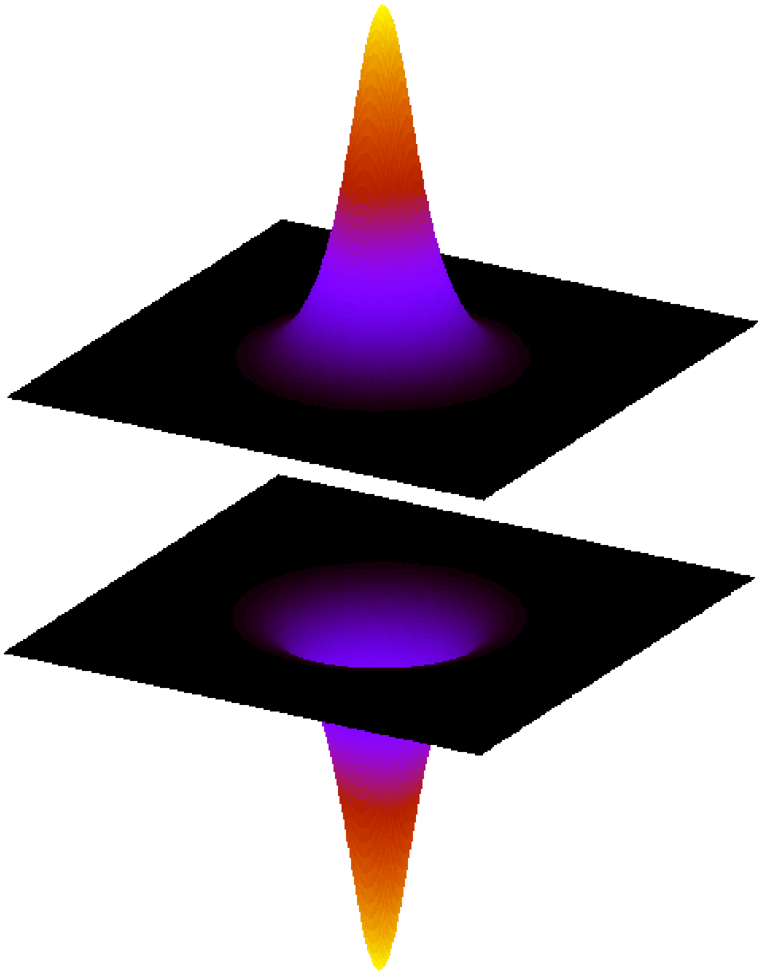
QMC calculations on biexcitons in bilayer systems



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Outline

- What are excitons and biexcitons?
- Why are they interesting?
- Experimental setup / the bilayer system
- QMC calculations
- Conclusions

Excitons

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.

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

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

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

This will occur when the de Broglie wavelength, $\lambda = \sqrt{2\pi h^2/Mk_BT}$, is comparable to the interparticle separation, $n^{-1/2}$.

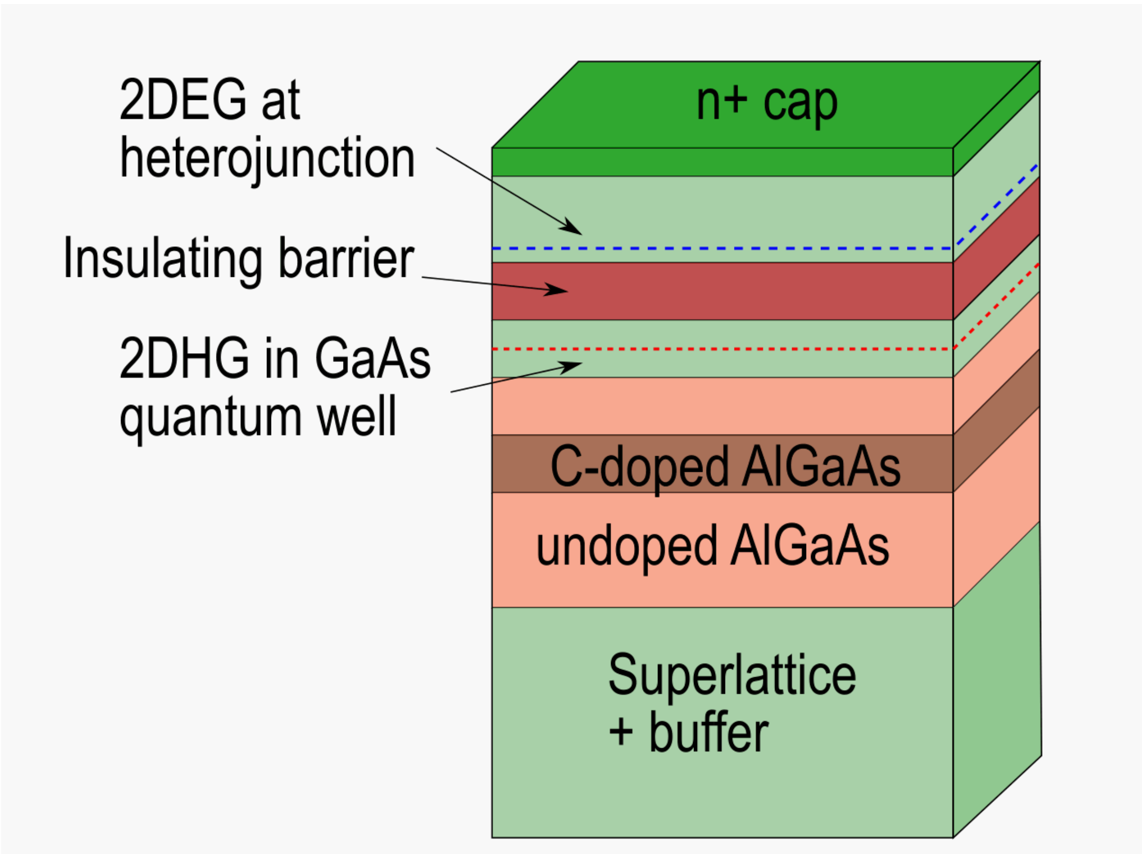
$$T_t = 2\pi h^2 n/Mk_B \approx 3K$$

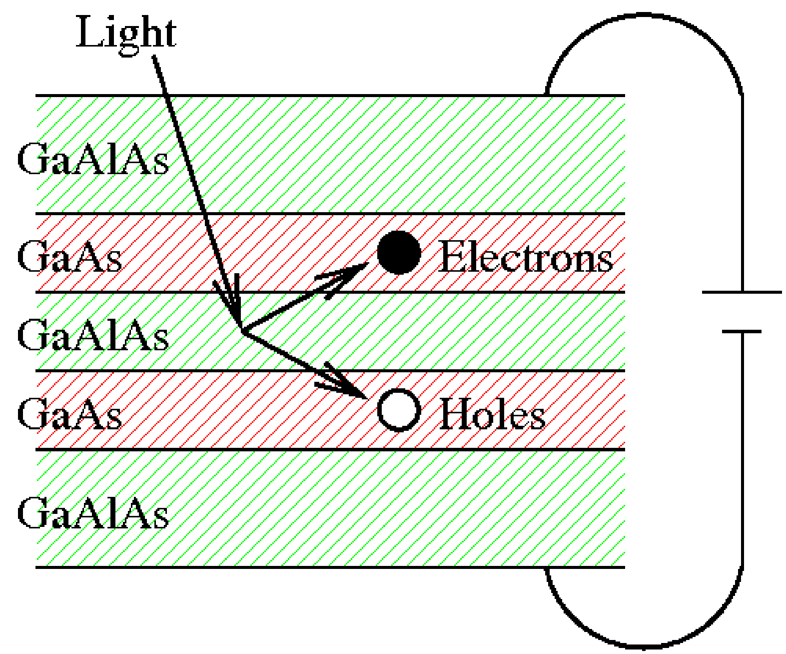
Well within experimental reach!

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

Other experimental problems persist...

The CQW system



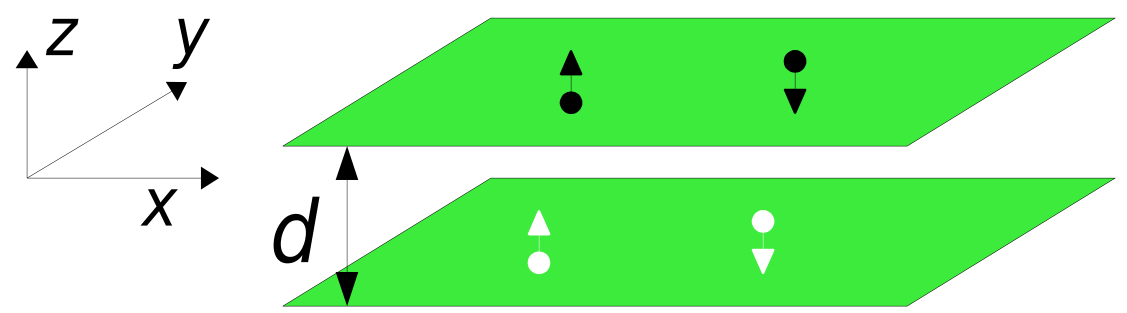


The experimental systems are designed to inhibit recombination while still allowing significant interactions between layers

(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:

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

The trial wavefunction

$$
\begin{aligned}
\Psi &= \Psi_{ee}\Psi_{hh}\Psi_{eh} \\
\Psi_{ee} &= \exp\left[\frac{c_1 r_{12}}{1+c_2 r_{12}}\right] \\
\Psi_{hh} &= \exp\left[\frac{c_3 r_{ab}}{1+c_4 r_{ab}}\right] \\
\Psi_{eh} &= \exp\left[\left(\frac{c_5 r_{1a}+c_6 r_{1a}^2}{1+c_7 r_{1a}}+\frac{c_5 r_{1b}+c_8 r_{1b}^2}{1+c_9 r_{1b}}+\frac{c_5 r_{2a}+c_8 r_{2a}^2}{1+c_9 r_{2a}}+\frac{c_5 r_{2b}+c_6 r_{2b}^2}{1+c_7 r_{2b}}\right)\right] \\
&+ \exp\left[\left(\frac{c_5 r_{1a}+c_8 r_{1a}^2}{1+c_9 r_{1a}}+\frac{c_5 r_{1b}+c_6 r_{1b}^2}{1+c_7 r_{1b}}+\frac{c_5 r_{2a}+c_6 r_{2a}^2}{1+c_7 r_{2a}}+\frac{c_5 r_{2b}+c_8 r_{2b}^2}{1+c_9 r_{2b}}\right)\right],
\end{aligned}
$$

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}

Diffusion Monte Carlo

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:

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

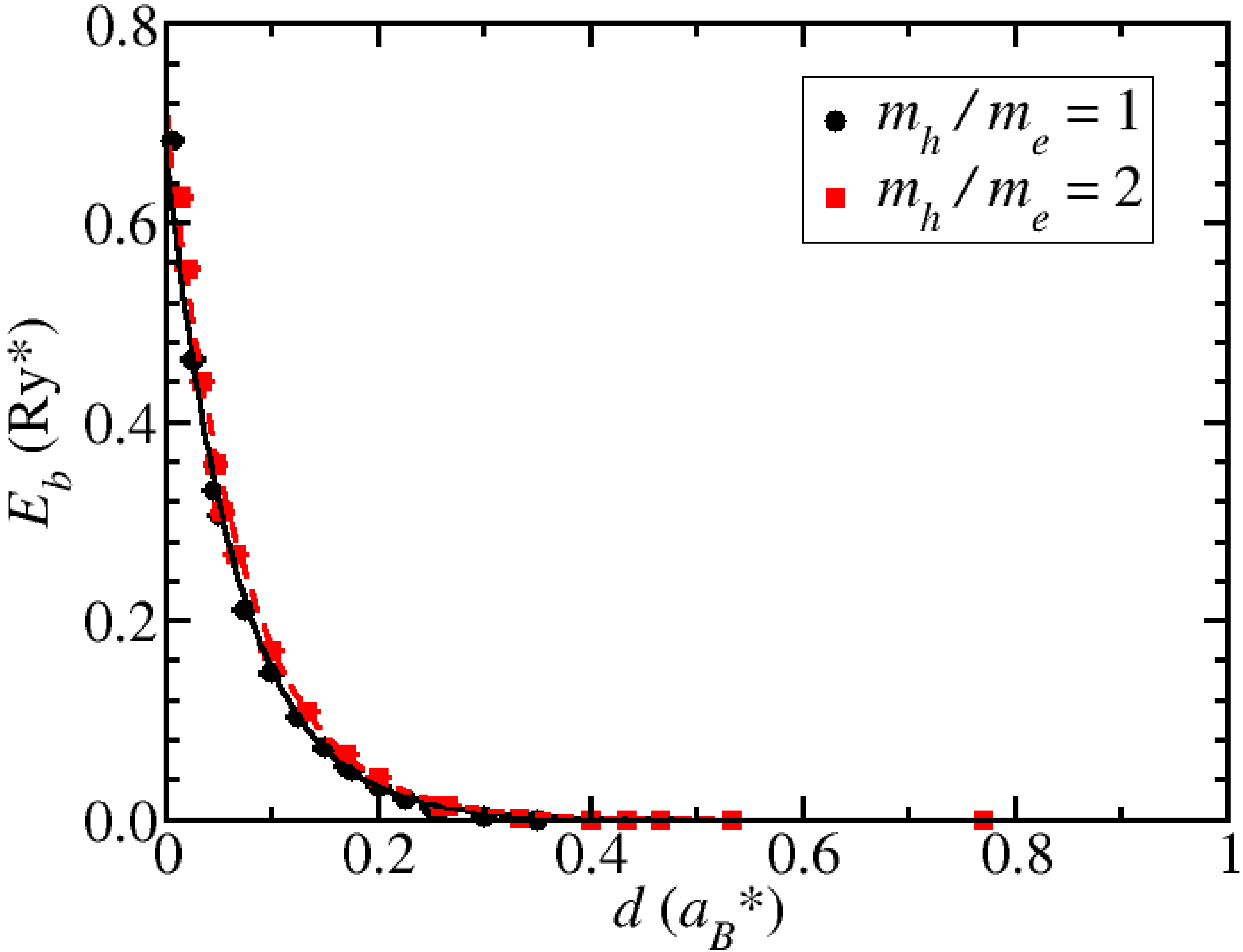
Propagation in imaginary time can project out the ground state component.
This is done in CASINO with drift-diffusion and branching dynamics.
Equivalent to solving the importance-sampled SE

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

with $f(\mathbf{R},\tau) = \Phi(\mathbf{R},\tau)\psi(\mathbf{R})$

Biexciton binding $2E_X - E_{XX}$

Robert Lee - QMC calculations on biexcitons in bilayer systems



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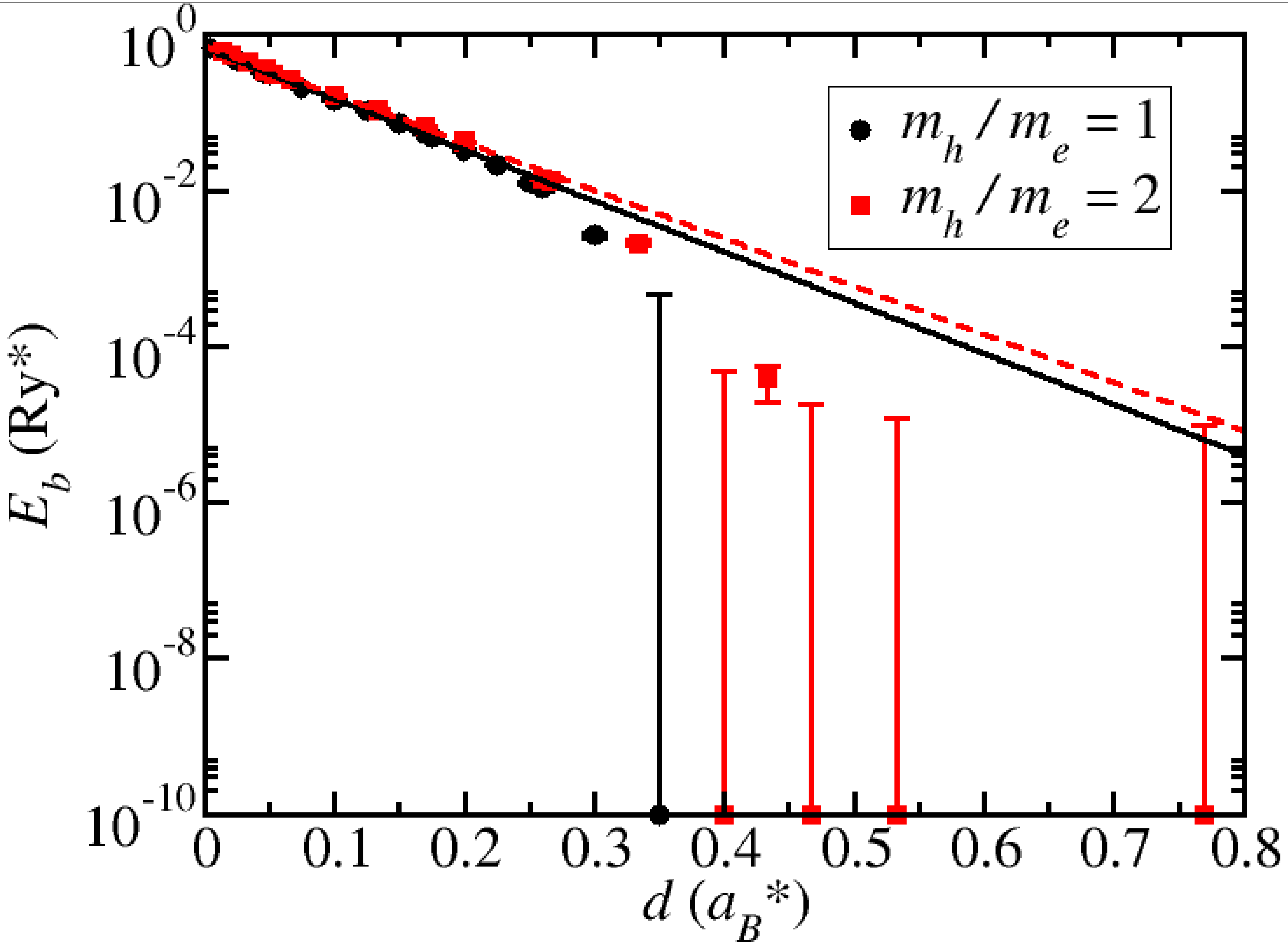

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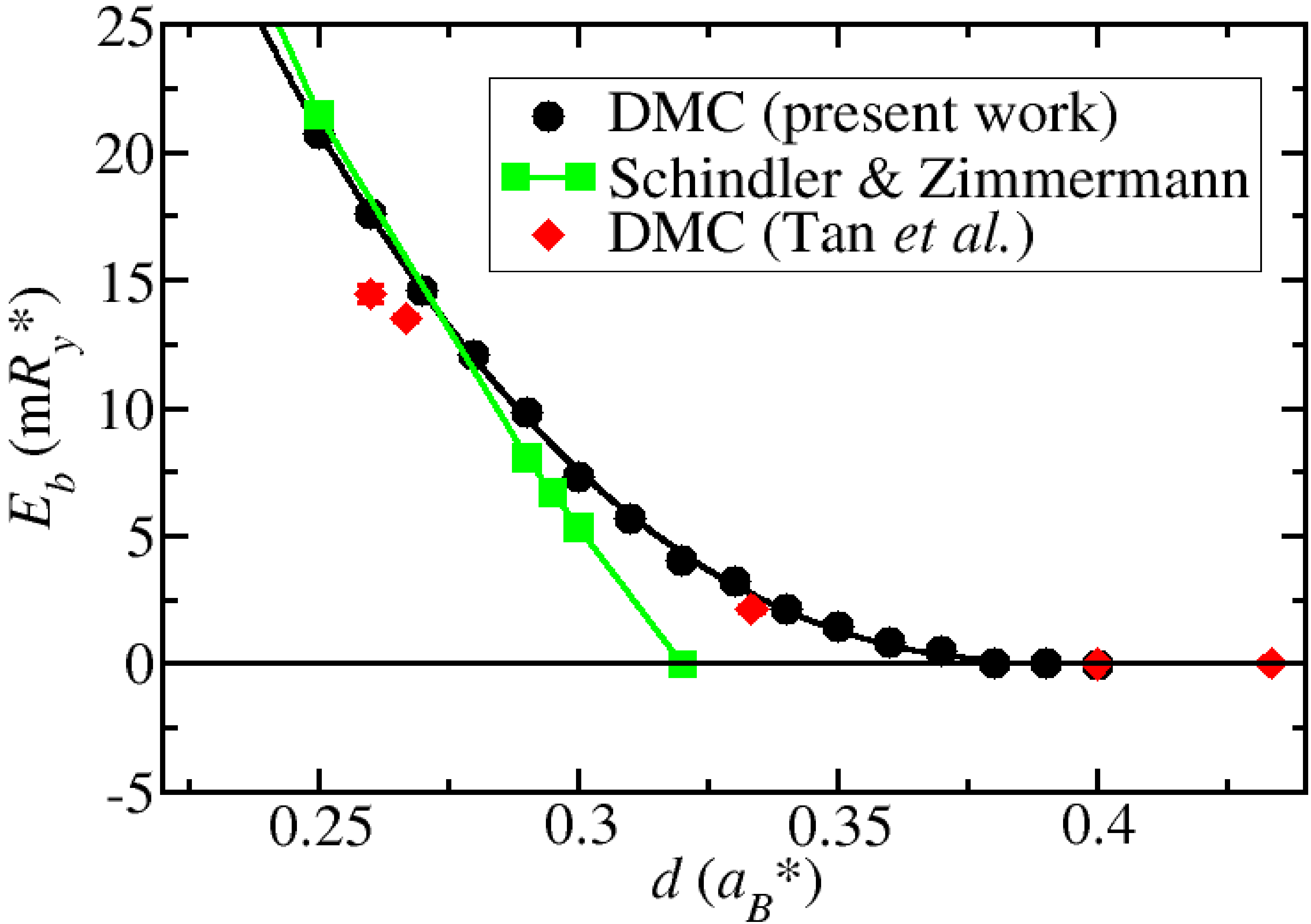

Biexciton stability

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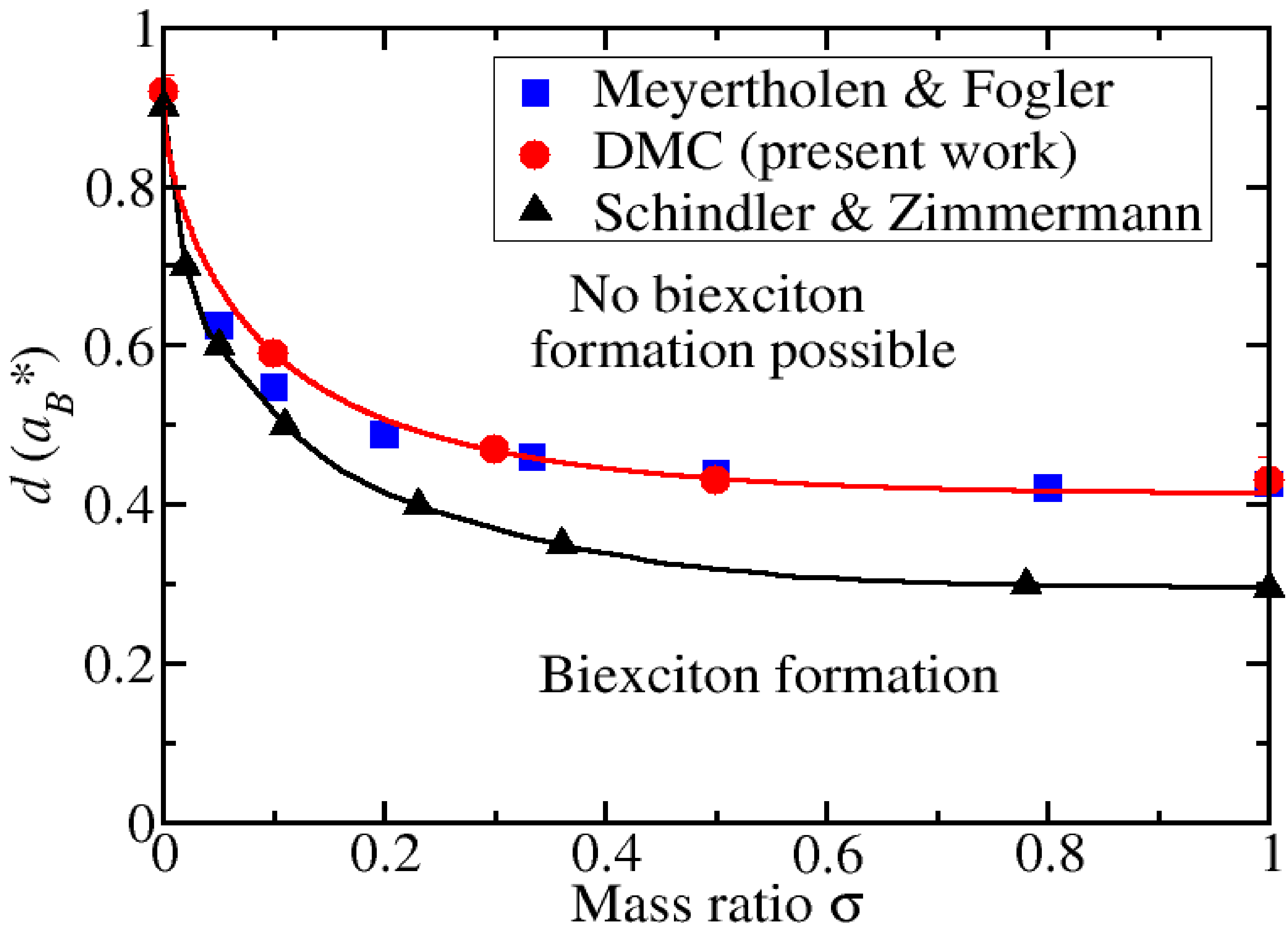


Exciton-exciton interaction

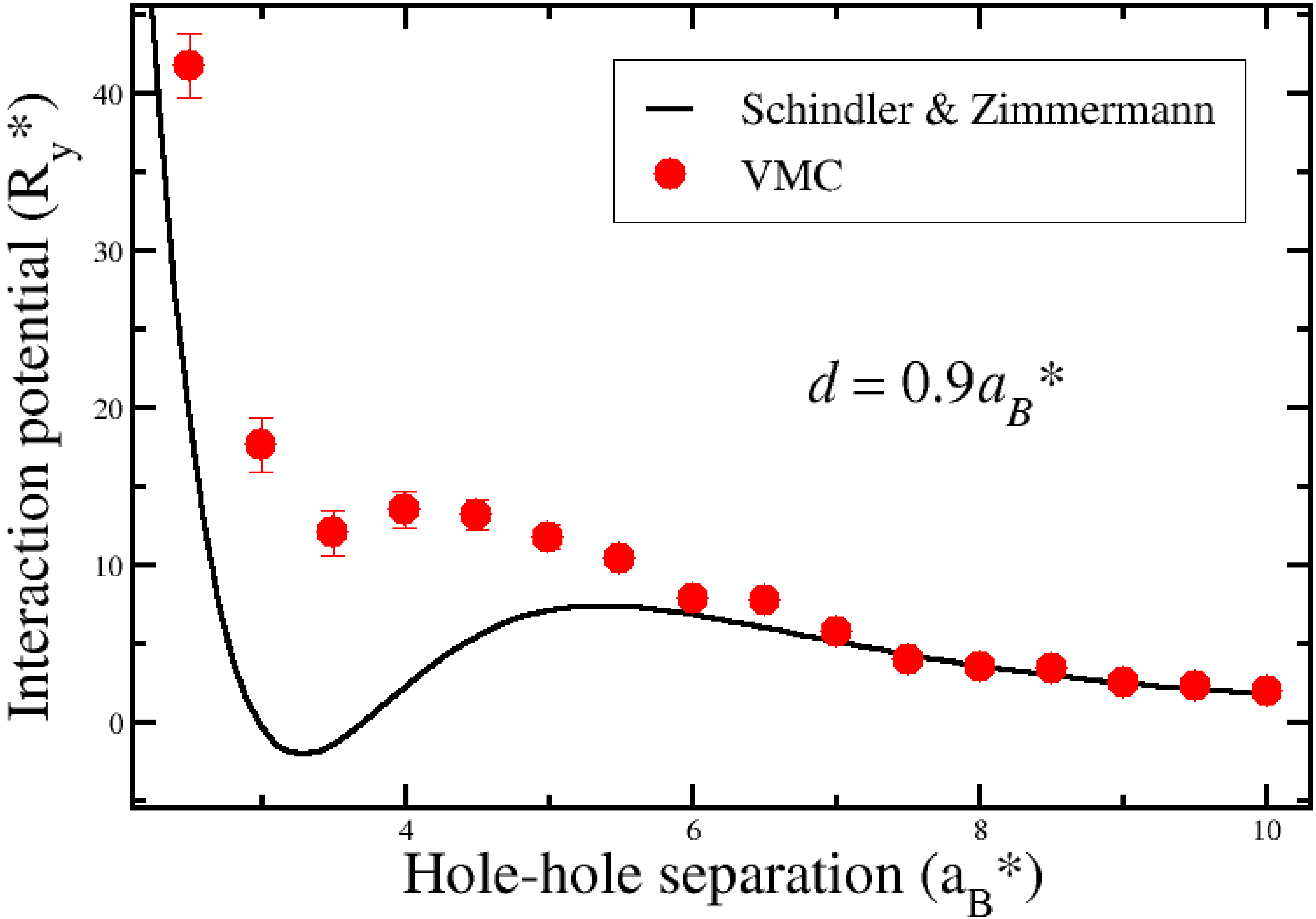
Constrain the centre-of-mass positions of two excitons. Then each exciton may be treated mathematically as a single particle. The two particles interact by the potential

$$\hat{V} = -\frac{1}{|\mathbf{r}_1|} - \frac{1}{|\mathbf{r}_2|} + \frac{1}{|\mathbf{R}_{cm} + \frac{m_\mu}{m_e}(-\mathbf{r}_2 + \mathbf{r}_1)|} + \frac{1}{|\mathbf{R}_{cm} + \frac{m_\mu}{m_h}(-\mathbf{r}_1 + \mathbf{r}_2)|}$$
$$- \frac{1}{|\mathbf{R}_{cm} - \frac{m_\mu}{m_h}\mathbf{r}_1 - \frac{m_\mu}{m_e}\mathbf{r}_2|} - \frac{1}{|\mathbf{R}_{cm} + \frac{m_\mu}{m_e}\mathbf{r}_1 + \frac{m_\mu}{m_h}\mathbf{r}_2|},$$

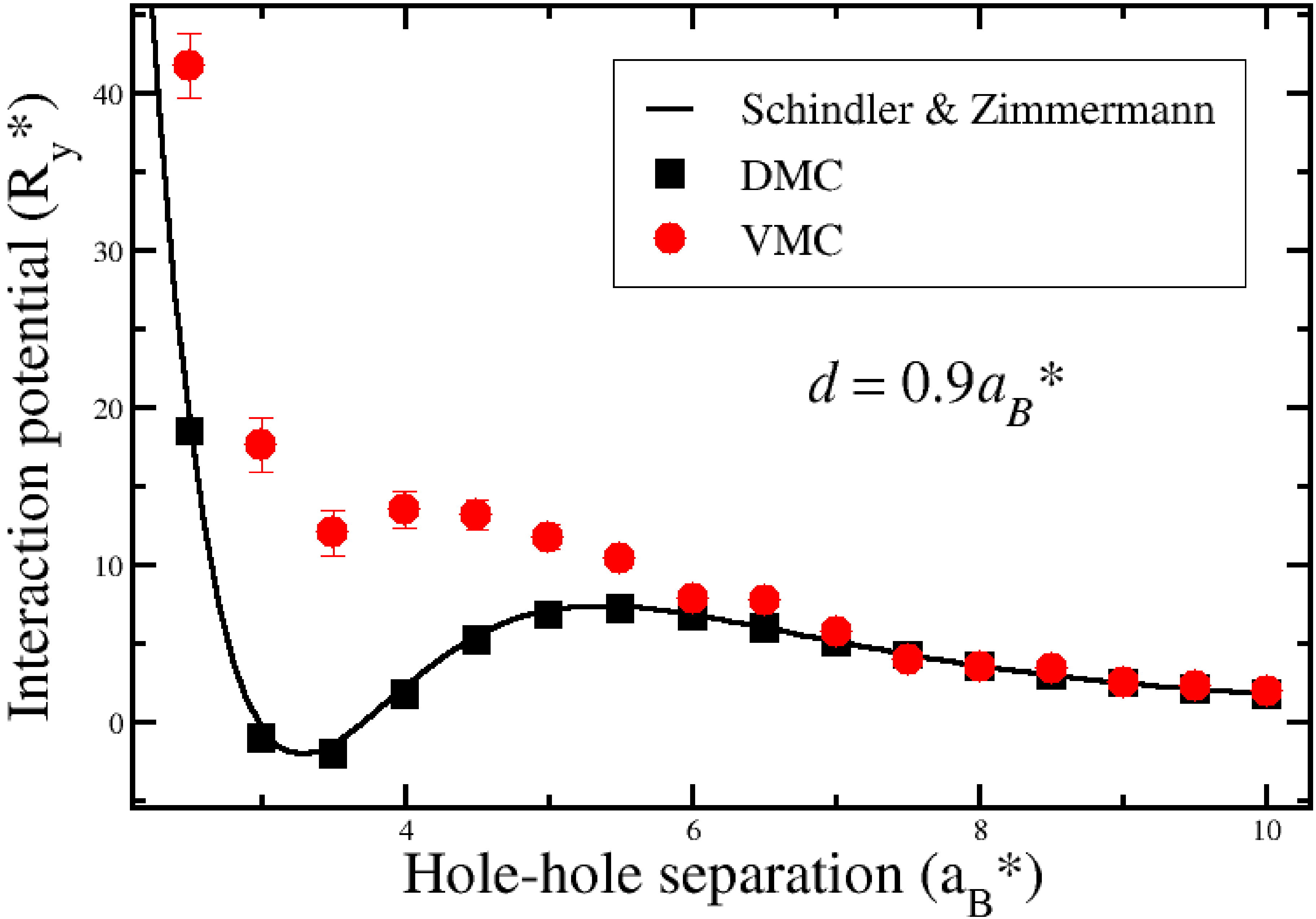
and have kinetic energy $\hat{T} = \frac{1}{2m_\mu}\left(\nabla_1^2 + \nabla_2^2\right)$,

So we can now treat $\mathbf{R}_{cm}$ as a parameter and investigate the exciton-exciton potential with $\sigma \neq 0$.

VMC versus DMC



VMC versus DMC



Pair dist. functions

Electron-hole PDF

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

Electron-electron PDF

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

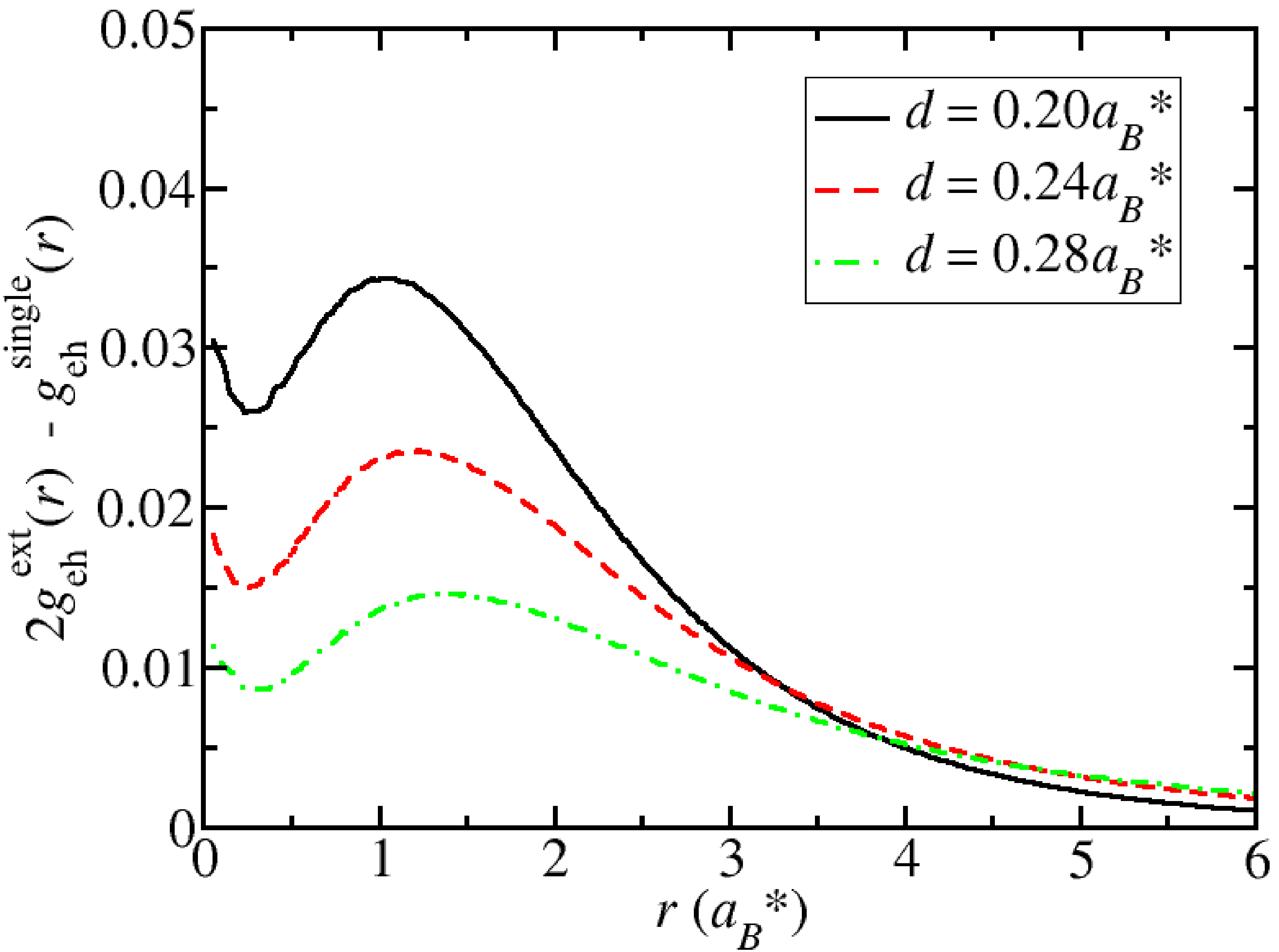
Extrapolated estimator

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

Normalization

$$\int_0^\infty 2\pi r g^{\mathrm{ext}}(r)\, dr = 1.$$

Pair dist. functions



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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