Introduction

HEG has been solved accurately using QMC including three-body and backflow effects. Wigner crystal by QMC solved using Gaussian trial function for 2D * and using a Padé Gaussian trial function for 3D †

There are still unresolved questions:
a) What role does correlation play ?
b) How good is the Gaussian basis for VMC and DMC? Can we improve upon it?
c) For 3D Ceperley and Alder report critical $r_s = 100 \pm 20$, while Ortiz, Harris and Ballone report $r_s = 65 \pm 10$

Why a mean field theory for Wigner Crystals?
a) Precise calculations
b) Possible starting point for DMC
c) Extra physical insight

*Rapisarda F. and Senatore G. *Aust. J. Phys* **49** 161 (1996)

†Ortiz G., Harris M. and Ballone P. *Phys. Rev. Lett.* **82** 5317 (1999)

HF Wigner crystal

Homogeneous electron gas
High density, unpolarised $\rightarrow$ low density polarised.
For HF at $r_s = 2.01$ 2D, 5.45 3D
For DMC at $r_s = \sim 26$ 2D, ~ 50 3D
$\Rightarrow$ For HEG, correlation is significant.

Convention is Wigner crystal ‘is quite outside the reach of the independent particle approximation’ (Ashcroft N.W. & Mermin N.D., *Solid State Physics* p.684)

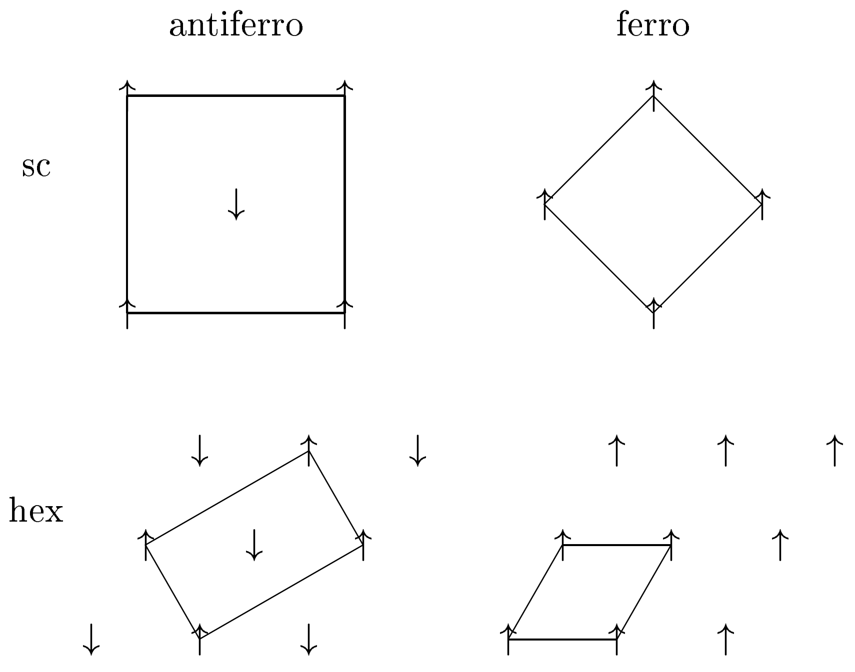
But, if orbitals of electrons overlap very little, as expected for a Wigner crystal, the correlation energy must be small and the e-e interaction dominated by the Hartree and exchange term.

2D HF

Spin constrained - unrestricted HF for chosen primitive unit cell to allow magnetic ordering

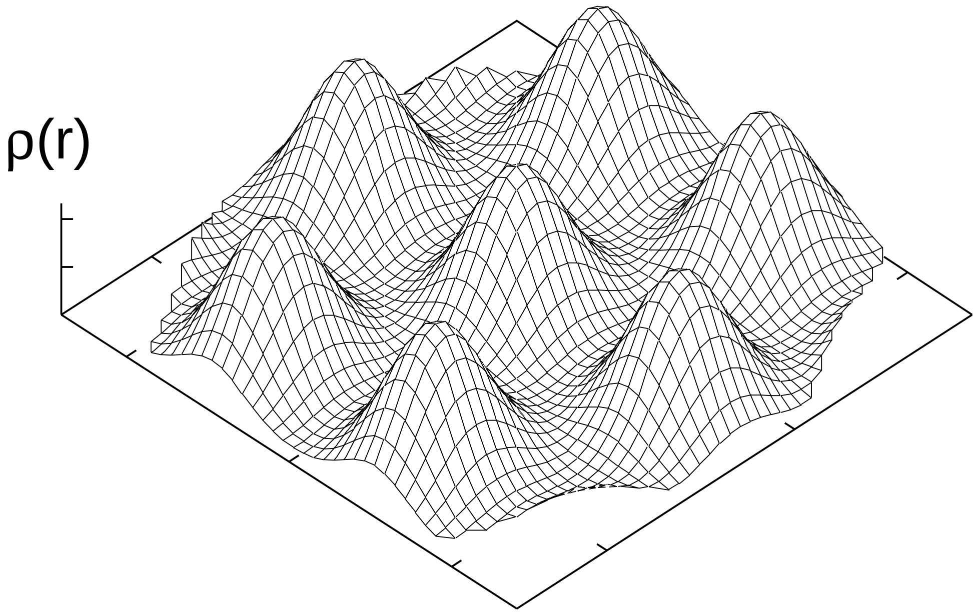
Plane wave basis UHF, $\pi r_s^2 = \frac{A}{N}$

2D square centred and hexagonal lattices - these have lowest Ewald energies.
unpolarised : one electron/unit cell
polarised : one each for $\uparrow$ and $\downarrow$ spin



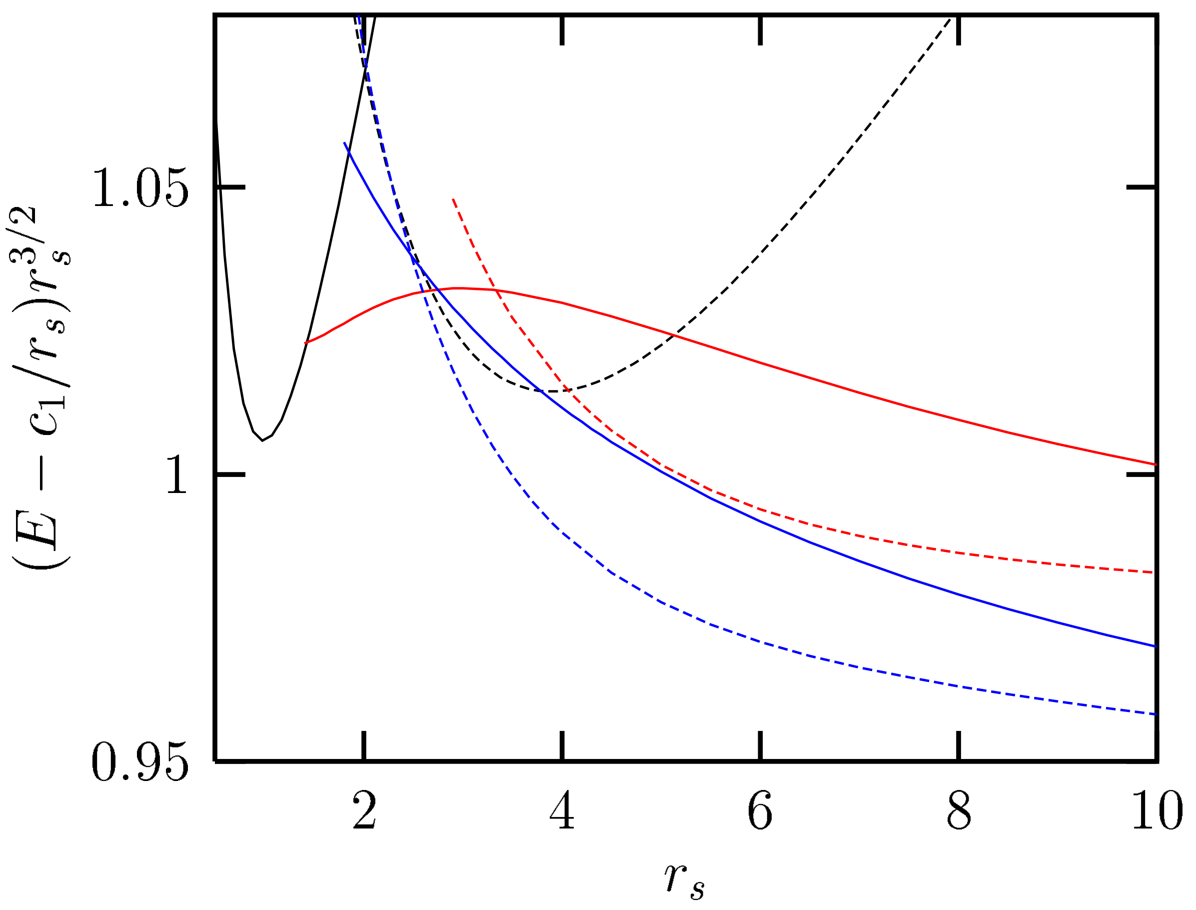
2D

F Hexagonal, $r_s = 10$



Strongly inhomogeneous: ratio ρ_{max}/ρ_{min} is:
17.1 for anti-ferromagnetic, 13.3 ferromagnetic

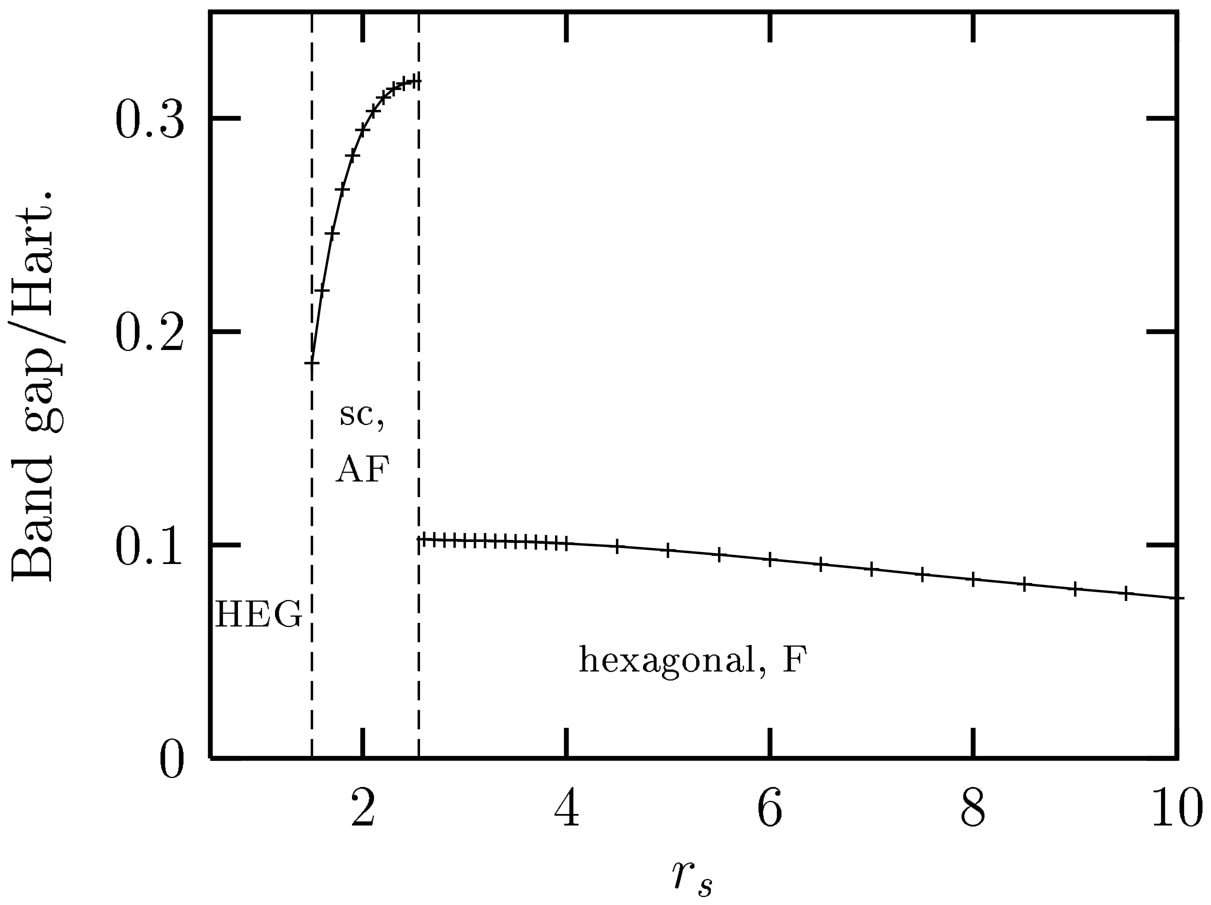
2D Energies



black	HEG
red	square centred
blue	hexagonal
solid	anti-ferromagnetic, unpolarised
dashed	ferromagnetic, polarised

c_1/r_s = Madelung energy for hexagonal lattice

2D Band gap



First order transitions:

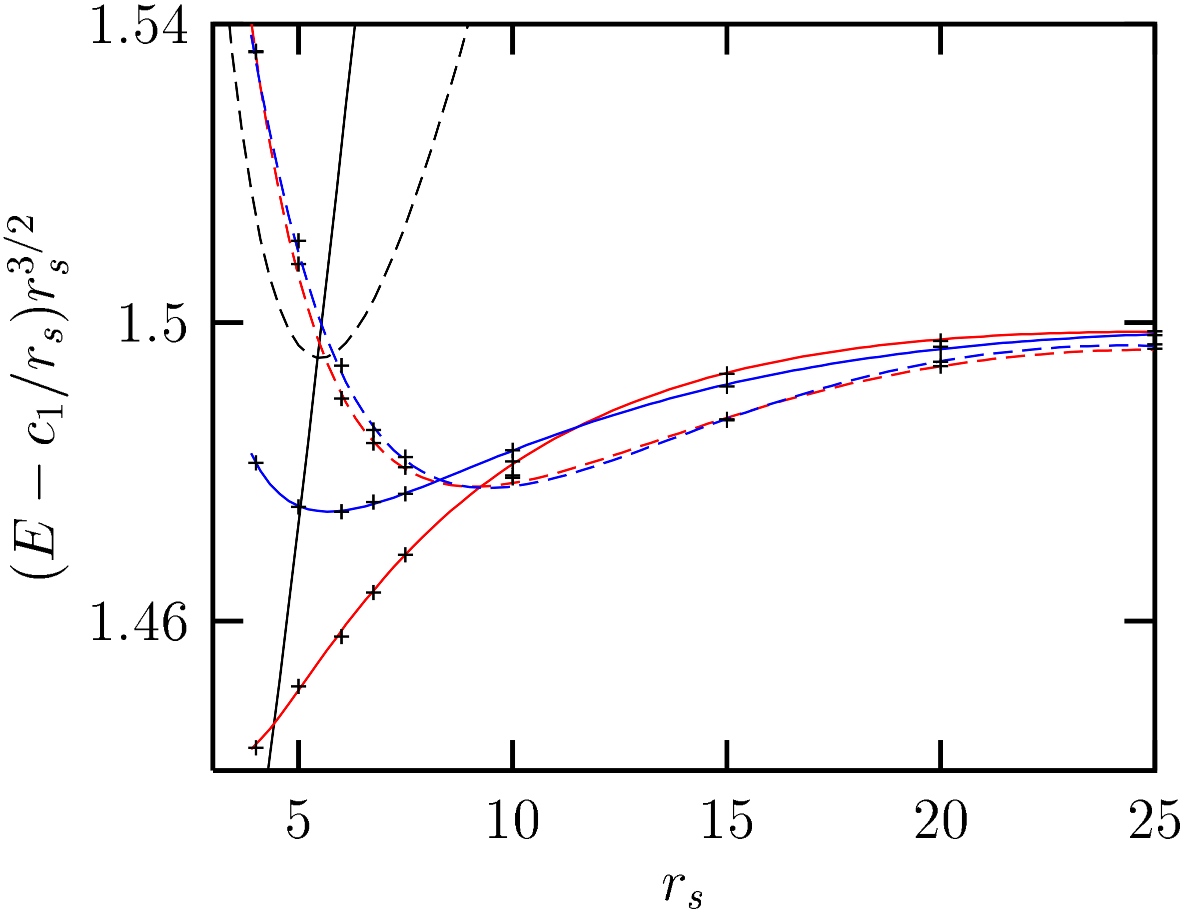
unpolarised HEG $\rightarrow$ sc AF crystal at $r_s = 1.4$

$\rightarrow$ hex F crystal at $r_s = 2.6$

n.b. DMC crystal phase is stable for $r_s > 35$

3D HF

Gaussian UHF, FCC and BCC lattice, $\frac{4\pi}{3}r_s^3 = \frac{\Omega}{N}$



black HEG
red BCC
blue FCC
solid anti-ferromagnetic, unpolarised
dashed ferromagnetic, polarised
$c_1/r_s =$ Madelung energy for BCC lattice

First order transitions:

unpolarised HEG $\rightarrow$ AF BCC crystal at $r_s = 4.5$

$\rightarrow$ F FCC crystal at $r_s = 9.5$

$\rightarrow$ F BCC at $r_s \sim 15$

n.b. For DMC crystal phase is stable for $r_s > 65 \sim 100$

Mean field theory, specifically unrestricted HF results in the Wigner crystallisation of the HEG with decreasing density.

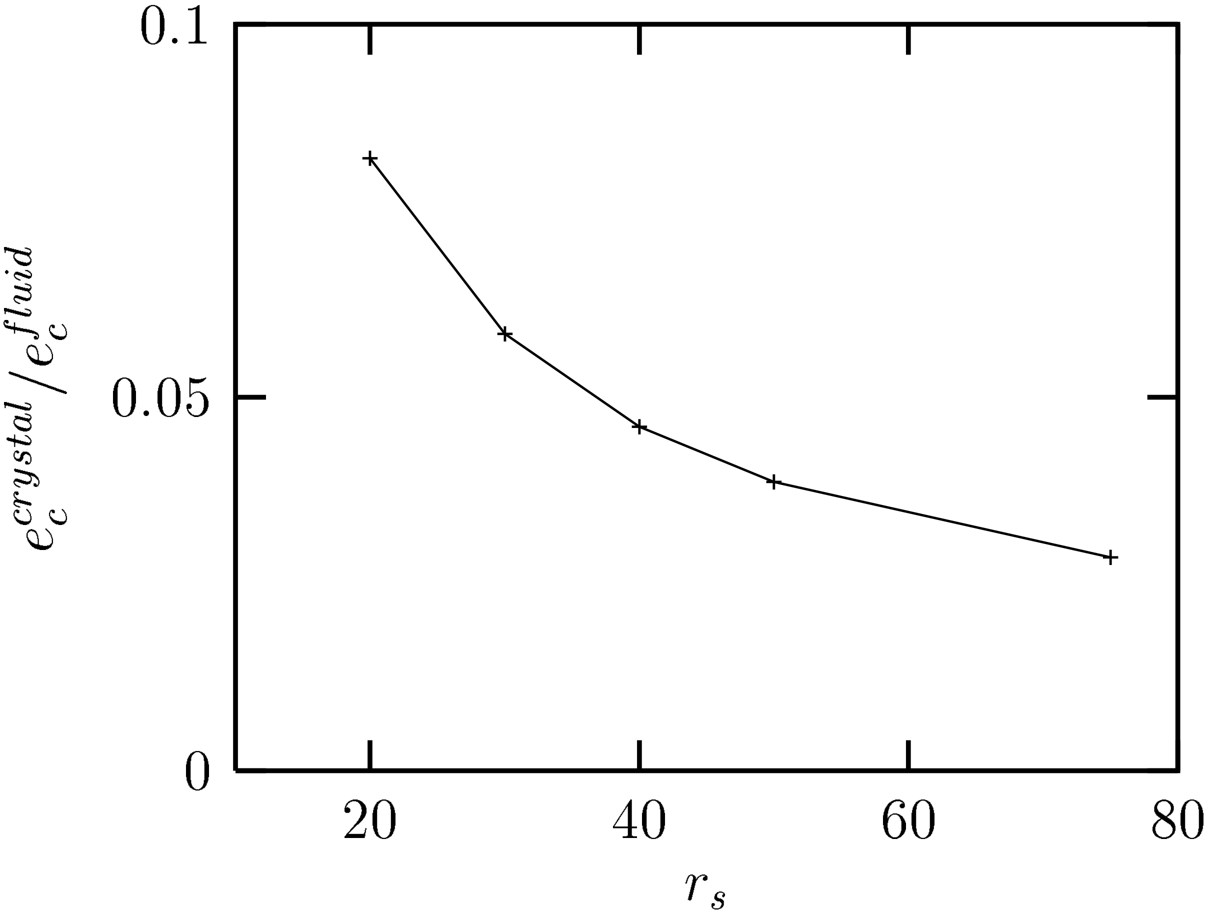
Why?

Absence of Self Interaction is crucial, and SI is not present in HF.
Electrons are kept apart by Hartree repulsion - suggests correlation should not be as important, at least for low densities in the region of interest.

Past work shows correlation energy is important for the HEG - is this the case for the Wigner crystal?

Examine $e_c = E_{DMC} - E_{HF}$ DMC for AF 2D case *

*Fluid e_c and Wigner E_{DMC} from Rapisarda F. and Senatore G. *Aust. J. Phys* **49** 161 (1996)



Correlation is smaller for the Wigner crystal than the HEG.

HF can be expected to provide a more accurate description of the Wigner crystal than the HEG.

3D, BCC

General asymptotic form:
$E = -\frac{c_1}{r_s} + \frac{c_2}{r_s^{3/2}} + \frac{c_3}{r_s^2} + O(\frac{1}{r_s^{5/2}})$

Term 1: Madelung energy, $c_1 = -0.89593$

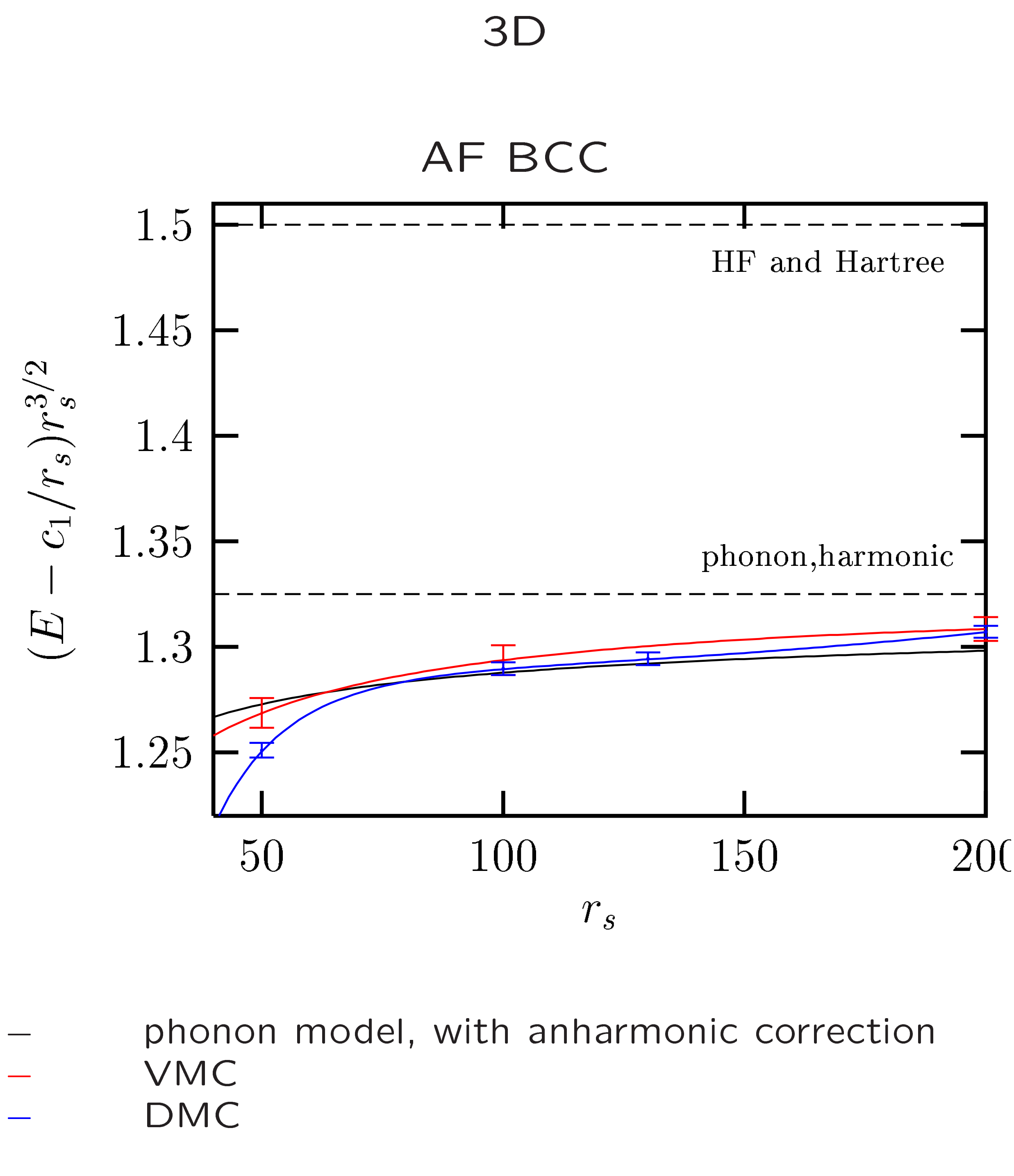
Term 2: 'Harmonic' energy. Zero point energy of harmonic oscillator

Term 3 and higher: anharmonic corrections

For Hartree and Hartree-Fock: $c_2 = 1.5$
. $c_3 \sim 0.0$

For Phonon model of Carr et al (includes 'phonon' correlation): $c_2 = 1.325$
. $c_3 = -0.73$

(Carr W.J. *et al*, Phys. Rev. **124**, 747 (1961).)



3D
AF BCC
1.5
1.45
1.4
1.35
1.3
1.25
HF and Hartree
phonon,harmonic
$(E - c_1/r_s)r_s^{3/2}$
50
100
150
200
r_s
phonon model, with anharmonic correction
VMC
DMC

3D AF BCC, $r_s = 100$

Calculation	E (Hart./e)
$E_{Hartree}$	-0.0074592932
E_{HF}	-0.0074592955
E_{phonon}, Harmonic *	-0.0076350000
E_{VMC} †	-0.007665(4)
E_{DMC} †	-0.007669(2)
E_{phonon} *	-0.0076715006

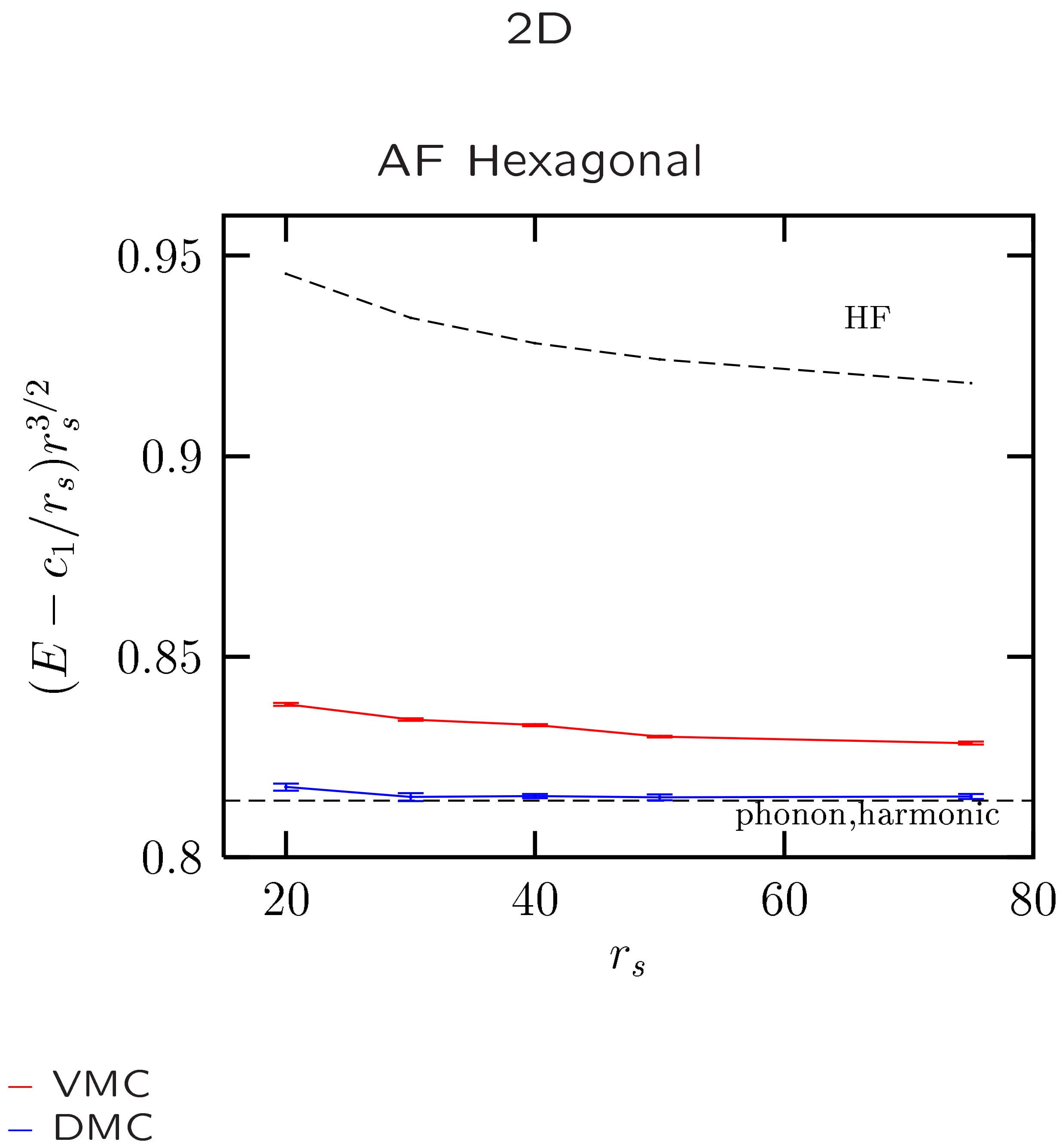
Energy due to exchange $\sim 10^{-9}\ Hart./e$

correlation $\sim 2.1 \times 10^{-4}\ Hart./e$

anharmonic correction $\sim 4 \times 10^{-5}\ Hart./e$

*Carr WJ *et al* *Phys. Rev.* **124** 747 (1961)

†Ceperley DM and Alder BJ *Phys. Rev. B* **45** 566 (1980)


2D
AF Hexagonal
$(E - c_1/r_s)r_s^{3/2}$
0.95
0.9
0.85
0.8
20
40
60
80
r_s
HF
phonon,harmonic
VMC
DMC

2D AF Hexagonal, $r_s = 40$

Calculation	E (Hart./e)
E_{HF}	-0.02398341
E_{VMC} †	-0.024360(1)
E_{DMC} †	-0.024430(1)
E_{phonon}, Harmonic *	-0.02443433

Energy due to exchange + phonon correlation= 4.5×10^{-4} $Hart./e$

*Bonsall L and Maradudin AA *Phys. Rev. B* **15** 1959 (1977)

†Rapisarda F and Senatore G *Aust. J. Phys.* **49** 161 (1996)

Can this ‘phonon’ correlation be included in the trial function?

Within phonon model wave function for distinguishable particles:

$$\Psi' = \mathrm{e}^{\sum_{ij}(\mathbf{r}_i-\mathbf{R}_i)A_{ij}(\mathbf{r}_j-\mathbf{R}_j)} \tag{1}$$

where $A_{ii} = A_{jj}$, or

$$\Psi' = \mathrm{e}^{\sum_{ij}(\mathbf{r}_i-\mathbf{R}_i)B_{ij}(\mathbf{r}_j-\mathbf{R}_j)} \prod_i \mathrm{e}^{-\alpha|\mathbf{r}_i-\mathbf{R}_i|^2} \tag{2}$$

where α is arbitrary and defines B_{ii}.

Anti-symmetrised version of this includes exchange, but is not in the standard ‘Jastrow-Slater’ form. A ‘Jastrow approximation’ to this takes the form

$$\Psi' = \left[\mathrm{e}^{\sum_{ij}(\mathbf{r}_i-\mathbf{R}_i)B_{ij}(\mathbf{r}_j-\mathbf{R}_j)}\right]_{sym} \prod_i \mathrm{e}^{-\alpha|\mathbf{r}_i-\mathbf{R}_i|^2} \tag{3}$$

with α chosen so the ‘Jastrow approximation’ is as good as possible.

Conclusion

1) UHF Wigner crystal solution exists
2) Energies are good - e_c of Wigner crystal is small. Suggests that we can use UHF for more complicated calculations
3) For 3D an accurate trial function must describe long range phonon correlations and anharmonic effects well
4) For 2D an accurate trial function must describe phonon correlations well, and anharmonic effects appear to be less important
5) These phonon modes suggest new trial functions for QMC calculations