BEC-BCS Crossover in Cold Atoms

(2 years later...)

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TTI 31st July 2009

Outline

- Theory
  - *Cold Atoms*
  - *BEC-BCS Crossover*
  - *Feshbach Resonance*
  - *Universal number*
- Previous Work
- Our method
  - *Modelling the interaction*
  - *Pairing wavefunctions*
  - *Multi-B in QMC*
- Problems
- Results
  - *Total Energy*
  - *Condensate fraction*

Theory

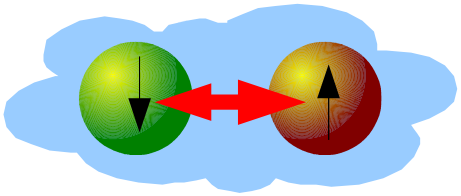
Cold Atoms

- Bose Gas
  - *BEC (1995)*
  - *Quantised Vortices*
  - *Propagation of solitons*
- Fermi Gas
  - *e.g. ^{6}Li, ^{40}K, ^{2}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* :

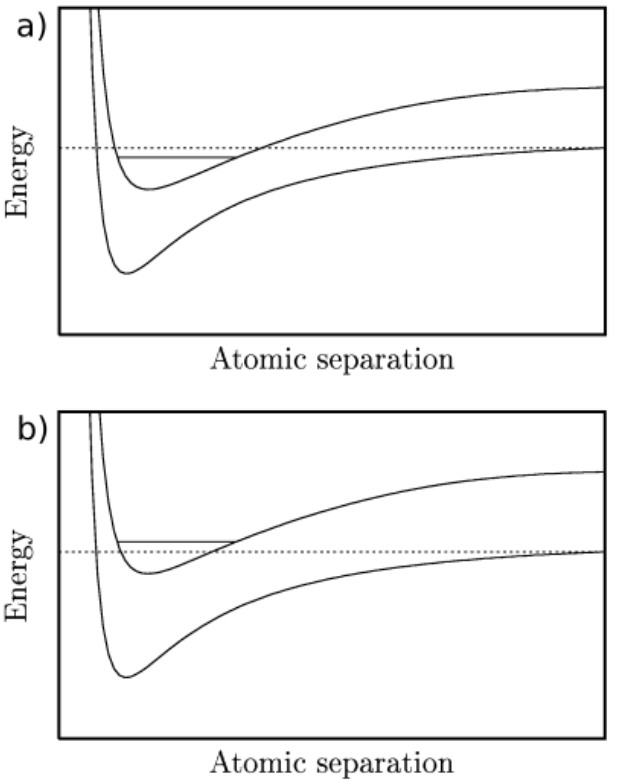
- Dilute : Interatomic potential range << Interparticle distance

- Strongly interacting : Scattering length >> Interparticle distance

- How would this occur?

Feshbach Resonance

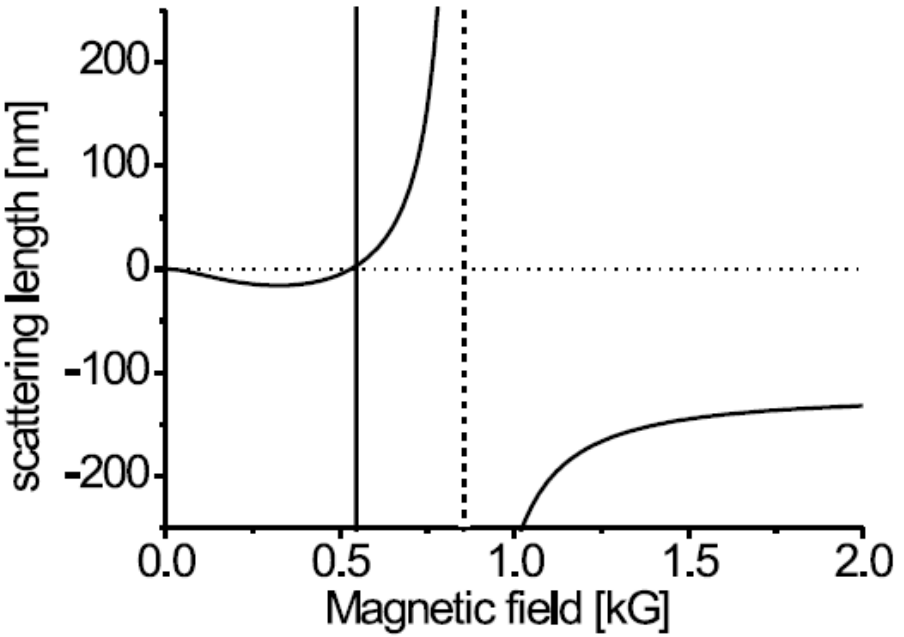
- 2 channels corresponding to different spin states
- *Open channel* (scattering process)
- *Closed channel* (bound state)
- *Resonance* occurs when Open and Closed channel energies are close
- Channel energies are *tuned* by a magnetic field



From Giorgini et al eprint cond-mat 0706.3360v1

Feshbach Resonance (2)

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



Resonances in ^{6}Li from Bourdel et al PRL 93 050401

Universal Number, ξ

- 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, ξ, is believed to be universal when $k_F R_0 << 1$ where R_0 is the effective range of interaction

- Throughout we measure the interaction strength in units of $1/k_F a$

Previous Work, ξ

- 2 previous studies using QMC,

  - *J. Carlson et al, PRL **91** 050401: 2003* $\xi = 0.44(1)$
  - *G.E. Astrakharchik et al, PRL **93** 200404: 2004* $\xi = 0.42(1)$
  - *S. Y. Chang et al, PRL **95** 080402: 2005* $\xi = 0.414(5)$
  - *J. Carlson et al, PRL **95** 060401: 2005* $\xi = 0.42(1)$

- Other methods,

  - *Nishida et al: eprint cond-mat/0607835: 2007* $\xi = 0.38(1)$

- Experiment

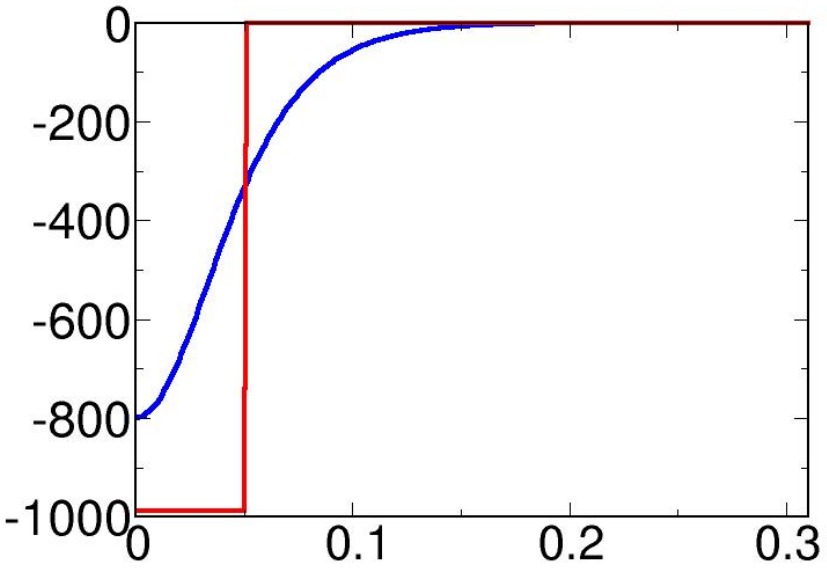
  - *Bartenstein et al PRL **92** 120401: 2004* $\xi = 0.32(10)$
  - *Partridge et al Science **311** 503: 2006* $\xi = 0.46(5)$

The Model

Modelling the Feshbach Resonance

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

Square Well



Pöschl-Teller

- 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, .

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

• 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 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 orbital have been tried

$$\phi = \sum_{i=1} C_i \exp(i(r\uparrow - r\downarrow))$$ *- Pairing Planewaves*

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

$$\phi = \sum_{i=0} \alpha_i (r\uparrow - r\downarrow)^i$$ *- 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)*

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

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

$$\Psi^{BF}\left(\boldsymbol{R}\right) = \mathrm{e}^{J(\boldsymbol{R})} \Psi_s\left(\boldsymbol{X}\right)$$

$$\boldsymbol{x}_i = \boldsymbol{r}_i + \xi_i\left(\boldsymbol{R}\right)$$

- We optimised the Jastrow, Backflow and orbital parameters using VMC and Energy Minimisation

- *Conclude using DMC*

September 2007

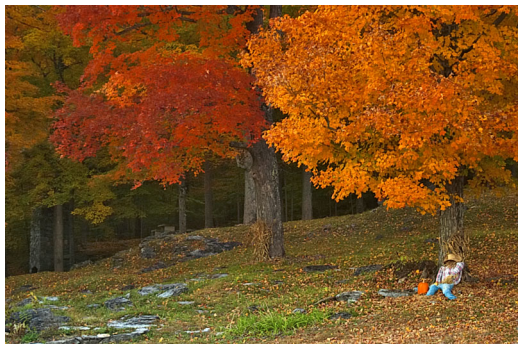
- Gaussians v Polynomials?
  - Gaussians are better orbitals alone – but polynomials are *much* faster

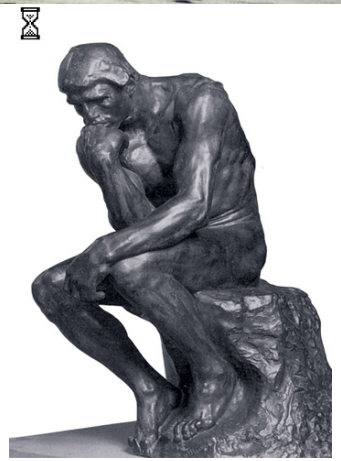
- Significant finite size errors,
  - 128 particles isn't really enough
  - Larger number of particles unfeasible

- General Bad Behaviour – won't minimise the energy in VMC properly with EMIN
  - Configurations can't “find” the sharp well
  - When things go a bit wrong, energy goes catastophically wrong
  - Sometimes ignores well altogether and goes to non-interacting wavefunction

- Finite width of the well still needs extrapolating to 0 (dilute limit)
  - If configs. have problems with finite well, how do we deal with an infinitely narrow one?

2 years pass...





Gaussians or Polynomials?

Gaussians or Polynomial Orbitals

- Yes, bare gaussian orbitals are better than polynomials

- But gaussians+J+B aren't as good as polynomials+J+B

- The total energy is strongly dependent on the short-range behaviour of the wavefunction. (that's where the well is!)

- The polynomial is better at this, if a planewave Jastrow is able to represent the long range behaviour

=> Use polynomials as they're much faster.

Finite Size Errors?

Baldereschi's Mean-Value Point

There is some point in the 1st BZ that gives the best approximation to an integral over all the BZ.

This is in terms of the first-failure star - the first G vector that gives rise to an error in the integration.

Further to this, Baldereschi minimises the error in the first-failure star.

The paper reports the Mean-Value (or Baldereschi) Points for SC, FCC and BCC.

In the old days, when you could only afford one k-point, the Baldereschi was the best.

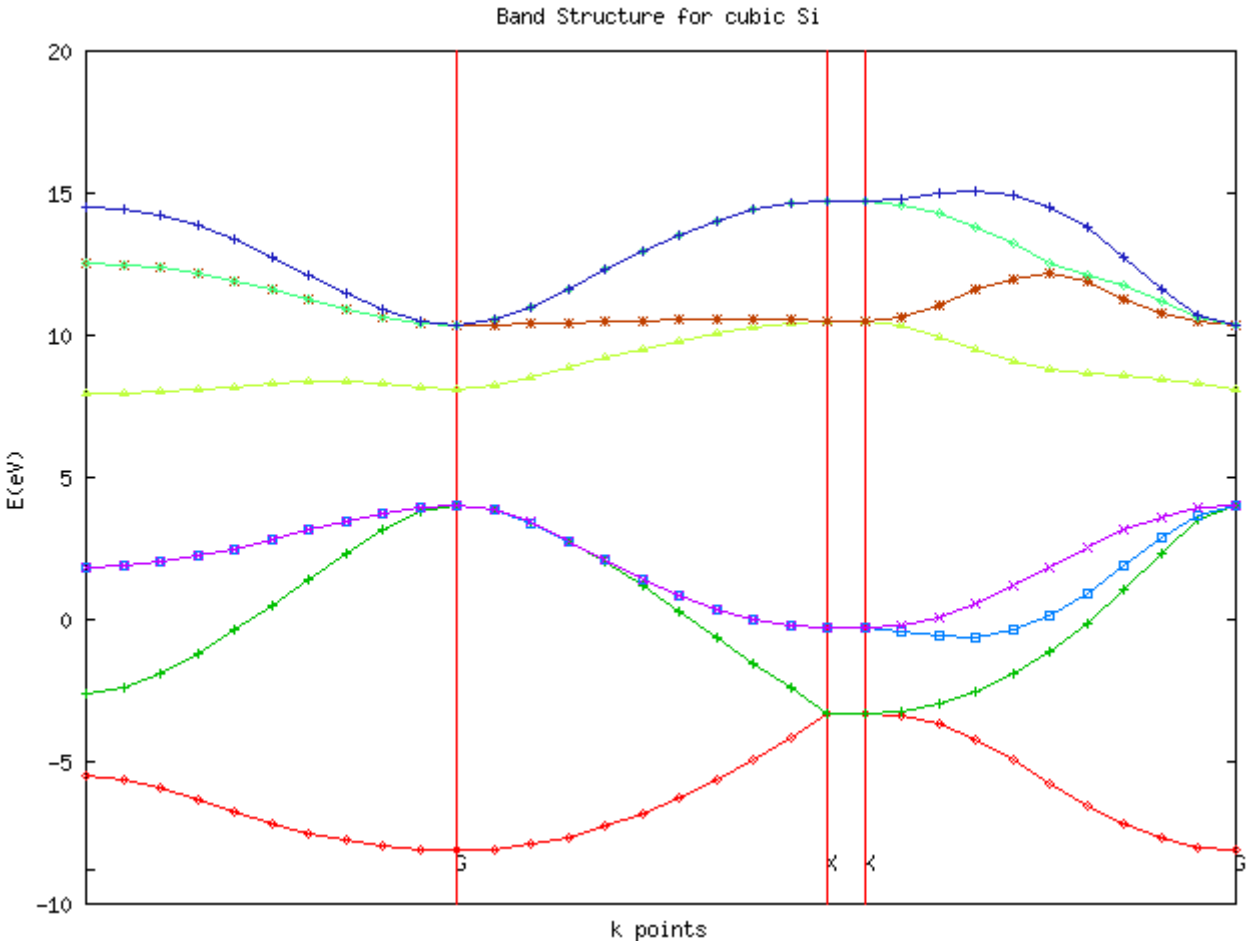
So what's so wrong with just using Γ (0,0,0)...

The Γ Point

Because of the curved nature of band structure, the Γ point and the BZ boundary are the furthest points from the mean value.

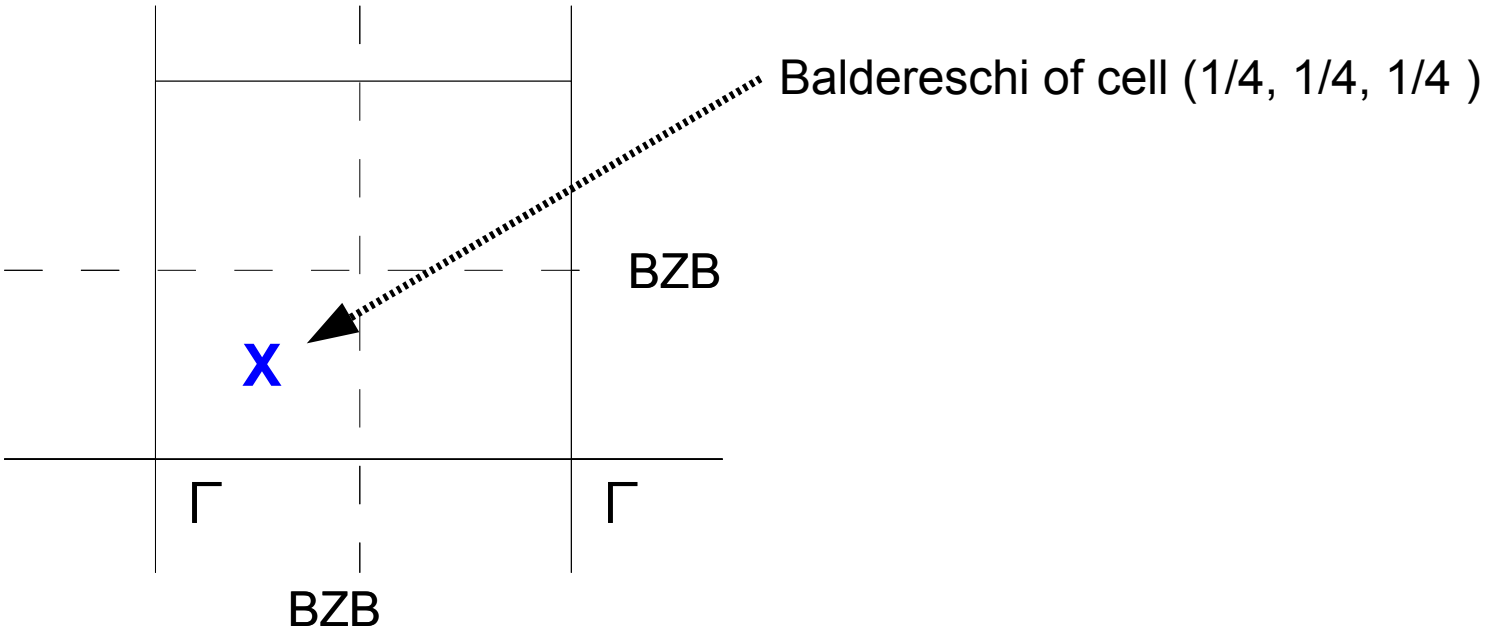
However, there is only 1 Γ point, but a whole boundary of BZ edge.

Hence Γ is always going to be the worst point.



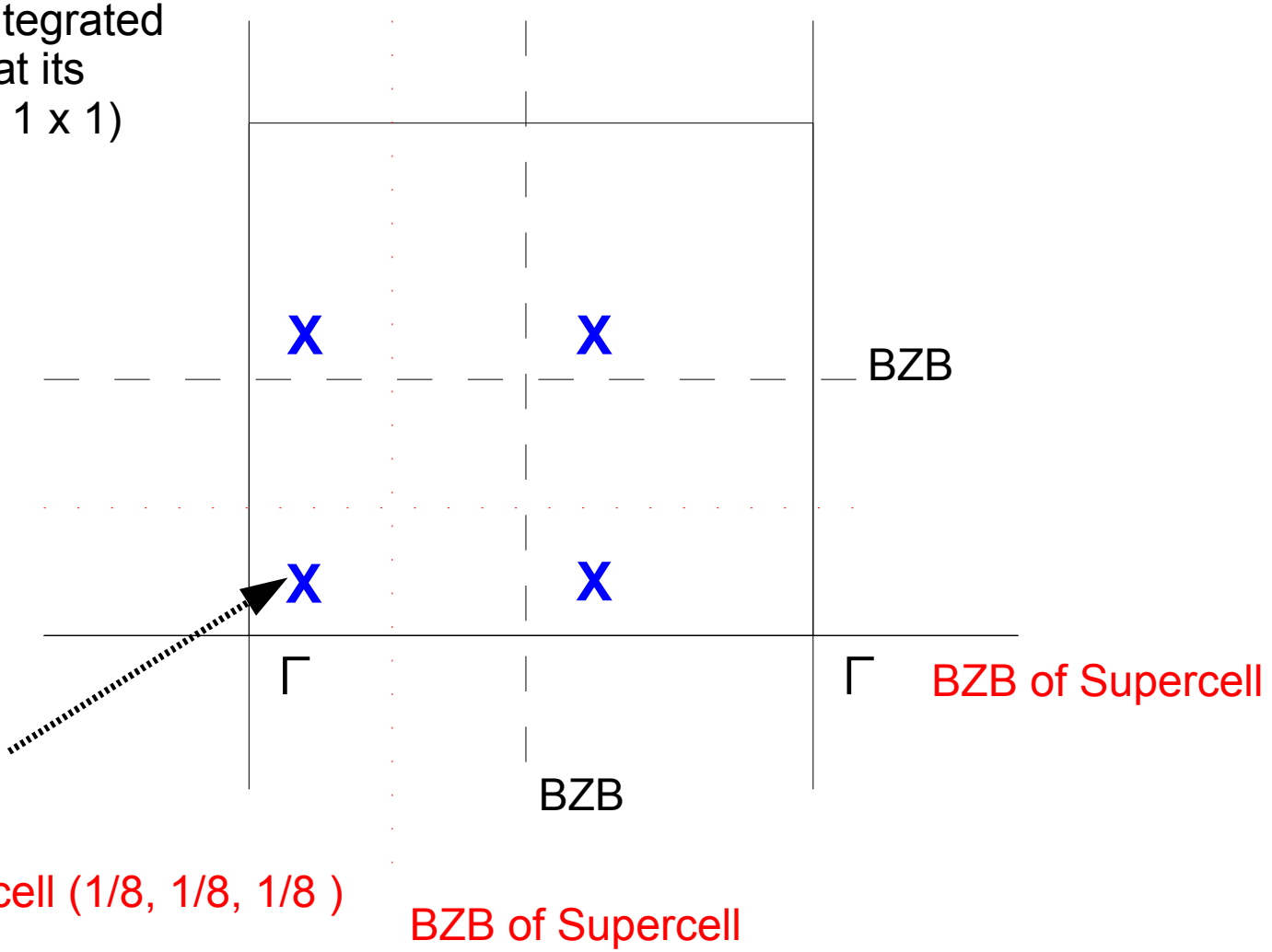
D.J. Chadi and M.L. Cohen, *Tight Binding Calculations of the Valence Bands of Diamond and Zincblende Crystals.* Phys. Stat. Sol. (b) **68**, 405 (1975).

128 particle cell



How?

We have effectively integrated the 1024 particle cell at its Baldereschi point (1 x 1 x 1)



Normal MP 2 x 2 x 2 grid, but centred on Baldereschi of super cell (1/8, 1/8, 1/8)

Bad Behaviour?

Bad Behaviour

- Due to the short-range nature of the well, if things go wrong, they go very wrong.

- Use Mean-Absolute Deviation from the Median (MADMIN) to minimise energy of VMC wavefunction.
  => Less weight placed on outliers

- Can't use EMIN for complex wavefunctions yet anyway!

- Train the wavefunciton by narrowing the well throughout the simulation.

Well Width Extrapolation

Well width extrapolation

- Make the well-width narrower, makes is more difficult for the wavefunctions to find.
- Changes cut-offs of polynomial parameters in orbitals, Jastrow and backflow
- Bad behaviour!

=>Can't use an easy to generate wavefunction as a 1st approximation to a difficult one. (Everything changes)

- But, it is the dilution that goes to zero not well width. So we can decrease the particle density instead
- Well width remains the same, so wavefunctions are a good approximation
- Cutoffs are a good approximation
- Makes Wigner-Seitz radius bigger, but that's the part of the cell that is less important for the energy.

Results

Results

- J. Carlson et al,	*(38 atoms)*	*2003*	*ξ = 0.44(1)*
- G.E. Astrakharchik et al,	*(66 atoms)*	*2004*	*ξ = 0.42(1)*
- S. Y. Chang et al,	*(14 atoms)*	*2005*	*ξ = 0.414(5)*
- J. Carlson et al,	*(66 atoms)*	*2005*	*ξ = 0.42(1)*

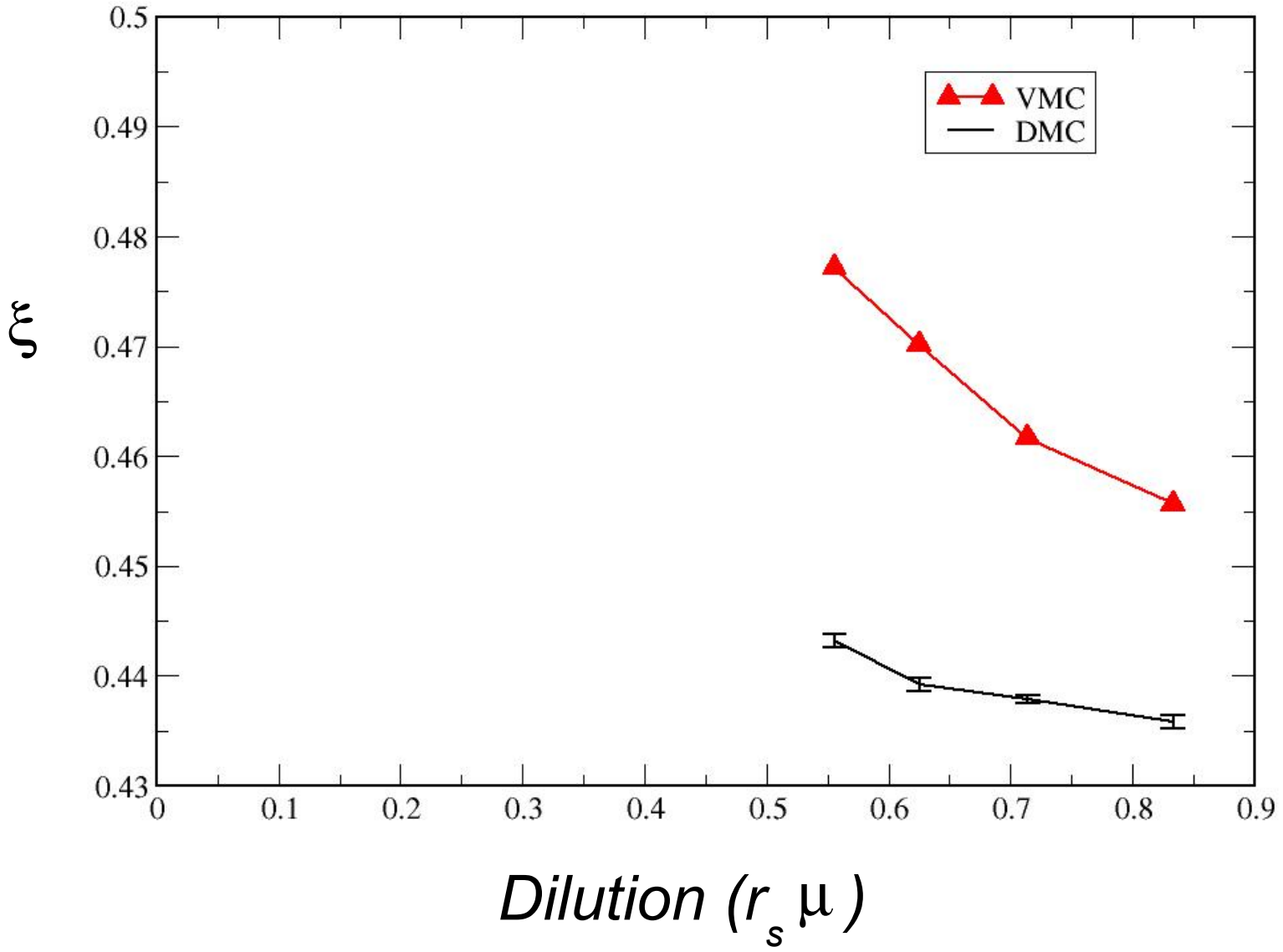
- Gamma point (128 atoms) *ξ = 0.4339(1)*

=> Good agreement at Gamma point.

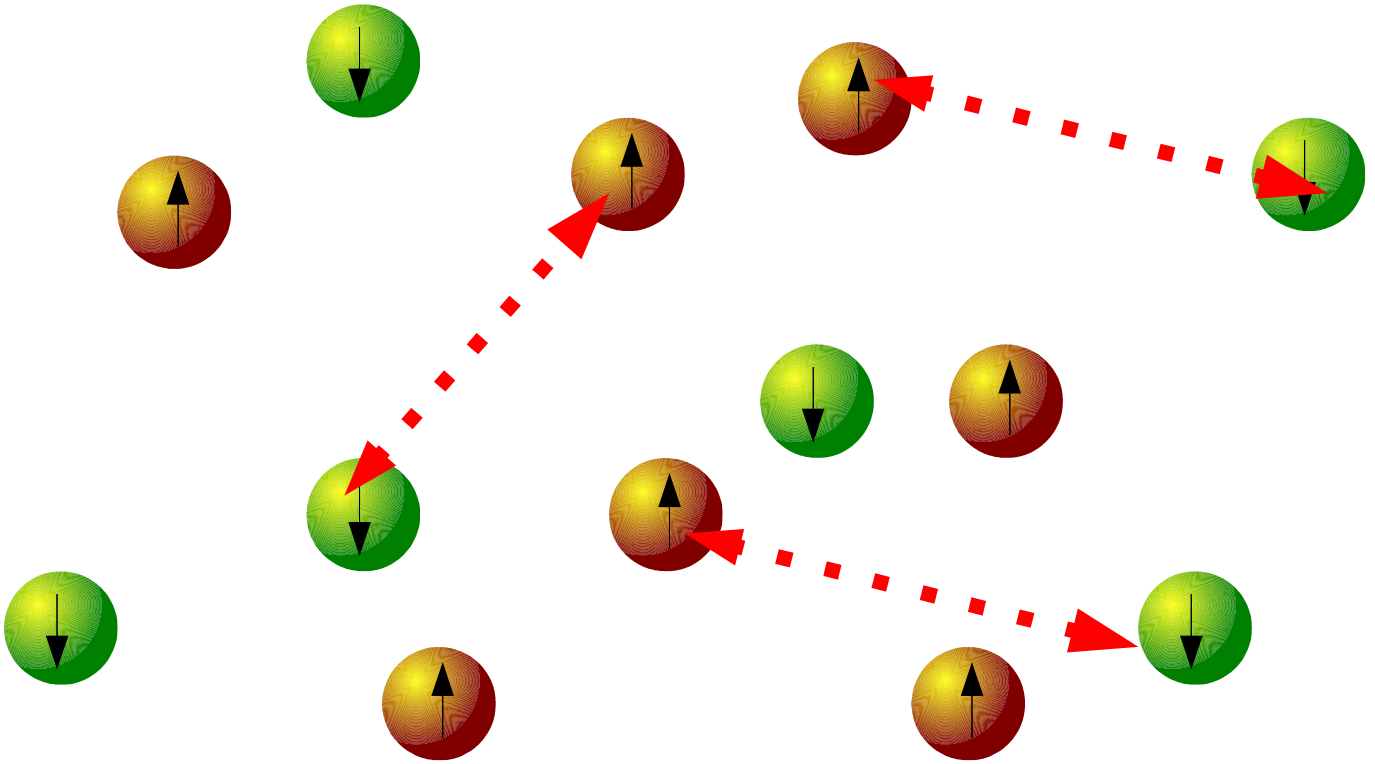
But...

- Multi-B 2x2x2 (1024 atoms) *ξ = 0.4783(2)*

Well width extrapolation



Condensate Fraction

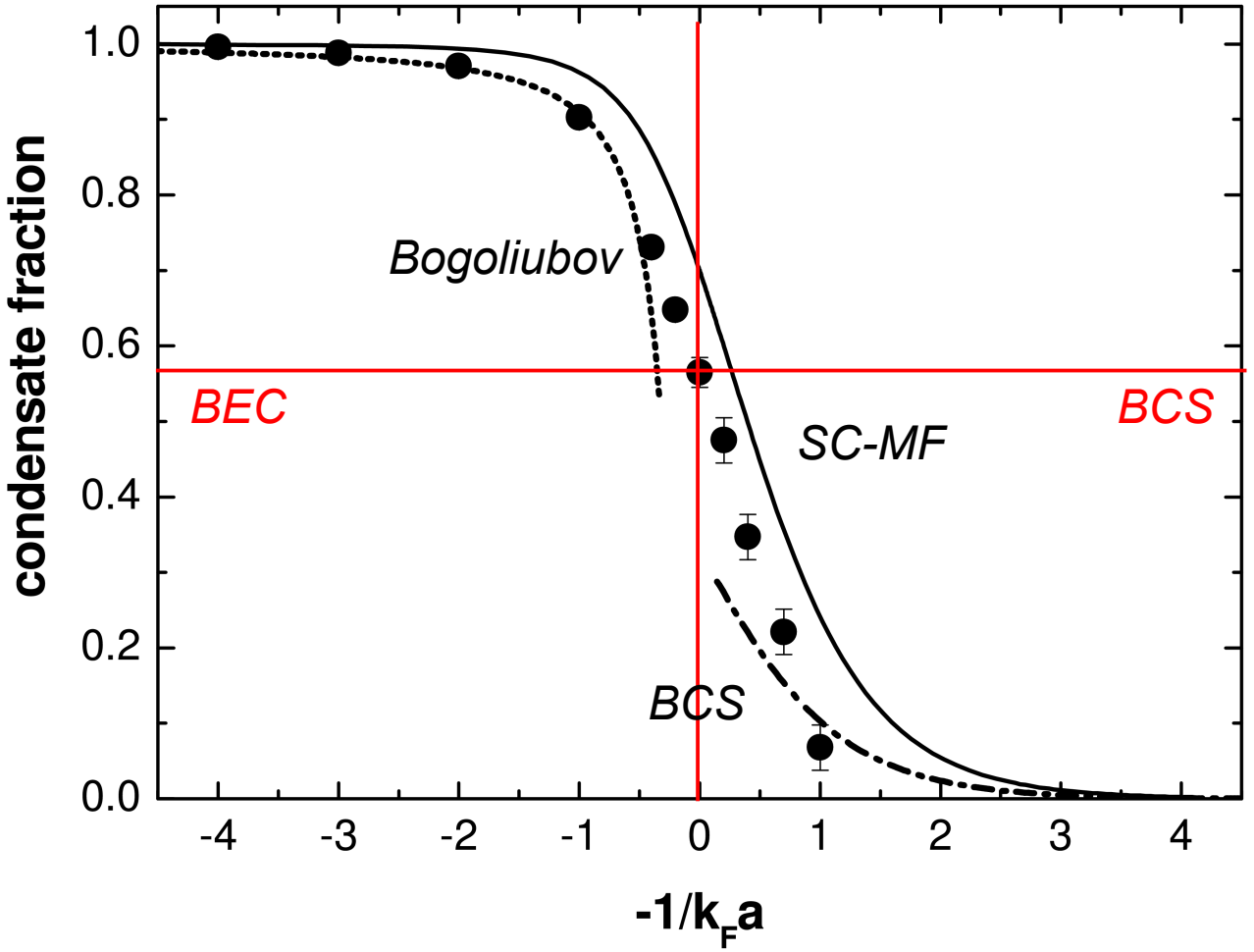


Example of Off-Diagonal Long-Range Order

Calculated from rotationally and translationally averaged two-body density-matrix

$$c = \frac{\Omega^2}{N} \lim_{r \to \infty} \rho \frac{TR}{2}(r)$$

Condensate Fraction



- [Astrakharchik *et al.* PRL **95** 23040 (2005)] *~0.58*

- *We obtain:* *Gamma* *0.512(9)*

  Multi-k-point *0.508(8)*

Conclusions

- *Baldereschi can get you better results*
- *K-point sampling is a good idea for QMC too at least for energies.*
- *Well-width extrapolation is the main problem*
- *Very difficult to do well*
- *Possible to overcome most of the technicalities in the end*

Acknowledgements

Richard Needs

Pablo Lopez Rios

Neil Drummond

Alexander Badinski

Matt Brown

Gareth Conduit