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SECOND EUROPEAN SUMMER SCHOOL on MICROSCOPIC QUANTUM MANY-BODY THEORIES and their APPLICATIONS

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QUANTUM SIMULATIONS
Model symmetric electron-hole bilayer

Part III

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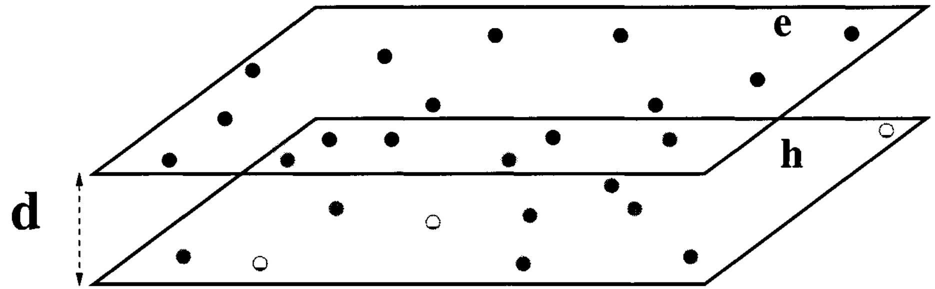
Model symmetric electron-hole bilayer

- $m_e = m_h$
- $N_e = N_h = N$
- B=T=0=thickness
- No inter–layer tunnelling



$$H = H^e + H^h \pm \sum_{i,j=1}^{N} \frac{e^2}{\sqrt{|\mathbf{r}_i^e - \mathbf{r}_j^h|^2 + d^2}},$$

$$H^a = -\frac{\hbar^2}{2m} \sum_{i=1}^{N} \nabla_i^{a\,2} + \frac{1}{2} \sum_{i \neq j}^{N} \frac{e^2}{|\mathbf{r}_i^a - \mathbf{r}_j^a|}$$

- r_s: $\pi r_s^2 a_B^2 = \frac{S}{N} = 1/n$; $\quad \gamma \equiv r_s a_B/d$=$(e^2/d)/(e^2/r_s a_B)$.

BCS Mean–field

- Determine the optimal $|\Psi\rangle$ (i.e., $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$) by minimizing $\langle\Psi|H|\Psi\rangle$, with

$$|\Psi\rangle = \prod_{\mathbf{k},\sigma}(u_{\mathbf{k},\sigma} + v_{\mathbf{k},\sigma} e^{\dagger}_{\mathbf{k},\sigma} h^{\dagger}_{\mathbf{k},\sigma})|0\rangle,$$

  and $e^{\dagger}_{\mathbf{k},\sigma}$, $h^{\dagger}_{\mathbf{k},\sigma}$ electron and hole creation operators.

- One defines a BCS (excitonic) orbital $\varphi(r)$ from

$$\varphi(\mathbf{k}) = v_{\mathbf{k}}/u_{\mathbf{k}}$$

  and a gap function

$$\Delta(\mathbf{k}) = u_{\mathbf{k}} v_{\mathbf{k}}$$

Wavefunctions for e-h layers

- The *Plasma nodes*:

$$\Psi_T(\mathbf{R}) = D_e^{\uparrow} D_e^{\downarrow} D_h^{\uparrow} D_h^{\downarrow} \mathbf{J},$$

$$\mathbf{J} = \prod_{i_e, j_h} exp[-u_{eh}(r_{i_e j_h})] \prod_{a=e,h} \prod_{i_a<j_a} exp[-u_{aa}(r_{i_a j_a})],$$

$$D_a^{\sigma} = det[\exp(i r_i^a \cdot k_j)],$$

and $u_{ab}(r)$ RPA pseudopotentials.

- The *Excitonic/BCS* nodes:

$$\Psi_T(\mathbf{R}) = D^{\uparrow\uparrow} D^{\downarrow\downarrow} \mathbf{J}$$

$$D^{\uparrow\uparrow} = det[\varphi(|\mathbf{r}_i^e - \mathbf{r}_j^h|)] = D^{\downarrow\downarrow}$$

- φ from the mean field solution [Zhu et al PRL **74** 1633, (1995)].

DMC Results for the e-h bilayer

Phase Diagram ($r_s = 1 \div 20$)

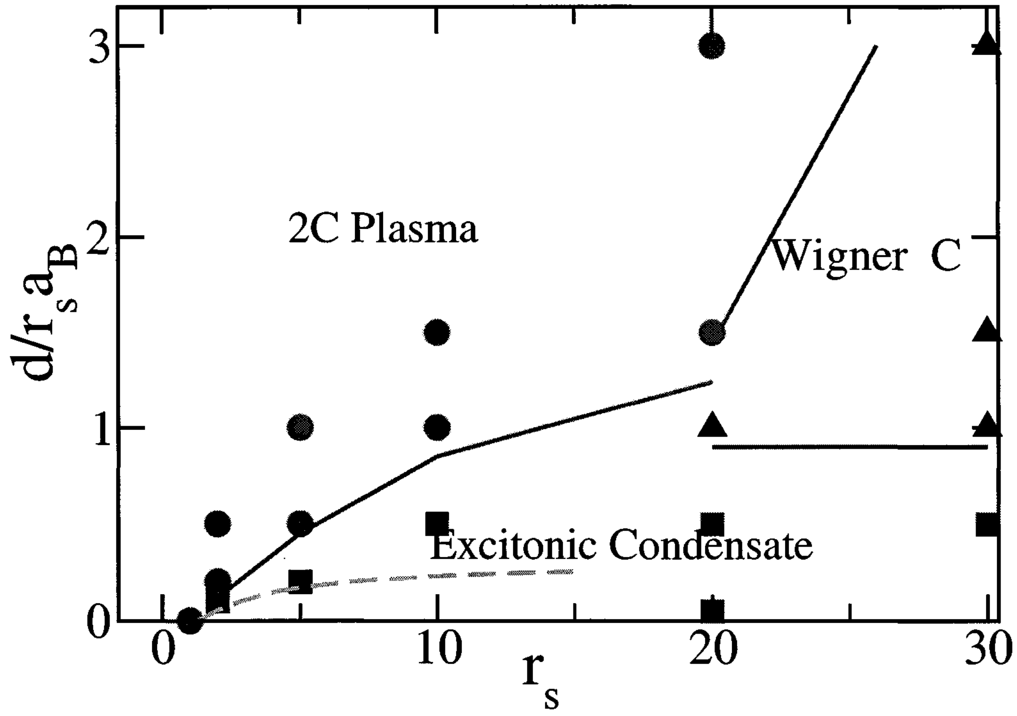
Correlation Functions ($r_s = 5$)

One-body density matrix $\Rightarrow$: $h^{(1)}(r)$

Two-body density matrix and Off-Diagonal Long Range OrderODLRO

Pair correlation functions $\Rightarrow$ $g_{e,e}(r), g_{e,h}(r), g_{h,h}(r)$

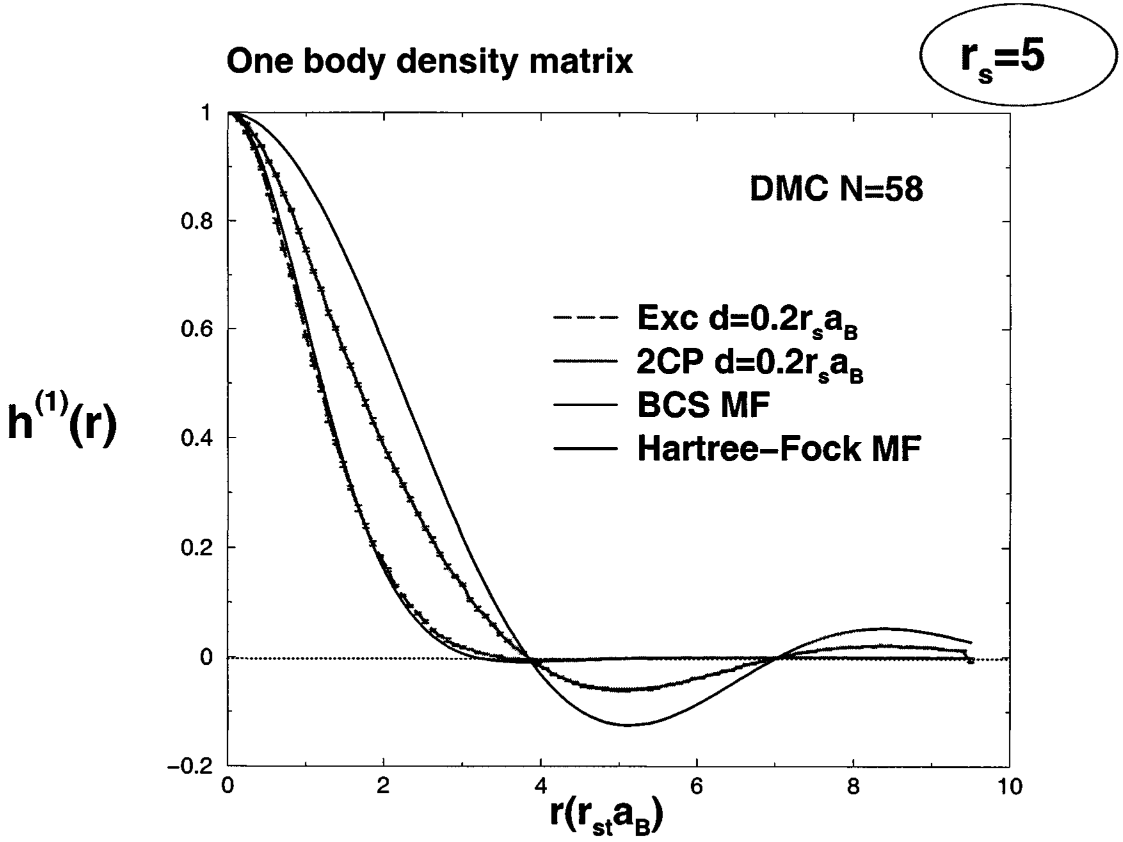
Phase diagram of the e-h bilayer



- Unpolarized Phases from extrapolated bulk DMC energy
- Energies of the Polarized Phases do not alter the phase diagram

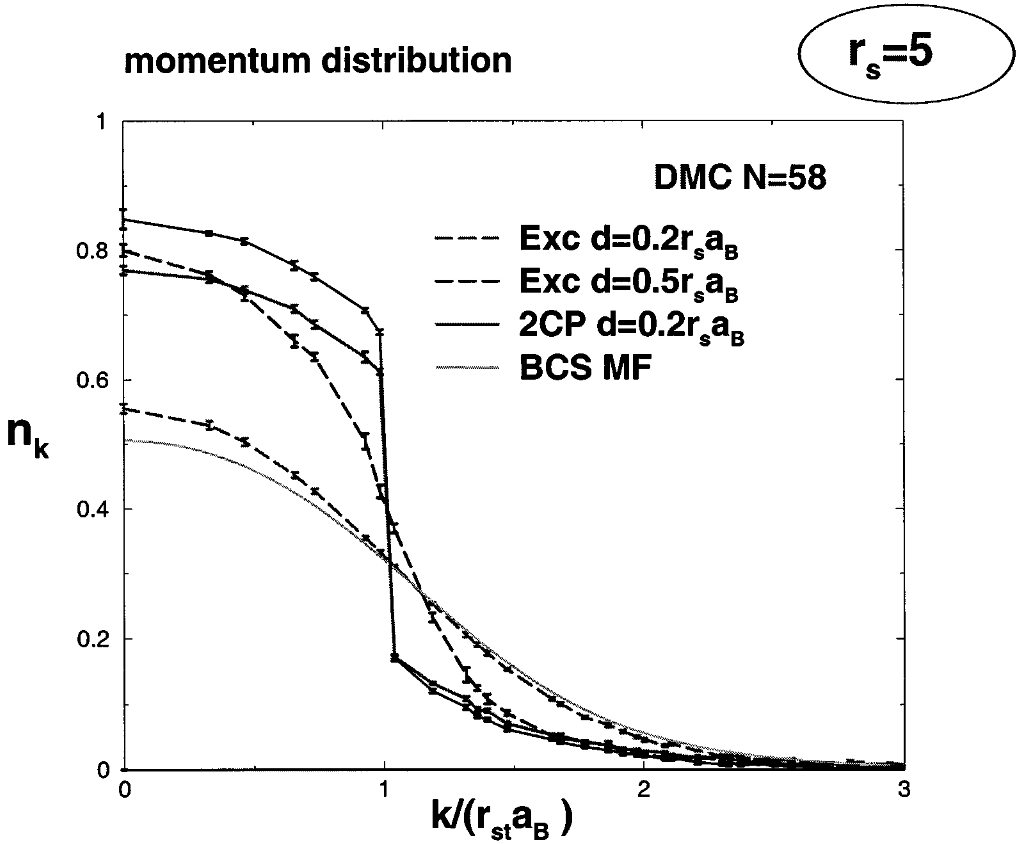
One body density matrix – r space

$$h^{(1)}_{e,e}(\vec{x}_1, \vec{x}'_1) = \frac{1}{n}\langle \phi^\dagger_e(\vec{x}_1)\phi_e(\vec{x}'_1)\rangle$$



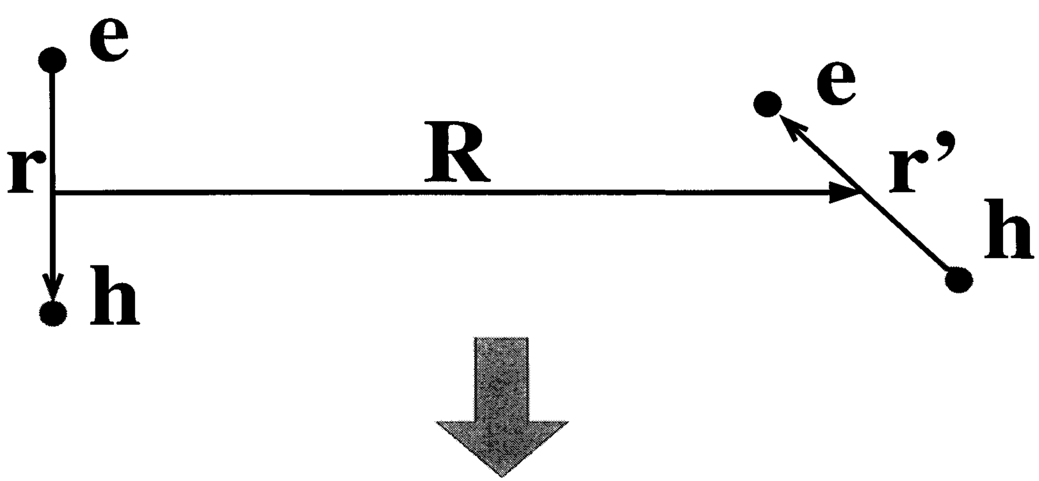
One body density matrix – k space

momentum distribution



Two body density matrix

$$h^{(2)}(\vec{x}'_e, \vec{x}'_h; \vec{x}_h, \vec{x}_e) = \langle \phi^\dagger(\vec{x}'_e)\phi^\dagger(\vec{x}'_h)\phi(\vec{x}_h)\phi(\vec{x}_e)\rangle$$



Asymptotic behaviour $\mathrm{R} >> \mathbf{r}, \mathbf{r}'$

Asymptotic behaviour: $\mathbf{R} >> \mathbf{r}, \mathbf{r}'$

- Normal State

$$h^{(2)}(\vec{x}'_e, \vec{x}'_h; \vec{x}_h, \vec{x}_e) \rightarrow n^2 h^{(1)}(\vec{x}'_e, \vec{x}_e) h^{(1)}(\vec{x}'_h, \vec{x}_h)$$

- BCS/Excitonic State: ODLRO

$$h^{(2)}(\vec{x}'_e, \vec{x}'_h; \vec{x}_h, \vec{x}_e) \rightarrow \Delta^*(\mathbf{r})\Delta(\mathbf{r}'),$$

in the BCS limit (r_s small), whith $\boldsymbol{\Delta}(\mathbf{r})$ the gap function or pair amplitude;

$$h^{(2)}(\vec{x}'_e, \vec{x}'_h; \vec{x}_h, \vec{x}_e) \rightarrow \alpha n \varphi^*(\mathbf{r})\varphi(\mathbf{r}'),$$

with $\varphi^*(\mathbf{r})$ the normalized excitonic wavefunction, in the excitonic limit (r_s large).

Projected two body density matrix

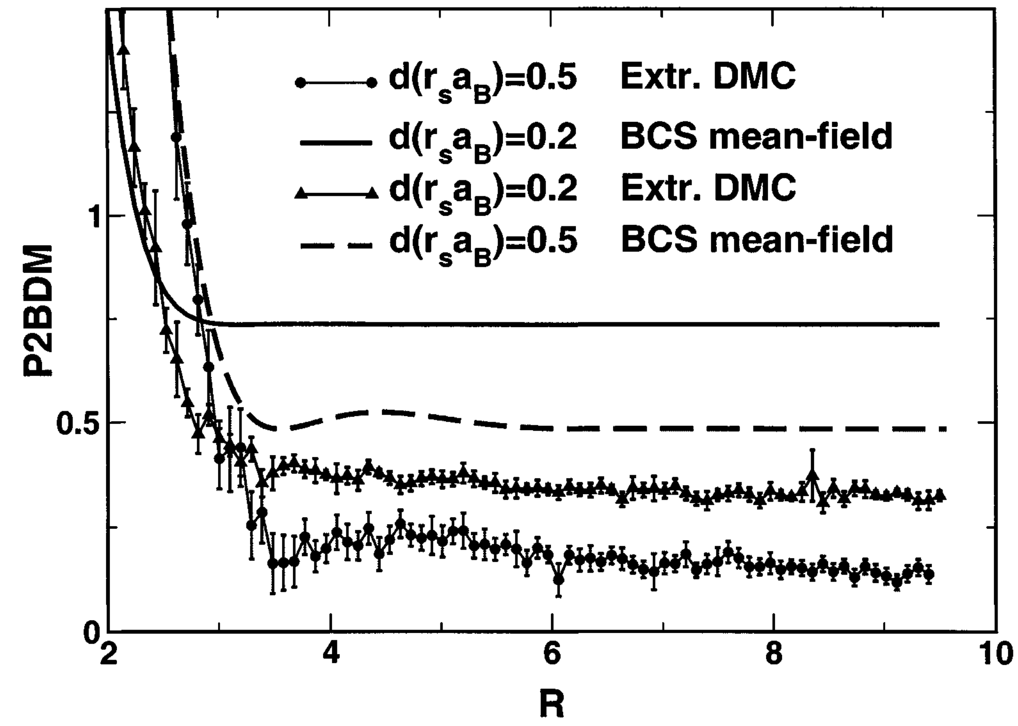
- ODLRO can be detected by looking at

$$f(\mathbf{R}) = \frac{1}{N}\int \frac{d\Omega_R}{2\pi}\int d\mathbf{r} h^{(2)}(0,\vec{r};\vec{R},\vec{R}+\vec{r})$$

$$\stackrel{\mathbf{R}\gg\mathbf{r},\mathbf{r}'}{\Longrightarrow} \frac{1}{n}\int \frac{d\Omega_R}{2\pi}\int d\mathbf{r}\alpha n|\tilde{\varphi}(\mathbf{r})|^2 \Longrightarrow \alpha$$

Two body density matrix: $r_s = 5$

- Projected two body density matrix



Conclusions: electron–hole bilayer

- Excitonic/BCS state is stable at small distances, with the plasma phase taking over at large distances and/or small r_s.
- BCS nodes yield a two-body density matrix that displays ODLRO, reduced with respect to the prediction of the BCS mean–field.
- The shortcoming of the BCS–like mean–field treatment are traced to the neglect of in–layers correlations.
- BCS–like mean–field yields stability of the Excitonic/BCS state everywhere and a consistent overestimate of the condensate and related properties.

Some extra references

Here some references in addition to the list given in the first lecture and to the those added in the following lectures.

- Magnetization Transition in the 2D egas:

  D. Varsano, S. Moroni e G. Senatore, Europhys. Lett. 53, 348 (2001).

  G.Senatore, S.Moroni, and D.Varsano, Sol. St. Comm. 119, 333 (2001).

- Quantum wires:

  A. Malatesta and G. Senatore, J. Phys. IV, Pr5 (2000)

- Electron–hole bilayer:

  S. De Palo, F. Rapisarda, and G. Senatore, to be published