25min./TTI2013

QMC study of bi-layer electron-hole system

Ryo Maezono,[1] Pablo Lopez Rios,[2] Tetsuo Ogawa,[3] and R.J. Needs[2]

[1] *School of Information Science, Japan Advanced Institute of Science and Technology, Asahidai 1-1, Nomi, Ishikawa 923-1292, Japan*

[2] *TCM Group, Cavendish Laboratory, University of Cambridge, J J Thomson Avenue, Cambridge CB3 0HE, United Kingdom*

[3] *Department of Physics, Osaka University, Machikaneyama-machi 1-1, Toyonaka, Osaka 560-0043, Japan*

(Dated: June 15, 2012)

Phys. Rev. Lett., accepted (2013).

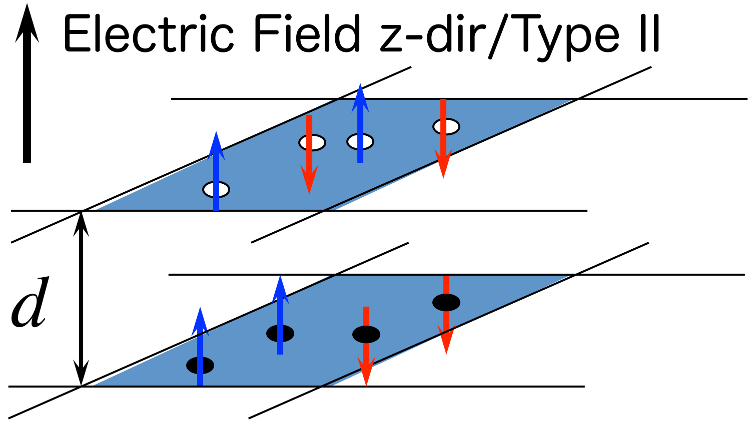
Ryo Maezono

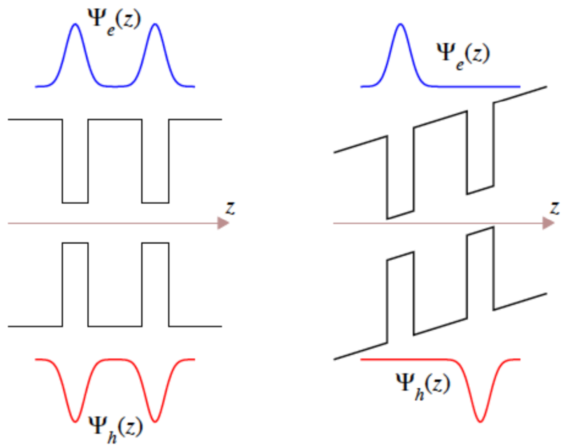
rmaezono@mac.com

School of Information Science,

Semi Conductor Bilayer

(Thermalization time~ 1ns)/(Lifetime~ Several μs)





d ~ 4-5nm ~ 100 a.u. e.g., AlAs/GaAs

m_h/m_e ~ 0.50 (heavier hole)

~ 0.09 (lighter hole)

L.V. Butov *et al.*, PRL**73**, 304(1994).

S. Yang, PRB 81, 115320(2010).

「Exciton formation」

Motivation

for Electron-Hole systems

- **DMC methodological**

  As a case with evaluations other than GS energy.

- **Foundation of Photonics** electronics → photonics

  Identifying where EH pairs stably exist.

- **Foundation of Solid state Physics**

  Electron Gas ; Exchange and Correlation

  ↓

  'Exciton' '2-comp. plasma'

  Elec.-Hole Gas ; Localization v.s. Delocalization

  Binding Screening

Laser & Semiconductors providing tractable experiments for Mott Tr.

Particle Density controlled by Laser Intensity

Two Component Plasma

in 3d-EH gas

Mott Criterion $r_S^{cr.} = 4\left(\frac{12}{\pi}\right)^{\frac{2}{3}} = 9.8$ Mott

(Exciton Bohr rad.) = (Screening length)

Keldish's droplet Keldish/68

Mean-field Th. Unstable Phase Brinkman-Rice/73

Correlation Methods Recover toward stability Vashista et.al./73

Higher Diagram, STLS etc.

Realistic Materials more Stable Combescot-Nozieres/72

Anisotropy, Multi-Valley...

Motivation

for Electron-Hole systems

- **DMC methodological challenge**

As a case with evaluations other than GS energy.

Analysis using Density Matrices, Pair Correlation Functions...

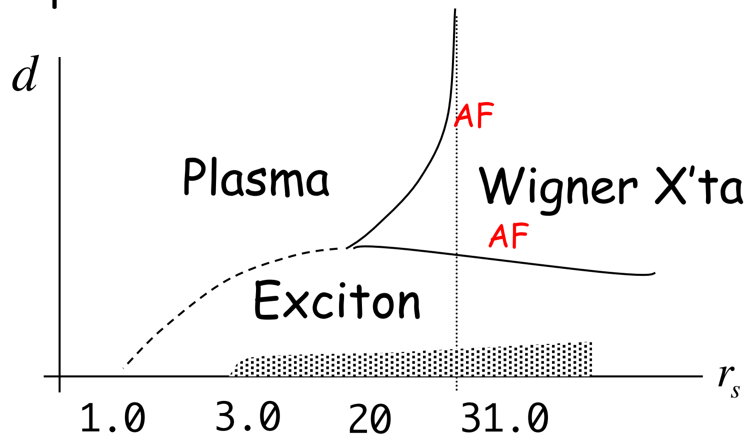
Firstly establishing implementations

for such a system that definitely shows the transition

between 2C plasma and Exciton phases

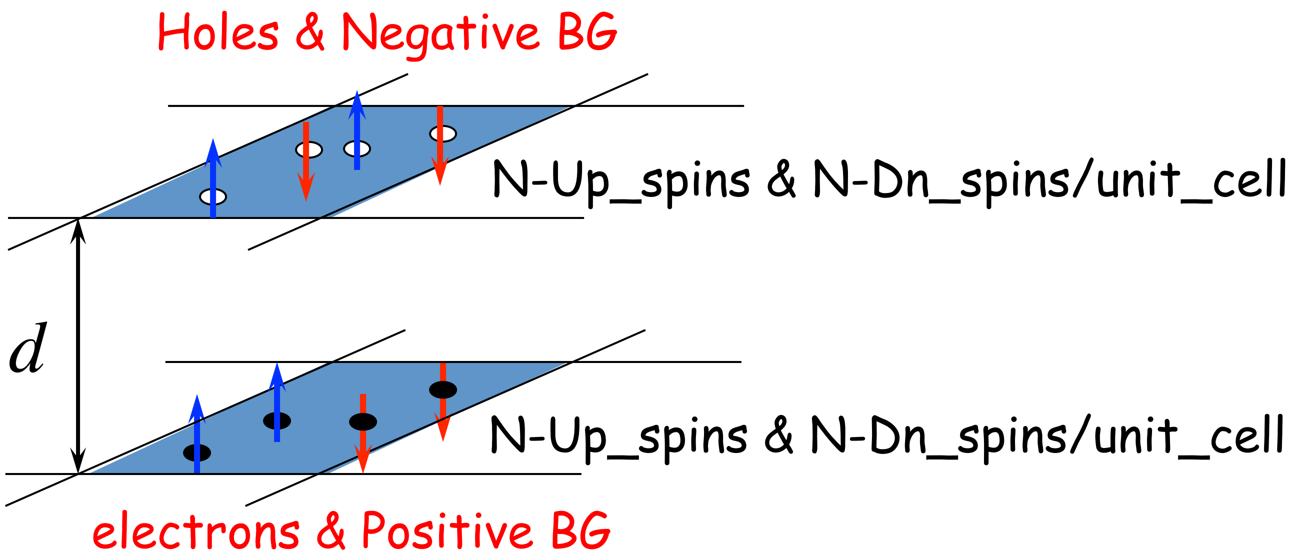
"Bilayer System"

Pablo L. Rios/Thesis (2001)



R. Maezono et.al., Phys. Rev. Lett., accepted (2013).

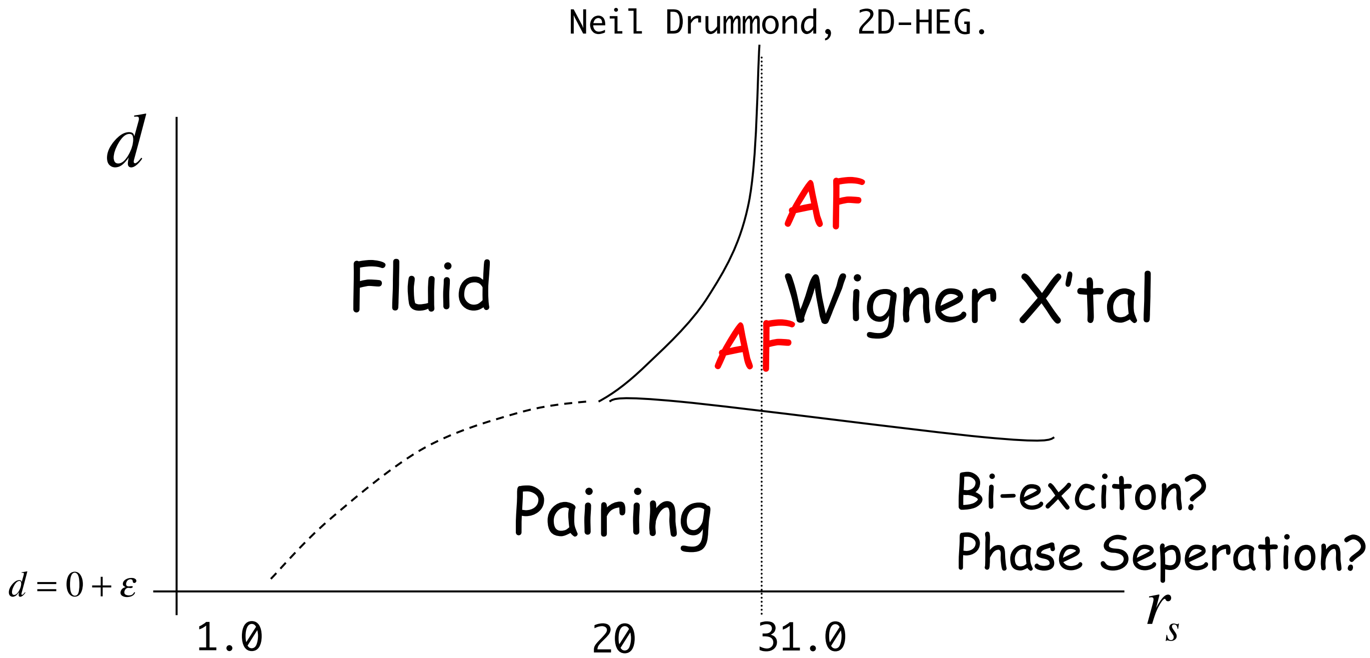
Model Bilayer



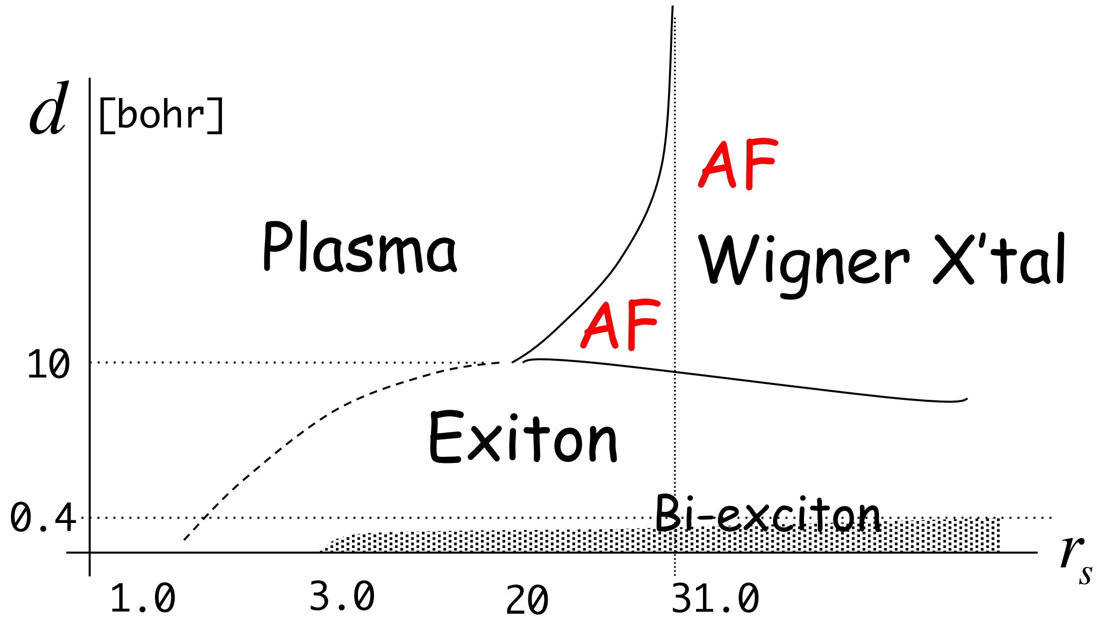
- (d, r_S) -plane Phase Diagram
- $m_h/m_e = 1.0$; Mass ratio fixed in the present study

Phase Diagram

... as predicted



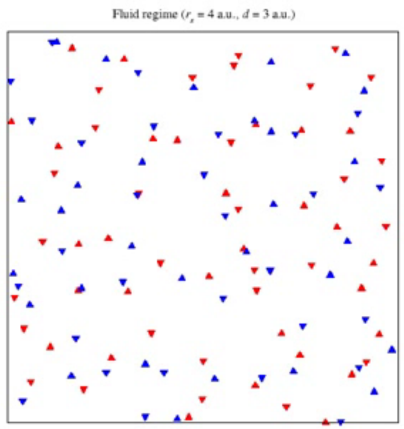
Bi-exciton captured



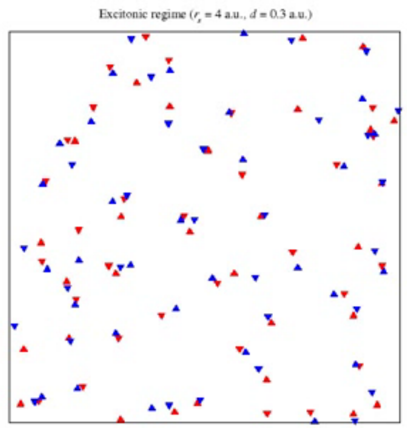
R. Maezono et.al., Phys. Rev. Lett., accepted (2013).

VMC config snapshot

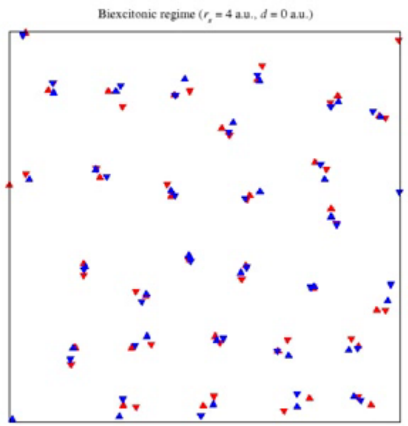
2C-Plasma
$d = 3$



Excitonic
$d = 0.3$

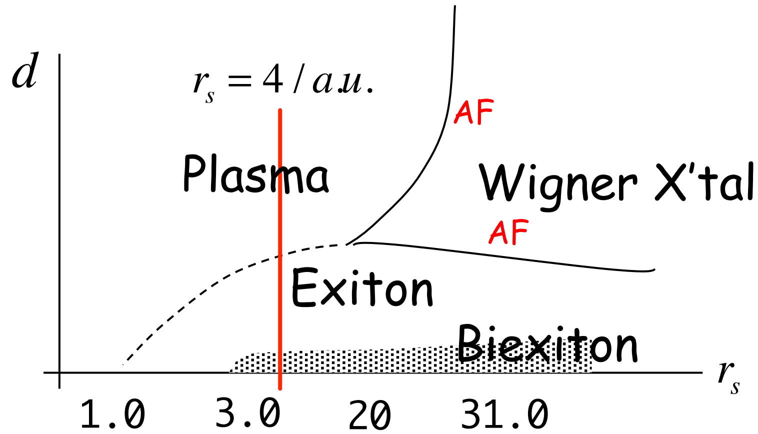


Bi-excitonic
$d = 0$



Red/Blue ; Elec./Hole

▲/▼ ; ↑spin/↓spin



Previous Studies

Analytic Approaches

BCS-type WF, mainly by Mean-field approached

- Yu. E. Lozovik et.al., Lett. **22**, 274 (1975).
- Xuejun Zhu, P. B. Littlewood, S. Hybersten, and T. M. Rice, Phys. Rev. Lett. **74**, 1633 (1995).
- P. B. Littlewood and Xuejun Zhu, Phys. Scr. **T68**, 56 (1996).
- Y. E. Lozovik and O. L. Berman, Phys. Scr. **55**, 491 (1997).

Difficult to describe global feature of Phase Diagram (as a matter of course)

Excitonic phase predicted stable at all the region

not able to reproduce 2C-Plasma at (d→large)

Study by QMC

Good at for Global Phase Diagram

→ Intermediate Regions about many-body correlations

Numerical Variational Approach

VMC & DMC

1） Phase Boundary identification

Order parameter via Density Matrices

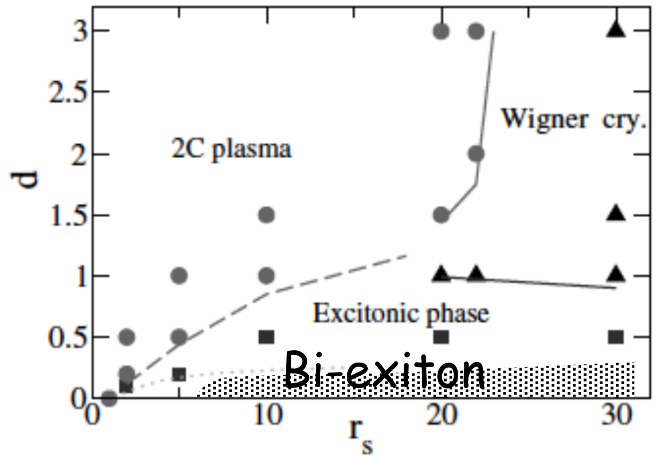
2） Internal spatial structure inside each phase

Pair Correlation Functions

De Palo's prev. Results

G. Senatore Group, PRL 88, 206401 ('02)

Successfully Described 2C plasma/Excitonic Phase Boundary



$[r_s*a_B]$

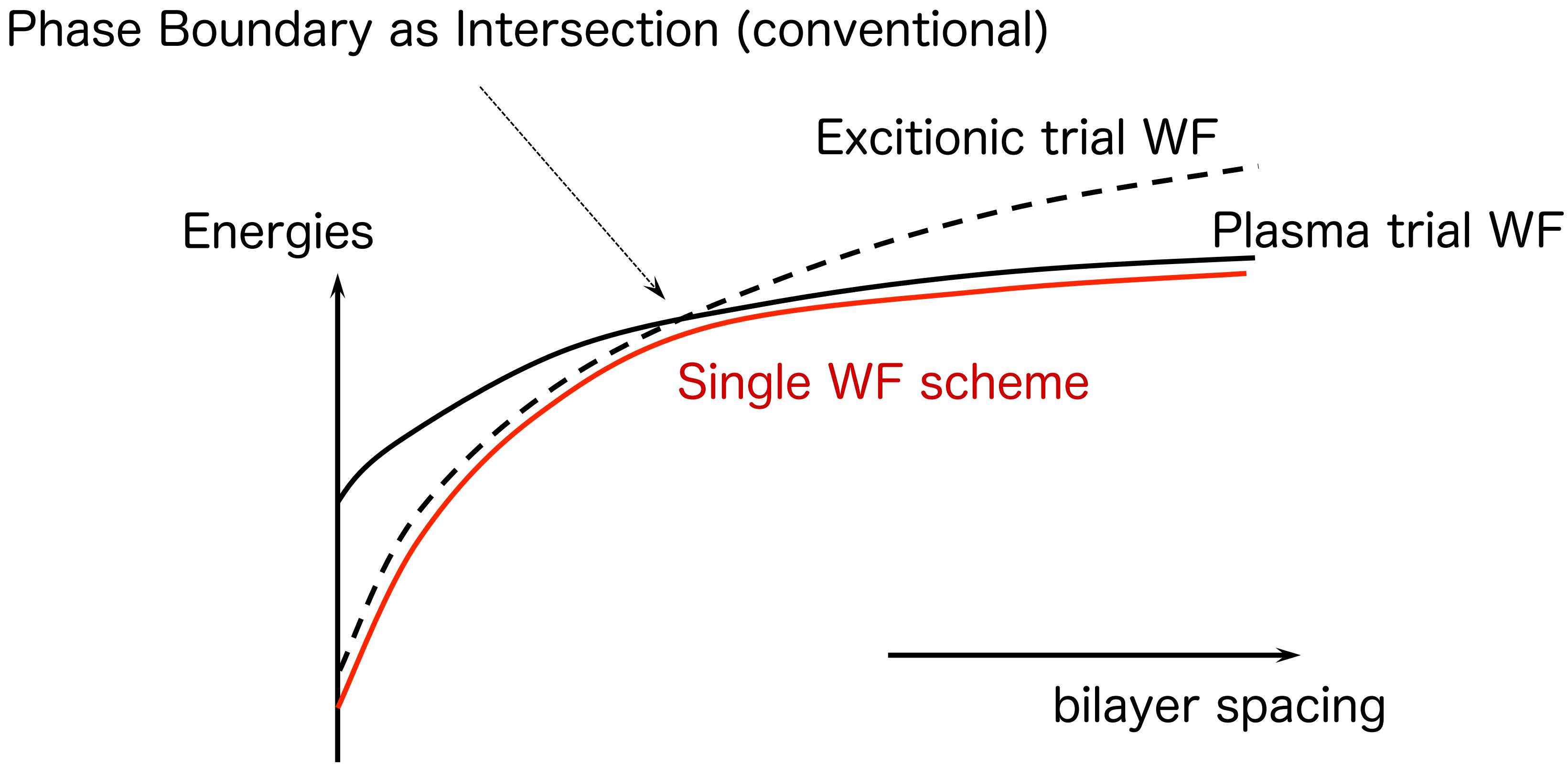
Our works

Order Parameter/Pair Correlation Function analysis

using Single Wave Function scheme

→ Successfully captured Biexcitonic phase.

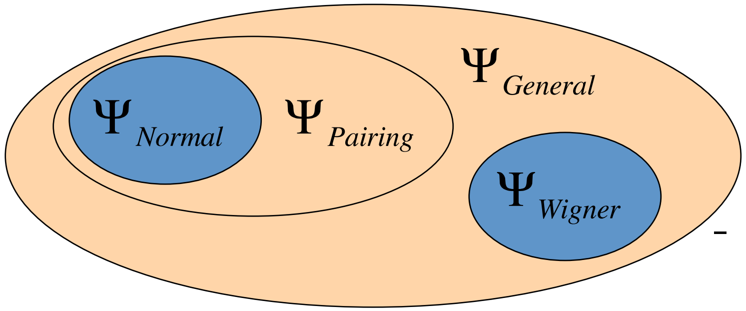
Multi WaveFunc. Scheme



SWF doesn't use 'energy intersection identification' for phase Boundary

Single WF scheme

Description using most general form of WF



- W. L. McMillan, Phys. Rev. 138, A442 (1965).

McMillan, ^4He VMC (Solid/Liquid phase transition)

possible to get Variational advantage, but

$$E\left[\Psi_{Normal}\right] > E\left[\Psi_{Pairing}\right]$$ no such identification possible.

→ Require direct evaluation of Order Parameter

to identify the Phase Boundary

Single WF scheme

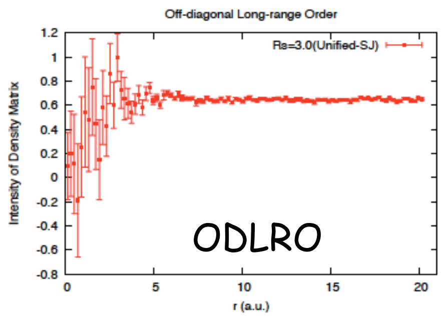
Phase Boundary by Order parameters

- Make use of Backflow Tr.

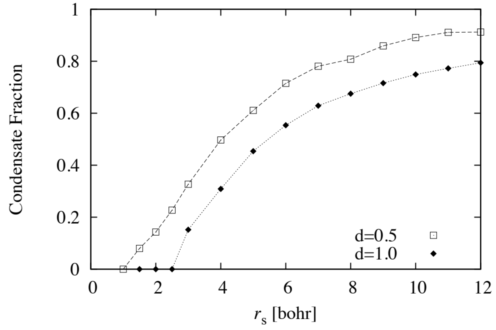
    Distinction between trial WFs becomes unclear when BF is used.

- Exciton Mott Transition details/ possibility of cross-over

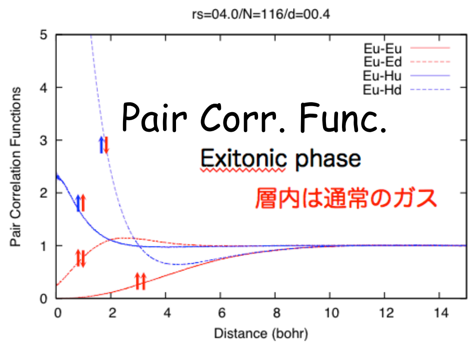
$$\lim_{|\vec{r}|\to\infty} \gamma_{eh}^{(2)}\left(\vec{r}_e, \vec{r}_h; \vec{r}_e + \vec{r}, \vec{r}_h + \vec{r}\right)$$



Order Parameter



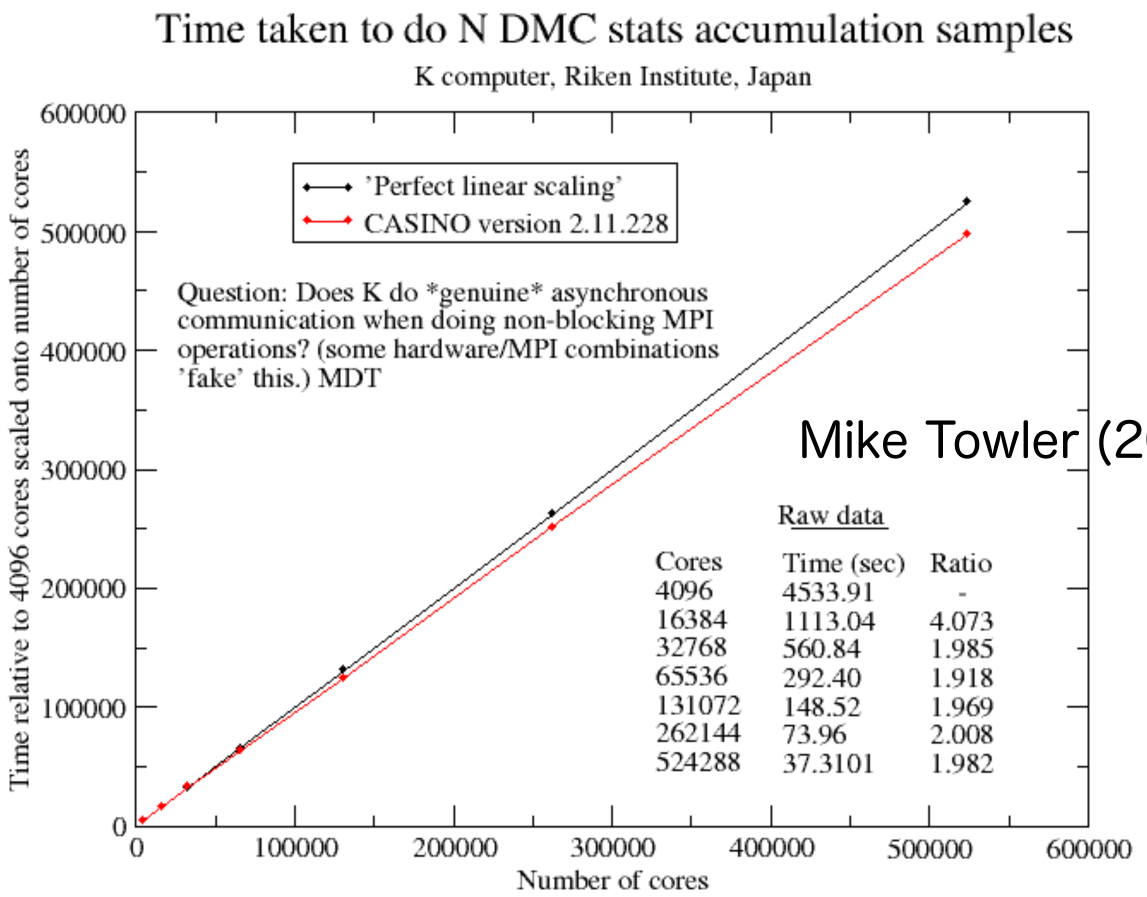
Exciton Formation occurs



Spatial structure the phase has

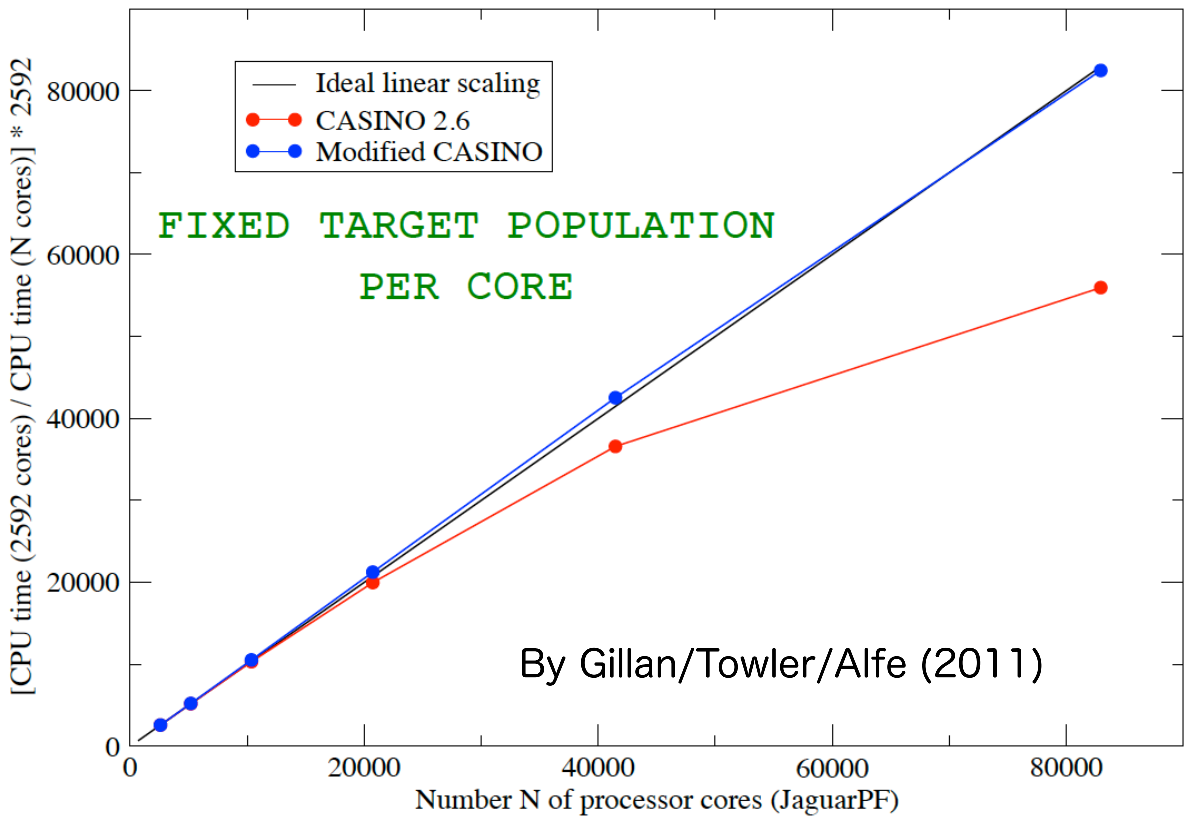
Strong Scaling on K

Hydrogen atom on graphene sheet



Mike Towler (2013).

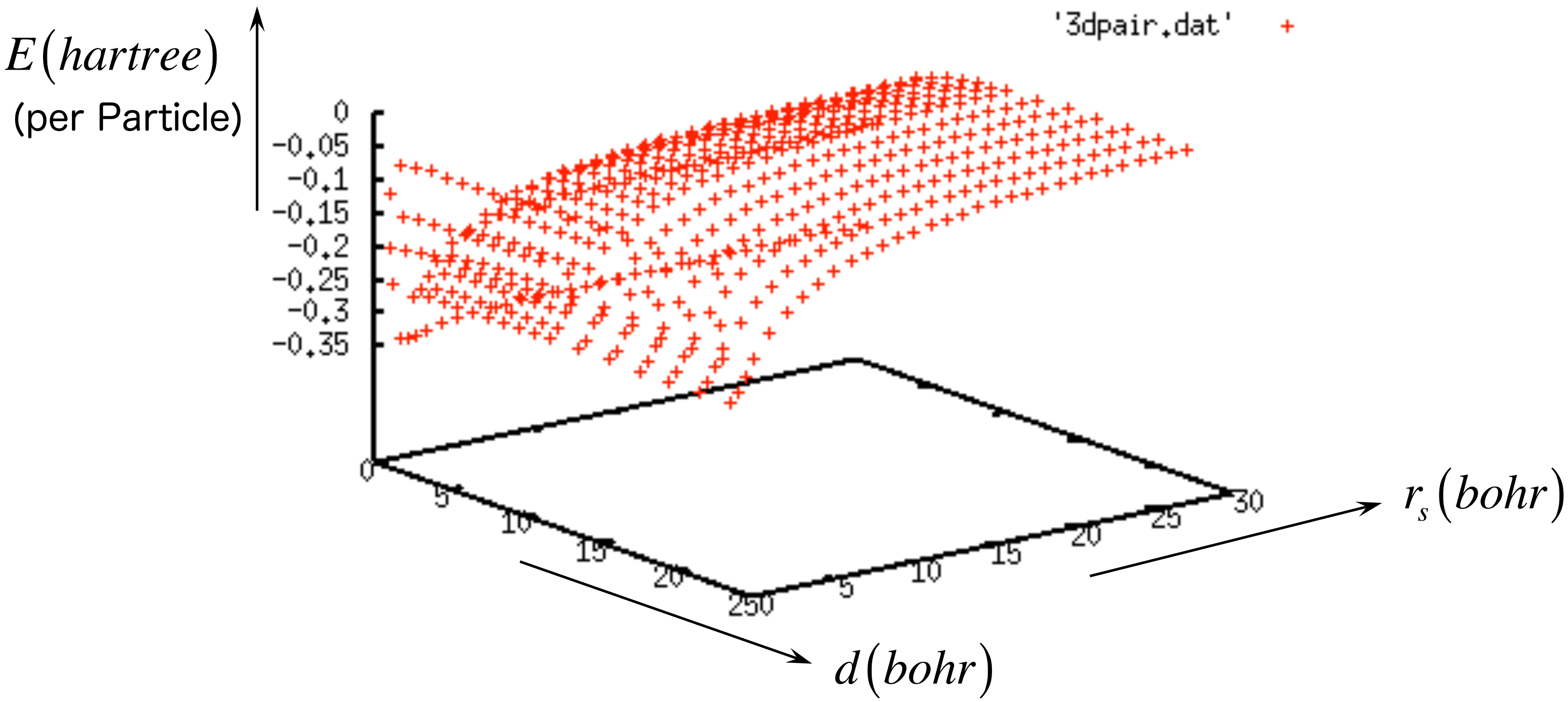
Scalability



Improved by replacing MPI_SEND --> MPI_ISEND

Results

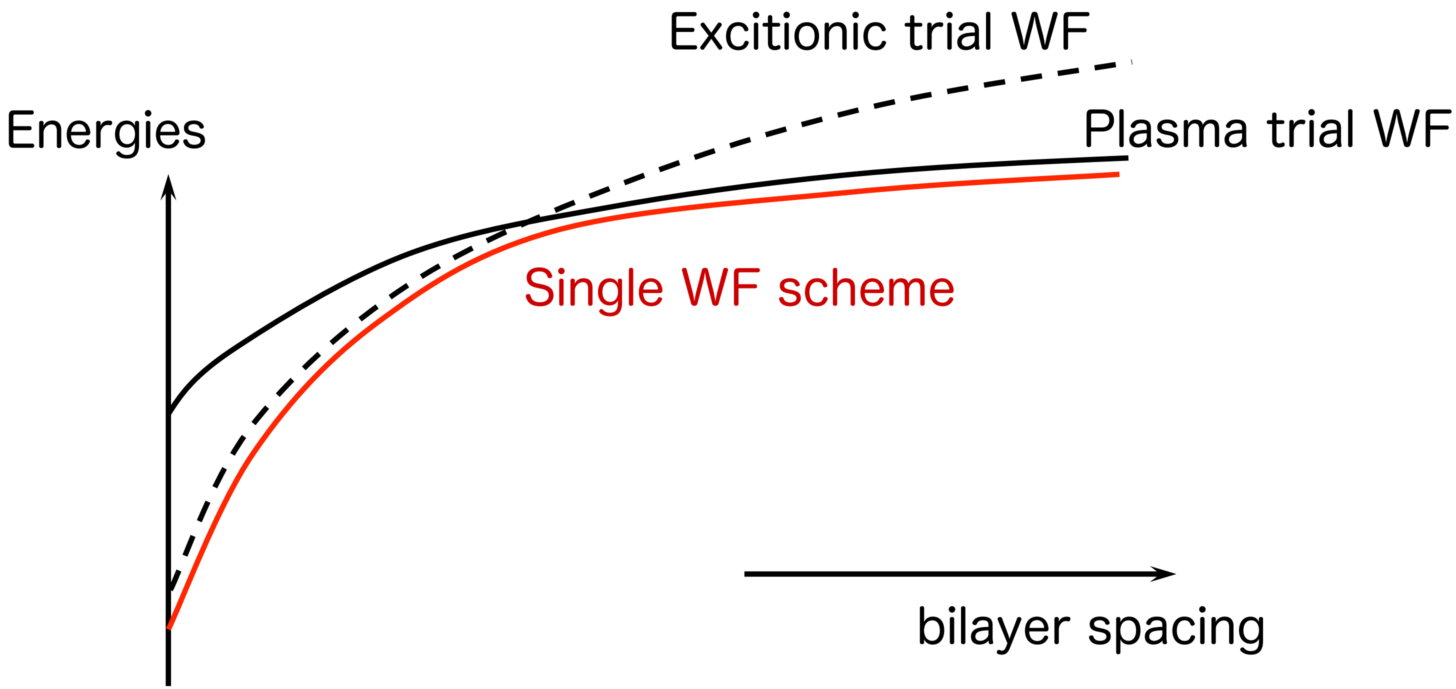
Global survey(1)



- Only for (PW and Poly)/VMC/N=116 (no PPW, Wigner...)

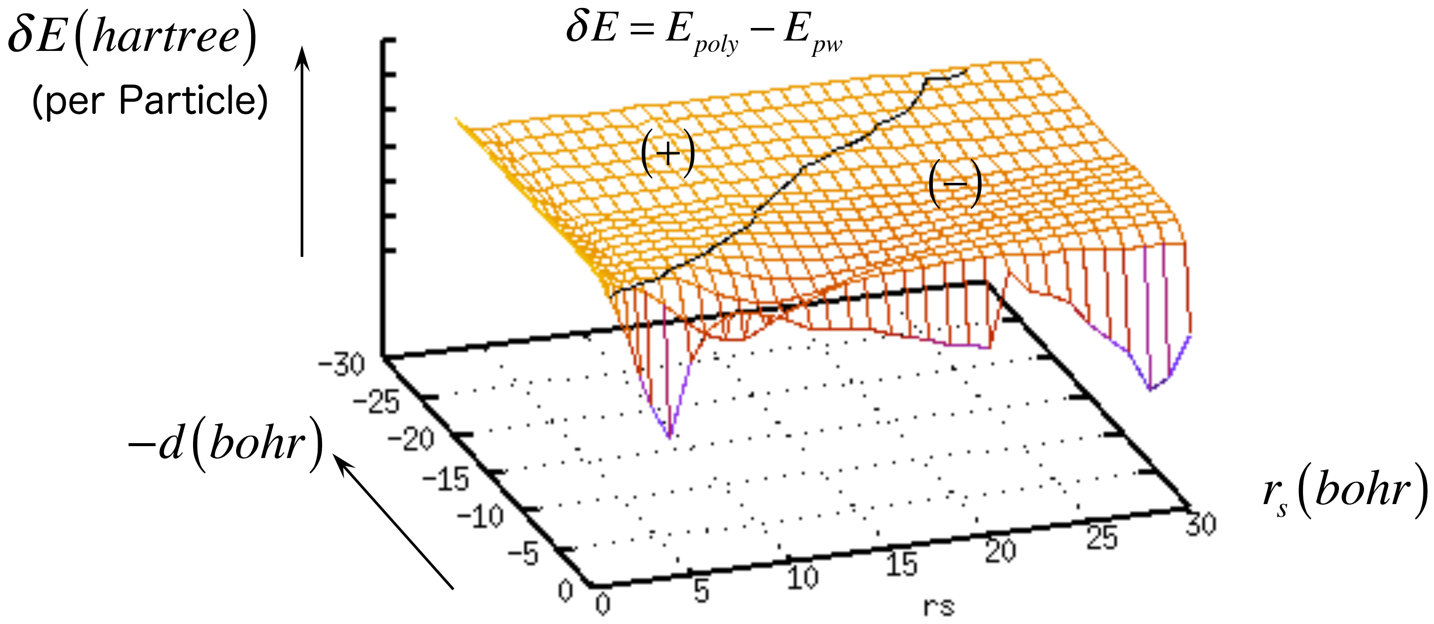
  --> To get reference values, first of all.

Multi WaveFunc. Scheme



SWF doesn't use 'energy intersection identification' for phase Boundary

Global survey(3)



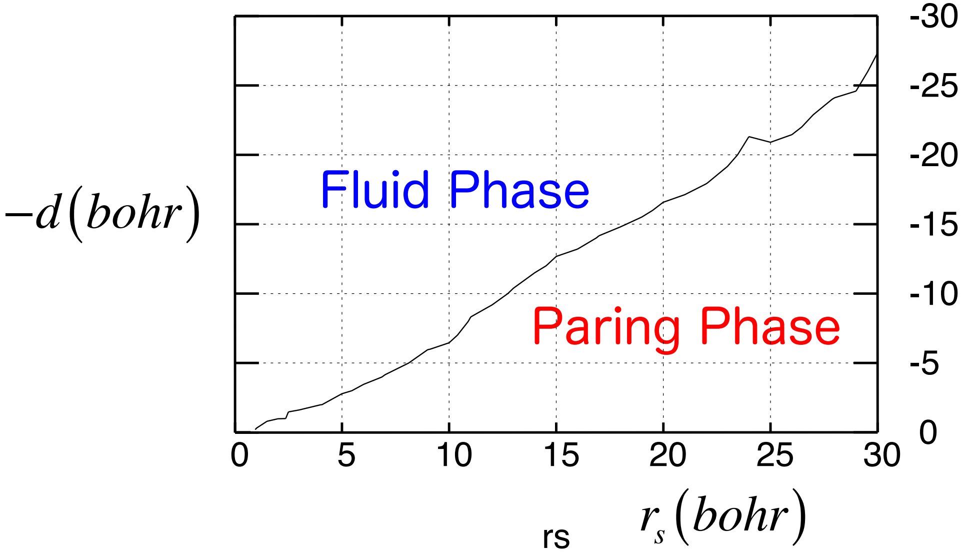
- Only for (PW and Poly)/VMC/N=116 (no PPW, Wigner...)

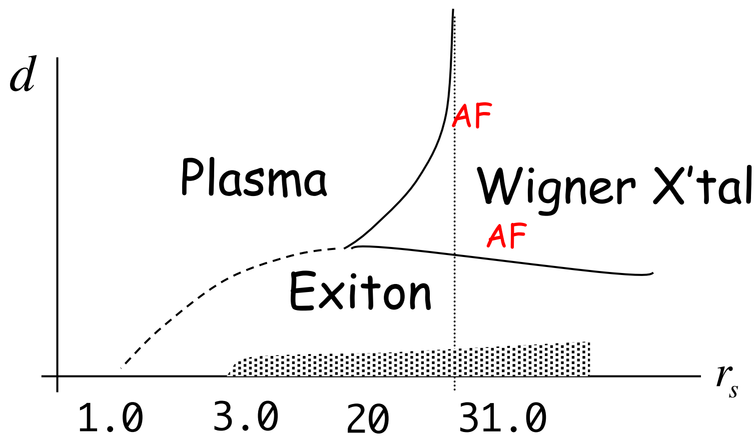
--> To get reference values, first of all.

Global survey(4)

VMC Phase Boundary estimated by Fluid and Paring Trial WF.

Possibility of Wigner X'tal phase not taken into account here.





De Palo's work

- DMC value at (rs=1.0, d=0.0)

  E = -0.417(4) De Palo *et.al.*, Phys. Rev. Lett. 88, 206401 (2002).

  E = -0.4236 (1) Our result by Paring WF.

- No Paring at rs=1.0 ?

  De Palo reports No Paring

  while our DMC shows Paring at smaller distance.

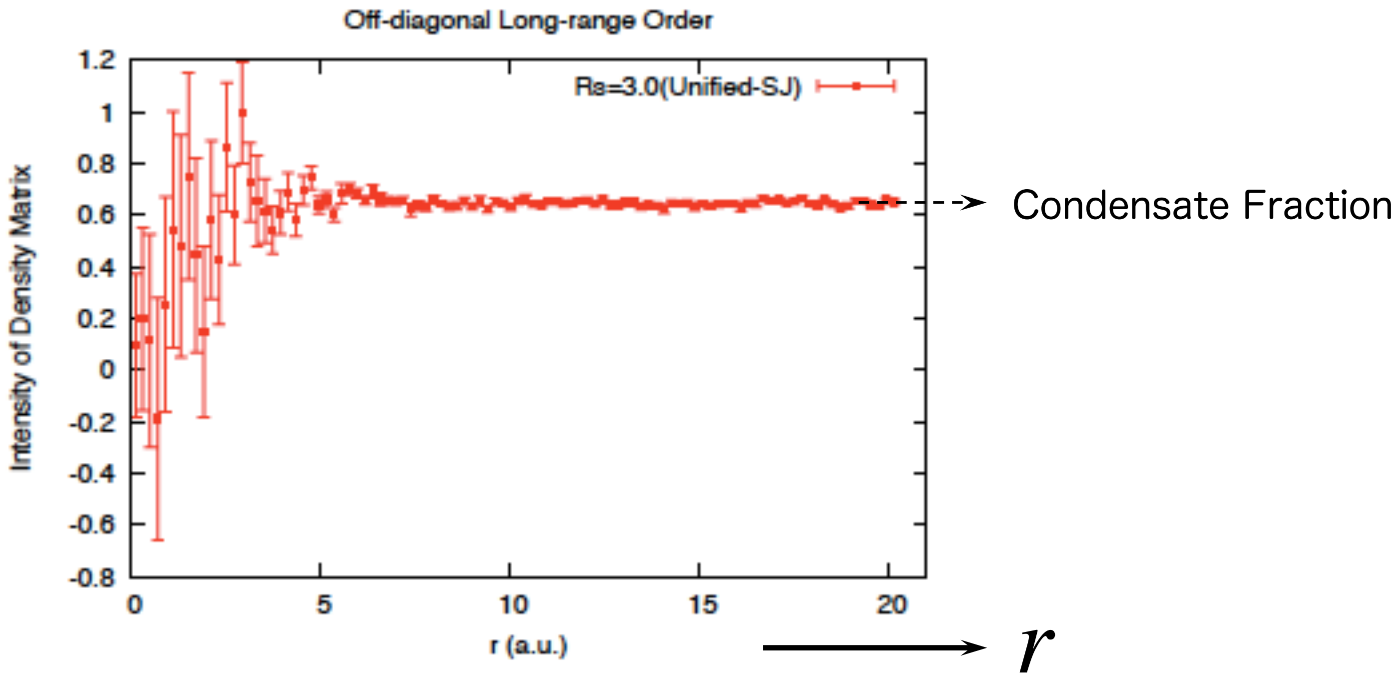
Order Parameter

Condensate Fraction for Exciton formation

(normalized into [0,1])

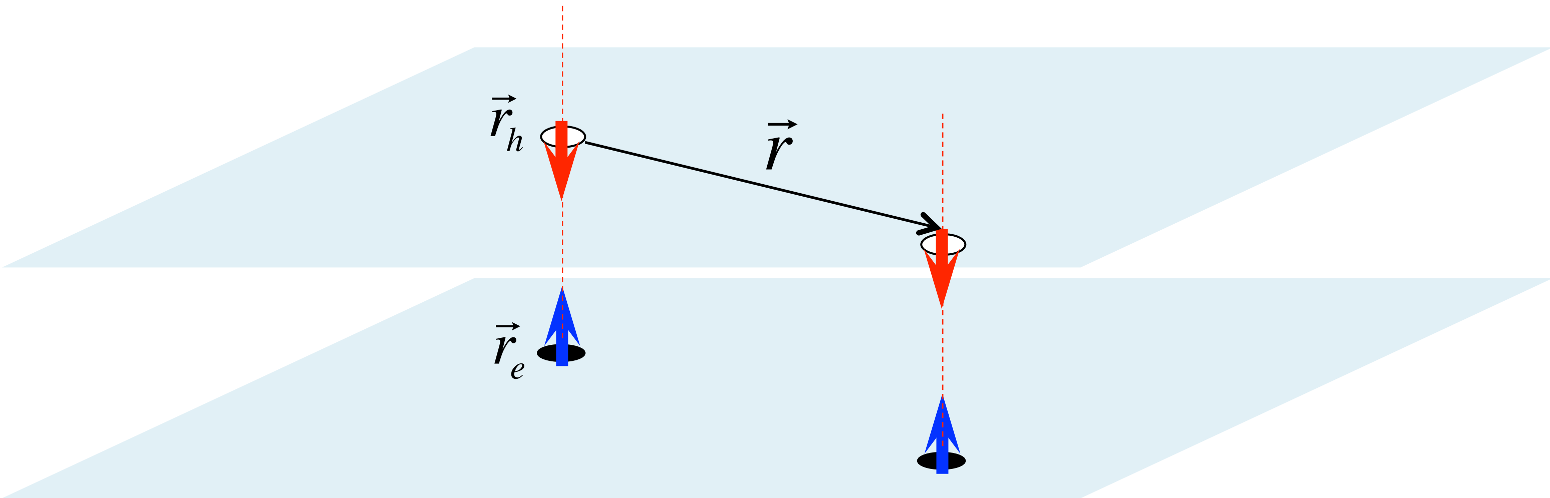
Correlation between pairs located $\vec{r}$ distance

$$\lim_{|\vec{r}|\to\infty} \gamma_{eh}^{(2)}(\vec{r}_e, \vec{r}_h; \vec{r}_e + \vec{r}, \vec{r}_h + \vec{r})$$



Phase Correlation

between different snapshots



Two-body Density Matrix

$$\gamma^{(2)}_{eh}\left(\vec{r}_e,\vec{r}_h;\vec{r}_e+\vec{r},\vec{r}_h+\vec{r}\right)=N_1\left(N_2-\delta_{12}\right)\frac{\int\left|\Psi\left(\vec{R}\right)\right|^2\frac{\Psi\left(\vec{r}_e+\vec{r},\vec{r}_h+\vec{r},\cdots,\vec{r}_N\right)}{\Psi\left(\vec{r}_e,\vec{r}_h,\cdots,\vec{r}_N\right)}d\vec{r}_3\cdots d\vec{r}_N}{\int\left|\Psi\left(\vec{R}\right)\right|^2 d\vec{R}}$$

Measure How much Cancellation

Quantum Condensation

Two-body DM

One-body vanishes for Fermion

$$\gamma_2(\vec{x}_1,\vec{x}_2;\vec{y}_1,\vec{y}_2)=\frac{1}{2}\gamma_1(\vec{x}_1,\vec{y}_1)\gamma_1(\vec{x}_2,\vec{y}_2)-\frac{1}{2}\cancel{\gamma_1(\vec{x}_1,\vec{y}_2)}\gamma_1(\vec{x}_2,\vec{y}_1)+\frac{1}{2}\chi^*(\vec{y}_2,\vec{x}_2)\chi(\vec{y}_1,\vec{x}_1)$$

$$\chi(\vec{x},\vec{x}')=\langle\Psi_0|\psi(\vec{x}')\psi(\vec{x})|\Psi_0\rangle$$ should be non-zero for Condensation

For Slater Det. Ψ, it vanishes and then γ_2 is decoupled by γ_1

→ No Condensation

Quantum Condensation requires many-body description

beyond Slater Determinant

e.g., Geminal WF → HFB theory

Density Matrix Sampling

many-body WF form

One-body DM：

$$\gamma^{(1)}\left(\vec{r}_1;\vec{r}_1'\right)=N_1\frac{\int\Psi^*\left(\vec{r}_1,\vec{r}_2,\cdots,\vec{r}_N\right)\Psi\left(\vec{r}_1',\vec{r}_2,\cdots,\vec{r}_N\right)d\vec{r}_2\cdots d\vec{r}_N}{\int\left|\Psi\left(\vec{R}\right)\right|^2 d\vec{R}}$$

$$=N_1\frac{\int\left|\Psi\left(\vec{R}\right)\right|^2\frac{\Psi\left(\vec{r}_1',\vec{r}_2,\cdots,\vec{r}_N\right)}{\Psi\left(\vec{r}_1,\vec{r}_2,\cdots,\vec{r}_N\right)}d\vec{r}_2\cdots d\vec{r}_N}{\int\left|\Psi\left(\vec{R}\right)\right|^2 d\vec{R}}$$

Two-body DM：

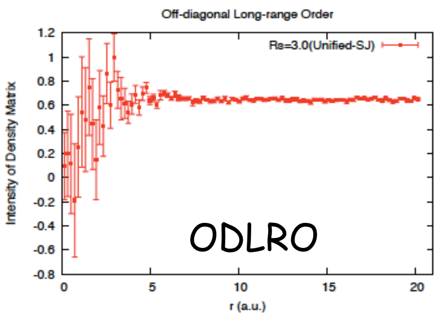
$$\gamma_{12}^{(2)}\left(\vec{r}_1,\vec{r}_2;\vec{r}_1',\vec{r}_2'\right)=N_1\left(N_2-\delta_{12}\right)\frac{\int\Psi^*\left(\vec{r}_1,\vec{r}_2,\cdots,\vec{r}_N\right)\Psi\left(\vec{r}_1',\vec{r}_2',\cdots,\vec{r}_N\right)d\vec{r}_3\cdots d\vec{r}_N}{\int\left|\Psi\left(\vec{R}\right)\right|^2 d\vec{R}}$$

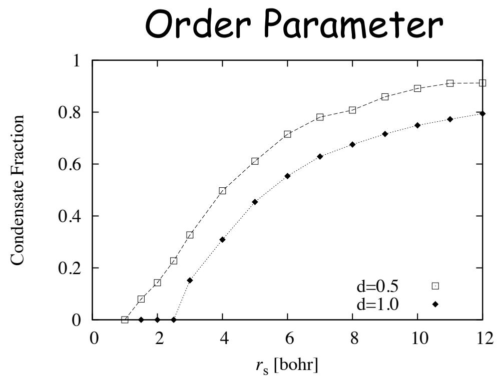
$$=N_1\left(N_2-\delta_{12}\right)\frac{\int\left|\Psi\left(\vec{R}\right)\right|^2\frac{\Psi\left(\vec{r}_1',\vec{r}_2',\cdots,\vec{r}_N\right)}{\Psi\left(\vec{r}_1,\vec{r}_2,\cdots,\vec{r}_N\right)}d\vec{r}_3\cdots d\vec{r}_N}{\int\left|\Psi\left(\vec{R}\right)\right|^2 d\vec{R}}$$

Order parameter

Condensate Fraction of Exciton

$$\lim_{|\vec{r}|\to\infty} \gamma_{eh}^{(2)}\left(\vec{r}_e, \vec{r}_h; \vec{r}_e + \vec{r}, \vec{r}_h + \vec{r}\right)$$

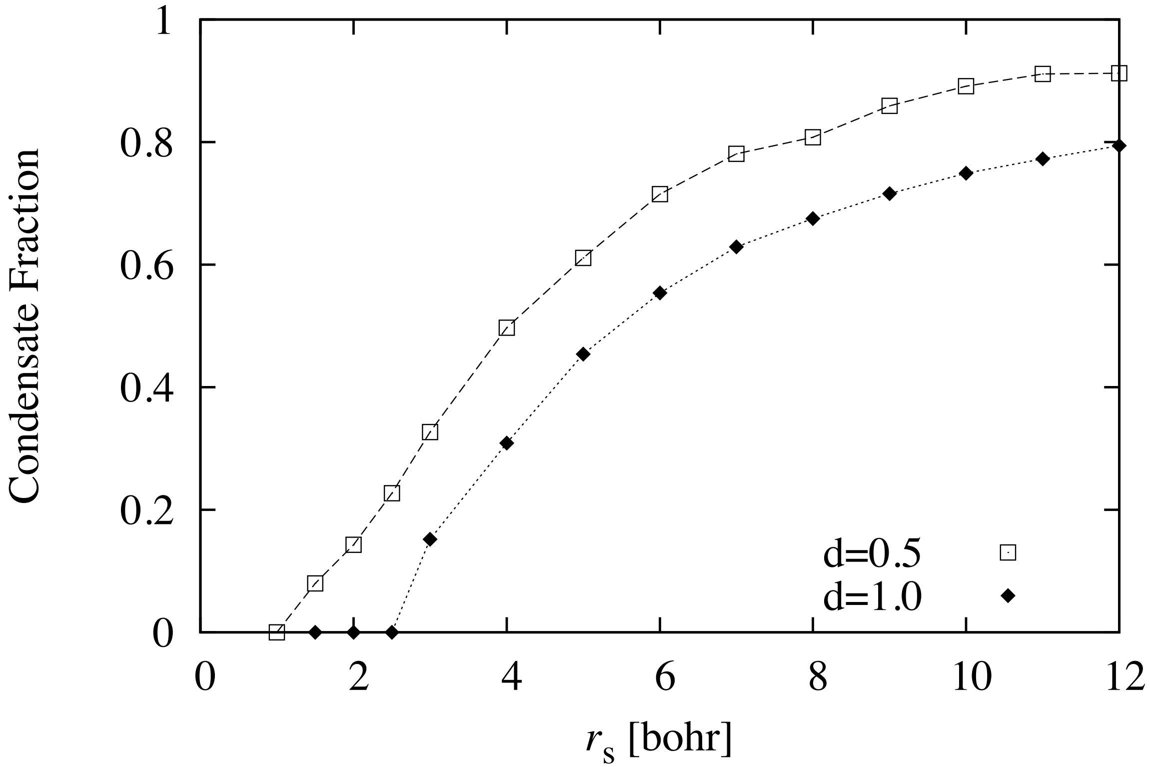


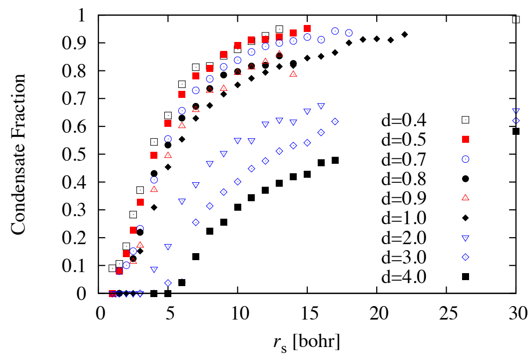


Exciton Formation occurs

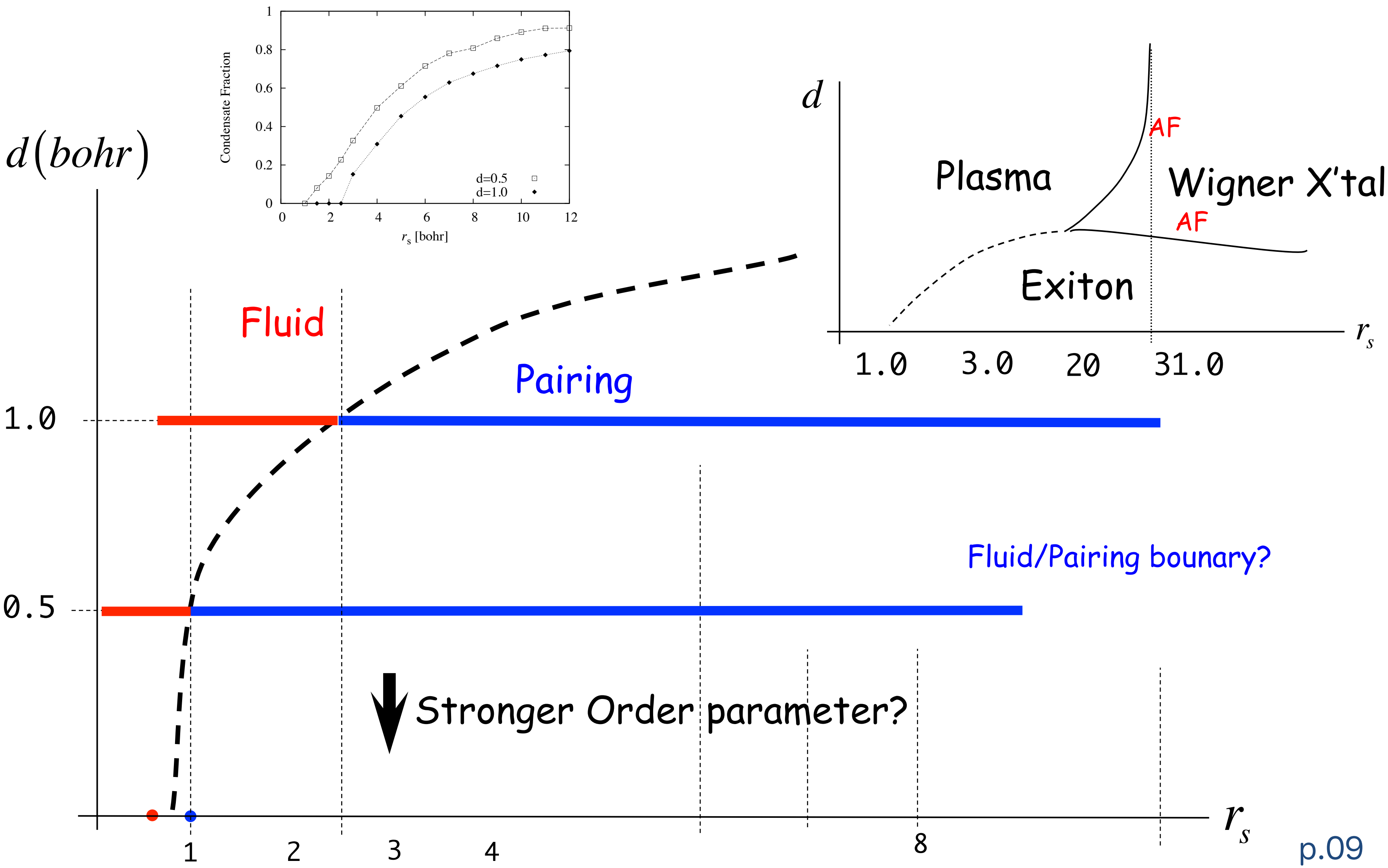
Order Parameter

Revised on 13 Sep. 2012.



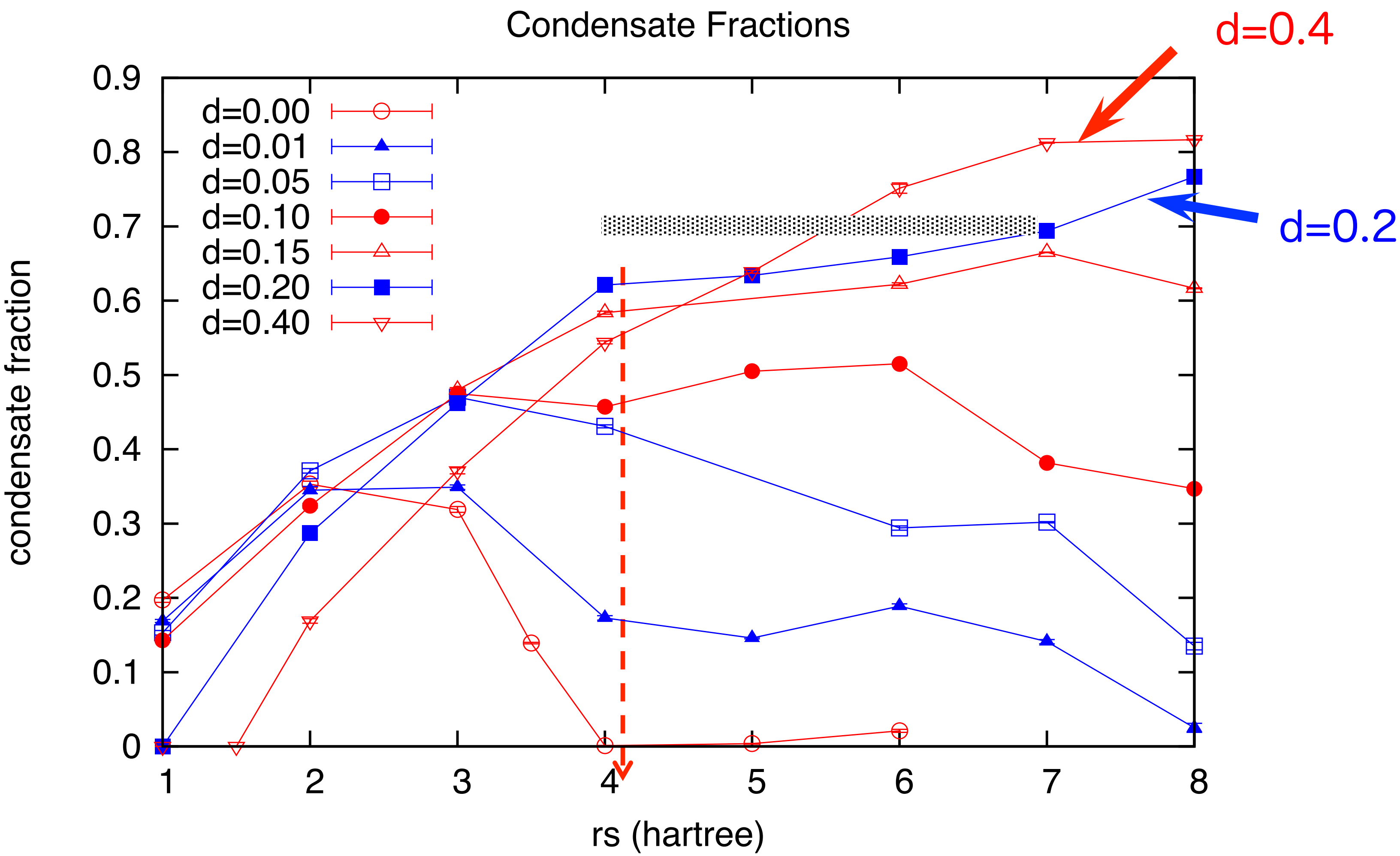


Phase Diagram

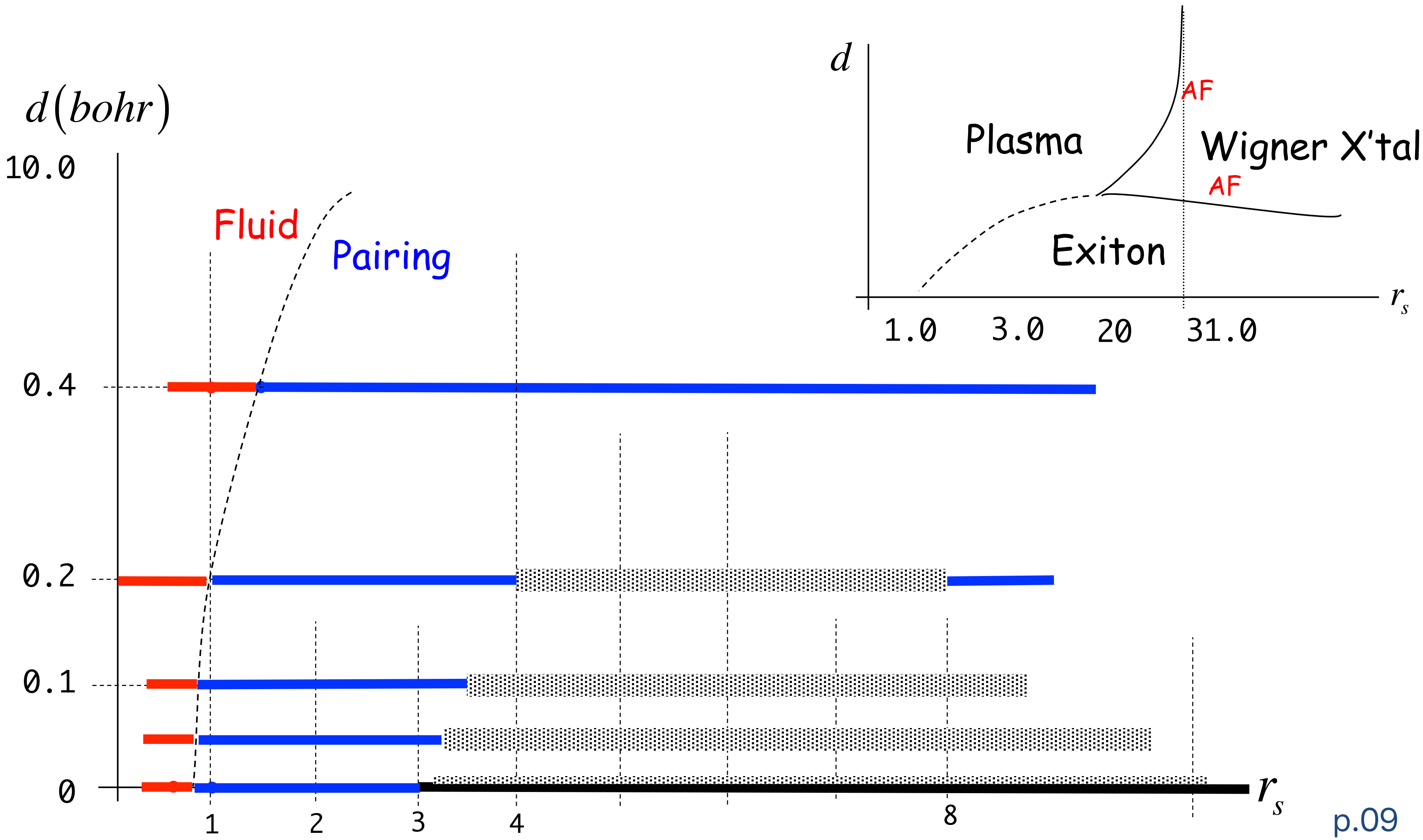


Dying-off behavior

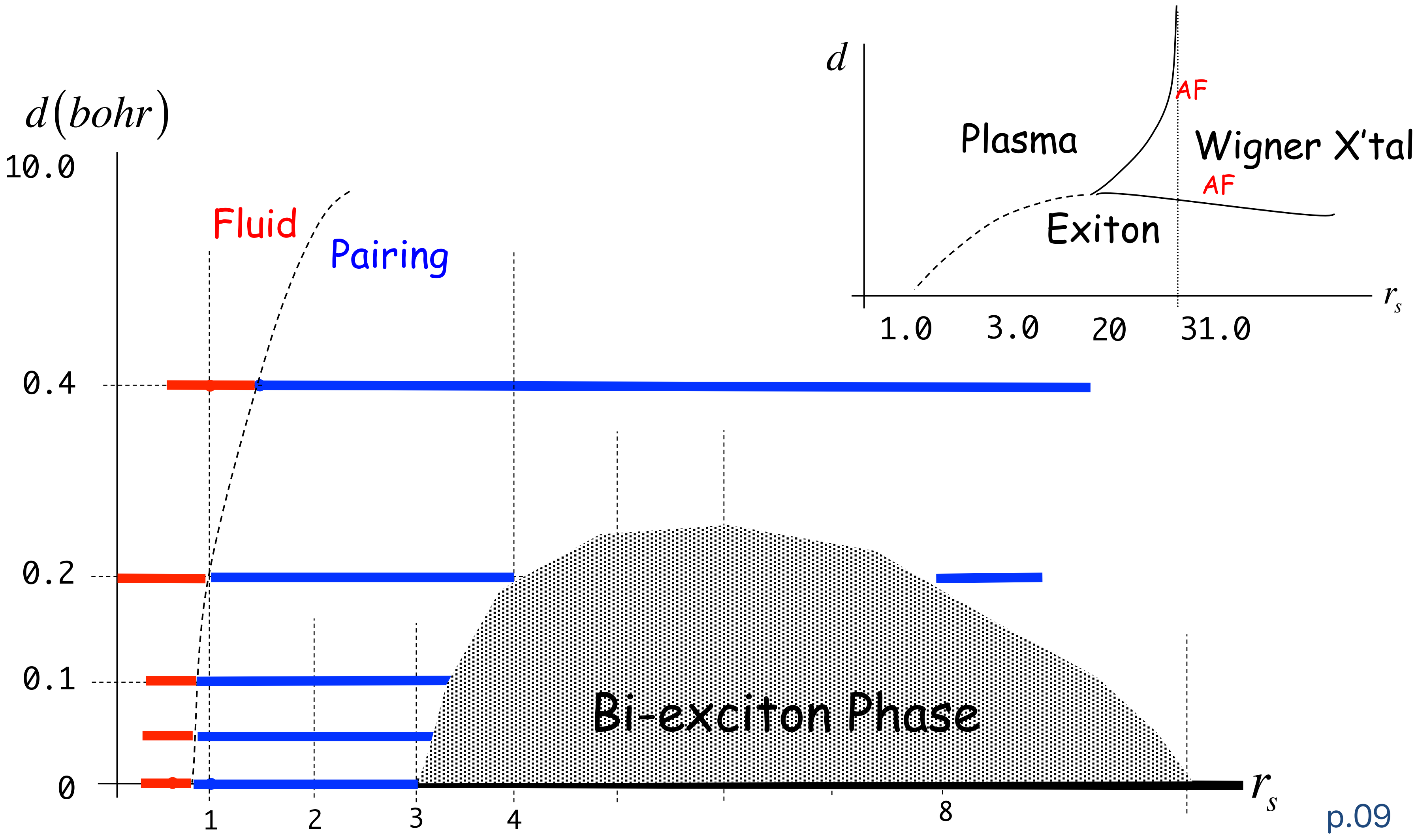
Revised on 22 May. 2012.



Dying-off behavior



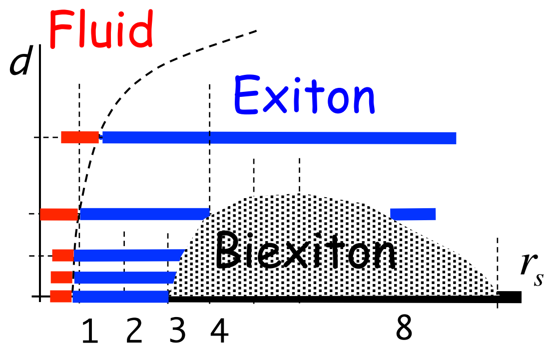
Dying-off



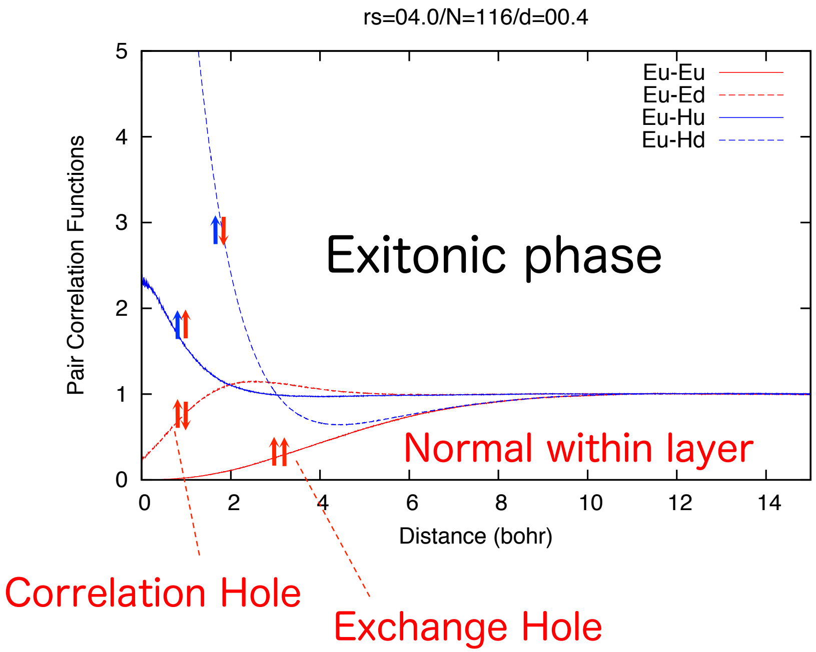
$d(bohr)$
10.0
0.4
0.2
0.1
0
Fluid
Pairing
Bi-exciton Phase
1
2
3
4
8
r_s
d
Plasma
Wigner X'tal
AF
AF
Exiton
1.0
3.0
20
31.0
r_s

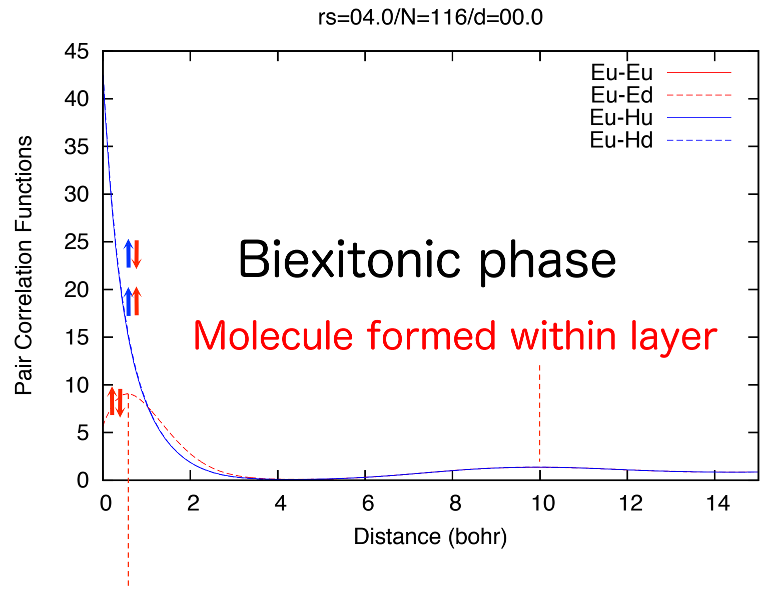
Pair Correlation Functions

PCF



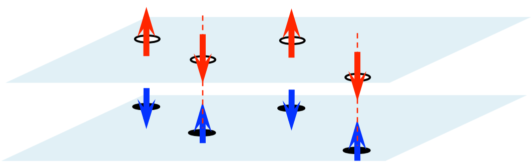
Different behaviors in Eu-Ed distributions.

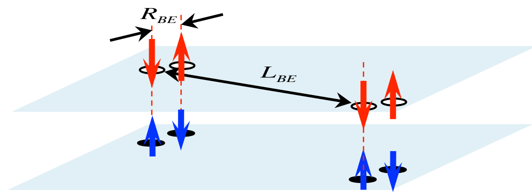




Biexiton Radius R_{BE}

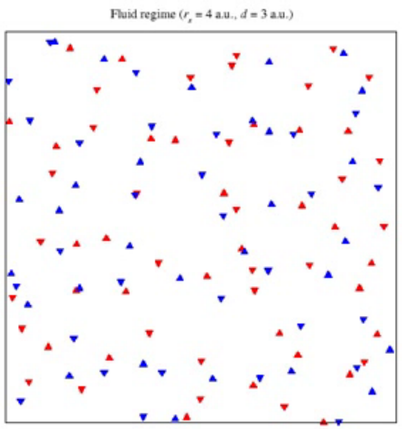
characteristic profile appears with peak.



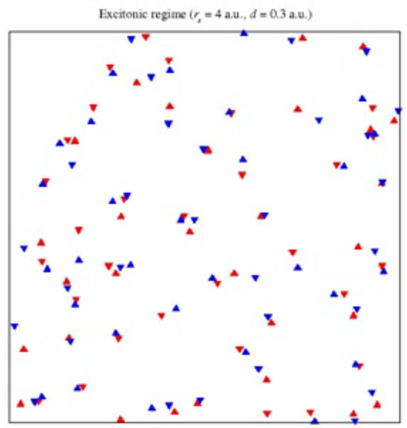


VMC config snapshot

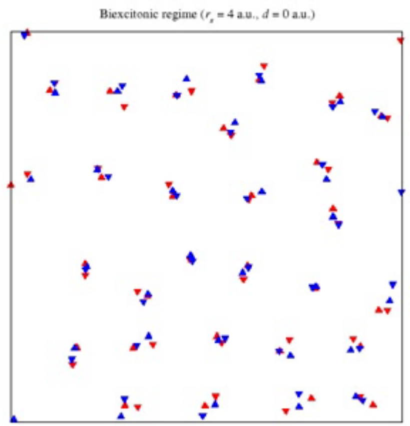
2C-Plasma
$d = 3$



Excitonic
$d = 0.3$

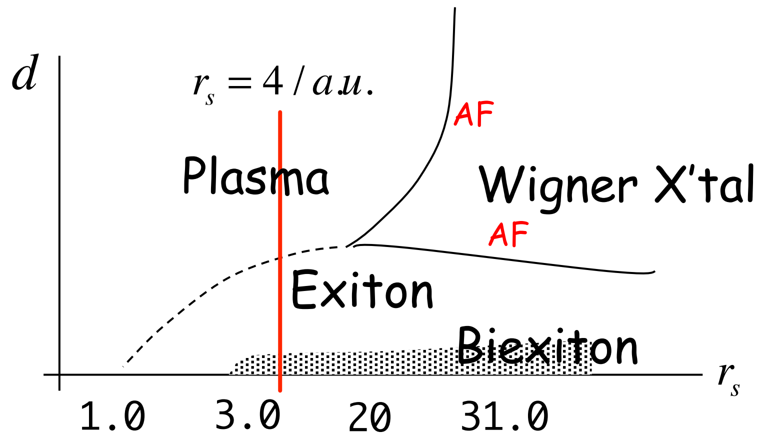


Bi-excitonic
$d = 0$



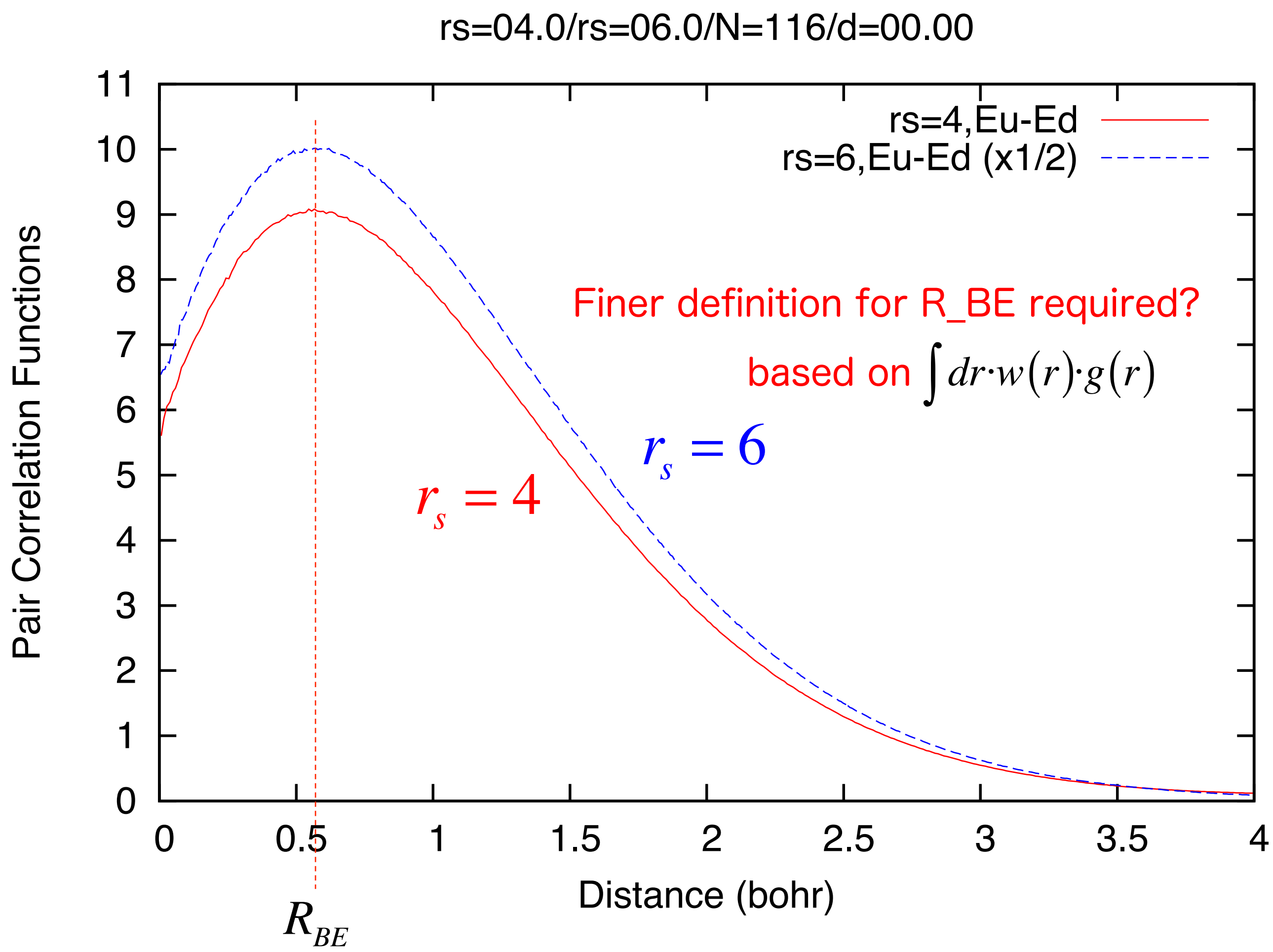
Red/Blue ; Elec./Hole

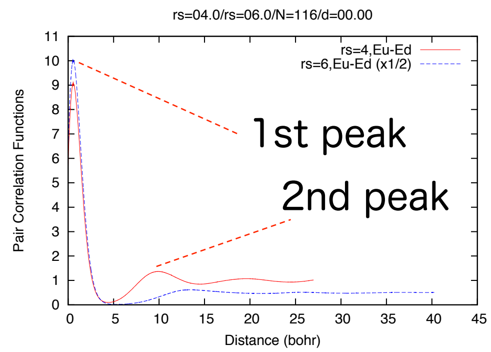
▲/▼ ; ↑spin/↓spin



Biexciton Radius

Revised on 20 May. 2012.

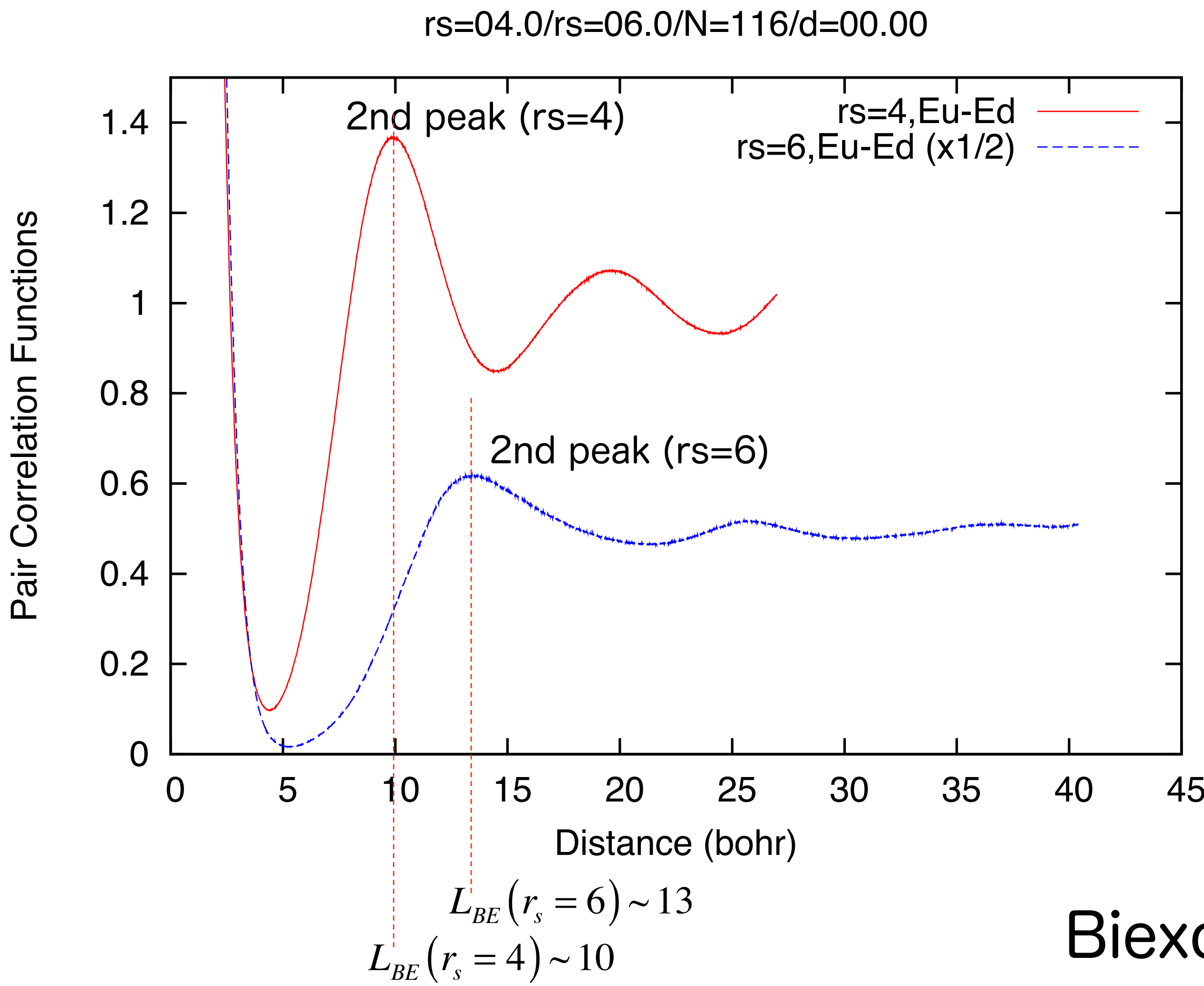


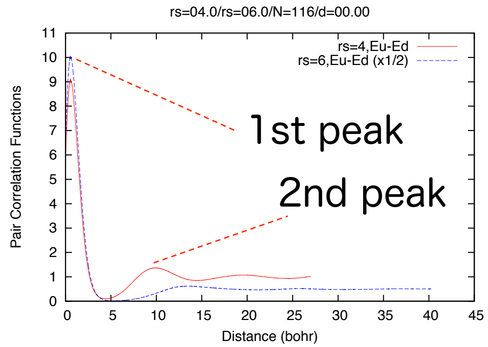


<Whole view>

Inter-Biexciton length

Revised on 18 May. 2012.





<Whole view>

Biexciton Gas