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Trion formation in coupled quantum well heterostructures

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Introduction

Outline

In this talk I shall be discussing:

- A small introduction to quantum Monte Carlo methods.
- A brief overview of coupled quantum wells and why they are important.
- The form of the trial wave function used.
- The (incomplete) results of my findings.

The results presented are incomplete as the project is still ongoing with calculations being run on the HEC as we speak.

Variational Principle

For a general Hamiltonian $\hat{H}$ and arbitrary wave function $\Psi(\mathbf{R})$, we have the *variational principle*:

$$\frac{\int \Psi^* \hat{H} \Psi \, \mathrm{d}\mathbf{R}}{\int |\Psi|^2 \, \mathrm{d}\mathbf{R}} \geq E_0 \tag{1}$$

where $\mathrm{d}\mathbf{R}$ is a 3N-dimensional integral.

This is the main tool used in quantum Monte Carlo methods. The other being Monte Carlo integration with the Metropolis-Hastings algorithm.

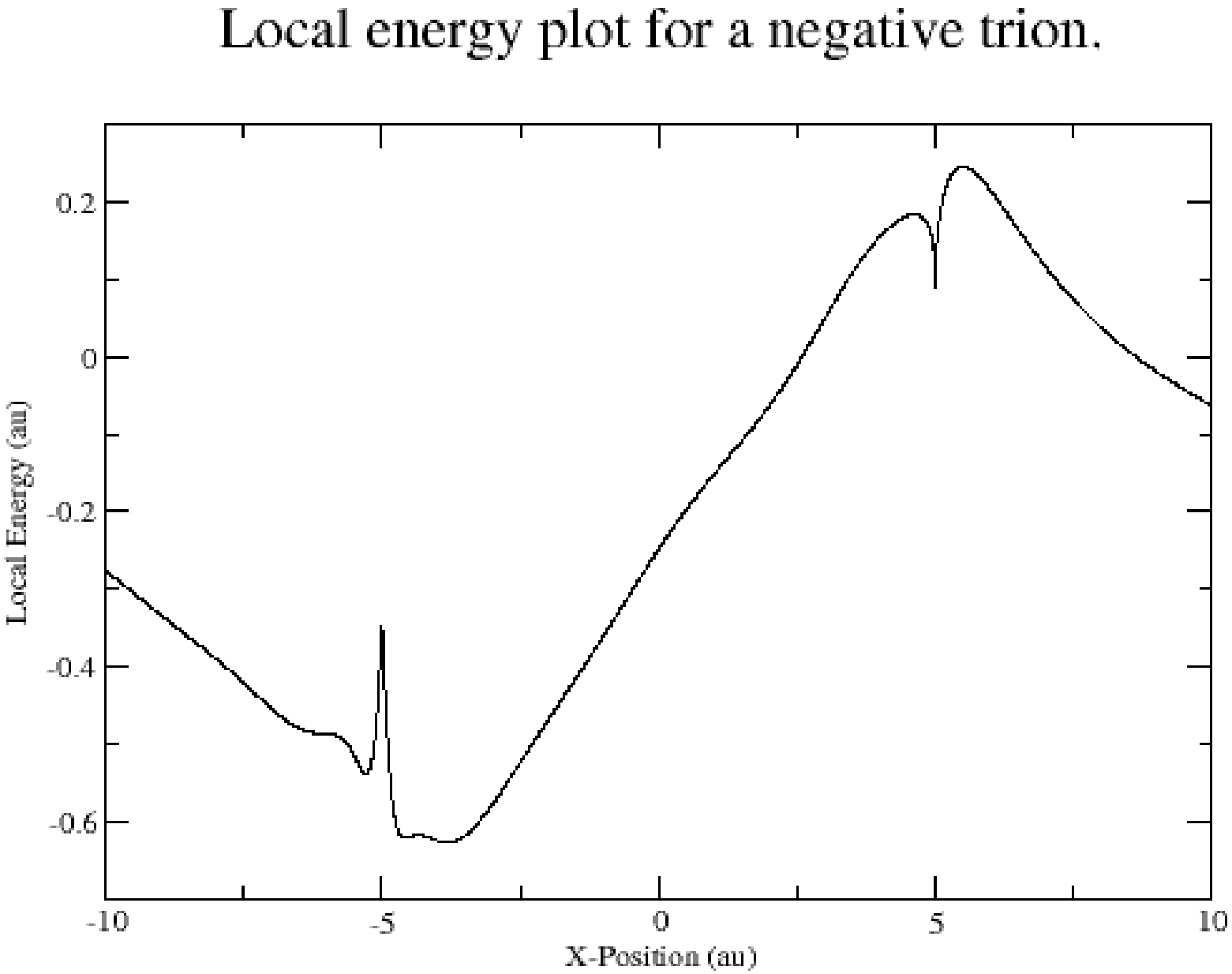
Local energy

Variational Monte Carlo involves accumulating averages of the so-called local energy:

$$\langle E_L \rangle = \frac{\int |\Psi|^2 \, E_L \, \mathrm{d}\mathbf{R}}{\int |\Psi|^2 \, \mathrm{d}\mathbf{R}} \tag{2}$$

where $E_L = \Psi^{-1} \hat{H} \Psi$ is the local energy.

If the wave function used was an eigenstate of the Hamiltonian, the local energy would be constant throughout space.


Local energy plot for a negative trion.
0.2
0
-0.2
-0.4
-0.6
Local Energy (au)
-10
-5
0
5
10
X-Position (au)

Quantum Monte Carlo

VMC

Variational Monte Carlo uses the Metropolis-Hastings to generate sets of electron coordinates distributed as $|\Psi|^2$ and averages the local energies to create an estimate for the energy.

DMC

Diffusion Monte Carlo uses the imaginary-time Schrödinger equation to project out the ground state wave function of the system.

$$-\frac{\mathrm{d}\Psi}{\mathrm{d}t} = (\hat{H} - E_T)\Psi \tag{3}$$

where excited states decay exponentially compared to the ground state.

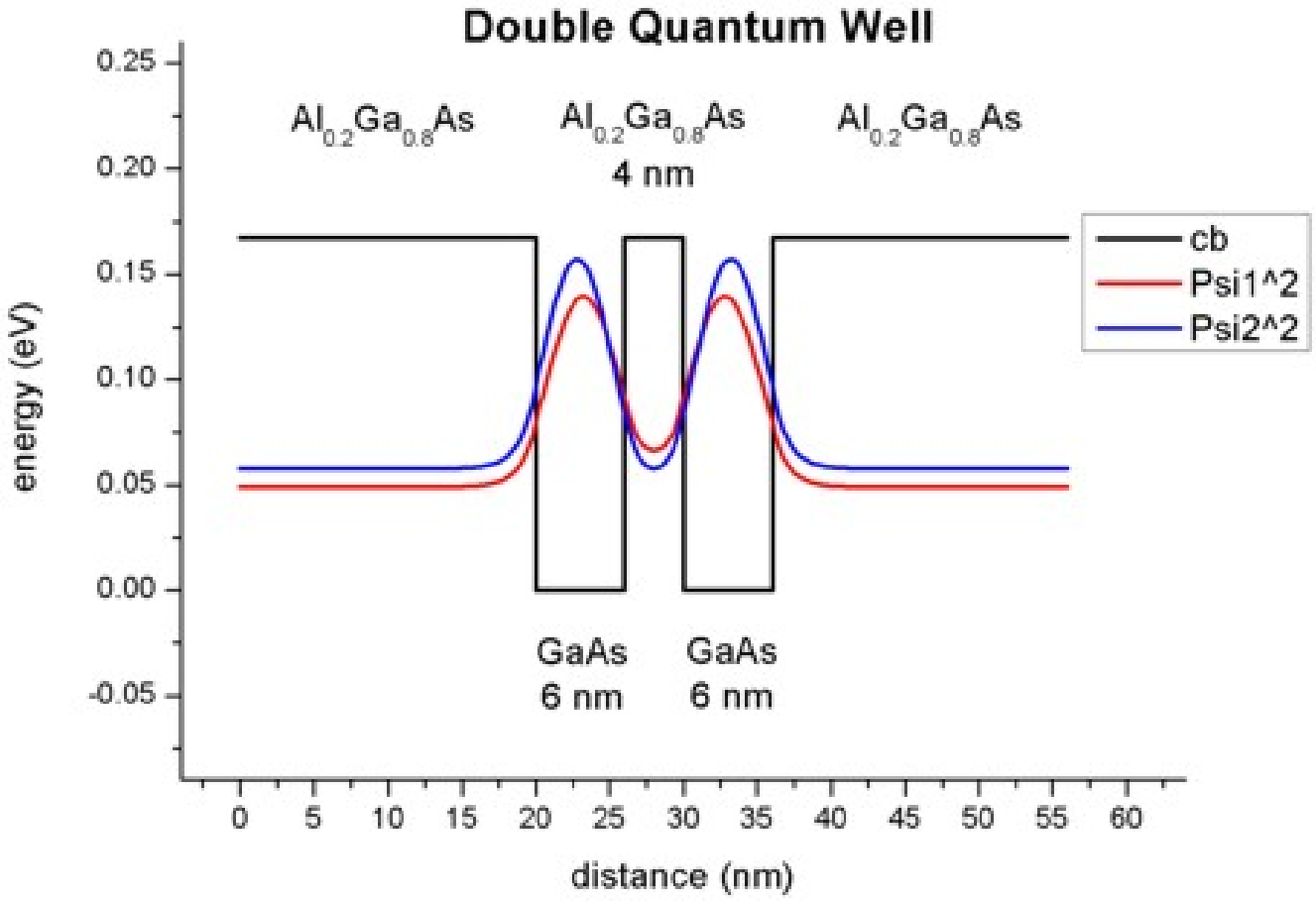
Trial Wave Functions

The accuracy of quantum Monte Carlo calculations is dependent on the accuracy of the trial wave function used. Thus it is important to design one which accurately describes the physics of the system, both short range and long range.

In VMC calculations the energy of the system depends on the trial wave function, whereas for nodeless systems, the DMC energy is independent of the trial wave function.

Coupled Quantum Wells

Quantum wells are thin layered semiconductors in which we can observe and control many quantum effects. They derive most of their special properties from the spatial confinement of the charge carriers; electrons and holes[1].



Coupled Quantum Wells

Bose-Einstein Condensate

Experimentalists have long been looking for excitonic Bose-Einstein condensates in coupled quantum wells due to their long lifetimes in bilayer systems.

Trial Wave Function

The trial wave function used in the VMC and DMC calculations was as follows:

$$\Psi = \Psi_{ee}\Psi_{eh_1}\Psi_{eh_2} \tag{4}$$

$$\Psi_{ee} = \exp\left\{\frac{c_1 r_{12}}{1 + c_2 r_{12}} + \frac{1}{2}\left(e^{-c_6 r_{12}^2} - 1\right)\log\left(r_{12}\right)\right\} \tag{5}$$

$$\Psi_{eh_1} = \exp\left\{\frac{c_3 r_{1a} + c_4 r_{1a}^2}{1 + c_5 r_{1a}}\right\}, \quad \Psi_{eh_2} = \exp\left\{\frac{c_3 r_{2a} + c_4 r_{2a}^2}{1 + c_5 r_{2a}}\right\} \tag{6}$$

where c_1 - c_6 are optimisable parameters.

Trial Wave Function

Parameters c_1 - c_6

The parameters are free to take any value subject to a few constraints:

- The value of c_1 is fixed by the electron-electron Kato cusp conditions.
- We require $c_2 > 0$ so th at Ψ is well behaved.
- The value of c_3 is fixed by the electron-hole cusp conditions when the layer separation is 0 and is set to 0 for non-zero separation.
- We require $c_4 < 0$ to make sure the wave function decays exponentially when an electron is pulled away.
- We require $c_5 > 0$ so that Ψ is well behaved.
- We require $c_6 > 0$ so that the long range behaviour of the system is satisfied.

Trial Wave Function

Long Range Behaviour

The wave function was designed to exhibit the correct behaviour as an electron or hole is pulled away from the system.

Electron Pulled Away

The wave function tends to:

$$\Psi \to A\frac{1}{\sqrt{r_{12}}}\exp\left\{-kr_{12}\right\}\exp\left\{\frac{c_3 r_{2a}+c_4 r_{2a}^2}{1+c_5 r_{2a}}\right\}\to 0 \tag{7}$$

Hole Pulled Away

The wave function tends to:

$$\Psi \to \exp\left\{c_1 r_{12}1+c_2 r_{12}+\frac{1}{2}\left(e^{-c_6 r_{12}^2}-1\right)\log\left(r_{12}\right)\right\}\exp\left\{2\frac{c_4}{c_5}r_{1a}\right\}\to 0 \tag{8}$$

Results

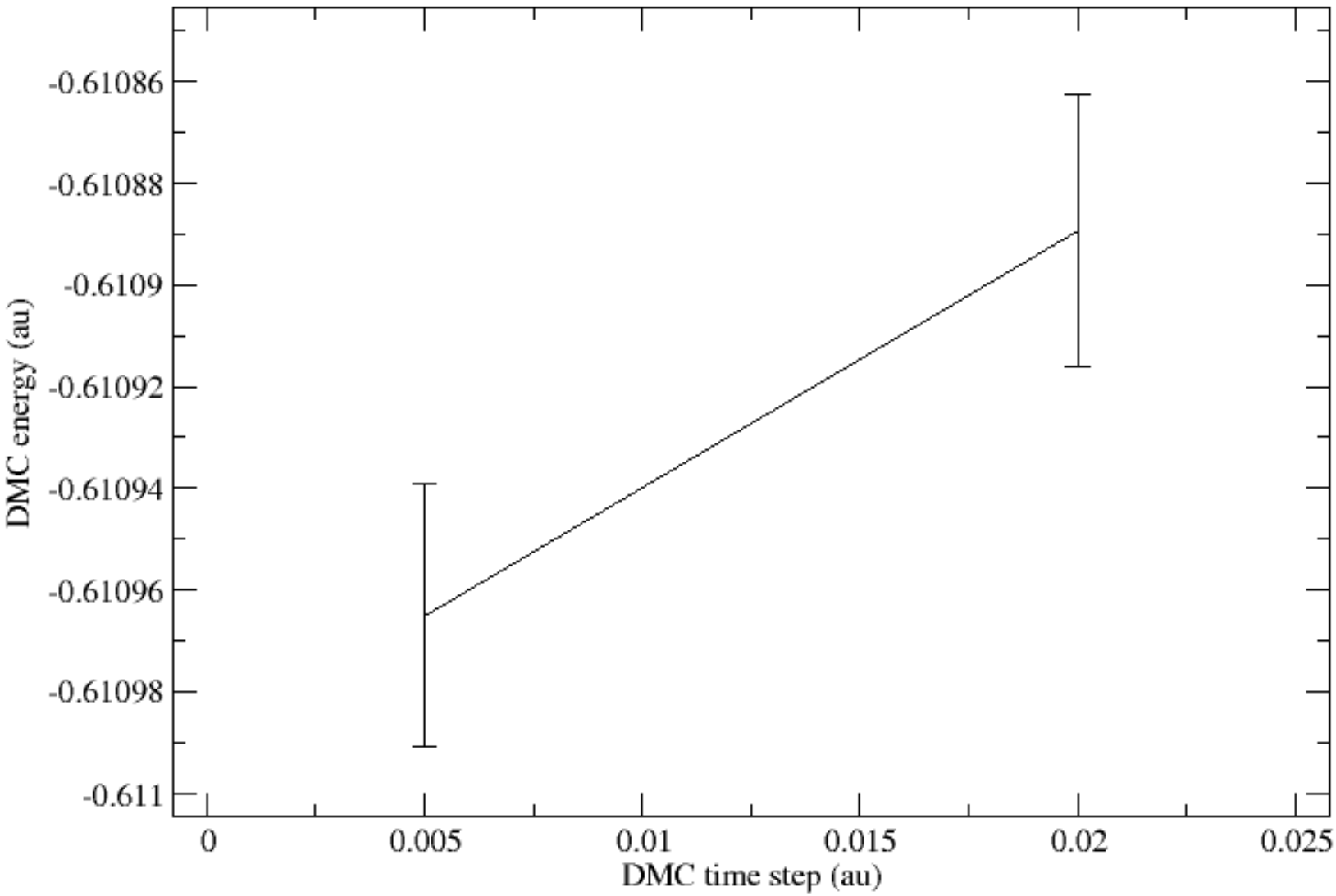
Outline

The plan is to produce a grid of points of trion energies and binding energies at different layer separations and mass ratios and to fit a curve to these results to predict the separation at which the trion becomes unbound. The grid of points consists of:

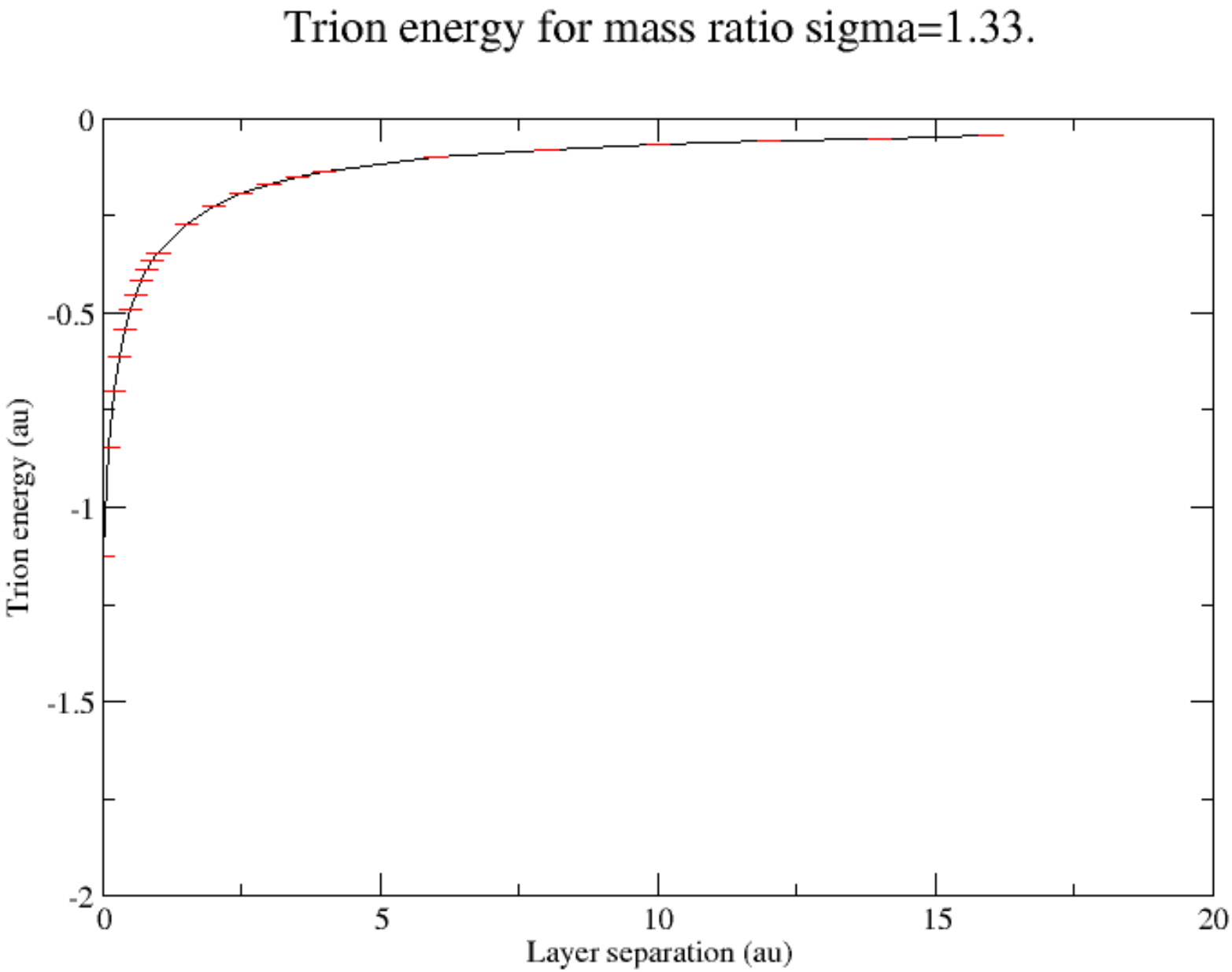
- Layer separations of from 0 to 16 (au).
- Mass ratios of 0.25, 0.5, 0.75, 1 and the infinitely heavy cases.

Results

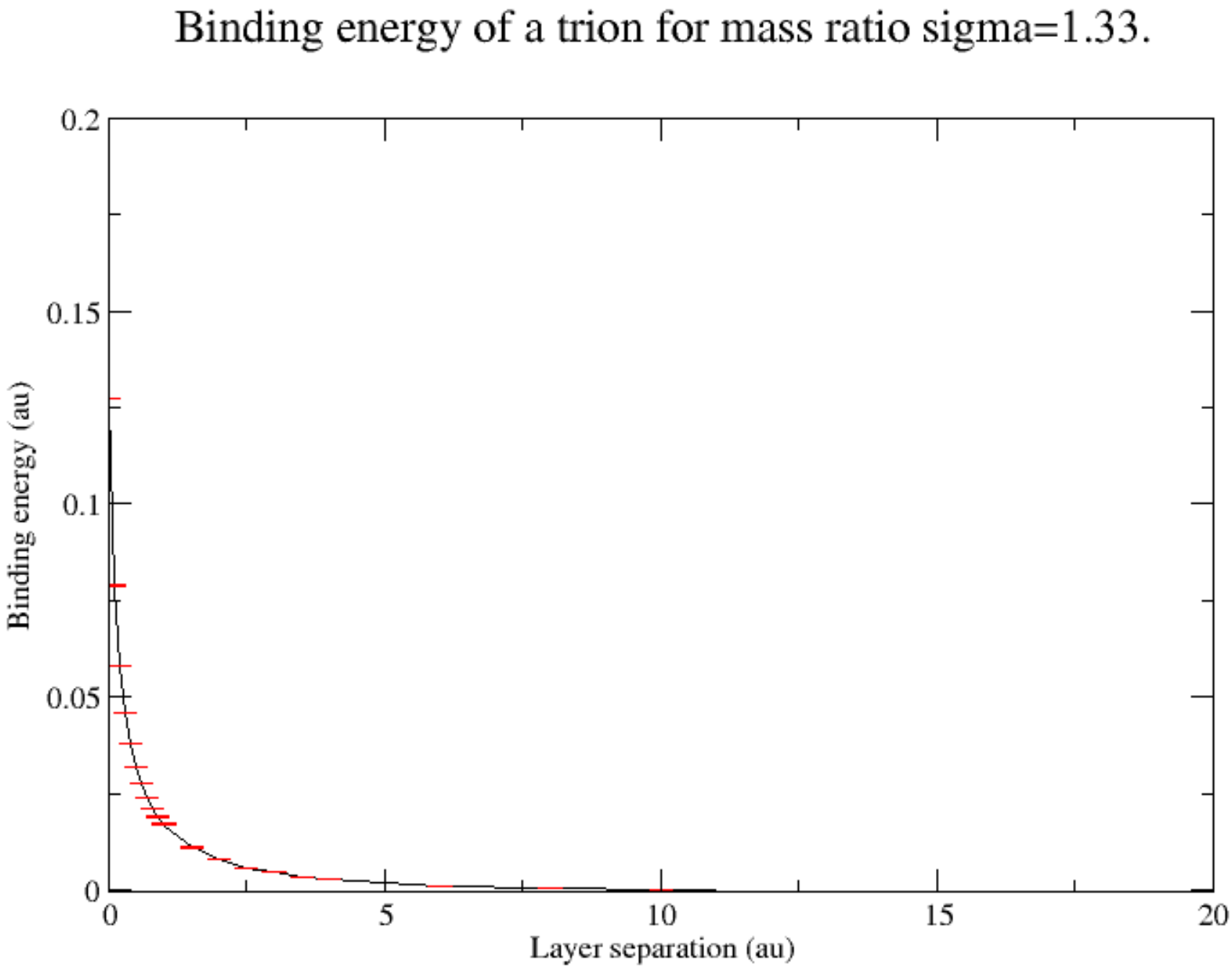
Representation of extrapolation to zero time step and infinite population.



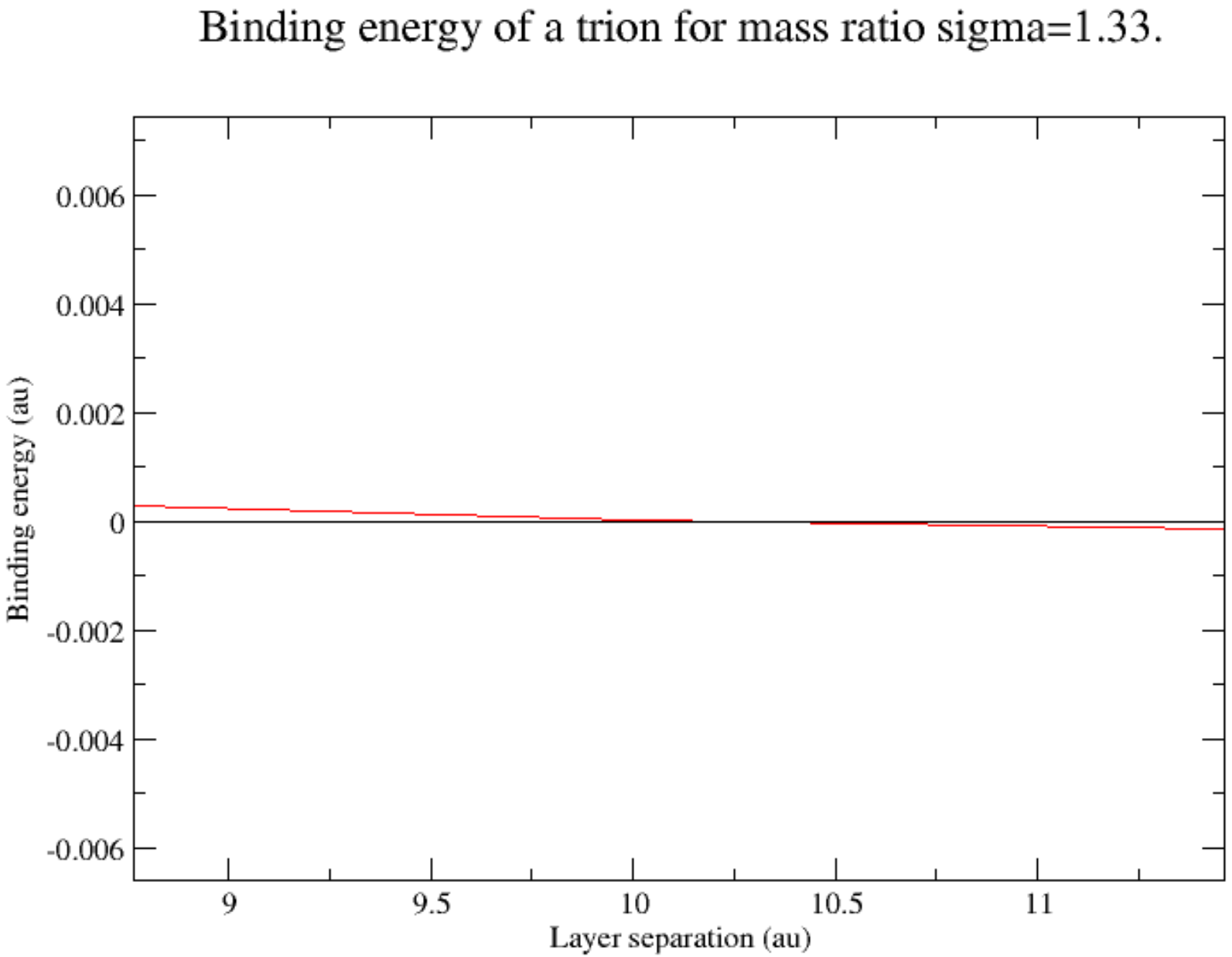
Results


Trion energy for mass ratio sigma=1.33.
Trion energy (au)
Layer separation (au)
0
-0.5
-1
-1.5
-2
0
5
10
15
20

Results


Binding energy of a trion for mass ratio sigma=1.33.
Binding energy (au)
Layer separation (au)
0.2
0.15
0.1
0.05
0
0
5
10
15
20

Results


Binding energy of a trion for mass ratio sigma=1.33.
0.006
0.004
0.002
0
-0.002
-0.004
-0.006
Binding energy (au)
9
9.5
10
10.5
11
Layer separation (au)

Summary

Conclusion

The critical layer separation for a trion is much higher (10) than that of the biexciton. This is an unexpected result as the geometry of the biexciton (4 particles) was expected to lead to more stable configurations that the trion (3 particles).

Thank you for taking the time to listen, any questions are welcomed.

Bibliography


Stefan Birner (2016). Double Quantum well. Available online at: http://www.nextnano.com/nextnano3/tutorial/1Dtutorial_DoubleQW.htm.