# **QMC for Cold Atoms and Neutron Matter** Thermodynamic and transport properties

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In the Autumn of 2003 Joaquín Drut walked into my office asking whether he can work with me. I suggested we try together QMC for cold atoms.

All I knew about QMC at the time was that:

- many people do it and that they used random numbers to calculate infinite dimensional integrals
- there was a very challenging problem still largely unsolved in theoretical physics
   The properties of the unitary Fermi gas!
   The Bertsch MBX Challenge
- As I did not know better we started with the grand canonical QMC (hard), instead of T=0 microcanonical QMC (much easier)
- Soon Piotr Magierski joined us, and later others.

# Besides pure theoretical curiosity, cold atom physics is related to neutron stars physics!



Gezerlis and Carlson, Phys. Rev. C 77, 032801(R) (2008)

## **Dilute Fermion Matter**

The ground state energy is given by such a function:

$$E_{gs} = f(N, V, \hbar, m, a, r_0)$$

Taking the scattering length to infinity and the range of the interaction to zero, we are left with:

$$E_{gs} = F(N, V, \hbar, m) = \frac{3}{5} \varepsilon_F N \times \xi$$
$$\frac{N}{V} = \frac{k_F^3}{3\pi^2}, \qquad \varepsilon_F = \frac{\hbar^2 k_F^2}{2m}$$

Pure number Beretsch parameter What George Bertsch essentially asked in 1999 is:

# What is the value of $\xi$ ?! Is it positive?

But he wished to know the properties of the system as well: *The system turned out to be superfluid* !

$$E_{gs} = \frac{3}{5} \varepsilon_F N \times \xi \qquad \Delta = \varepsilon_F \times \zeta$$
$$\xi = 0.372(5), \qquad \zeta = 0.45(5)$$

Now these results are a bit unexpected.

 ✓ The energy looks almost like that of <u>a non-interacting system</u>! (there are no other dimensional parameters in the problem)
 ✓ The system has <u>a huge pairing gap</u>!
 ✓ This system is a very strongly interacting one, since the <u>elementary cross section is huge</u>!



Fig. 2: Vortices in a strongly interacting gas of fermionic atoms on the BEC- and the BCS-side of the Feshbach resonance. At the given field, the cloud of lithium atoms was stirred for 300 ms (a) to 500 ms (b-h) followed by an equilibration time of 500 ms. After 2 ms of ballistic expansion, the magnetic field was ramped to 735 G for imaging (see text for details). The magnetic fields were (a) 740 G, (b) 766 G, (c) 792 G, (d) 812 G, (e) 833 G, (f) 843 G, (g) 853 G and (h) 863 G. The field of view of each image is  $880 \ \mu m \times 880 \ \mu m$ .

#### Zweirlein et al. Nature <u>435</u>, 1047 (2005)

The initial Bertsch's Many Body challenge has evolved over time and became the problem of <u>Fermions in the Unitary Regime</u>. (part of the BCS-BEC crossover problem)

# In cold old gases one can control the <u>strength</u> of the interaction at will!

The system is very dilute, but strongly interacting!



# Phases of a two species dilute Fermi system in the BCS-BEC crossover Normal atomic (plus a few molecules) phase **Strong interaction** weak interaction **between dimers** weak interaction **Molecular BEC and between fermions** Atomic+Molecular **BCS Superfluid** Superfluids 1/aa<0 a>0

no 2-body bound state

shallow 2-body bound state

# Finite Temperatures Grand Canonical Path-Integral Monte Carlo

$$\hat{H} = \hat{T} + \hat{V} = \int d^3x \left[ \psi_{\uparrow}^{\dagger}(\vec{x}) \left( -\frac{\hbar^2 \Delta}{2m} \right) \psi_{\uparrow}(\vec{x}) + \psi_{\downarrow}^{\dagger}(\vec{x}) \left( -\frac{\hbar^2 \Delta}{2m} \right) \psi_{\downarrow}(\vec{x}) \right] - g \int d^3x \ \hat{n}_{\uparrow}(\vec{x}) \hat{n}_{\downarrow}(\vec{x})$$
$$\hat{N} = \int d^3x \left[ \hat{n}_{\uparrow}(\vec{x}) + \hat{n}_{\downarrow}(\vec{x}) \right], \qquad \hat{n}_s(\vec{x}) = \psi_s^{\dagger}(\vec{x}) \psi_s(\vec{x}), \qquad s = \uparrow, \downarrow$$

Trotter expansion

$$Z(\beta) = \operatorname{Tr} \exp\left[-\beta\left(\hat{H} - \mu\hat{N}\right)\right] = \operatorname{Tr} \left\{\exp\left[-\tau\left(\hat{H} - \mu\hat{N}\right)\right]\right\}^{N_{\tau}}, \qquad \beta = \frac{1}{T} = N_{\tau}\tau$$

$$E(T) = \frac{1}{Z(T)} \operatorname{Tr} \hat{H} \exp\left[-\beta \left(\hat{H} - \mu \hat{N}\right)\right]$$
$$N(T) = \frac{1}{Z(T)} \operatorname{Tr} \hat{N} \exp\left[-\beta \left(\hat{H} - \mu \hat{N}\right)\right]$$

No approximations so far, except for the fact that the interaction is not well defined!

Recast the propagator at each time slice and put the system on a 3D-spatial lattice, in a cubic box of side L=N<sub>s</sub>l, with periodic boundary conditions

$$\exp\left[-\tau\left(\hat{H}-\mu\hat{N}\right)\right] \approx \exp\left[-\tau\left(\hat{T}-\mu\hat{N}\right)/2\right] \exp\left(-\tau\hat{V}\right) \exp\left[-\tau\left(\hat{T}-\mu\hat{N}\right)/2\right] + O(\tau^3)$$

Discrete Hubbard-Stratonovich transformation

$$\exp(-\tau \hat{V}) = \prod_{\vec{x}} \sum_{\sigma_{\pm}(\vec{x})=\pm 1} \frac{1}{2} \Big[ 1 + \sigma_{\pm}(\vec{x}) A \hat{n}_{\uparrow}(\vec{x}) \Big] \Big[ 1 + \sigma_{\pm}(\vec{x}) A \hat{n}_{\downarrow}(\vec{x}) \Big], \qquad A = \sqrt{\exp(\tau g) - 1}$$

 $\sigma$ -fields fluctuate both in space and imaginary time

$$\frac{m}{4\pi\hbar^2 a} = -\frac{1}{g} + \frac{mk_c}{2\pi^2\hbar^2}, \qquad k_c < \frac{\pi}{l}. \qquad \mathbf{r}_{eff} = \frac{4}{\pi k_c}$$

Running coupling constant g defined by the lattice constant



 $\delta p >$ 

L

**Momentum space** 



$$Z(T) = \exp\left(-\beta H\right) = \int \prod_{\vec{x},\tau} D\sigma(\vec{x},\tau) \operatorname{Tr} \hat{U}(\{\sigma\}), \quad \beta = \frac{1}{T}, \quad 0 \le \tau \le \beta$$
$$\hat{U}(\{\sigma\}) = T_{\tau} \prod_{\tau} \exp\{-\tau[\hat{h}(\{\sigma\}) - \mu]\} \qquad \text{One-body evolution} \text{operator in imaginary time}$$

$$E(T) = \int \frac{\prod D\sigma(\vec{x}, \tau) \operatorname{Tr} \hat{U}(\{\sigma\})}{Z(T)} \frac{\operatorname{Tr} \left[\hat{H} \hat{U}(\{\sigma\})\right]}{\operatorname{Tr} \hat{U}(\{\sigma\})}$$

 $\operatorname{Tr} \hat{U}(\{\sigma\}) = \{\det[1 + \hat{U}(\{\sigma\})]\}^2 = \exp[-S(\{\sigma\})] > 0 \text{ No sign problem!}$ 

$$n_{\uparrow}(\vec{x},\vec{y}) = n_{\downarrow}(\vec{x},\vec{y}) = \sum_{k,l < k_c} \varphi_{\vec{k}}(\vec{x}) \left[ \frac{\hat{U}(\{\sigma\})}{1 + \hat{U}(\{\sigma\})} \right]_{\vec{k} \ \vec{l}} \varphi_{\vec{l}}^*(\vec{y}), \quad \varphi_{\vec{k}}(\vec{x}) = \frac{\exp(i\vec{k} \cdot \vec{x})}{\sqrt{V}}$$

All traces can be expressed through these single-particle density matrices



Bulgac, Drut, and Magierski PRL <u>96</u>, 090404 (2006), PRA <u>78</u>, 023625 (2008)



$$E_{\text{phonons}}(T) = \frac{3}{5} \varepsilon_F N \frac{\sqrt{3}\pi^4}{16\xi_s^{3/2}} \left(\frac{T}{\varepsilon_F}\right)^4$$
$$E_{\text{quasi-particles}}(T) = \frac{3}{5} \varepsilon_F N \frac{5}{2} \sqrt{\frac{2\pi\Delta^3 T}{\varepsilon_F^4}} \exp\left(-\frac{\Delta}{T}\right)$$
$$\Delta = \left(\frac{2}{e}\right)^{7/3} \varepsilon_F \exp\left(\frac{\pi}{2k_F a}\right)$$

#### PHYSICAL REVIEW A 85, 051601(R) (2012)



FIG. 2. (Color online) Energy  $E/E_{\rm FG}$  (red dots), as obtained by Ku *et al.* [8]. Our AFQMC results extrapolated to infinite volume are shown by open black circles. The results for  $N_x = 8$  (open blue squares) were obtained with the DMC algorithm in Ref. [9]. The green square shows the QMC result of Ref. [20] for  $\xi$  at T = 0. The inset shows the vicinity of the superfluid phase transition at  $T_c/\epsilon_F \simeq 0.15$ .

FIG. 4. (Color online) Density  $n(\mu,T)$  of the UFG (red circles) as obtained by Ku *et al.* [8], normalized to the density  $n_0(\mu,T)$  of a noninteracting Fermi gas. The notation for the AFQMC results is identical to Fig. 2. The diagrammatic MC results of Refs. [21,22] (solid up and down triangles) and the Bold Diagrammatic MC results of Ref. [23] are shown as well (solid squares). The inset shows the vicinity of the superfluid phase transition at  $T_c/\epsilon_F \simeq 0.15$ .

## Critical temperature for superfluid to normal transition



Bulgac, Drut, and Magierski, Phys. Rev. A 78, 023625 (2008)

Amherst-ETH: Hard and soft bosons: Burovski et al. Phys. Rev. Lett. <u>101</u>, 090402 (2008) Pilati et al. PRL <u>100</u>, 140405 (2008)



## Matsubara propagator, spectral function and linear response

$$G(\vec{p},\tau) = \frac{1}{Z} \operatorname{Tr} \left\{ \exp\left[-\left(\beta - \tau\right)\left(H - \mu N\right)\right] \psi^{\dagger}(\vec{p}) \exp\left[-\tau\left(H - \mu N\right)\right] \psi(\vec{p}) \right\}$$
$$= -\frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega A(\omega, \vec{p}) \frac{\exp(-\omega\tau)}{1 + \exp(-\omega\beta)}$$
$$\frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega A(\omega, \vec{p}) = 1, \quad \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega A(\omega, \vec{p}) \frac{1}{1 + \exp(\omega\beta)} = n(\vec{p}), \quad A(\omega, \vec{p}) \ge 0$$

$$\chi_{s} = \lim_{p \to 0} \frac{1}{V} \int_{0}^{\beta} d\tau \left\langle s_{z}(\vec{p}, \tau) s_{z}(-\vec{p}, 0) \right\rangle, \qquad s_{z}(\vec{p}, \tau) = n_{\uparrow}(\vec{p}, \tau) - n_{\downarrow}(\vec{p}, \tau)$$



Singular value decomposition and maximum entropy method reconstruction of the spectral function





Chen et al, Low Temp. Phys. 32, 406 (2006)







$$G(p,\tau) = \frac{1}{Z} \operatorname{Tr} \left\{ \exp\left[-\left(\beta - \tau\right)\left(H - \mu N\right)\right] \psi^{\dagger}(p) \exp\left[-\tau\left(H - \mu N\right)\right] \psi(p) \right\}$$
$$= -\frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega A(p,\omega) \frac{\exp(-\omega\tau)}{1 + \exp(-\omega\beta)}$$









Using photoemission spectroscopy to probe a strongly interacting Fermi gas Stewart, Gaebler, and Jin, Nature, <u>454</u>, 744 (2008)



# KSS conjecture

[Kovtun, Son, Starinets, PRL (2005)]



#### Bound has been proposed on the basis of string theory.

Valid for large class of (string) theories

Saturated for the case of strongly coupled theory.

### Slide from a talk given by G. Wlazlowski

1.0

1.5

2.0

He near λ–transitior

QGP

3.0

String theory

2.5

$$\begin{split} G_{\Pi}(\vec{q},\tau) &= \frac{1}{V} \left\langle \Pi_{\vec{q}}^{(xy)}(\tau) \Pi_{-\vec{q}}^{(xy)}(0) \right\rangle \\ \Pi_{0}^{(xy)} &= \sum_{\vec{p},\sigma} p_{x} p_{y} a_{\sigma}^{\dagger}(\vec{p}) a_{\sigma}(\vec{p}) \\ \Pi_{\vec{q}}^{(xy)}(\tau) &= e^{-\tau(H-\mu N)} \Pi_{\vec{q}}^{(xy)} e^{\tau(H-\mu N)} \\ G_{\Pi}(0,\tau) &= \frac{1}{\pi} \int_{0}^{\infty} d\omega \ \eta(\omega) \omega \frac{\cosh\left[\omega(\tau-\beta/2)\right]}{\sinh(\omega\beta/2)} \\ \int_{0}^{\infty} d\omega \left[ \eta(\omega) - \frac{C}{15\pi\sqrt{\omega}} \right] &= \frac{\varepsilon}{3} - \frac{C}{12\pi a}, \ \eta(\omega) \ge 0 \\ n(p) &\approx \frac{C}{p^{4}} \ \text{when } (p \to \infty) \\ E &= TS - pV + \mu N \\ \frac{S(x,y)}{N} &= \frac{\xi(x,y) - \zeta(x,y) + \frac{C(x,y)y}{6\pi Nk_{F}}}{6\pi Nk_{F}}, \\ \text{where } x &= \frac{T}{\varepsilon_{F}}, \ y = \frac{1}{k_{F}a}, \ E = \frac{3}{5} \varepsilon_{F} \xi(x,y), \ \mu = \varepsilon_{F} \zeta(x,y) \end{split}$$





$$\eta = \alpha \hbar n$$



Joseph, Elliott, and Thomas, Phys. Rev. Lett. 115, 020406 (2015)









Shear viscosity at and near unitarity





#### High temperature kinetic theory

Bluhm and Schäfer, Phys. Rev. A 90, 063615 (2014)

$$t = \frac{T}{\varepsilon_F}, x = \frac{1}{k_F a}$$
$$z = \frac{n\lambda^3}{2} \text{ (fugacity)}$$

Expansion to order 
$$O\left(\left(\frac{\lambda}{a}\right)^2\right)$$
 and  $O\left(z\frac{\lambda}{a}\right)$ 



$$\chi_{s} = \lim_{p \to 0} \frac{1}{V} \int_{0}^{\beta} d\tau \left\langle s_{z}(\vec{p}, \tau) s_{z}(-\vec{p}, 0) \right\rangle, \qquad s_{z}(\vec{p}, \tau) = n_{\uparrow}(\vec{p}, \tau) - n_{\downarrow}(\vec{p}, \tau)$$

## **Spin susceptibility**





$$j_{s} = j_{\uparrow} - j_{\downarrow} = \sigma_{s} \dot{F} \quad \text{- spin conductivity}$$

$$\Gamma_{sd} = \frac{n}{\sigma_{s}}, \ \sigma_{s} \ge 0$$

$$G_{s}^{jj}(\vec{q},\tau) = \frac{1}{V} \left\langle \left[ j_{q\uparrow}^{z}(\tau) - j_{q\downarrow}^{z}(\tau) \right] \left[ j_{q\uparrow}^{z}(0) - j_{q\downarrow}^{z}(0) \right] \right\rangle$$

$$\vec{j}_{s} = -D_{s} \vec{\nabla} \left( n_{\uparrow} - n_{\downarrow} \right) \quad \text{- spin drag}$$

$$D_{s} = \frac{\sigma_{s}}{\chi_{s}} \quad \text{(Einstein relation)}$$

$$D_{s} \approx v\lambda \sim 1 \quad \text{(kinetic theory)}$$

## Now back to realistic Nuclear Physics



Somebody else's slidee

Entem and Machleidt parameterization of the NN and NNN interaction with  $\Lambda$ =414 MeV/c

- NN phase shifts up to lab energies 200 MeV with  $\chi^2/DOF = 1.44$
- Binding energy and lifetime of <sup>3</sup>H

- Empirical nuclear matter saturation point and critical point of liquid-gas phase transition

see Corragio et al, Phys. Rev. C 75, 024311 (2007) Phys. Rev. C 87, 014322 (2013) Machleidt and Entem, Phys. Rep. 503, 1 (2011) Microcanonical QMC at T=0  $\Delta \tau = 0.1 \text{ MeV}^{-1}$  and about 300 imaginary time steps

$$\Delta x = \frac{\pi \hbar}{\Lambda} = 1.5 \text{ fm and } \Lambda = 414 \text{ MeV/c}$$

$$N_x = N_y = N_z = 10, 12, 14, 16$$

$$N_{\text{part}} = 38 - 340 \text{ neutrons}$$
(previous "record" in nuclear physics  $\approx 100 \text{ neutrons}$ )
$$\langle \psi | O | \psi \rangle^{\text{cont}} \approx \langle \psi | O | \psi \rangle \frac{\langle \psi_0 | O | \psi_0 \rangle^{\text{cont}}}{\langle \psi_0 | O | \psi_0 \rangle}$$

$$f(p,p') = \exp\left(-\left(\frac{p}{\Lambda}\right)^{20} - \left(\frac{p'}{\Lambda}\right)^{20}\right), \quad \Lambda = 414 \text{ Mev/c}$$

$$H = T + V_{\text{evol}} + (V - V_{\text{evol}})$$
$$V = V_{2N} + V_{3N}$$

$$\psi(\tau \to \infty) \propto \exp(-\tau H_{evol})\psi_0$$

$$V_{\text{evol}} = \sum_{\alpha = \pi, \sigma, \omega} \frac{V_{\alpha}}{m_{\alpha}^2 + q^2} f(q), \quad f(q) = \exp\left(-\left(\frac{q}{\Lambda}\right)^{30}\right)$$

$$\chi^{2} = \sum_{i,j} w^{(j)} \left[ \delta^{j}_{\text{EFT}}(E_{i}) - \delta^{j}_{\text{evol}}(E_{i}) \right]^{2} + \alpha \left[ E^{\text{pert}}_{\text{EFT}} - E^{\text{pert}}_{\text{evol}} \right]^{2}, \quad j = \text{s- and p-waves}$$



FIG. 1 (color online). Momentum-space evolution potentials [see Eq. (4)] employed in the imaginary-time propagation of the trial wave function, corresponding to different densities. In the inset is shown the expectation values of the evolution potential (red solid circles) and the two-body chiral potential (blue squares) computed for the density n = 0.011 fm<sup>-3</sup>.



FIG. 2 (color online). Occupation probabilities of neutron matter as a function of momentum for selected densities.

- Gezerlis, Tews, Epelbaum, Gandolfi, Hebeler, Nogga, and Schwenk, Phys. Rev. Lett. 111, 032501 (2013) AFQMC/GFMC with two-body NN–interaction LO+NLO+N<sup>2</sup>LO

Roggero, Mukherjee, and Pederiva,
 Phys. Rev. Lett. 112, 221103 (2014)
 CIMC with two-body NN-interaction LO+NLO+N<sup>2</sup>LO

- Gezerlis and Carlson, Phys. Rev. C 77, 032801(R) (2008) GFMC with s-wave part of AV18 NN–interaction





Energy/nucleon, chemical potential, and <u>self-energy (preliminary)</u>.



<u>Preliminary! Effective mass  $m^*/m \approx 1(0.1)$ </u>

NN (up to N<sup>3</sup>LO) and NNN (N<sup>2</sup>LO), Wlazłowski et al, PRL 113, 182503 (2014)



### **Neutron matter at finite temperatures**



A)  $T = 0.06 \epsilon_F$ , B)  $T = 0.08 \epsilon_F$ , C)  $T = 0.1 \epsilon_F$ , D)  $T = 0.12 \epsilon_F$ Wlazlowski and Magierski, PRC 83, 012801 (2011), Int. J. Mod. Phys. E20, 569 (2011)

 $T_c = 0.09 \epsilon_{F,} \quad \Delta = 0.25 \epsilon_{F,} \quad \underline{\Delta/T_c} = 2.8$ 





A)  $T = 0.06 T_F$ , B)  $T = 0.08 T_F$ , C)  $T = 0.1 T_F$ , D)  $T = 0.12 T_F - Tc = 0.09 T_F$ Wlazlowski and Magierski, PRC 83, 012801 (2011), Int. J. Mod. Phys. E18, 919 (2010)



Seki and Abe, J. Phys. Conf. Proc. 321, 012037 (2011), PRC 79, 054002 and 054003 (2009)

## What LQCD can do for low energy nuclear physics?

In order to move from phenomenology to a truly microscopic theory one needs to:

- Determine the nn-interaction with a  $p_c \approx 400-500$  MeV/c.
- Determine the np-interaction with a  $p_c \approx 400-500$  MeV/c. Even though nn- and pn-interactions can be extracted from phase shifts, they have to be reproduced by LQCD for us to have confidence in 3-nucleon interactions.
- Determine the 3n-interaction with a  $p_c \approx 400-500$  MeV/c.
- Determine the 2n1p-interaction with a  $p_c \approx 400-500$  MeV/c.
- Estimate the importance of four-nucleon interactions with a p<sub>c</sub>≈ 400-500 MeV/c, and that includes 4n, 3n1p, 2n2p, and hope that they are not important. Otherwise we will have to include them too.

Binding energies of nuclei should be predicted hopefully with an accuracy better than <u>1 MeV per nucleus</u> (which is better than 0.1% for heavy nuclei, where the binding energy is about 1.6 GeV) and radii with an accuracy of at least 0.05 fm (thus about 1% for heavy nuclei)!

Only then LQCD interactions are going to replace the phenomenological ones! If solid information about these interactions are provided we can try to establish if the correct properties of finite nuclei, especially those of medium and heavy nuclei, of the neutron matter, and the saturation properties of the nuclear matter can be obtained, and subsequently move and compute other nuclear observables.

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