MB31 - TRENTO

F. Pederiva

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L. Colletti (high school teacher)

(A. Yu Illarionov)

Activities

- Nuclear structure: hypernuclei and hyperon physics (talk D. Lonardoni). Neutron stars
- Accurate response functions for many-body systems from Integral Transforms (talk A. Roggero)
- Low-dimensional electron systems: spin-orbit (Rashba) interactions, inhomogeneous systems.

SNM & PNM @ T > 0

A. Yu. Illarionov, S. Gandolfi, K.E. Schmidt, S. Fantoni, N. Bassan, F.P.

We propose a MIXED APPROACH based on:

Variational evaluation of the finite temperature corrections by means of a Fermi – HyperNetted Chain calculation;

Application of the corrections to theT=0 equation of state computed with the DDI

The variational calculations are based on the Gibbs-Bogoliubov inequality:

$$F(\rho,T) \leq F_V(\rho,T) = \mathrm{Tr}\,(\rho_V H) - TS_V(\rho,T)$$

where ρ_v is the thermal density matrix defined by:

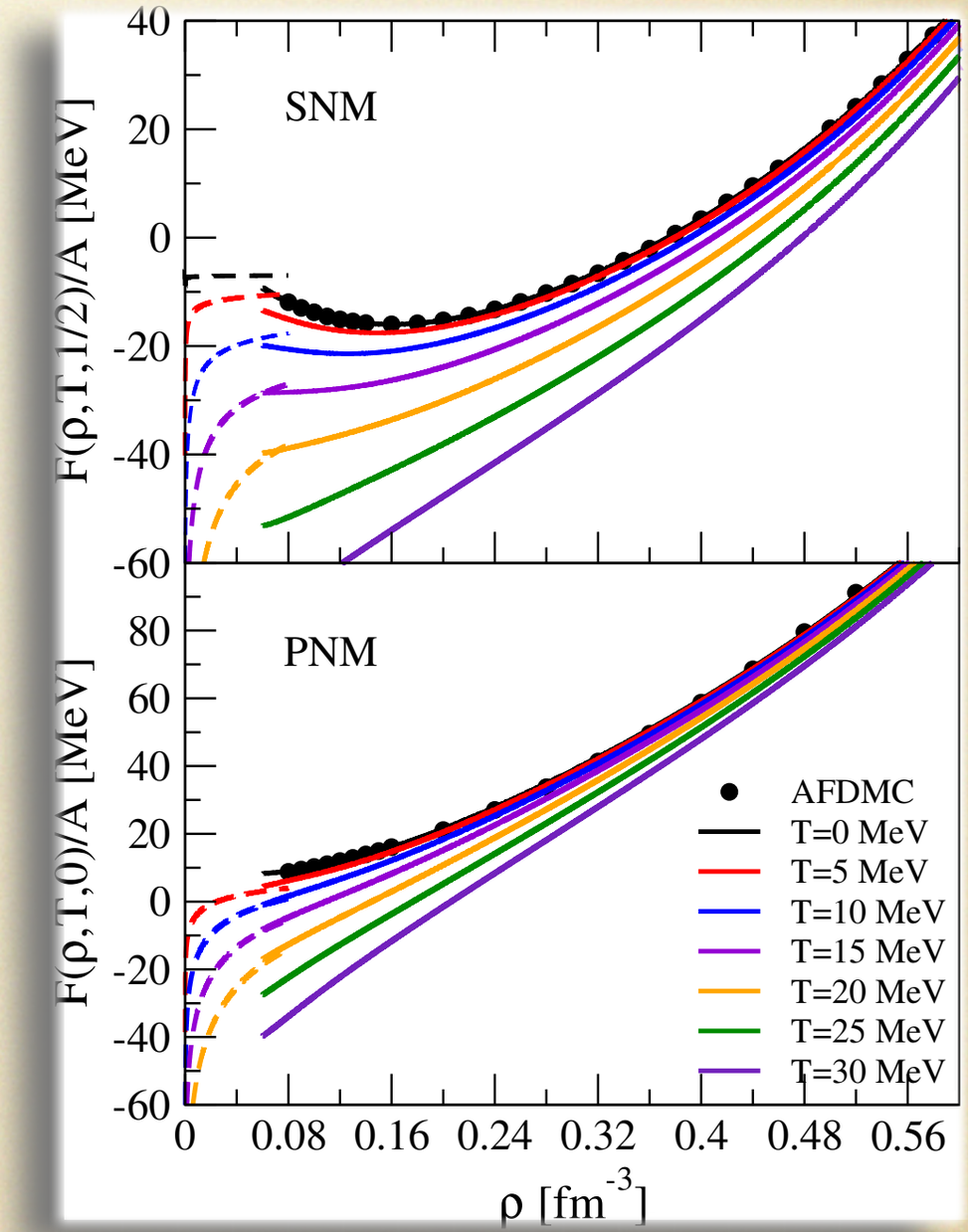
$$\rho_V = \frac{\exp(-\beta H_V)}{\mathrm{Tr}(-\beta H_V)} \qquad \beta = 1/K_B T$$

In FHNC calculations H_v is chosen in such a way that:

$$H_V|\Psi_i\,[n_i(\mathbf{k})]\rangle = \left[\sum_{\mathbf{k}} n_i(\mathbf{k})\epsilon_V(\mathbf{k},\rho,T)\right]|\Psi_i\,[n_i(\mathbf{k})]\rangle$$

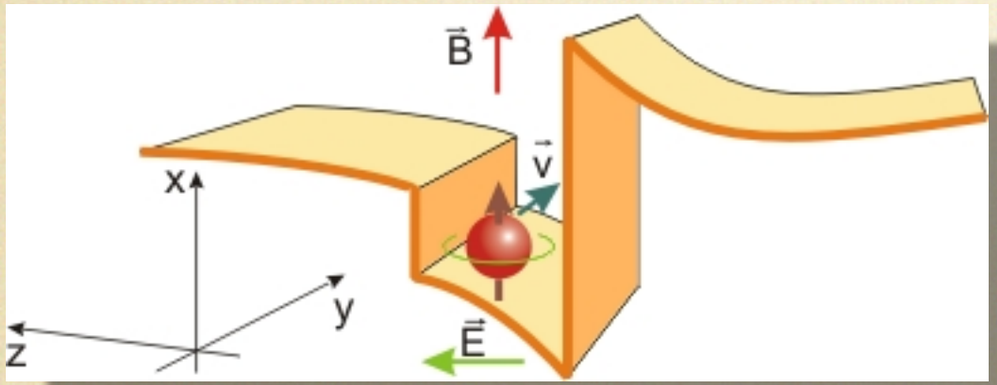
where the Ψ_i are correlated basis states, function of the occupation numbers n(k), and the function ε_V introduces the temperature dependence

$$\epsilon(\mathbf{k},\rho,T) = \frac{\hbar^2 k^2}{2m\left[1 + A(\rho,T)\exp\left(-B(\rho,T)k^2\right)\right]} \quad \sim 0$$

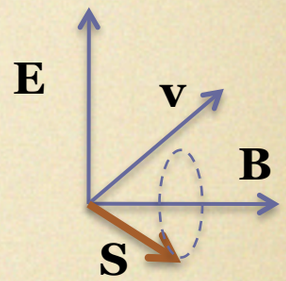


Many electron systems

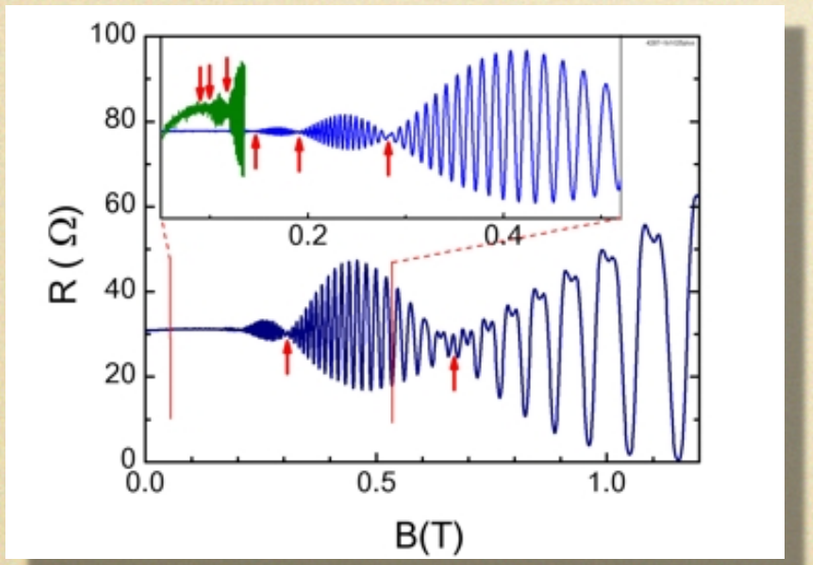
Topic: Rashba interactions / spin orbit
(E. Lipparini, A. Ambrosetti, F.P.)

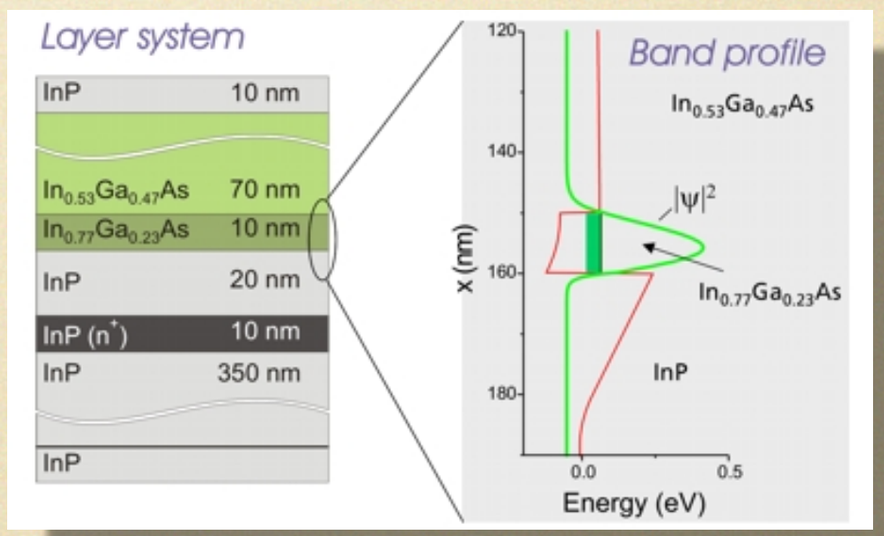


Electrons confined in a 2D quantum well are subject to the effect of an electric field **E** perpendicular to the plane containing the electrons if the confining potential is ***asymmetric***

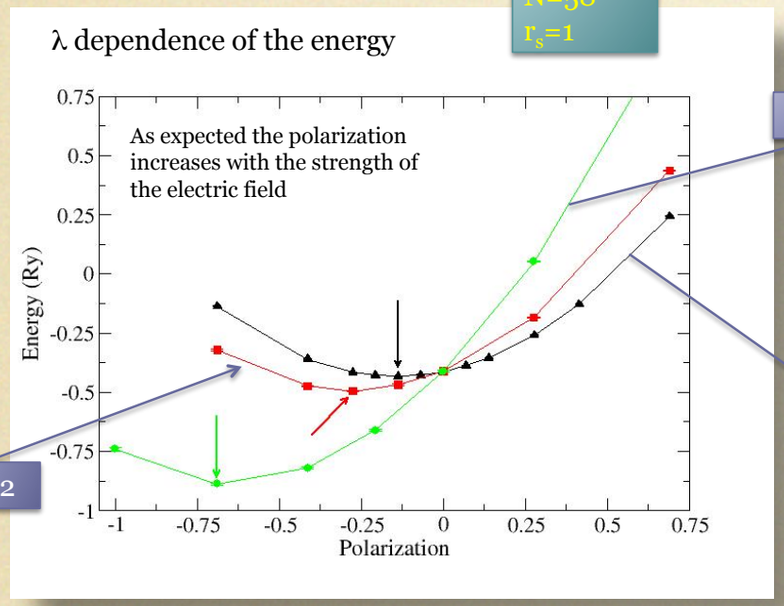


$$V_{Rashba} = \frac{\lambda}{\hbar}\sum_{i=1}^{N}\left[p_i^x\sigma_i^y - p_i^y\sigma_i^x\right] \propto \vec{S}\cdot\vec{B}$$





Many electron systems

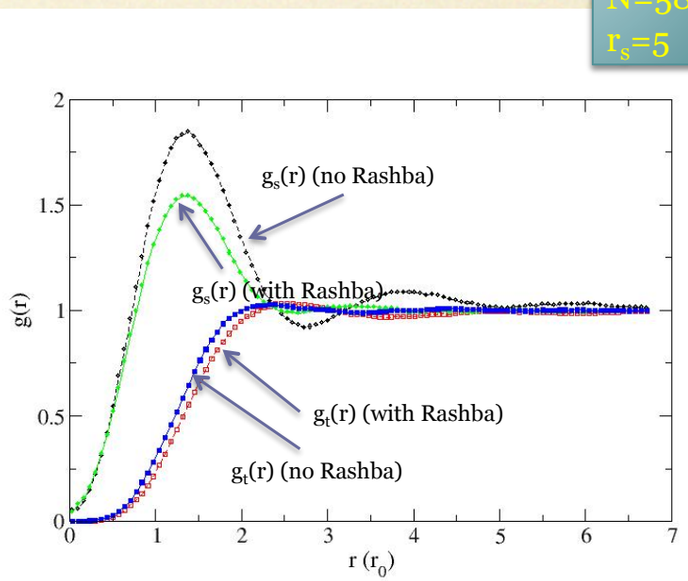


N=58
r_s=1

λ=0.5

λ=0.1

λ=0.2



N=58
r_s=5

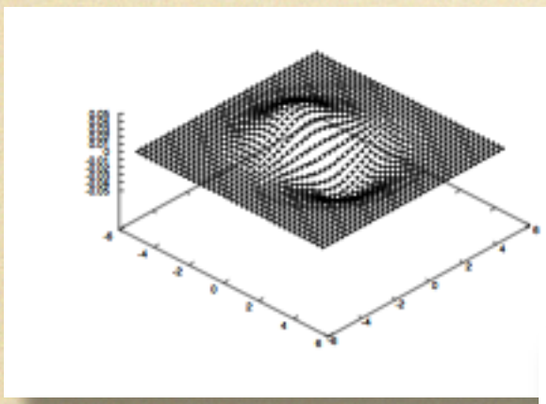
It is possible to compute pair distribution functions in the spin-singlet and spin-triplet channels.

$$g_c(r) = N\sum_{i<j}\frac{\langle\Psi|\delta(|r_i - r_j|)|\Psi\rangle}{\langle\Psi\|\Psi\rangle}$$

$$g_\sigma(r) = N\sum_{i<j}\frac{\langle\Psi|\delta(|r_i - r_j|)\vec{\sigma}_i\cdot\vec{\sigma}_j|\Psi\rangle}{\langle\Psi\|\Psi\rangle}$$

$$g_s(r) = \frac{1}{4}\left[g_c(r) - g_t(r)\right]$$

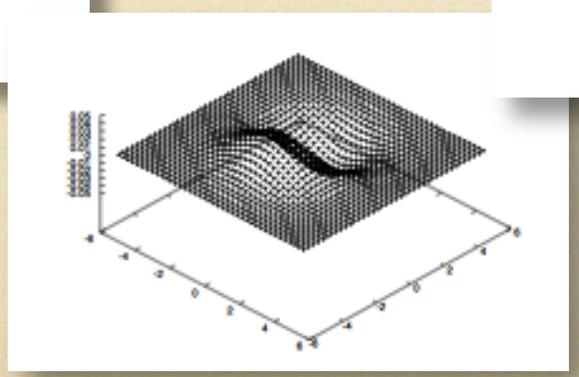
$$g_s(r) = \frac{1}{4}\left[3g_c(r) + g_t(r)\right]$$

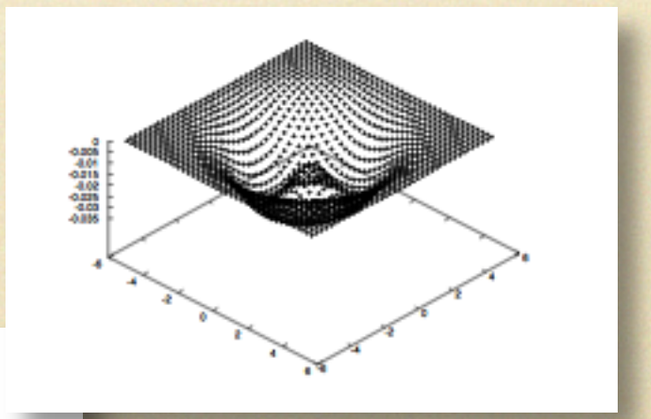


x component:
broken symmetry

N=3
ω=0.28 λ=0.1

y component:
broken symmetry





z component :
circular symmetry

Future extensions

- Atoms and solids (A. Ambrosetti, L. Mitas)
- Ultracold Atoms

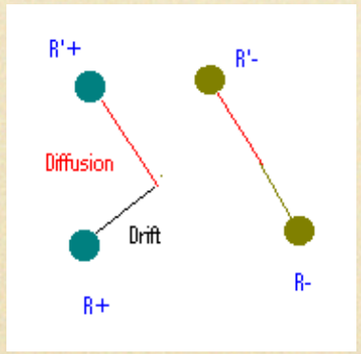
QMC Algortihms

Sign Problem **(shall thou have no uncontrolled approximations....)**

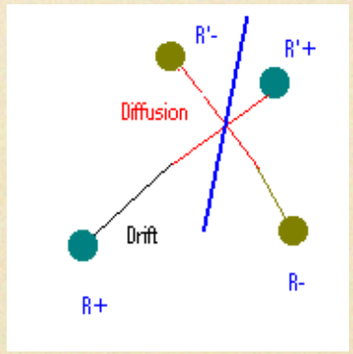
(M.H. Kalos, A. Roggero)

Still work in progress. We are exploration the possibility that the plus/minus symmetry in the Diffusion Monte Carlo algorithm is broken by choosing a position-dependent dynamics of pairs of signed walkers.

PARALLEL DYNAMICS



REFLECTED DYNAMICS



$$E_0^A \approx \frac{\sum_i \hat{H}\Psi_T^A(R^+) - \sum_i \hat{H}\Psi_T^A(R^-)}{\sum_i \Psi_T^A(R^+) - \sum_i \Psi_T^A(R^-)}$$

"Exact" propagations can be performed in simple discretized models

QMC Algortihms

Inhomogeneous Fermion Systems

(M.H. Kalos, F. Calcavecchia, F.P.)

Variational Monte Carlo calculations based on Shadow Wave Functions would be an extremely powerful method to address inhomogeneous Fermion matter (think of the NS crust). However, this algorithm suffers of a severe sign problem too.

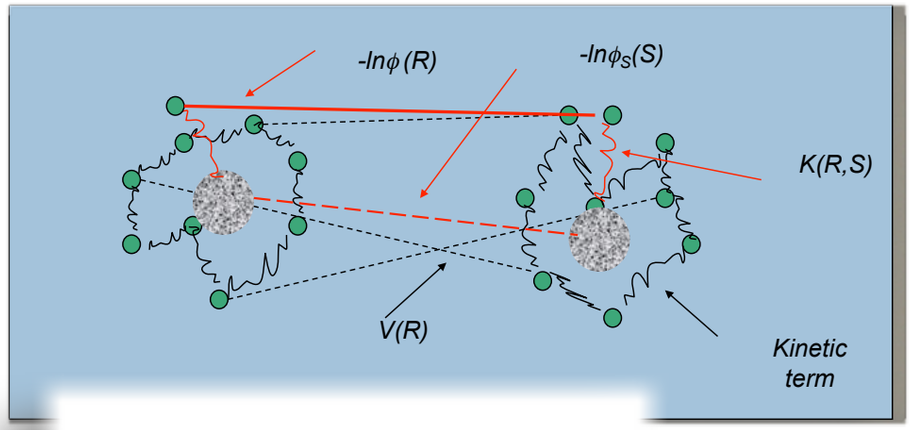
$$\Psi_T^A(R) = \Phi_r(R)\int K(R,S)D_\uparrow(S_\uparrow)D_\downarrow(S_\downarrow)\Phi_s(S)dS$$

$$\frac{\langle\Psi_T^A|O(R)|\Psi_T^A\rangle}{\langle\Psi_T^A\|\Psi_T^A\rangle} = \frac{1}{\langle\Psi_T^A\|\Psi_T^A\rangle}\iiint dRdSdS'\,O(R)|\varphi_r(R)|^2\Xi(R,S,S') =$$

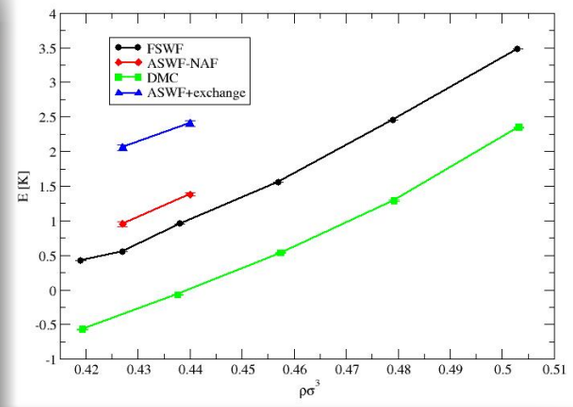
$$= \frac{1}{\langle\Psi_T^A\|\Psi_T^A\rangle}\iiint dRdSdS'\,O(R)|\varphi_r(R)|^2\frac{\Xi(R,S,S')}{|\Xi(R,S,S')|}|\Xi(R,S,S')| =$$

This is a "weight" W(R,S,S')=±1

This is positive, and we can sample from it



$\rho\sigma^3$	E/N(54)	T/N(54)	E/N(53)	T/N(53)
0.419	0.422(1)	23.947(1)	0.69(1)	23.71(3)
0.427	0.548(2)	24.608(1)	0.78(8)	24.6(2)
0.438	0.955(1)	26.005(2)	1.26(1)	25.76(3)
0.457	1.556(1)	27.986(2)	1.844(8)	28.05(2)
0.479	2.455(1)	30.482(2)	2.801(7)	30.60(2)
0.503	3.481(1)	32.487(2)	4.127(7)	32.35(2)



p eople p eople interaction

- Alessandro L., Omar (Crust)
- Giampaolo (AFDMC for nuclei, wavefunctions)
- More?