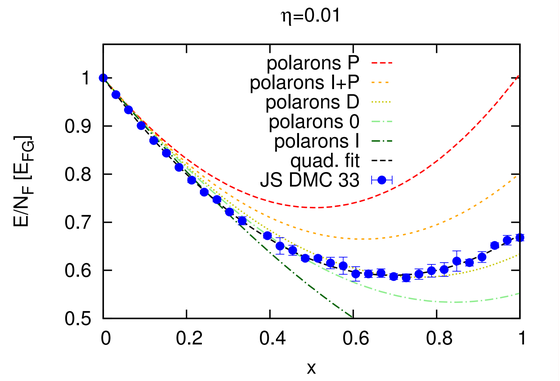


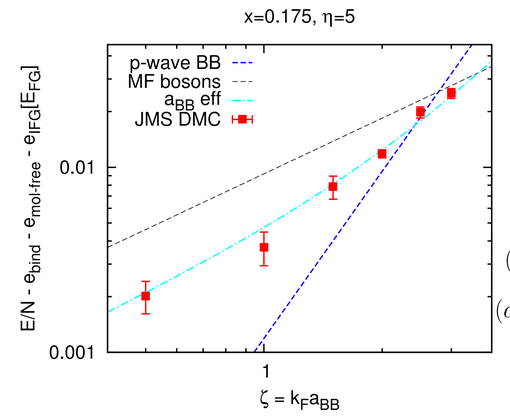


— Energy per particle from QMC —

- Extreme limits compatible with energy functionals
- **Polaronic regime**: A from T-matrix
  (0) $F = 0$
  (P) $F \propto \zeta\left(\frac{\partial A}{\partial\varepsilon_F}\right)^2$
  (I) $F \propto -\left(\frac{\partial A}{\partial\varepsilon_F}\right)^2$
  (D) $F \propto \zeta D(\eta)$
- **Molecular regime**
  – M^* from T-matrix (Combescot et al. EPL 2009)

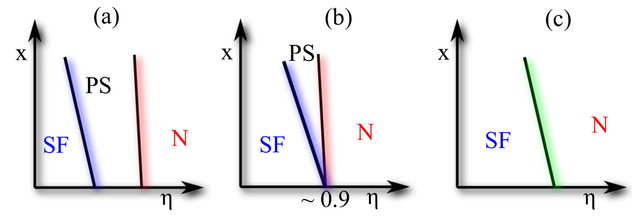
— Energy at unitarity as a function of x —
Good quadratic fit (at least) up to $x = 1$





— Dependence on ζ (Molecular regime) —
(MF) $\frac{\Delta E}{E_{FG}} = \frac{10}{9\pi}\zeta x^2$
(p-wave) $\frac{\Delta E}{E_{FG}} = \frac{\beta^3}{3\pi}x^{8/3}$, with $\beta = k_F a_p$ (assume $a_p \propto a_{BB}$)
(a_{BB} eff) $\frac{\Delta E}{E_{FG}} = \frac{1}{2}\frac{10}{9\pi}\zeta_{eff}x^2\left(1 + \sqrt{x}\zeta_{eff}^{3/2}\frac{128}{15\pi\sqrt{6\pi}}\right)$
$\zeta_{eff} = 0.85(4)\zeta$

— Tentative phase diagram, small x —
We cannot consider case (c)
Case (b) allows direct observation of transition avoiding phase separation



— Conclusions and perspectives —

- Important role of x^2 coefficient in the bosonic polarons functional
- New wavefunction for composite fermions
- Useful comparison to T-matrix calculations
- Unveiled polaron-molecule transition ($x = 0$)
- Need for interpretation of interaction between molecules
- Investigation of condensate fraction in molecular branch
- Role of mass imbalance