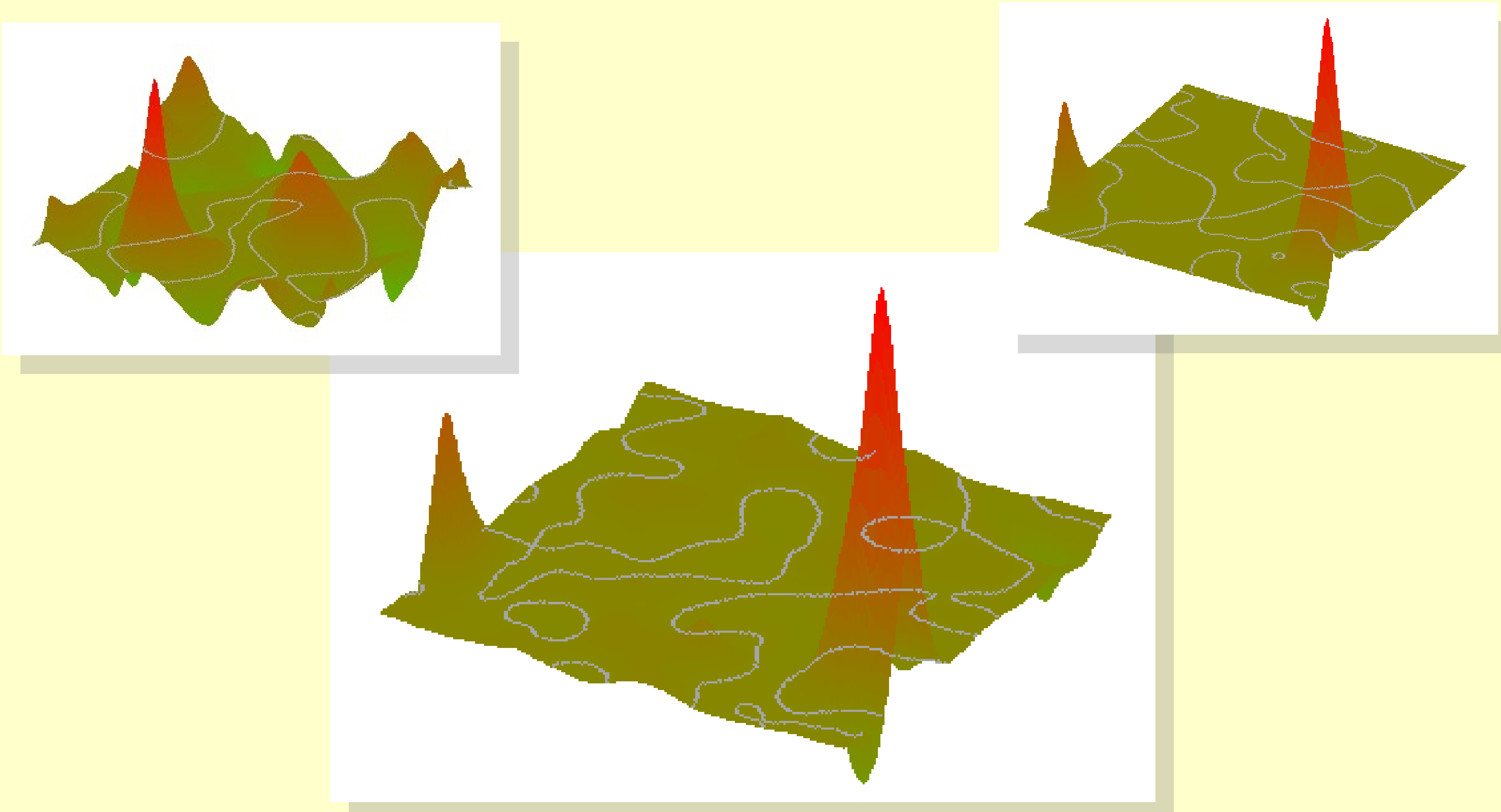
QMC study of electron-hole systems



Pablo López Ríos
University of Cambridge

QMC study of electron-hole systems

The quantum Monte Carlo method can determine the total energy of an assembly of quantum particles to a high degree of accuracy.

- In variational Monte Carlo (VMC), a trial wave function $\Psi_T(\mathbf{R})$ is used to evaluate an upper bound to the exact ground-state energy E_0.

$$E_{VMC} = \sum_{i=1}^{M} \frac{\hat{H}(\boldsymbol{R}_i)\Psi_T(\boldsymbol{R}_i)}{\Psi_T(\boldsymbol{R}_i)} \simeq \frac{\int |\Psi_T(\boldsymbol{R})|^2 \frac{\hat{H}(\boldsymbol{R})\Psi_T(\boldsymbol{R})}{\Psi_T(\boldsymbol{R})} d\boldsymbol{R}}{\int |\Psi_T(\boldsymbol{R})|^2 d\boldsymbol{R}} \geq E_0$$

- In diffusion Monte Carlo (DMC), imaginary-time propagation is used to project out the higher-energy components of $\Psi_T(\mathbf{R})$.

- For fermions, the *fixed-node approximation* is required. It is equivalent to constraining the *nodal surface* of the DMC wave function to equal that of $\Psi_T(\mathbf{R})$.

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The following are typical fermionic trial wave functions:

- $\Psi_T(\mathbf{R})=\Psi_S(\mathbf{R})$ (*Slater* or *Hartree-Fock* type)

  where $\Psi_S(\mathbf{R})$ is a Slater determinant (or a multi-determinant expansion) of suitable one-particle orbitals. With a single determinant, there are **no correlation effects**.

- $\Psi_T(\mathbf{R})=e^{J(\mathbf{R})}\Psi_S(\mathbf{R})$ (*Slater-Jastrow* type)

  where $e^{J(\mathbf{R})}$ is a Jastrow correlation factor containing optimizable parameters.

- $\Psi_T(\mathbf{R})=e^{J(\mathbf{R})}\Psi_S[\mathbf{X}(\mathbf{R})]$ (*Slater-Jastrow-backflow* type)

  where $\mathbf{X}(\mathbf{R})$ is a set of collective coordinates containing optimizable parameters.

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Key points:

- The quality of $\Psi_T(\mathbf{R})$, and in particular of its nodal surface, is paramount for the accuracy of the results.

- The Jastrow factor is the most important tool to improve upon $\Psi_S(\mathbf{R})$, but it does not change its nodes.

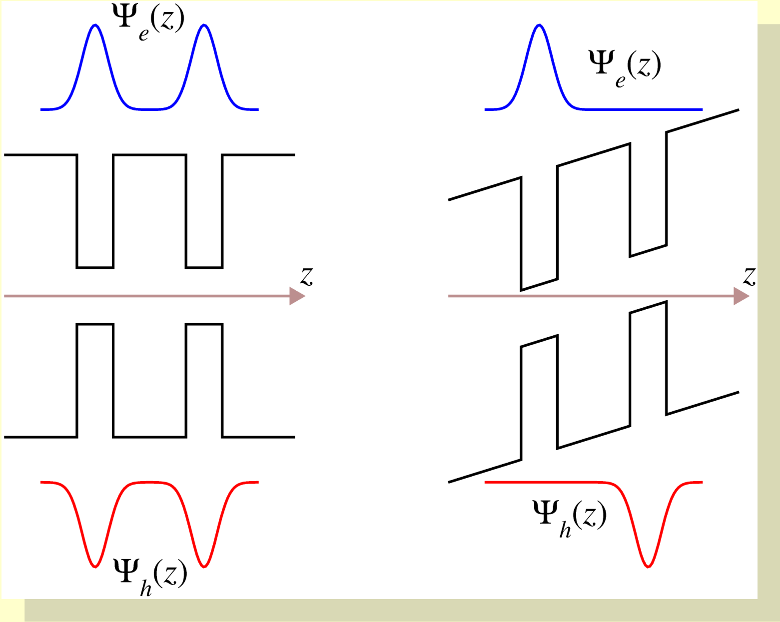
- There are ways to modify the nodal surface of $\Psi_S(\mathbf{R})$: orbital optimization, backflow transformations, multideterminant expansions, multi-Pfaffian wfns, etc. This is a very active area of research.

QMC study of electron-hole systems

The electron-hole system is a model for excited semiconductors.

- It is the simplest model system after the homogeneous electron gas, yet its phase diagram remains largely unknown.

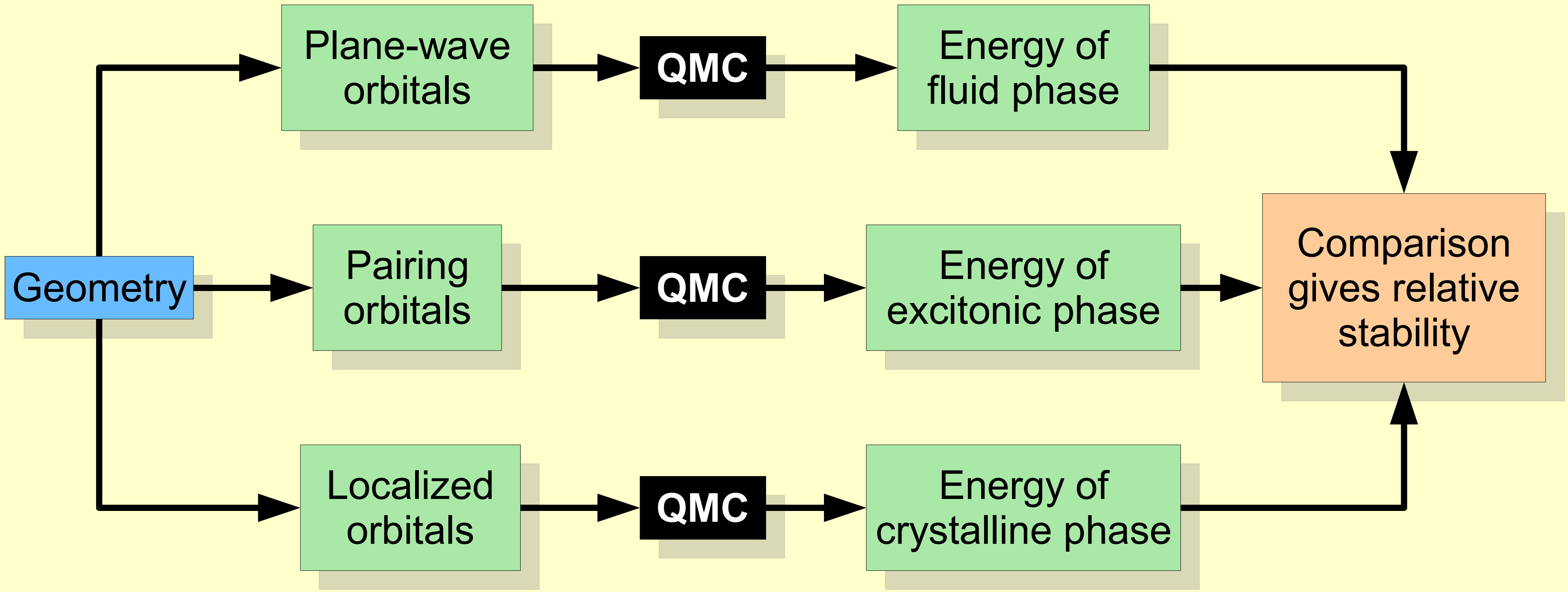
- Some electron-hole systems, such as the two-dimensional bilayer, can be recreated experimentally and display very interesting properties.



- The aim of this work is to determine the phase diagram of electron-hole systems using QMC, to a greater degree of accuracy than previous studies.

QMC study of electron-hole systems

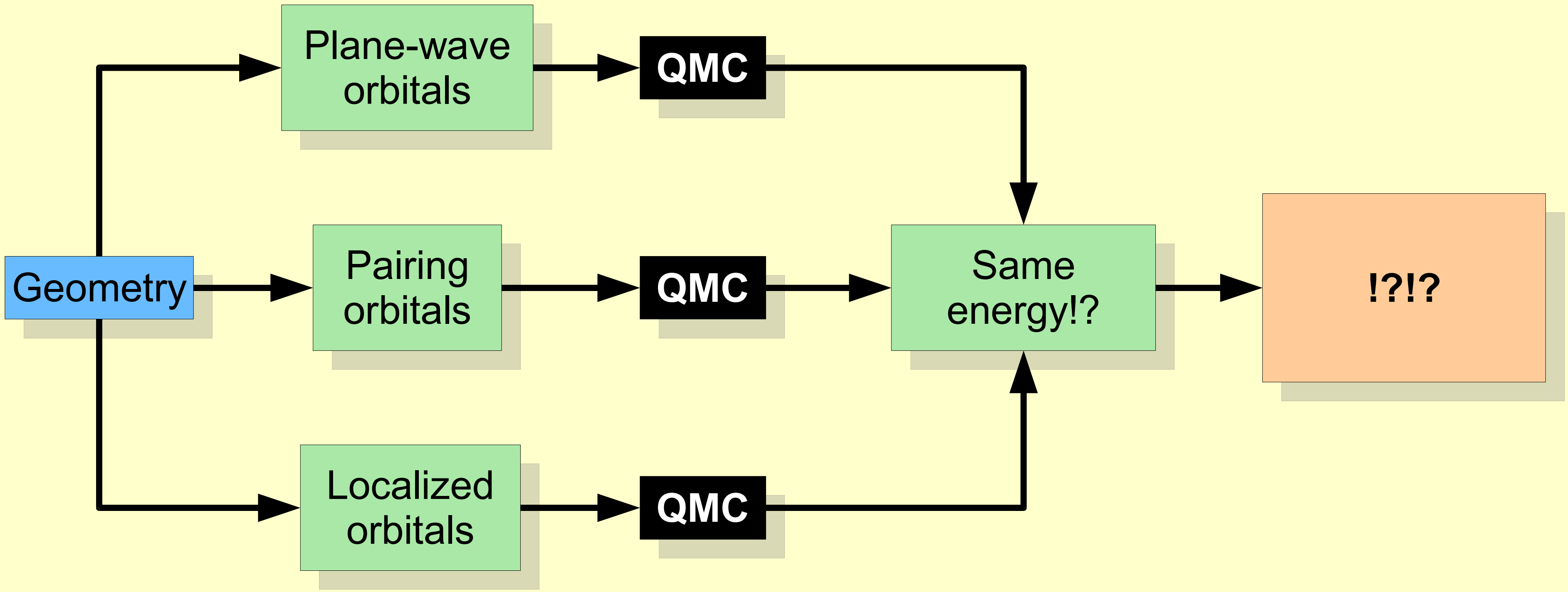
Previous QMC studies have made use of the following scheme:



"**Nodal argument**": different orbitals give different nodes give different energies. Hence there is a correspondence between phase/orbitals (input) and energies (output).

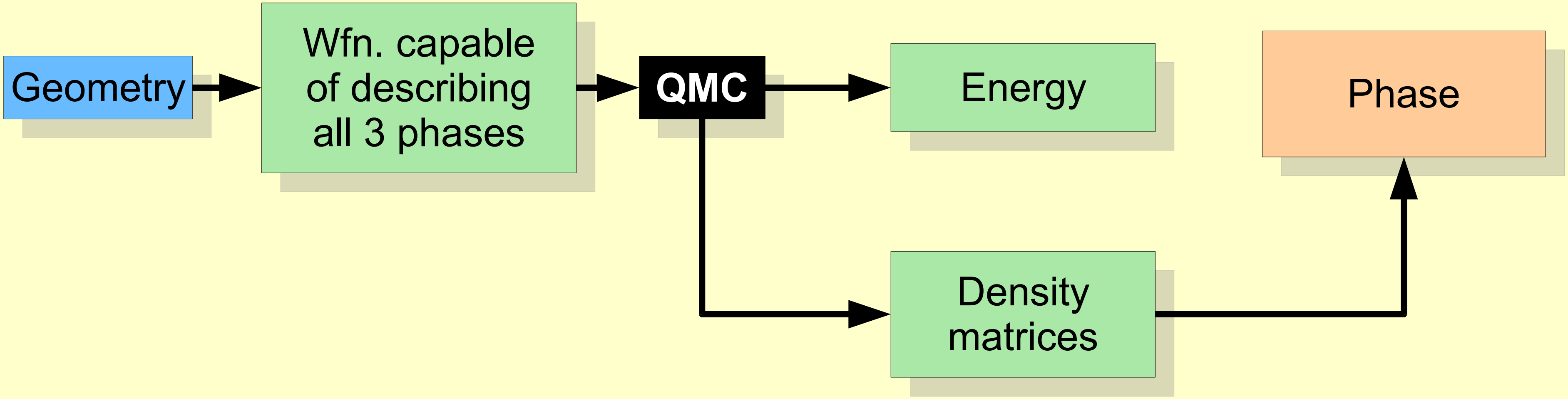
QMC study of electron-hole systems

However, in the limit of a perfect wave function:



QMC study of electron-hole systems

An appropriate approach is:



And on the plus side, this requires fewer calculations.

QMC study of electron-hole systems

The wave functions are formed using products of Slater determinants:

$$D[\phi]=\begin{vmatrix} \phi_{11} & \phi_{12} & \cdots & \phi_{1N} \\ \phi_{21} & \phi_{22} & \cdots & \phi_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ \phi_{N1} & \phi_{N2} & \cdots & \phi_{NN} \end{vmatrix}$$

with:

Pairing: $\phi_{ij}=\phi_L(\boldsymbol{e}_i-\boldsymbol{h}_j)$ $\Rightarrow$ $\Psi_S=D_{e\uparrow h\downarrow}D_{e\downarrow h\uparrow}$

Fluid: $\phi_{ij}=e^{i\boldsymbol{k}_j\cdot\boldsymbol{r}_i}$ $\Rightarrow$ $\Psi_S=D_{e\uparrow}D_{e\downarrow}D_{h\uparrow}D_{h\downarrow}$

Crystal: $\phi_{ij}=\phi_C(\boldsymbol{r}_i-\boldsymbol{R}_j)$ $\Rightarrow$ $\Psi_S=D_{e\uparrow}D_{e\downarrow}D_{h\uparrow}D_{h\downarrow}$

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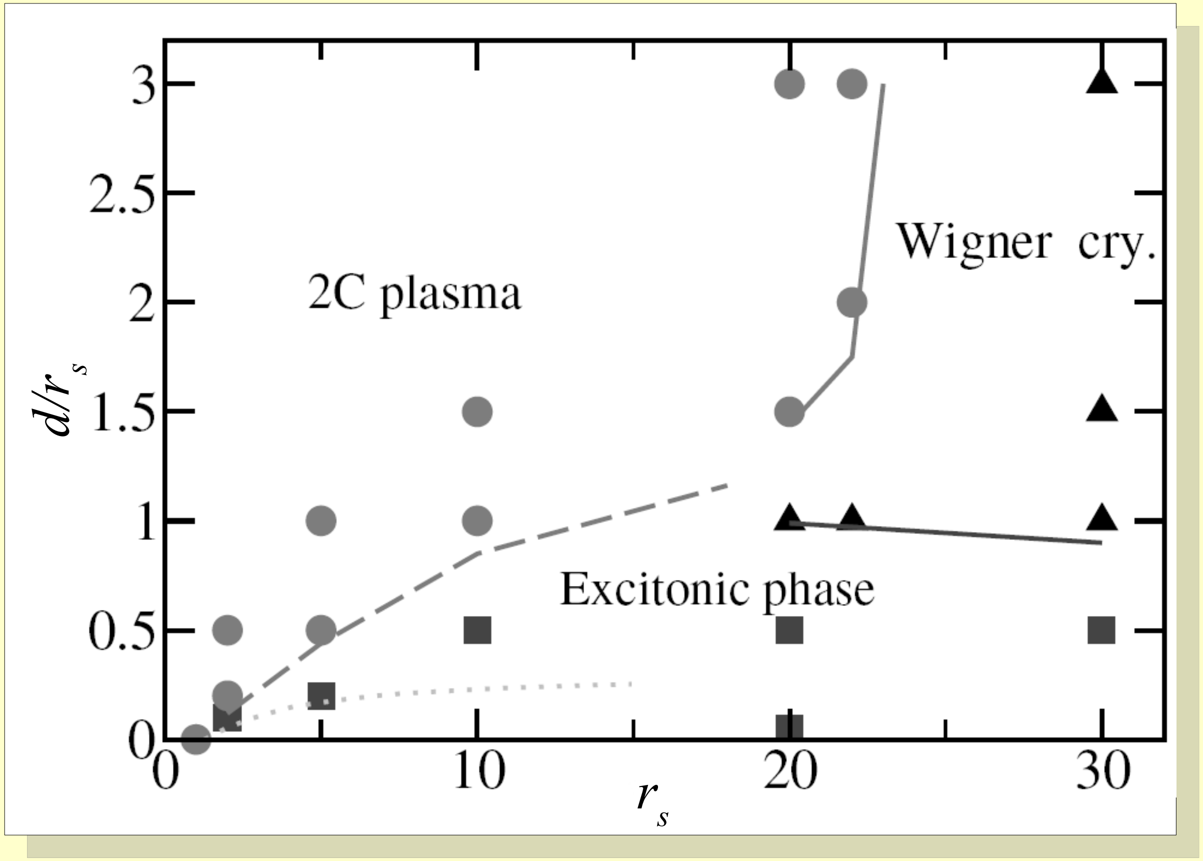
QMC study of electron-hole systems

The phase diagram of the symmetric 2D electron-hole bilayer has already been studied.



S. de Palo *et al*, Phys. Rev. Lett. **88**, 206401 (2002)

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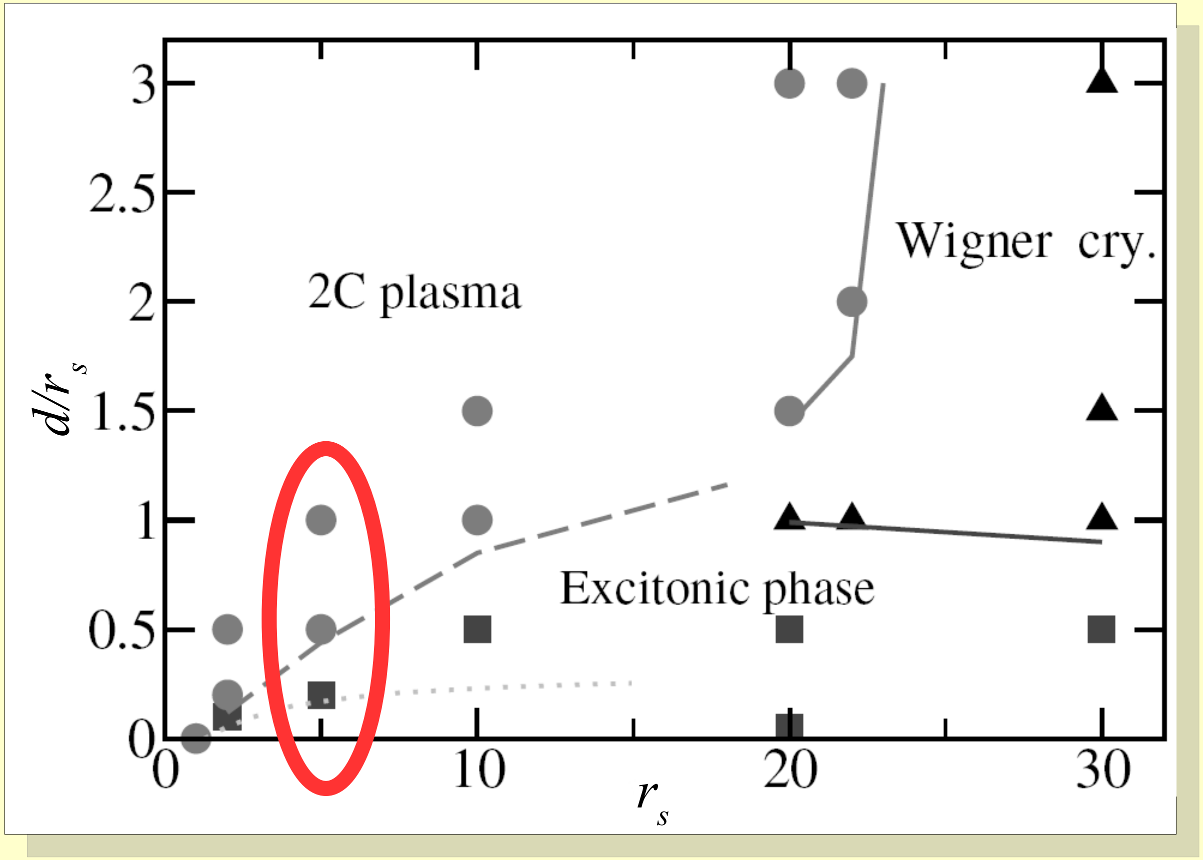

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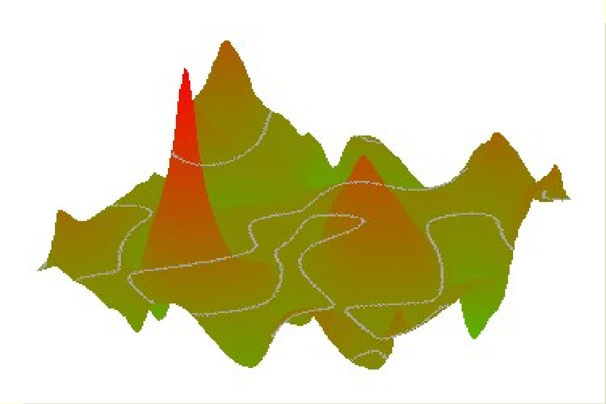
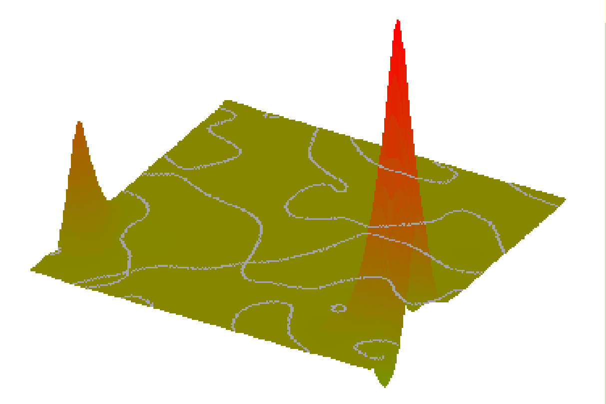
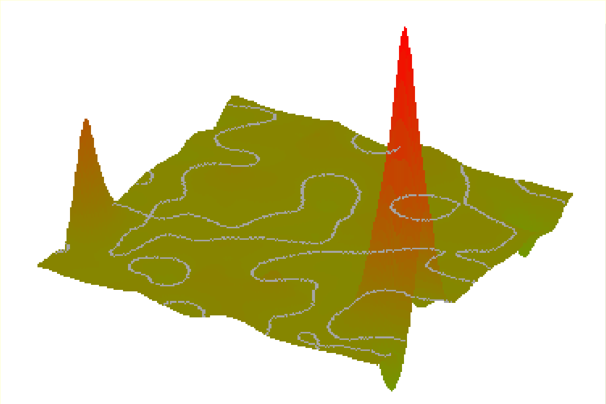


Fluid, E=-0.17879(3) a.u.

$r_s=5,\ d=1$

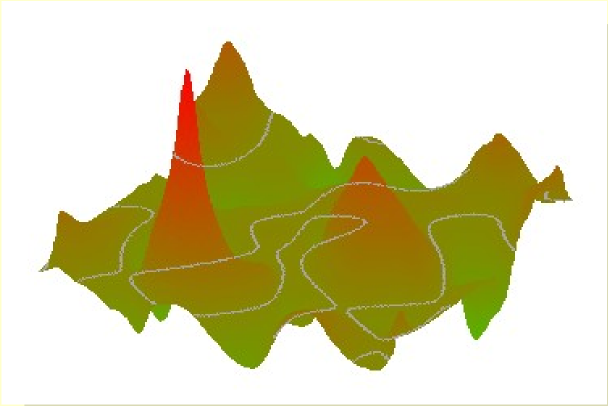


Exponential, E=-0.18937(3) a.u.



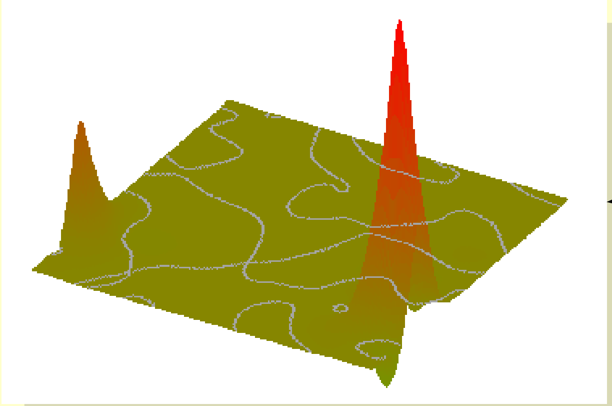
Exponential+PWs, E=-0.18979(3) a.u.

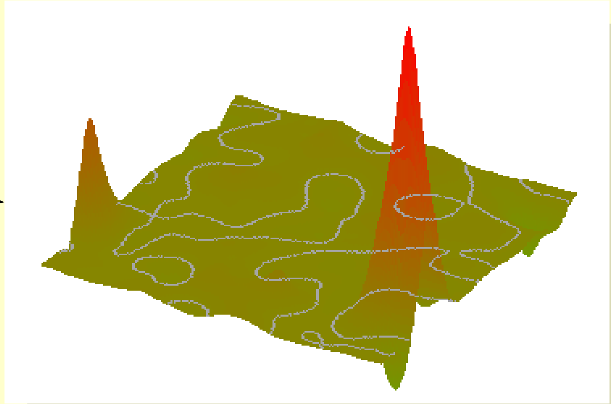
QMC study of electron-hole systems



r_s=5, d=1

Is the "nodal argument" reliable?





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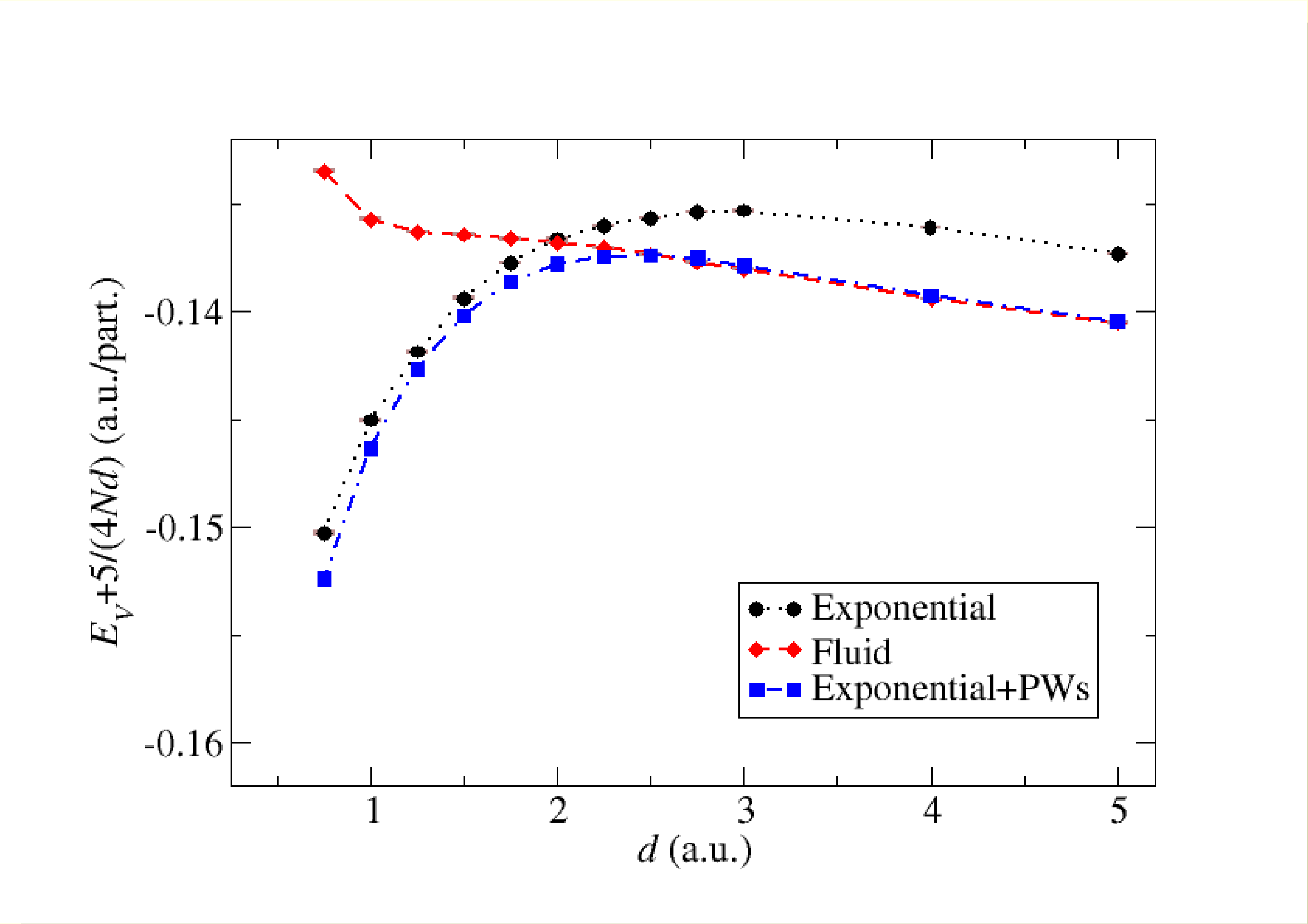
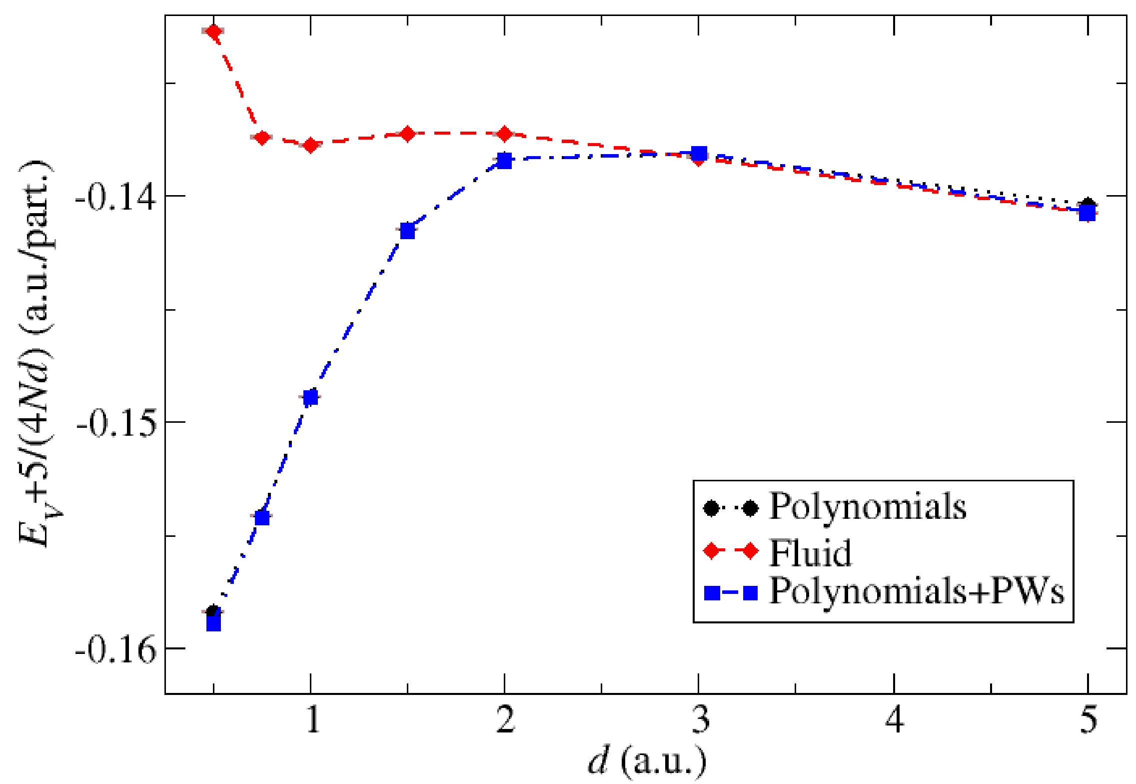


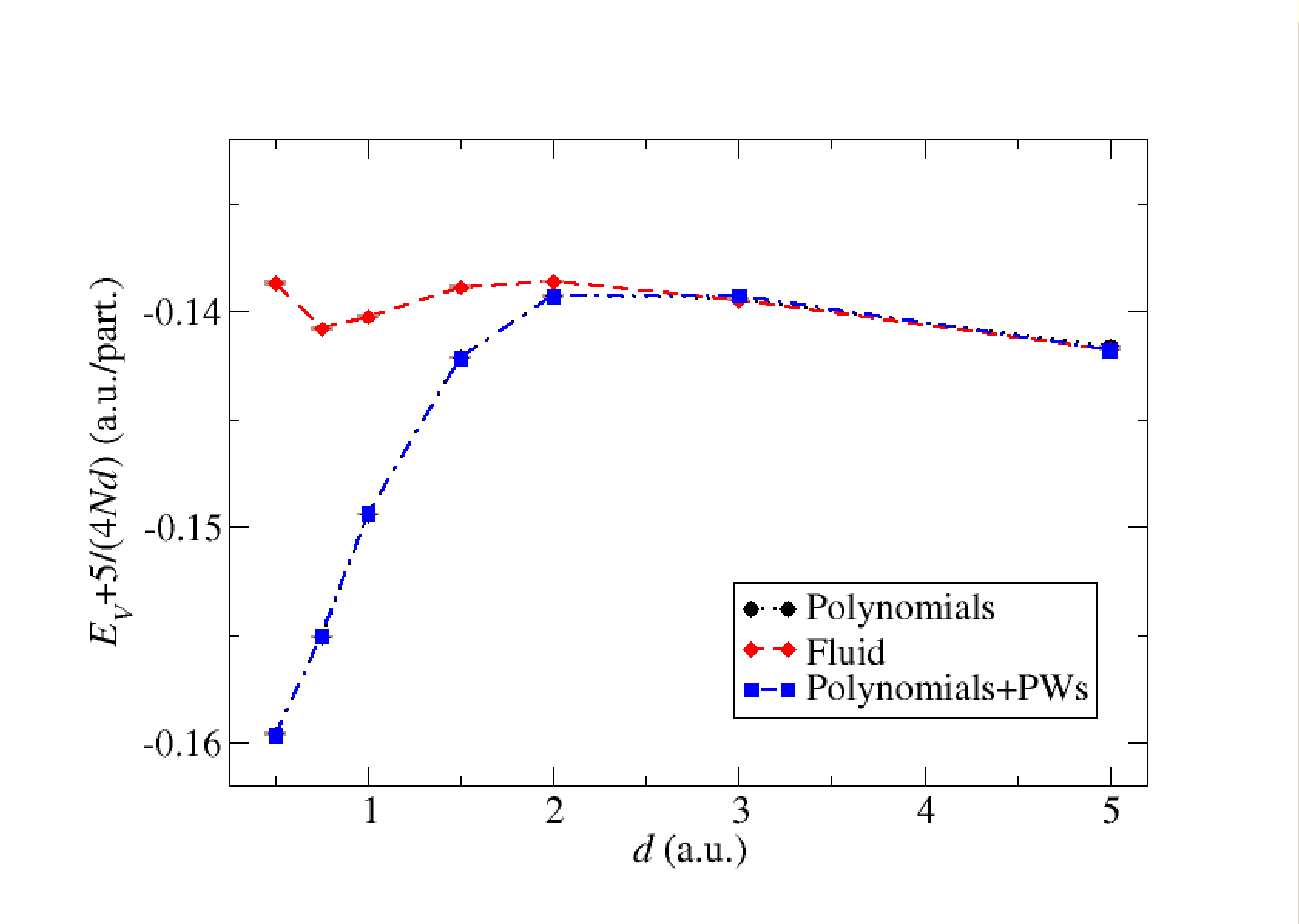
VMC results [variance minimization]

QMC study of electron-hole systems



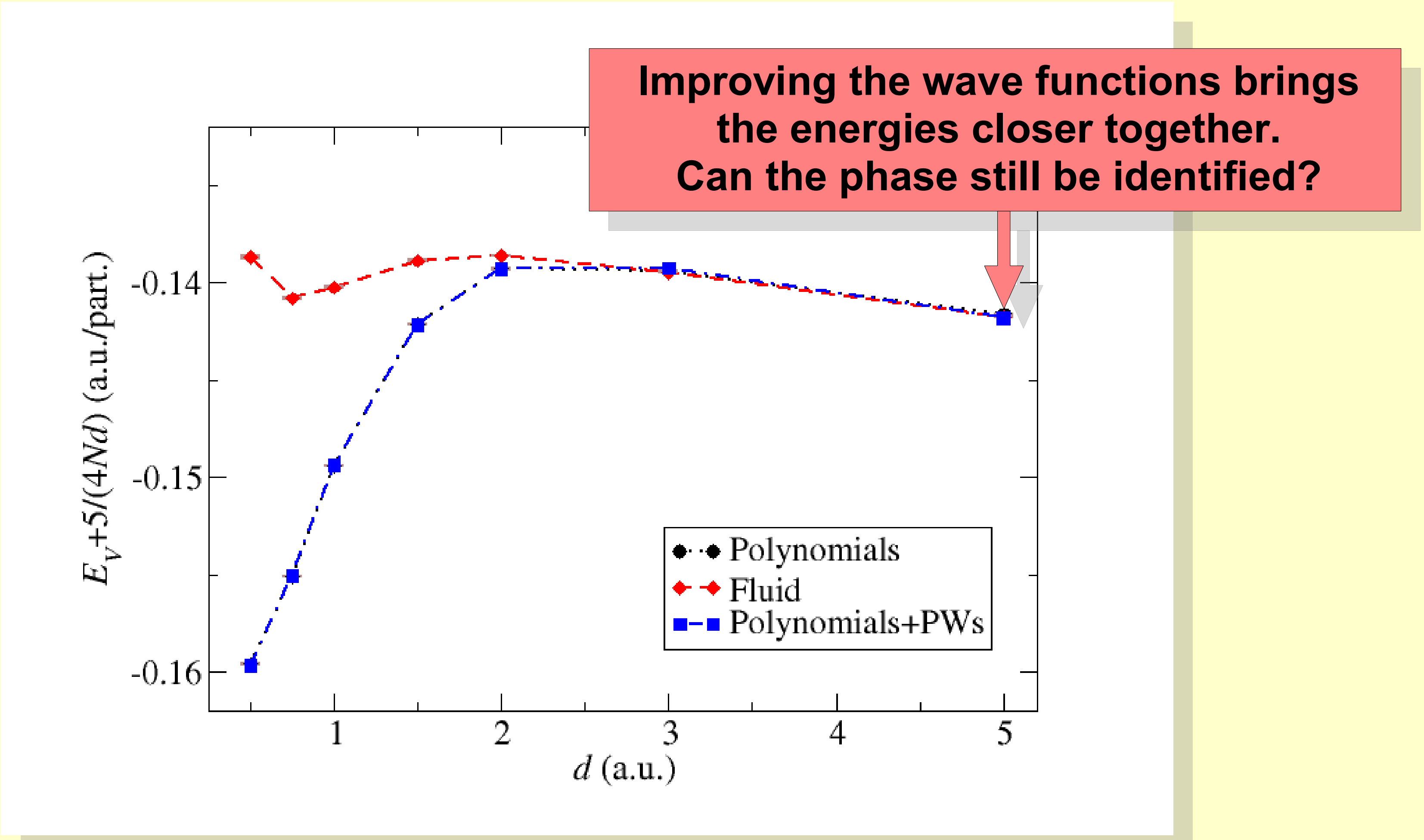
VMC results [energy minimization]

QMC study of electron-hole systems



BF-VMC results [energy minimization]

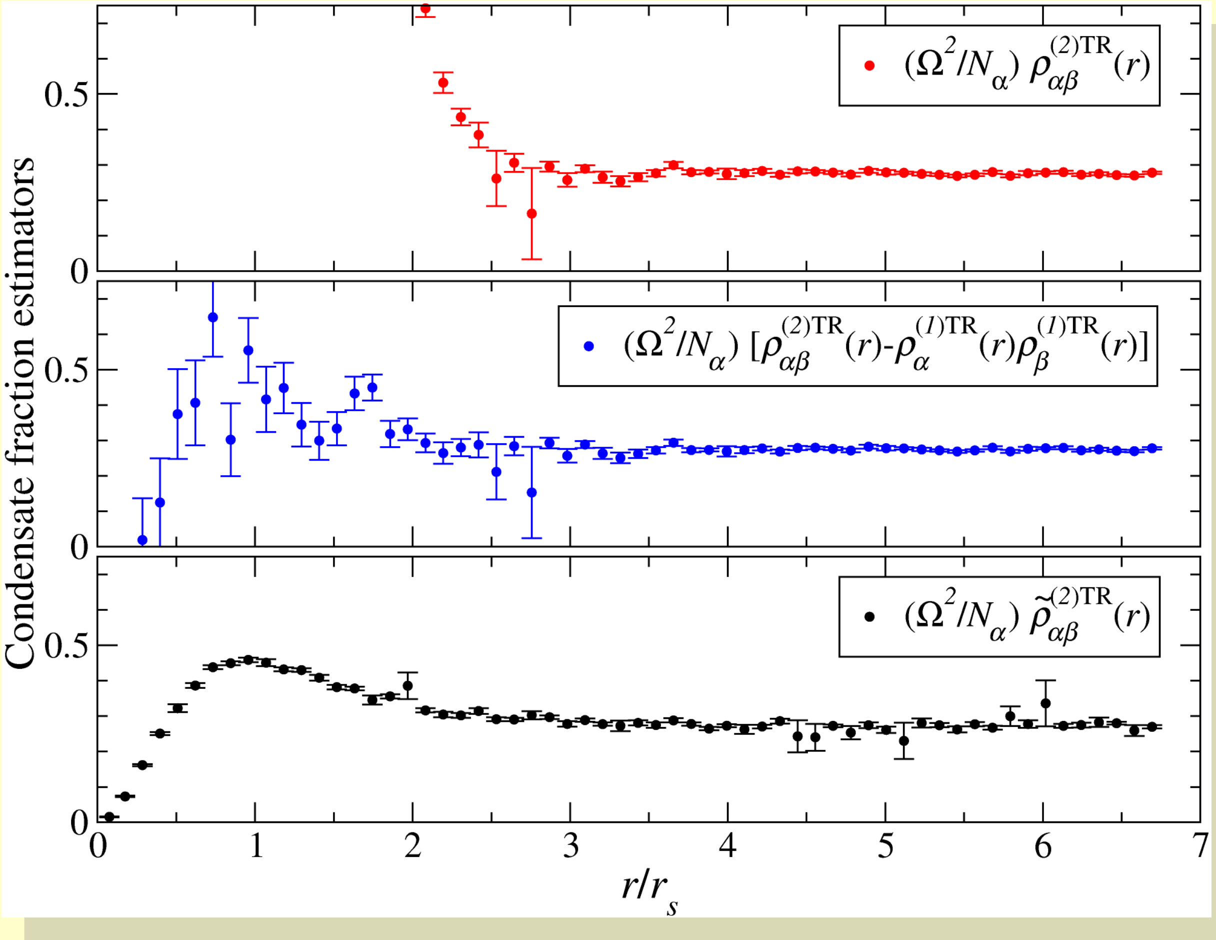
QMC study of electron-hole systems



BF-VMC results [energy minimization]

QMC study of electron-hole systems

The asymptotic behaviour of the two-body density matrix can be used to determine the phase:



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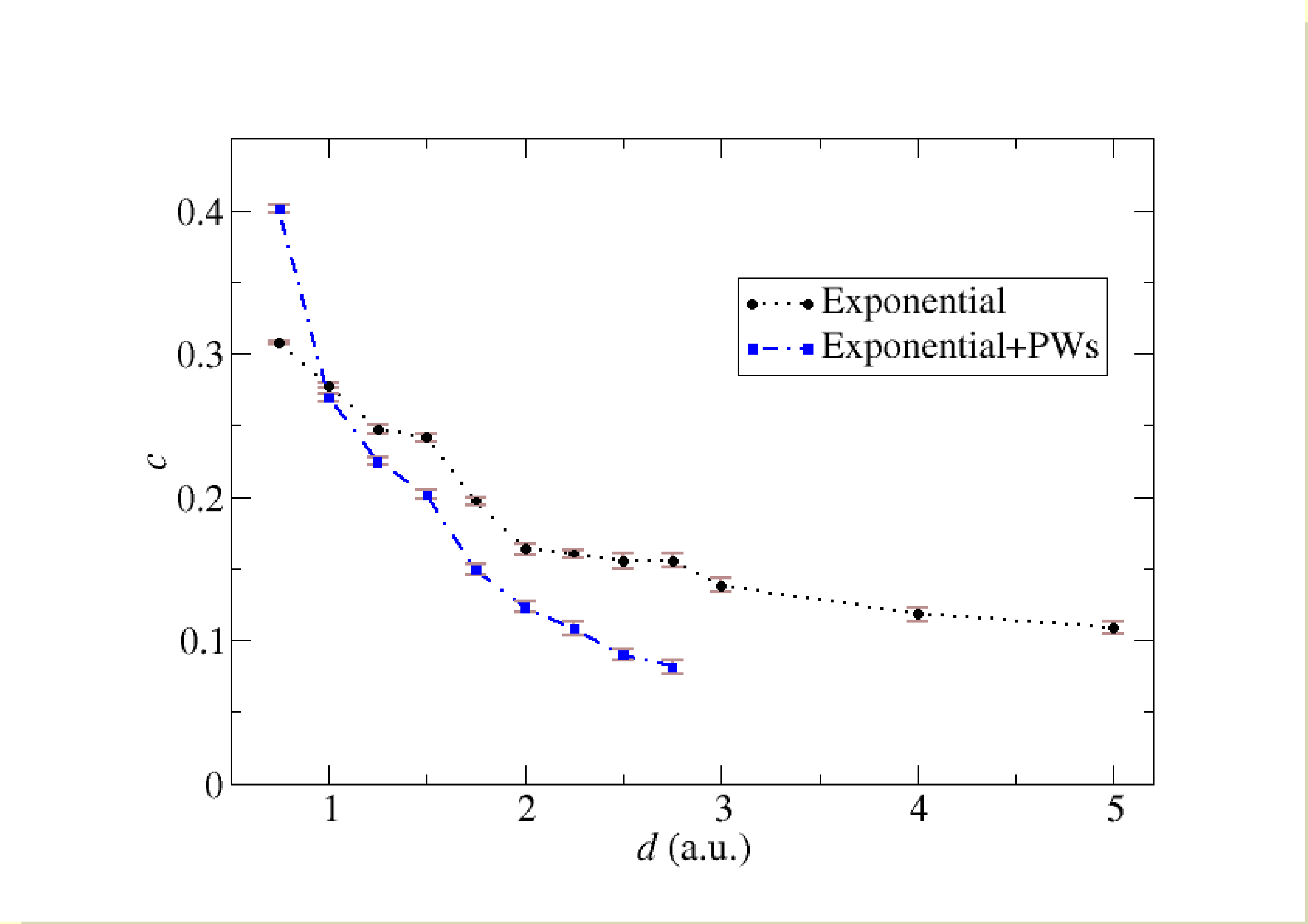
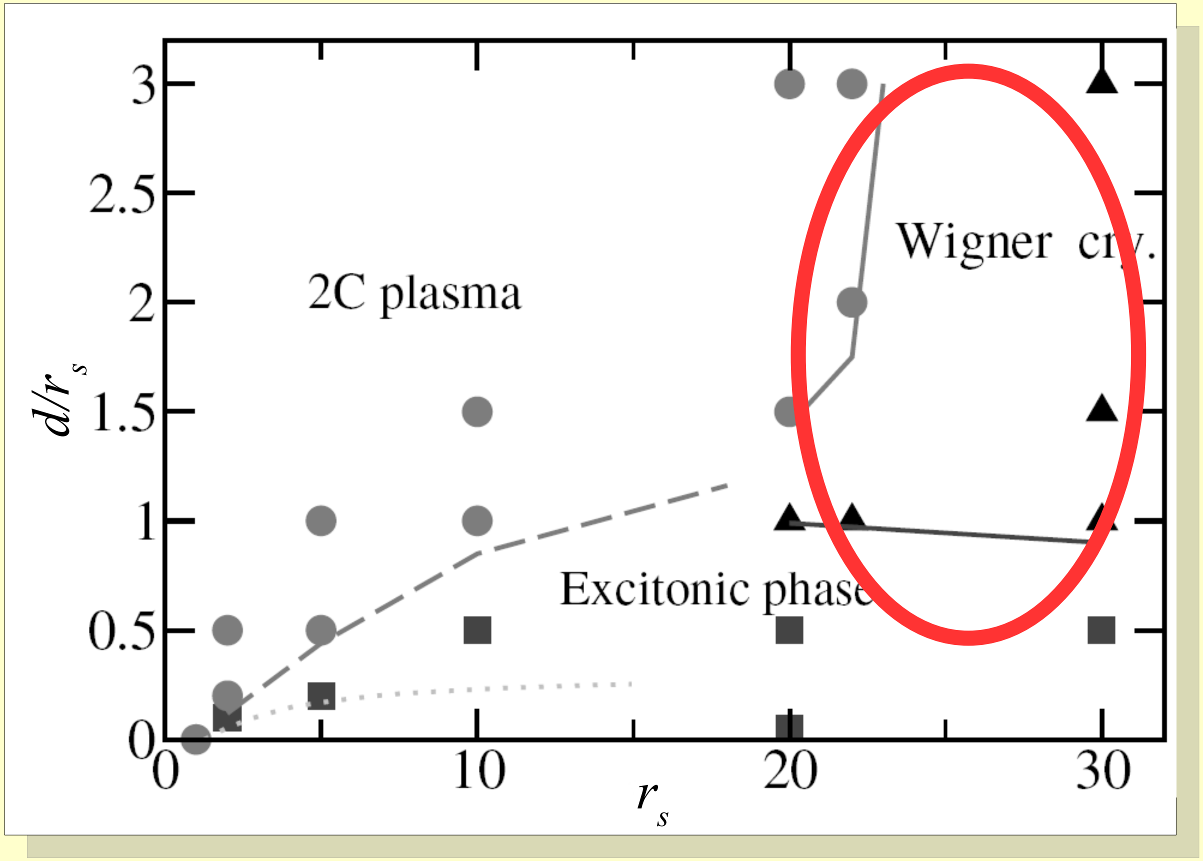


QMC study of electron-hole systems

How about the crystalline phase?



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$$\Gamma_{ij}=\phi(\boldsymbol{e}_i,\boldsymbol{h}_j)+\sum_{l=0}^{L}\psi(\boldsymbol{e}_i-\boldsymbol{R}_l)\psi(\boldsymbol{h}_j-\boldsymbol{R}_l)$$

$$\Psi_S=D_{e\uparrow h\downarrow}D_{e\downarrow h\uparrow}$$

with:

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Conclusions and further work:

- Improvements over previous QMC calculations are possible. Need a different approach involving:
  - More general wave functions.
  - Expectation values of density-matrix related objects.
- Robust wave-function optimization is a key element to get results efficiently.
- Real test: compare against experiment.