Phase diagram of the symmetric electron-hole bilayer

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In preparation

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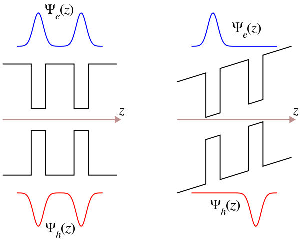
The model system

- Experimental setup: double-well heterojunction + electric field



- Model defined by:
  - two parallel infinite layers of infinitesimal width
  - separation d
  - in-layer density parameter r_s
  - electron-hole mass ratio $m_h/m_e = 1$

Expected phases

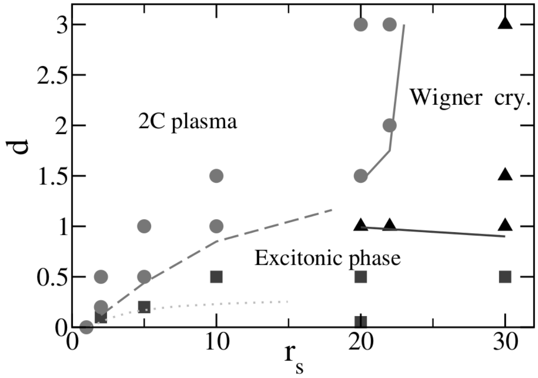
- $d \gg r_s$: recovers the 2D HEG phase diagram (fluid at low r_s, Wigner crystal at high r_s)
- $d \lesssim r_s$: exciton formation
- $d \lesssim 0.38$ a.u.: biexciton formation possible [1]

(NB, we ignore the Wigner crystal phase at this stage of the study, and concentrate on $r_s \leq 10$)

[1] R. M. Lee, N. D. Drummond, and R. J. Needs, Phys. Rev. B **79**, 125308 (2009).

De Palo et al. (2002)

Phase determined comparing energies obtained with different wave functions, each representing a phase [2]



[2] S. De Palo, F. Rapisarda, and G. Senatore, Phys. Rev. Lett. **88**, 206401 (2002)

A single wave function

Form of Ψ_S

$$\Psi_S = \det\left[\phi(\mathbf{e}_i^{\uparrow} - \mathbf{h}_j^{\downarrow})\right] \det\left[\phi(\mathbf{e}_i^{\downarrow} - \mathbf{h}_j^{\uparrow})\right]$$

Form of pairing orbital

$$\phi(\mathbf{r}) = \sum_{l=1}^{n_{\rm PW}} p_l \cos(\mathbf{k}_l \cdot \mathbf{r}) + f(r;L) \sum_{m=0}^{n_{\rm poly}} c_m r^m$$

- Describes pure fluid phase when $n_{\rm PW} = N$, $p_l \neq 0$ and $c_m = 0$
- Describes pure excitonic phase when $p_l = 0$
- Phase determined by computing e–h condensate fraction (from two-body density matrix) and pair-correlation functions

Why use a single wave function?

- Associating phases and wave functions involves either:
  - limiting the flexibility of the wave function, or
  - risking obtaining a wrong result

  (the "*magic backflow*" argument)

- Describes region near boundary

- Single calculation per point in (r_s, d)

$d \to 0$ and the e–h Kato cusp condition

- At $d = 0$ we impose e–h Kato cusp condition $(\Gamma_{eh} = -1)$
- At $d > 0$ we impose e–h cusplessness $(\Gamma_{eh} = 0)$
- Not a smooth change! Hard to study $d \to 0$

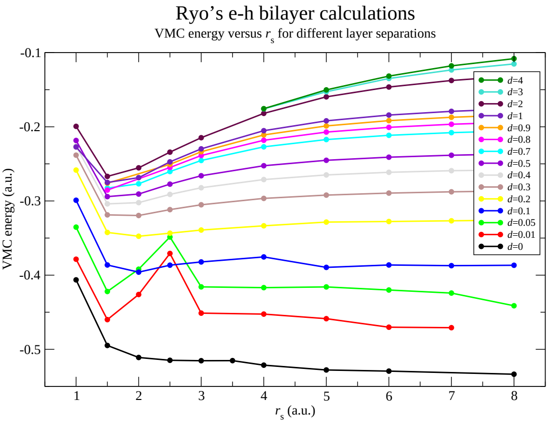
The quasi-cusp Jastrow term $(d > 0)$

$$Q(r) = \Gamma_{eh} \left[\sqrt{r^2 + z^2} - \sqrt{L^2 + z^2} \right] g(r/L)$$

$$g(x) = 1 - 6x^2 + 8x^3 - 3x^4$$

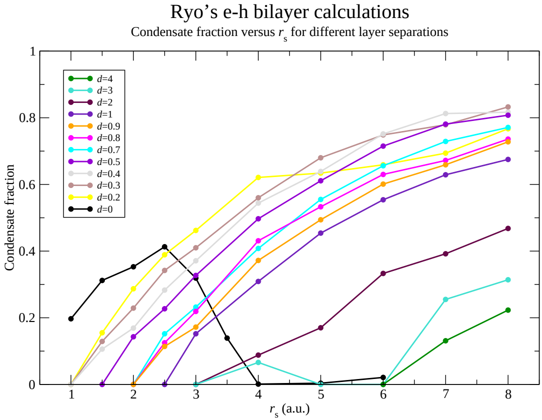
(Plane-cone intersection, if you're wondering)

Behaviour of the energy



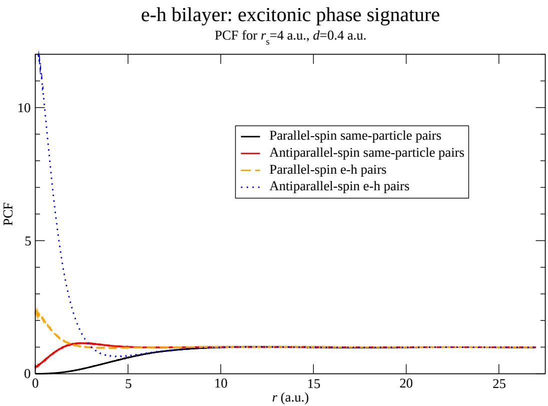
- Behaviour at $r_s = 1$ is correct, uninteresting, also in HEG
- Four odd-looking points are human error (now corrected)

Behaviour of the condensate fraction

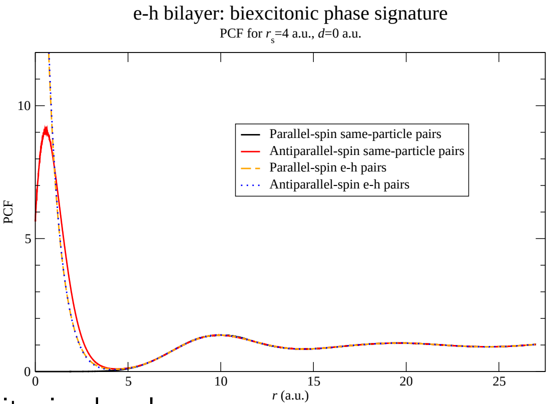


- What's with the condensate fraction at $d = 0$?

Pair-correlation function in the excitonic phase



Pair-correlation function in the “problematic” region



- Biexcitonic phase!
- Jastrow factor is likely responsible for biexciton description
- Phase onset at $d \sim 0.2$, consistent with Lee et al. [3]

[3] R. M. Lee, N. D. Drummond, and R. J. Needs, Phys. Rev. B **79**, 125308 (2009).

Summary

- More robust scheme than associating wave functions to phases
- Excellent results, unsought appearence of biexcitonic phase
- In progress:
  - Pretty plots
  - Investigation of finite size effects
- Future work:
  - Include Wigner crystal: geminal-type wave function (thanks Pascal!), static structure factor detects phase
  - More experimentally-relevant mass ratios
  - Similar scheme for HEG?

End

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