



# BEC-BCS Crossover in Cold Atoms

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# Outline

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- Theory
  - *Cold Atoms*
  - *BEC-BCS Crossover*
  - *Feshbach Resonance*
  - *Universal number,  $\xi$*
- Previous Work
- Our method
  - *Modelling the interaction*
  - *Pairing wavefunctions*
- **(Results)**
  - *Total Energy*
  - *Condensate fraction*
- Future work

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# Theory

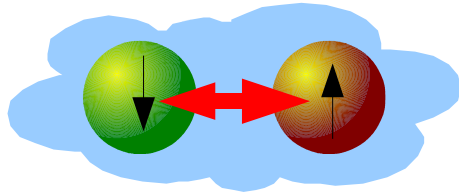
# Cold Atoms

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- Bose Gas
  - *BEC (1995)*
  - *Quantised Vortices*
  - *Propagation of solitons*
- Fermi Gas
  - e.g.  ${}^6\text{Li}$ ,  ${}^{40}\text{K}$ ,  ${}^2\text{H}$
- Vary the interaction strength between fermionic atoms...

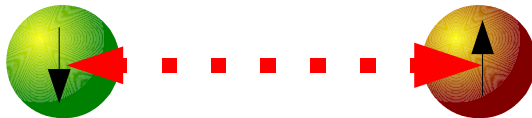
# BEC-BCS crossover

- Strong pairing :



- Atoms form molecules of up and down spin
- These molecules are bosonic
- Bosonic molecules condense into BEC

- Weak pairing :



- Atoms interact over a long range
- BCS theory

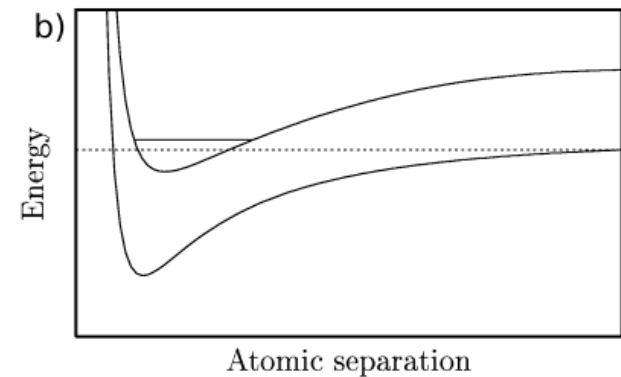
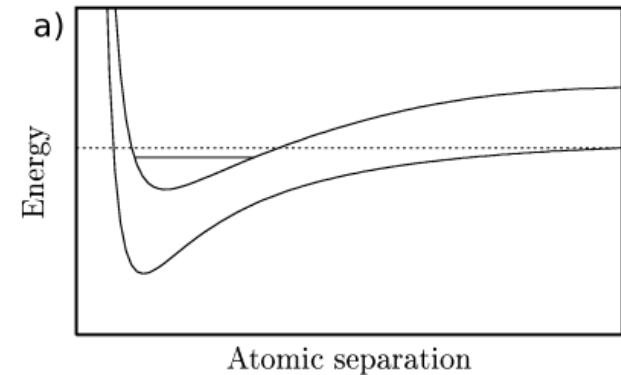
- Interesting point at *unitarity* :

- Dilute : Interatomic potential range  $\ll$  Interparticle distance
- Strongly interacting : Scattering length  $\gg$  Interparticle distance

- How would this occur?

# Feshbach Resonance

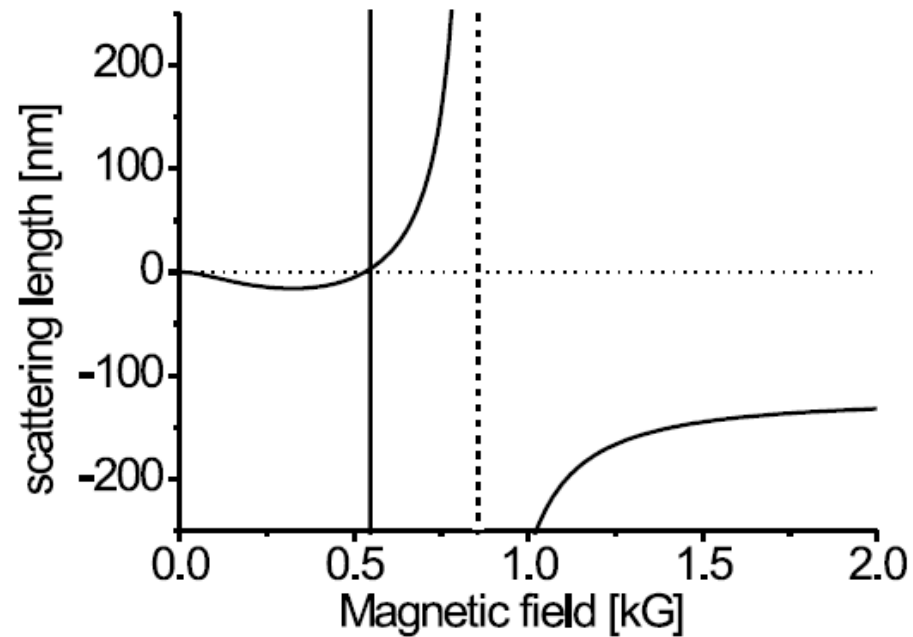
- 2 channels corresponding to different spin states
- *Open channel* (scattering process)
- *Closed channel* (bound state)
- *Resonance* occurs when Open and Closed channel energies are close
- Channel energies are *tuned* by a magnetic field



*From Giorgini et al eprint cond-mat  
0706.3360v1*

# Feshbach Resonance (2)

- The *s*-wave scattering length,  $a$ , diverges at resonance



*Resonances in  ${}^6\text{Li}$  from Bourdel et al PRL  
93 050401*

# Universal Number, $\xi$

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- At resonance the only relevant energy scale is that of a non-interacting gas

$$E_I = \xi E_{FG} = \xi \frac{3 k_F^2}{10 m}$$

- This value,  $\xi$ , is believed to be universal when  $k_F R_0 \ll 1$  where  $R_0$  is the effective range of interaction
- Throughout we measure the interaction strength in units of  $1/k_F a$



# Previous Work

- 2 previous studies using QMC,

- J. Carlson et al, *PRL 91 050401*:  $\xi = 0.44(1)$

- G.E. Astrakharchik et al, *PRL 93 200404*:  $\xi = 0.42(1)$

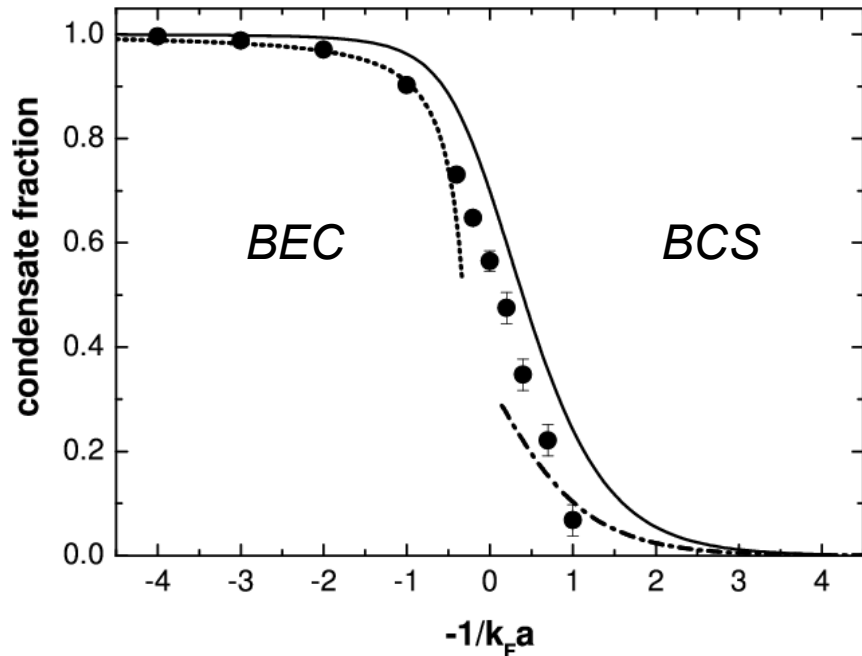
*Symbols - QMC*

*(Dot - Bogoliubov*

*Dot-Dashed BCS theory*

*Black line SC-MF)*

*From Astrakharchik et al PRL 95 230405.*



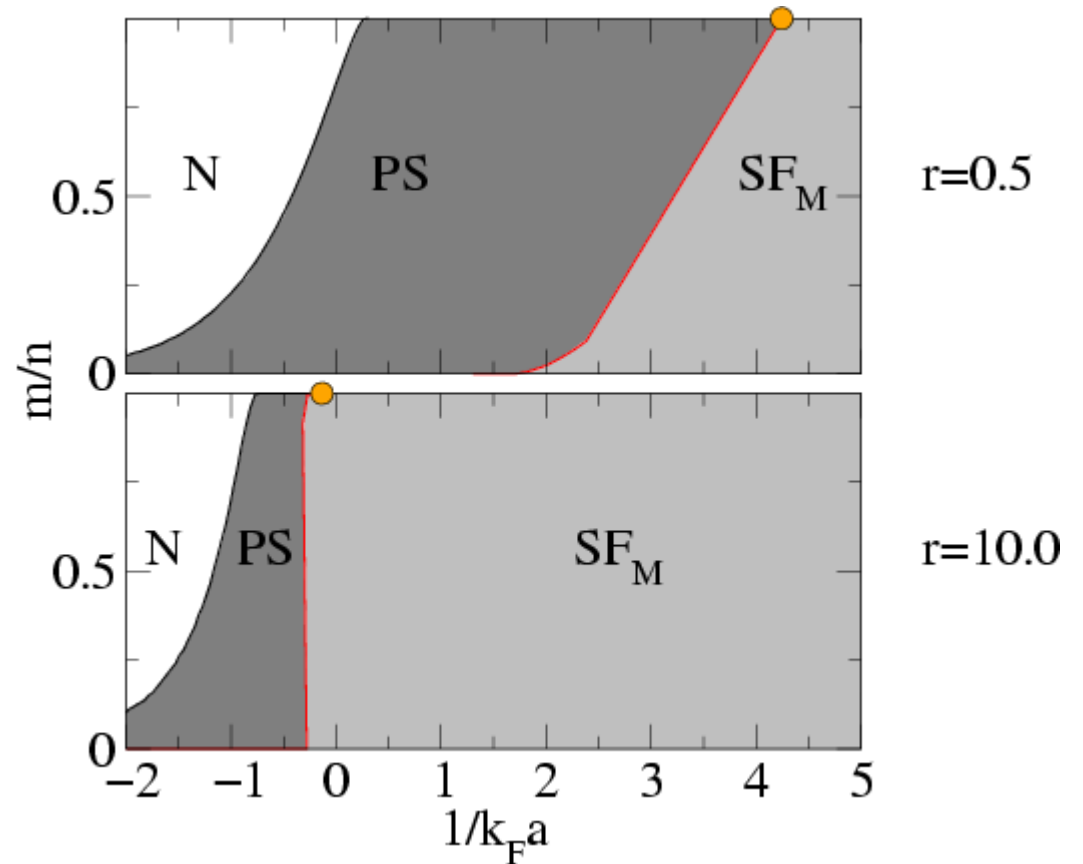
- Other methods,

- Nishida et al: *eprint cond-mat/0607835*  $\xi = 0.38(1)$

# This Work

- Unequal particle numbers / unequal masses

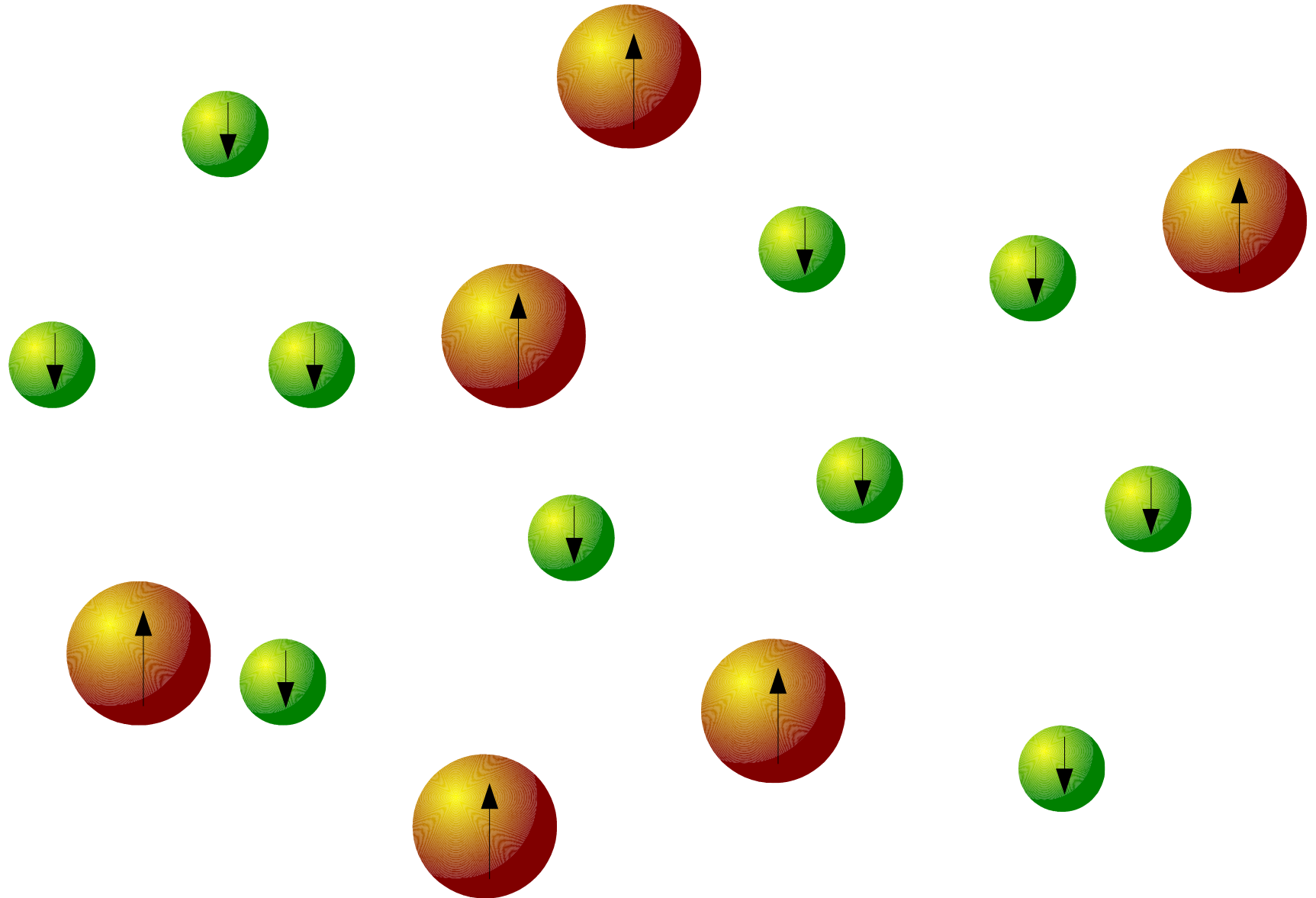
$r = m_{\downarrow}/m_{\uparrow}$   
 $n = \text{density of particles}$   
 $m = \text{magnetisation}$



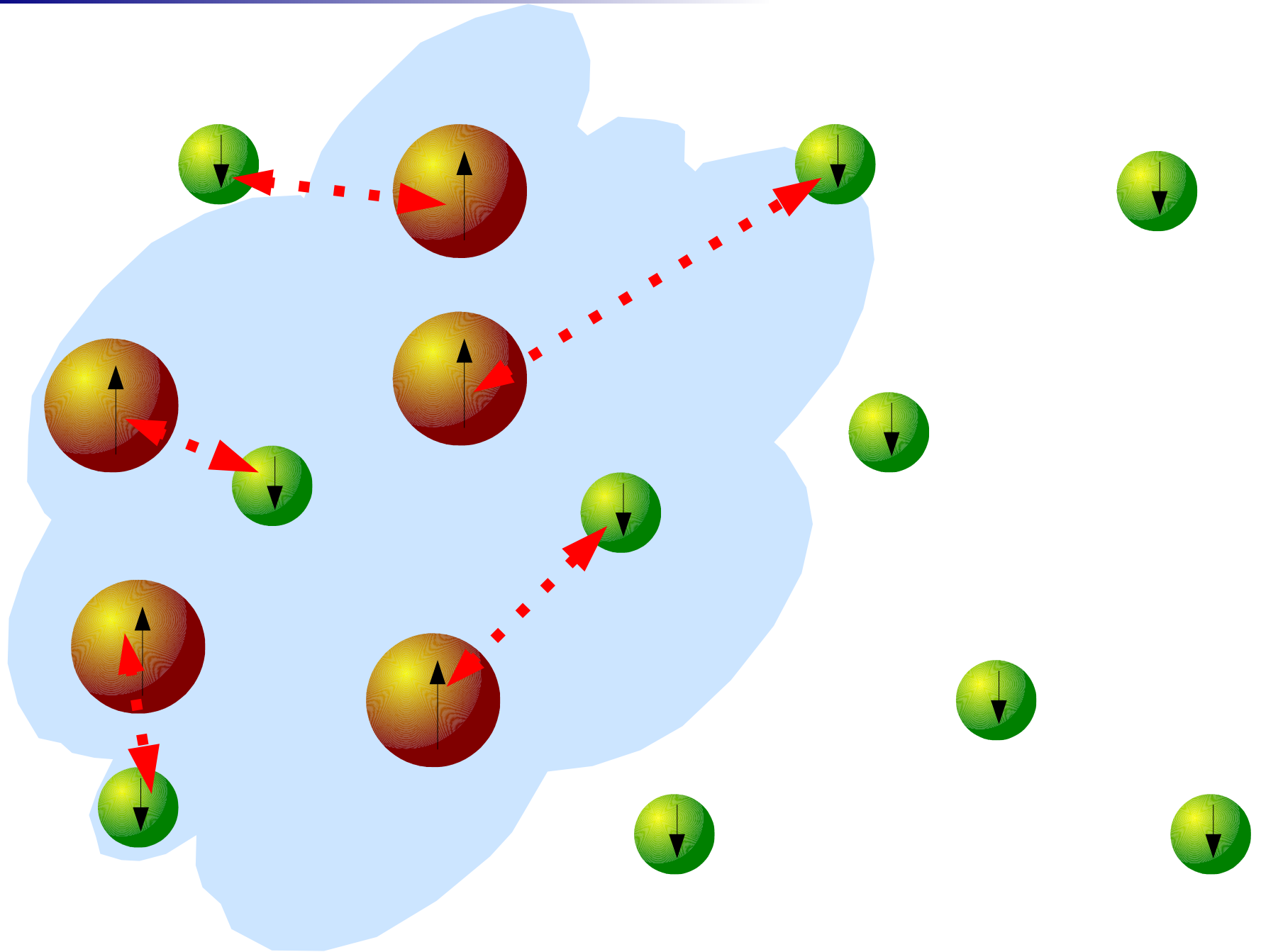
From Parish et al, PRL 98 160402 (2007)

# Normal Phase

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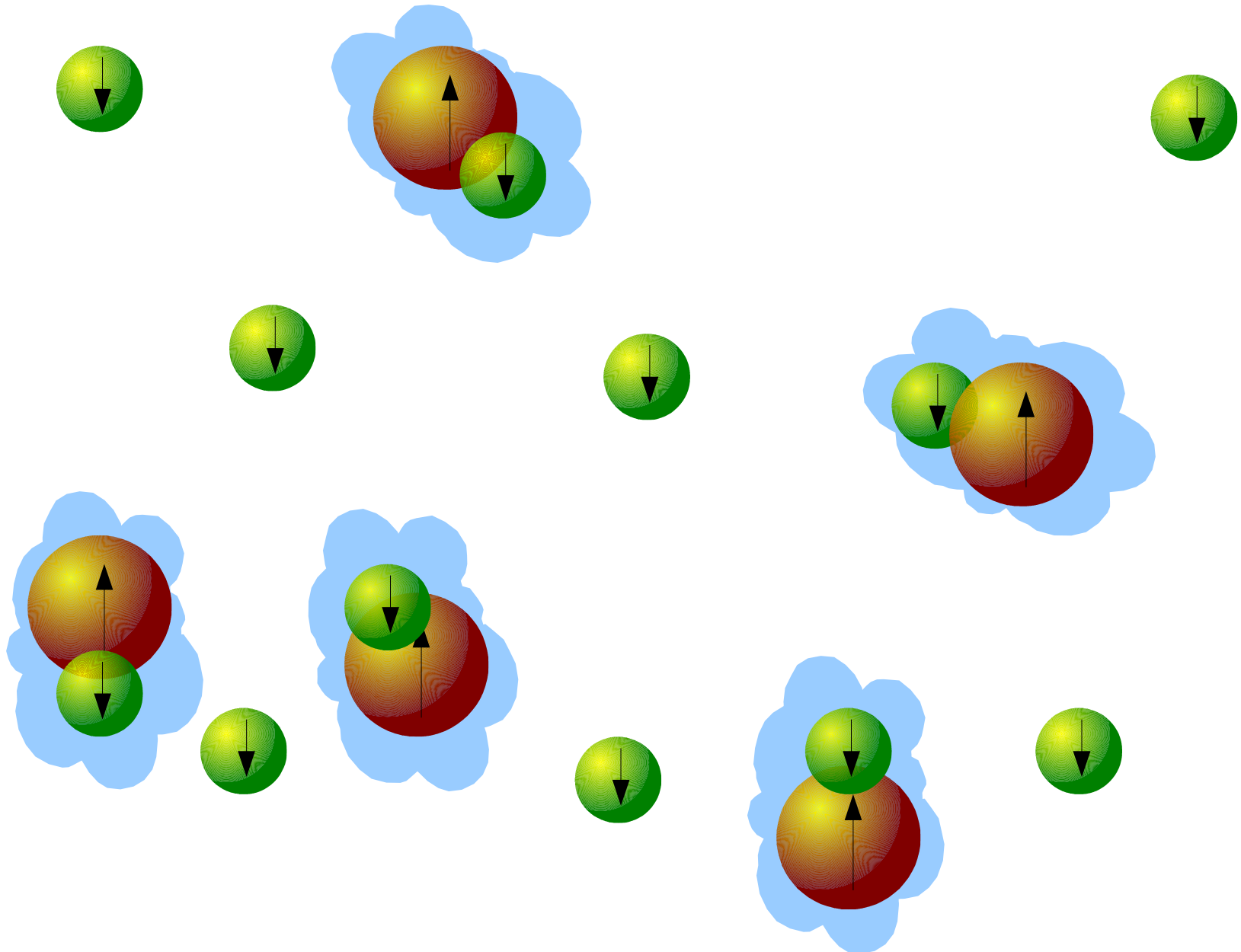


# Phase Separated



# Magnetised Superfluid

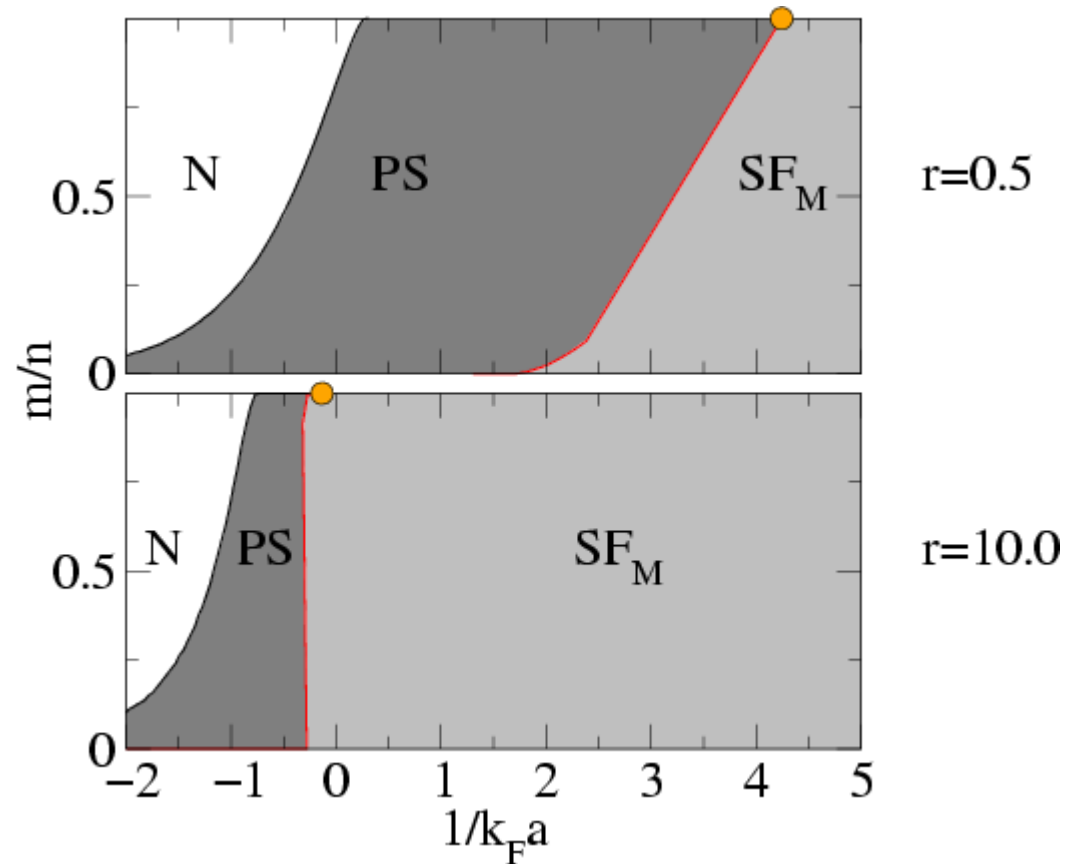
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# This Work

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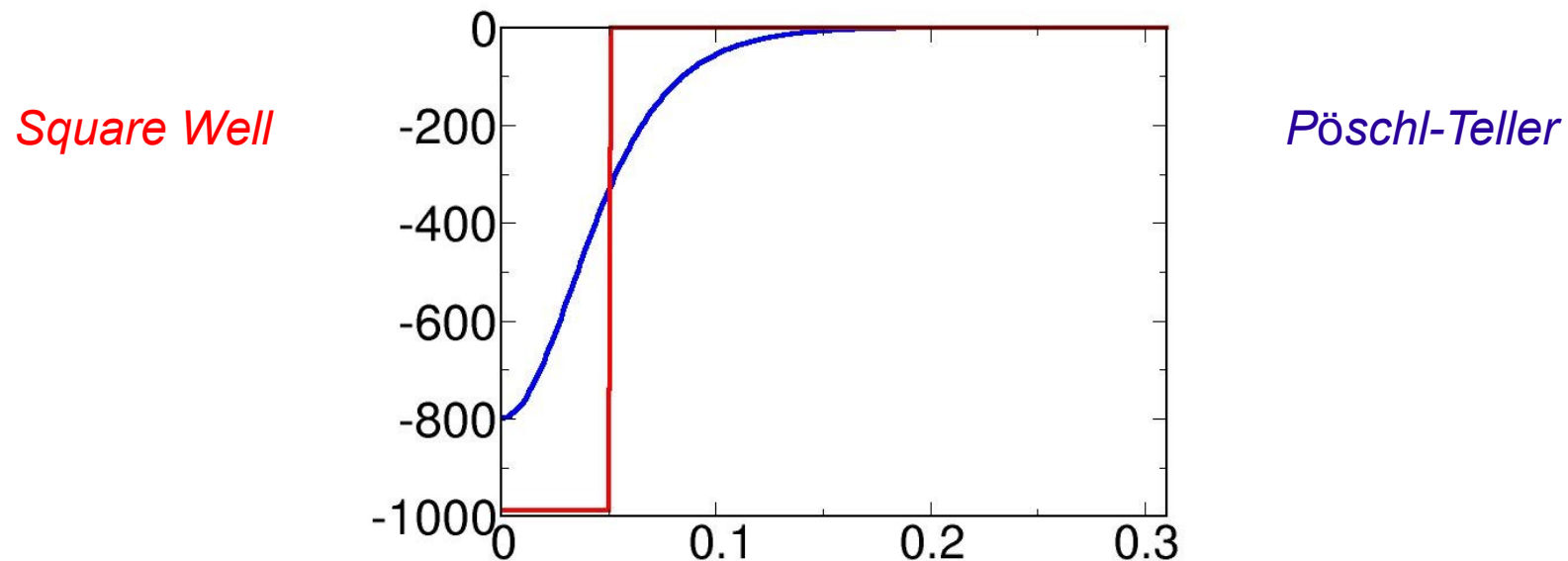
From Parish et al, PRL 98 160402 (2007)

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# The Model

# Modelling the Feshbach Resonance

- Pauli-Exclusion Principle for parallel spin
- As interatomic potential  $\ll$  atom spacing, the exact form of the interaction is unimportant
- 2 types of interaction normally used...



- We use the Pöschl-Teller



# Pairing Wavefunctions

- In QMC for a spin-independent operator we normally use a product of *Slater determinants*, one containing  $n$  up-spin and one  $m$ , down-spin one-particle orbitals,  $\phi$ .

$$\Psi = e^J \begin{vmatrix} \phi_1(r_{1\uparrow}) & \cdots & \phi_n(r_{1\uparrow}) \\ \vdots & \ddots & \vdots \\ \phi_1(r_{n\uparrow}) & \cdots & \phi_n(r_{n\uparrow}) \end{vmatrix} \begin{vmatrix} \phi_1(r_{1\downarrow}) & \cdots & \phi_m(r_{1\downarrow}) \\ \vdots & \ddots & \vdots \\ \phi_1(r_{m\downarrow}) & \cdots & \phi_m(r_{m\downarrow}) \end{vmatrix}$$

- However, we want a wave function that explicitly describes pairing

## Pairing Wavefunctions (2)

- We now use only one *Slater determinant*. It contains only one type of orbital,  $\phi$ , which is a function of the distance between up and down particles

$$\Psi = e^J \begin{vmatrix} \phi(r_{1\uparrow} - r_{1\downarrow}) & \cdots & \phi(r_{1\uparrow} - r_{n\downarrow}) \\ \vdots & \ddots & \vdots \\ \phi(r_{n\uparrow} - r_{1\downarrow}) & \cdots & \phi(r_{n\uparrow} - r_{n\downarrow}) \end{vmatrix}$$

- 3-types of  $\phi$  have been tried

$$\phi = \sum_{i=1} C_i \exp(i(r\uparrow - r\downarrow)) \quad - \textit{Pairing Plane-waves}$$

$$\phi = \sum_{i=1} g_i \exp(\beta_i (r\uparrow - r\downarrow)^2) \quad - \textit{Pairing Gaussians}$$

$$\phi = \sum_{i=0} \alpha_i (r\uparrow - r\downarrow)^i \quad - \textit{Pairing Polynomials}$$

- And combinations of the above

# Jastrow factor + Backflow

- Jastrow factor of *Drummond et al PRB 70 235119 (2004)* (CASINO users, that's a Jastrow  $U + P$ )

$$J = \sum_{l=1}^L \alpha_l r_{ij}^l + \sum_A a_A \sum_{G_A} \cos(G_A \cdot r_{ij})$$

- Backflow corrections of *López Ríos et al PRE 74 066701 (2006)*

$$\Psi^{BF}(\mathbf{R}) = e^{J(\mathbf{R})} \Psi_s(\mathbf{X})$$

$$\mathbf{x}_i = \mathbf{r}_i + \xi_i(\mathbf{R})$$

- We optimise the Jastrow, Backflow and orbital parameters using VMC and *energy minimisation* (Umrigar et al PRL 98 110201 (2007))

- *Conclude using DMC*

# Pairing Wavefunctions (3)

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- Polynomial of order 20 + Jastrow U (Polynomial)  $E_{\text{VMC}} = 0.650(4)$
- Gaussian  $E_{\text{VMC}} = 0.664(2)$
- Gaussian + Jastrow U  $E_{\text{VMC}} = 0.5195(6)$
- Gaussian + Jastrow U + Backflow (Eta)  $E_{\text{VMC}} = 0.4745(1)$
- Gaussian + Jastrow U + Backflow (Eta) + Jastrow P  $E_{\text{VMC}} = 0.4605(2)$

$E_{\text{DMC}} \sim 4\%$  lower

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# Results

# Present state

- Testing our ideas and CASINO with reproducing the value of  $\xi$

- *J. Carlson et al PRL 91 050401:*  $\xi = 0.44(1)$

- *G.E. Astrakharchik et al PRL 93 200404:*  $\xi = 0.42(1)$

- *This work (to date)*

VMC

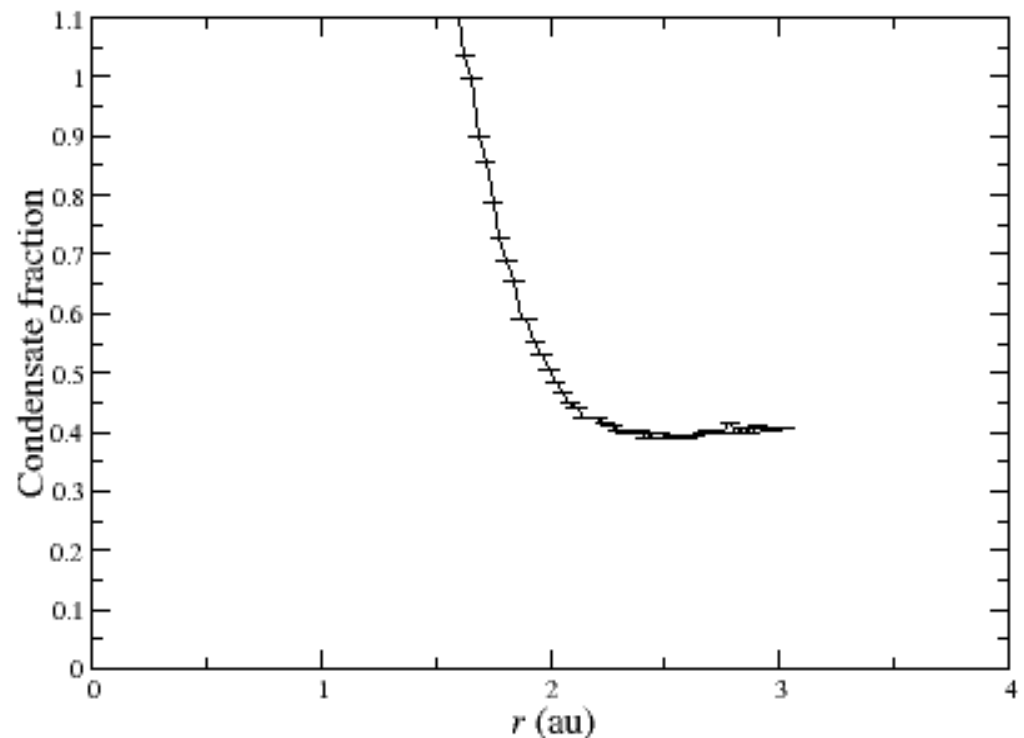
$\xi \sim 0.45$

DMC

$\xi \sim 0.44$  ( and still  $\downarrow$  )

- *Condensate fraction:*

*$\sim 0.4$  – not right yet!*



# Where next?

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- Verify / improve on  $\xi$
- Calculate 1- and 2-body density matrices
- Calculate condensate fraction
- Move on to varied mass system

# Acknowledgements

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- Pablo Lopez-Rios
- Richard Needs
- Ben Simons
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