QMC with biexcitons

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Contents

Excitons are bound electron-hole pairs which may be created by shining light onto semiconductors. They can also recombine and release their energy as photons.

Useful units for this system are the exciton Bohr radius,

$$a_B^* = \frac{4\pi\epsilon_0\epsilon\hbar^2}{\mu_{eh}e^2} ,$$

where $\mu_{eh} = m_e m_h/(m_e + m_h)$ is the reduced mass, and the exciton Rydberg,

$$Ry^* = \frac{\mu_{eh}e^4}{2(4\pi\epsilon_0\epsilon)^2\hbar^2}$$

In the low-density limit, $na_B^D \ll 1$ (n is the exciton density, $a_B = a_B^*$ is the exciton Bohr radius and D is the dimensionality), excitons are weakly interacting bosons - BEC believed to be possible!

Transition from classical to quantum gas occurs when the de Broglie wavelength, λ, is comparable to the interparticle separation, $n^{-1/2}$ (in 2D),

$$\lambda = \sqrt{2\pi h^2 / M k_B T}$$

Now for excitons...

$$M = m_e + m_h \approx M_{atom} \times 10^{-6}$$

$$T_t = 2\pi h^2 n / M k_B \approx 3K$$

The problem with realising this in experiments is finite exciton lifetimes.

Butov Group 2007, University of California, http://physics.ucsd.edu/lvbutov/index.html

An experimental setup for extended exciton lifetimes is the coupled-quantum-well system.

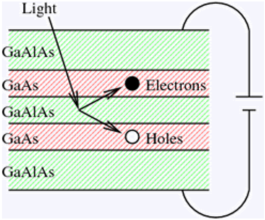
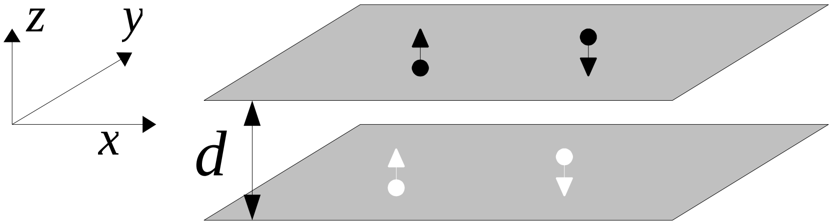


Image from Jonathan Keeling's personal webpage - http://www.tcm.phy.cam.ac.uk/jmjk2/

The bilayer model:
Layers of semiconductor are modelled as infinite, 2D parallel planes. Electrons and holes are free to move within the planes and their effective masses are isotropic.



Parameters: ϵ, d, m_e, m_h
Calculations here have 2 electrons in one layer and 2 holes in the other.

The trial wavefunction is

$$\Psi(\mathbf{R}) = \mathrm{e}^{J(\mathbf{R})}\Psi_{ee}\Psi_{hh}\Psi_{eh} \ ,$$

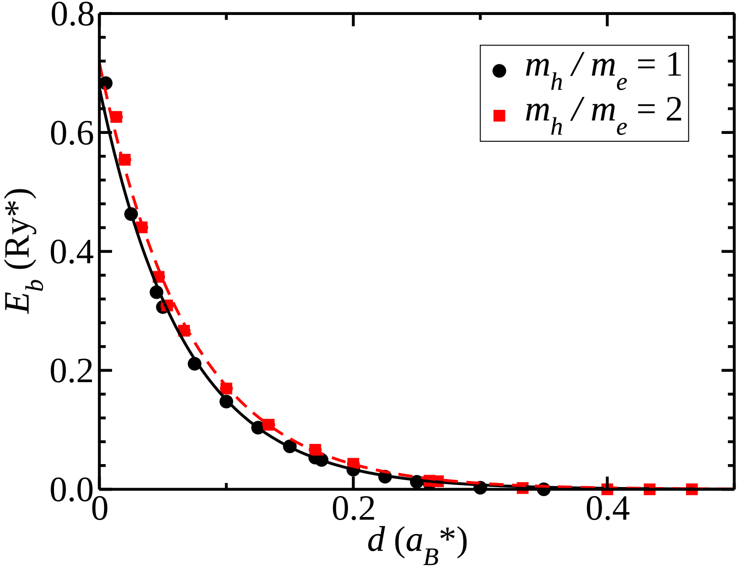
with Ψ_{ee} and Ψ_{hh} of the form

$$\exp\left[\frac{c_1 r}{1 + c_2 r}\right] \ ,$$

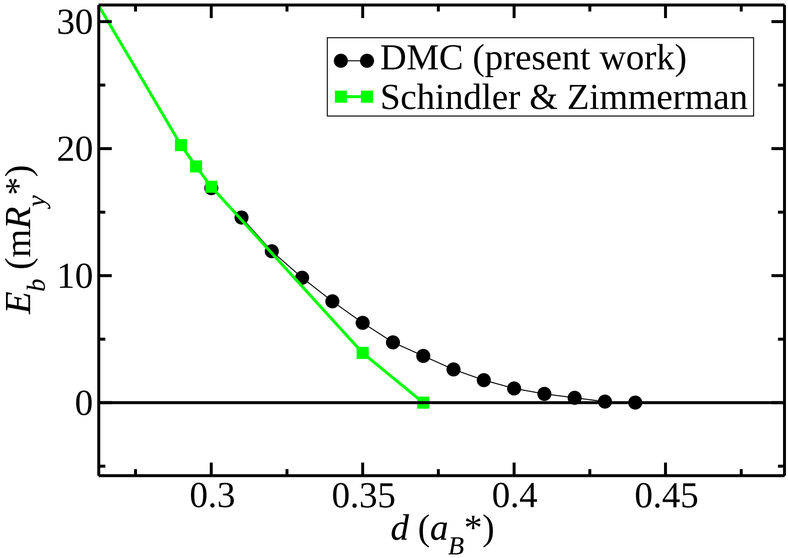
and Ψ_{eh} constructed from cuspless exponentials

$$\exp\left[\frac{d_1 r + d_2 r^2}{1 + d_3 r}\right] \ ,$$

M. Y. J. Tan, N. D. Drummond, and R. J. Needs, Phys. Rev. B **71**, 033303 (2005).

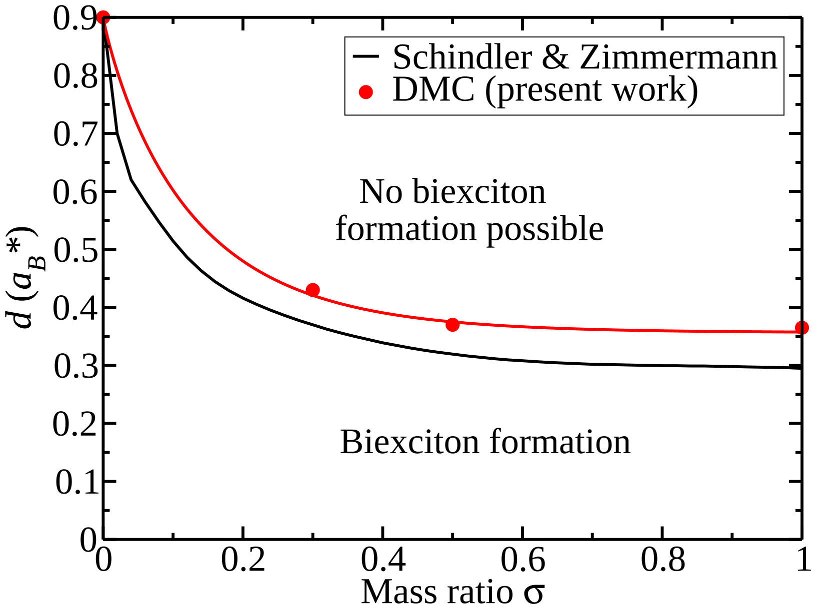


M. Y. J. Tan, N. D. Drummond, and R. J. Needs, Phys. Rev. B **71**, 033303 (2005).



$\sigma = 0.3$

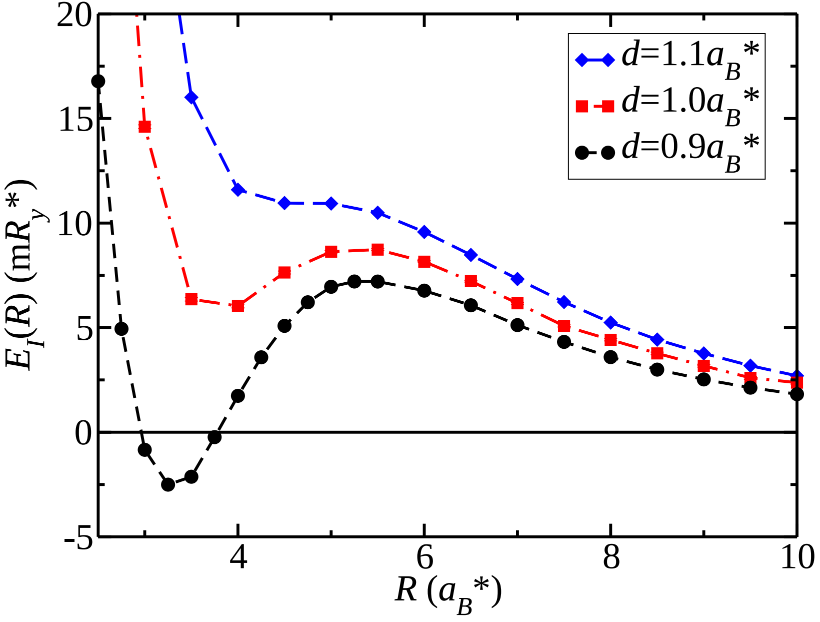
C. Schindler and R. Zimmermann, Phys. Rev. B **78**, 045313 (2008).


Schindler & Zimmermann
DMC (present work)
No biexciton
formation possible
Biexciton formation
$d\ (a_B^*)$
Mass ratio σ
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
0.2
0.4
0.6
0.8
1

Constrain hole positions in space. Then we are just modelling two electrons moving in an external $1/r$ potential with two sources. The Hamiltonian is

$$\begin{aligned}\hat{H} &= \frac{1}{2\mu}\left(\nabla_1^2 + \nabla_2^2\right) - \frac{1}{r_1} - \frac{1}{r_2} + \frac{1}{R} \\ &\quad + \frac{1}{|\mathbf{R} - \mathbf{r}_1 + \mathbf{r}_2|} - \frac{1}{|\mathbf{R} - \mathbf{r}_1|} - \frac{1}{|\mathbf{R} + \mathbf{r}_2|},\end{aligned}$$

where $\mathbf{R}$ is the hole-hole separation, which we may choose.

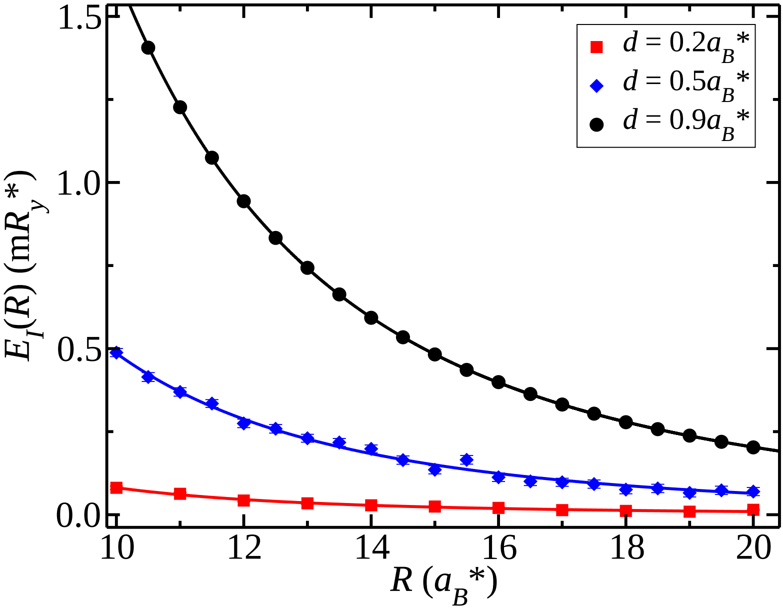


d=1.1a_B*
d=1.0a_B*
d=0.9a_B*
$E_I(R)$ (mR_y*)
R (a_B*)
20
15
10
5
0
-5
4
6
8
10

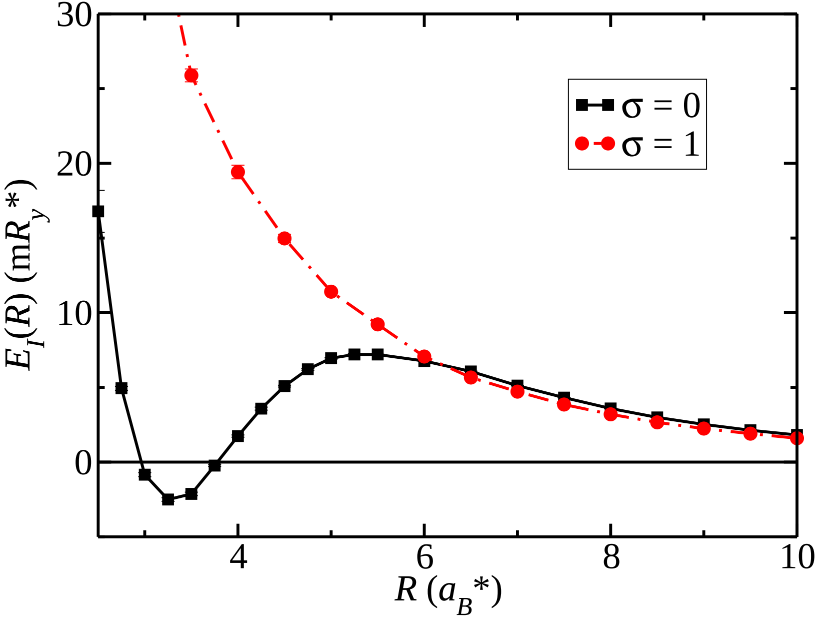
Constrain center-of-mass instead of hole positions. The Hamiltonian may be written as

$$\begin{aligned}\hat{H} &= \frac{1}{2\mu}\left(\nabla_1^2 + \nabla_2^2\right) - \frac{1}{r_1} - \frac{1}{r_2} \\ &\quad + \frac{1}{\left|\mathbf{R} + \frac{\mu}{m_e}(-\mathbf{r}_2 + \mathbf{r}_1)\right|} + \frac{1}{\left|\mathbf{R} + \frac{\mu}{m_h}(-\mathbf{r}_1 + \mathbf{r}_2)\right|} \\ &\quad - \frac{1}{\left|\mathbf{R} - \frac{\mu}{m_h}\mathbf{r}_1 - \frac{\mu}{m_e}\mathbf{r}_2\right|} - \frac{1}{\left|\mathbf{R} + \frac{\mu}{m_e}\mathbf{r}_1 + \frac{\mu}{m_h}\mathbf{r}_2\right|},\end{aligned}$$

where $\mathbf{R}$ is the center-of-mass separation - a parameter that we may fix to investigate the exciton-exciton interaction.



$d = 0.2a_B*$
$d = 0.5a_B*$
$d = 0.9a_B*$
$E_I(R)$ (mR_y*)
R (a_B*)
0.0
0.5
1.0
1.5
10
12
14
16
18
20



30
20
10
0
4
6
8
10
$E_I(R)$ (mR_y*)
R (a_B*)
σ = 0
σ = 1

Pair-distribution functions

Electron-electron

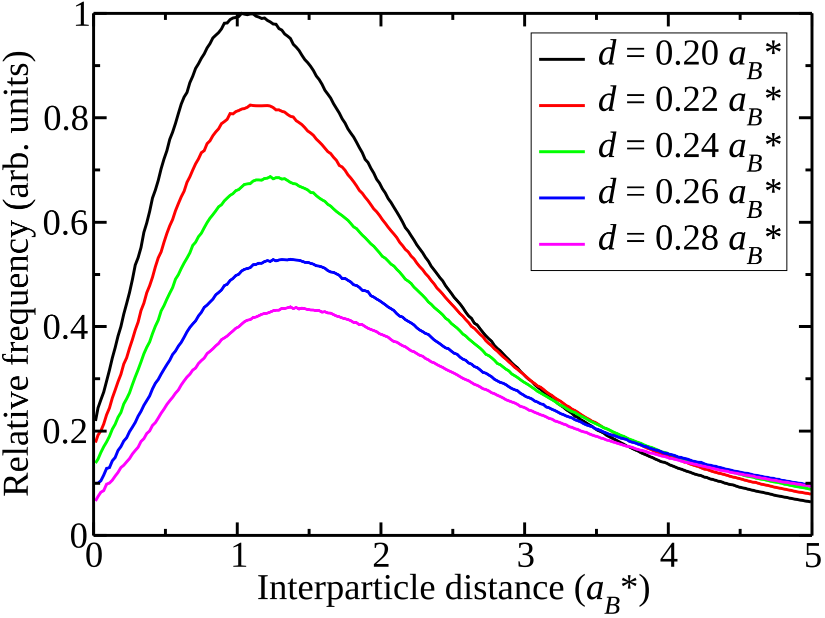
$$g_{\mathrm{ee}}(r) = \frac{1}{2\pi r} \left\langle \delta(|\mathbf{r}_{\mathrm{e}\uparrow} - \mathbf{r}_{\mathrm{e}\downarrow}| - r) \right\rangle \ ,$$

Electron-hole

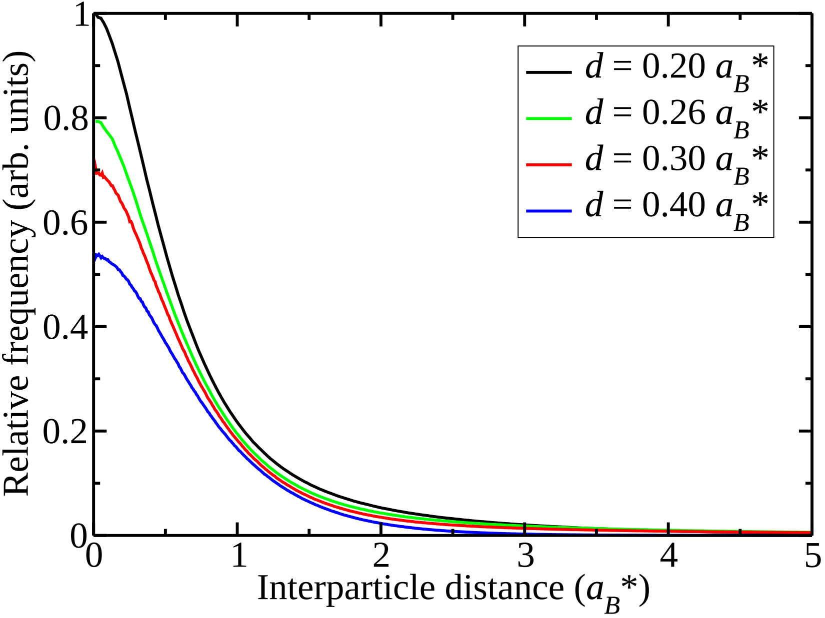
$$g_{\mathrm{eh}}(r) = \frac{1}{8\pi r} \left\langle \sum_{\sigma_{\mathrm{e}},\sigma_{\mathrm{h}} \in \{\uparrow,\downarrow\}} \delta(|\mathbf{r}^{\parallel}_{\mathrm{e}\sigma_{\mathrm{e}}} - \mathbf{r}^{\parallel}_{\mathrm{h}\sigma_{\mathrm{h}}}| - r) \right\rangle \ ,$$

Extrapolated estimator

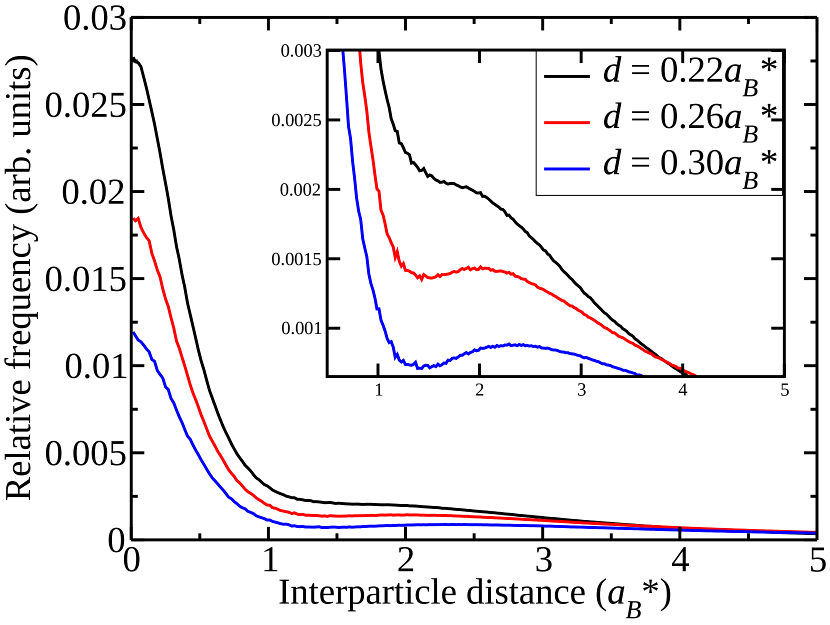
$$g^{\mathrm{ext}} = 2g^{\mathrm{DMC}} - g^{\mathrm{VMC}}$$



Relative frequency (arb. units)
Interparticle distance (a_B*)
0
0.2
0.4
0.6
0.8
1
0
1
2
3
4
5
d = 0.20 a_B*
d = 0.22 a_B*
d = 0.24 a_B*
d = 0.26 a_B*
d = 0.28 a_B*



$d = 0.20\ a_B^*$
$d = 0.26\ a_B^*$
$d = 0.30\ a_B^*$
$d = 0.40\ a_B^*$
Relative frequency (arb. units)
Interparticle distance (a_B^*)
0
0.2
0.4
0.6
0.8
1
0
1
2
3
4
5



Relative frequency (arb. units)
Interparticle distance (a_B*)
0.03
0.025
0.02
0.015
0.01
0.005
0
0
1
2
3
4
5
0.003
0.0025
0.002
0.0015
0.001
$d = 0.22a_B$*
$d = 0.26a_B$*
$d = 0.30a_B$*

Conclusions

- We have more accurately calculated biexciton binding energies over a range of system parameters.
- We may therefore plot the region of biexciton stability more accurately.
- By constraining exciton centers-of-mass, we may investigate the exciton-exciton interaction as a function of σ and d, and also reproduce previous results as a limiting case (by putting $\sigma = 0$).
- Pair-distribution functions reveal biexciton sizes and the retention of individual exciton identities.

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