QMC calculations on biexcitons in bilayer systems

Robert Lee
Outline

- What are excitons and biexcitons?
- Why are they interesting?
- Experimental setup / the bilayer system
- QMC calculations
- Conclusions
Excitons are bound electron-hole pairs, formed in semiconductors when an electron is excited into the conduction band and interacts with a hole (the absence of an electron) in the valence band.

In the low density limit, \( na_B^D \ll 1 \), excitons may be treated as weakly interacting, neutral bosons. Thus BEC is predicted at low temperatures.

This will occur when the de Broglie wavelength, \( \lambda = \sqrt{2\pi \hbar^2 / M k_B T} \), is comparable to the interparticle separation, \( n^{-1/2} \).

\[
a_B^* = \frac{4\pi \varepsilon_0 \varepsilon \hbar^2}{\mu_{eh} e^2}, \\
R_y^* = \frac{\mu_{eh} e^4}{2(4\pi \varepsilon_0 \varepsilon)^2 \hbar^2}
\]

\[ T_t = 2\pi \hbar^2 n / M k_B \approx 3K \quad \text{Well within experimental reach!} \]

(noting that \( M = m_e + m_h \approx M_{atom} \times 10^{-3} \) )  

Other experimental problems persist...
The CQW system

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The experimental systems are designed to inhibit recombination while still allowing significant interactions between layers.

(Left) Courtesy of Joanna Waldie  (Right) Jonathan Keeling http://www.tcm.phy.cam.ac.uk/~jmjk2/
The bilayer system

- Idealized 2d layers
- Electron & hole masses are isotropic
- Two like-charge but opposite-spin particles in each layer

The Schrödinger equation for a biexciton is then:

\[
\left[ -\frac{1}{1+\sigma} \left( \nabla_1^2 + \nabla_2^2 \right) - \frac{\sigma}{1+\sigma} \left( \nabla_a^2 + \nabla_b^2 \right) + \frac{2}{r_{12}} + \frac{2}{r_{ab}} - \frac{2}{r_{1a}} - \frac{2}{r_{1b}} - \frac{2}{r_{2a}} - \frac{2}{r_{2b}} \right] \Psi = E_{XX} \Psi ,
\]
The trial wavefunction

\[ \Psi = \Psi_{ee} \Psi_{hh} \Psi_{eh} \]

\[ \Psi_{ee} = \exp \left[ \frac{c_1 r_{12}}{1 + c_2 r_{12}} \right] \]

\[ \Psi_{hh} = \exp \left[ \frac{c_3 r_{ab}}{1 + c_4 r_{ab}} \right] \]

\[ \Psi_{eh} = \exp \left[ \left( \frac{c_5 r_{1a} + c_6 r_{1a}^2}{1 + c_7 r_{1a}} \right) + \frac{c_5 r_{1b} + c_8 r_{1b}^2}{1 + c_9 r_{1b}} + \frac{c_5 r_{2a} + c_8 r_{2a}^2}{1 + c_9 r_{2a}} + \frac{c_5 r_{2b} + c_6 r_{2b}^2}{1 + c_7 r_{2b}} \right] \]

+ \exp \left[ \left( \frac{c_5 r_{1a} + c_8 r_{1a}^2}{1 + c_9 r_{1a}} \right) + \frac{c_5 r_{1b} + c_6 r_{1b}^2}{1 + c_7 r_{1b}} + \frac{c_5 r_{2a} + c_6 r_{2a}^2}{1 + c_7 r_{2a}} + \frac{c_5 r_{2b} + c_8 r_{2b}^2}{1 + c_9 r_{2b}} \right] , \]

VMC - Variational estimate of the ground state energy

\[ E \approx \frac{\int_0^\infty d\mathbf{R} \; \Psi(\mathbf{R}) \; \hat{H} \; \Psi^*(\mathbf{R})}{\int_0^\infty d\mathbf{R} \; |\Psi(\mathbf{R})|^2} \approx \frac{1}{M} \sum_{i=1}^M E_L(\mathbf{R}_i) \]

Minimize \( E \) w.r.t. the parameters \( c_{1-9} \)
The imaginary-time Schrödinger equation:

\[
(\hat{H} - E_T)\Phi(\mathbf{R}, \tau) = -\frac{\partial \Phi(\mathbf{R}, \tau)}{\partial \tau},
\]

Any wavefunction may be constructed from the complete set of eigenfunctions:

\[
\Phi(\mathbf{R}, \tau) = \sum_{i=0}^{\infty} c_i \phi_i(\mathbf{R}) e^{(E_T - E_i)\tau},
\]

Propagation in imaginary time can project out the ground state component. This is done in CASINO with drift-diffusion and branching dynamics. Equivalent to solving the importance-sampled SE

\[
-\frac{1}{2} \nabla^2 f(\mathbf{R}, \tau) + \nabla \cdot (V(\mathbf{R}) f(\mathbf{R}, \tau)) + (E_L(\mathbf{R}) - E_T) f(\mathbf{R}, \tau) = -\frac{\partial f(\mathbf{R}, \tau)}{\partial \tau},
\]

with \( f(\mathbf{R}, \tau) = \Phi(\mathbf{R}, \tau)\psi(\mathbf{R}) \)
Biexciton binding $2E_x - E_{xx}$
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Biexciton stability

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No biexciton formation possible

$d (a_B^{*})$

Biexciton formation

Mass ratio $\sigma$
Constrain the centre-of-mass positions of two excitons. Then each exciton may be treated mathematically as a single particle. The two particles interact by the potential

\[
\hat{V} = -\frac{1}{|r_1|} - \frac{1}{|r_2|} + \frac{1}{|R_{cm} + \frac{m_\mu}{m_e}(-r_2 + r_1)|} + \frac{1}{|R_{cm} + \frac{m_\mu}{m_h}(-r_1 + r_2)|} - \frac{1}{|R_{cm} - \frac{m_\mu}{m_h}r_1 - \frac{m_\mu}{m_e}r_2|} - \frac{1}{|R_{cm} + \frac{m_\mu}{m_e}r_1 + \frac{m_\mu}{m_h}r_2|},
\]

and have kinetic energy

\[
\hat{T} = \frac{1}{2m_\mu} \left( \nabla_1^2 + \nabla_2^2 \right),
\]

So we can now treat $R_{cm}$ as a parameter and investigate the exciton-exciton potential with $\sigma \neq 0$. 
VMC versus DMC

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Interaction potential ($R_y^*$) vs. Hole-hole separation ($a_B^*$)

$d = 0.9a_B^*$
VMC versus DMC

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\[ d = 0.9a_B^* \]
Pair dist. functions

**Electron-hole PDF**

\[ g_{\text{eh}}(r) = \frac{1}{8\pi r} \left\langle \sum_{\sigma_e, \sigma_h \in \{\uparrow, \downarrow\}} \delta(|r_{e\sigma_e} - r_{h\sigma_h}| - r) \right\rangle , \]

**Electron-electron PDF**

\[ g_{\text{ee}}(r) = \frac{1}{2\pi r} \left\langle \delta(|r_{e\uparrow} - r_{e\downarrow}| - r) \right\rangle , \]

**Extrapolated estimator**

\[ g^{\text{ext}} = 2g^{\text{DMC}} - g^{\text{VMC}} \]

**Normalization**

\[ \int_0^\infty 2\pi r g^{\text{ext}}(r) \, dr = 1. \]
Pair dist. functions

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\[ 2g_{\text{ext}}^\text{single} (r) - g_{\text{eh}} (r) \]

- \( d = 0.20a_B^* \) (black solid line)
- \( d = 0.24a_B^* \) (red dashed line)
- \( d = 0.28a_B^* \) (green dotted line)

\( r \) (\( a_B^* \))

0 1 2 3 4 5 6
Summary

- Calculated accurate binding energies and the region of biexciton stability.
- Looked at the exciton-exciton interaction for a range of system parameters.
- Observed the size of a bound biexciton using pair distribution functions.
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