

Quantum Monte Carlo study of biexcitons and trions in quantum rings

David Thomas and Bharghav Garikipati

Supervisor: Dr. Neil Drummond

Lancaster University

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Overview

- 1 Introduction
- 2 Quantum Monte Carlo
- 3 Modifying CASINO
- 4 Testing
- 5 Calculations
- 6 Results

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Introduction

- Investigate binding energies of biexcitons and trions for various quantum rings, using quantum Monte Carlo (QMC) methods.
- GaSb rings embedded in GaAs semiconductors, with holes confined to the ring, and electrons excluded.
- Use a modified version the QMC code CASINO [1].

Quantum Rings

- Nanometre scale objects formed using methods such self assembly and molecular beam epitaxy.
- Binding energies of excitonic complexes affect photoluminescence properties of the rings.

Model of quantum rings

- Quantum ring, hard-wall boundary conditions such that confinement potential is $V_c = 0$ for holes inside the ring and $V_c = \infty$ if the hole is outside.
- Chosen a ring with rectangular cross section, figure

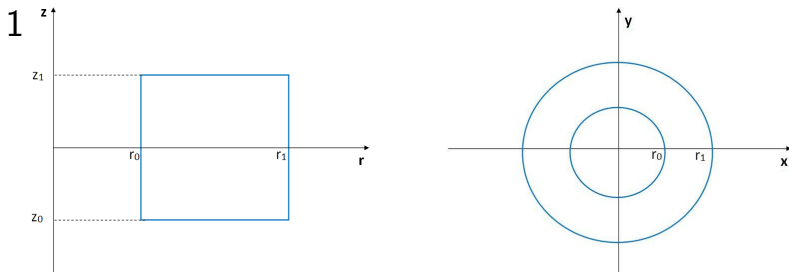


Figure 1: Left: Cross section of ring in cylindrical polar co-ordinates and Right: Top-down view of the ring, blue line is the ring boundary.

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Quantum Monte Carlo

- Variational Monte Carlo (VMC) is a stochastic method used to evaluate the expectation value of the Hamiltonian.
- Diffusion Monte Carlo (DMC) is a stochastic projector that evolves a wave function in imaginary time in order to project out the ground state component of the wave function.
- DMC is exact for these systems.

Variational Monte Carlo

- For a trial wave function Ψ_T , VMC evaluates the integral

$$E_V = \frac{\int |\Psi_T|^2 [\Psi_T^{-1} \hat{H} \Psi_T] d\mathbf{R}}{\int |\Psi_T|^2 d\mathbf{R}'}$$

by randomly sampling the probability space $|\Psi_T|^2 / \int |\Psi_T|^2 d\mathbf{R}'$, and evaluating the local energy $E_L = \Psi_T^{-1} \hat{H} \Psi_T$, at each sampling point.

- Averaging local energy over each sampling point gives E_V .

Diffusion Monte Carlo

- In DMC the wave function Ψ is evolved according to the imaginary-time Schrödinger equation¹

$$-\frac{\partial \Psi(\mathbf{R}, \tau)}{\partial \tau} = -\frac{1}{2} \nabla^2 \Psi(\mathbf{R}, \tau) + (V(\mathbf{R}) - E_T) \Psi(\mathbf{R}, \tau).$$

- This evolution projects out the ground-state component of the wave function.
- Simulate evolution by a diffusion and branching process.

¹In Hartree atomic units, $\hbar = |e| = m_e = 4\pi\epsilon_0 = 1$.

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Modifying CASINO

- CASINO not set up to deal with quantum rings, modification required.
- Need to come up with hole and electron orbitals, also needed is a Jastrow factor to take account of correlation.
- Hole orbitals will be ground-state solutions to the Schrödinger equation in the ring region.
- Electron Orbitals, have correct long and short range behaviour and variational freedom.
- Jastrow factor includes variational freedom.

Electron Orbitals - 1

- Divide up into regions, due to the square nature of the ring.

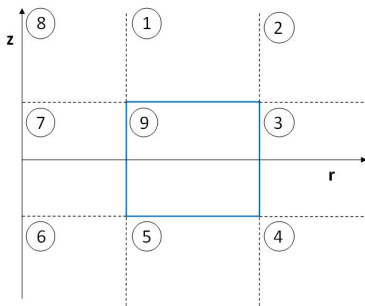


Figure 2: Regions 1-9 for electron orbitals.

- Orbitals should decrease linearly to zero on ring boundary and drop off exponentially at large distances.

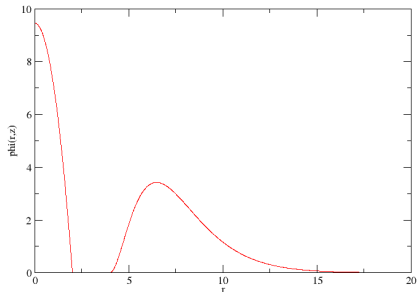
Electron Orbitals - 2

- Orbital should be smooth across each boundary, and its derivative should be zero at $r = 0$.
- For region 1 form of electron orbital is

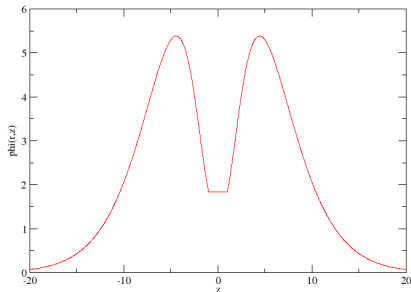
$$\phi_1 = (a_1(z - z_1) + b_1(z - z_1)^2)e^{-\frac{c_1(z-z_1)^2}{d_1(z-z_1)}}.$$

Electron Orbitals - 3

Plot of electron orbital along a line of constant z for $z_0 < z < z_1$



Plot of electron orbital along a long on constant r for $r > r_1$



Hole Orbitals - 1

- Hole orbitals are solutions to the free particle Schrödinger equation, that satisfy the boundary conditions:

$$\phi_h(z = z_0) = 0 = \phi_h(z = z_1)$$

$$\phi_h(r = r_0) = 0 = \phi_h(r = r_1)$$

Hole Orbitals - 2

- Hole Orbitals have the form of Bessel functions multiplied by a cosine function.

$$\phi_h = A \left(\frac{-J_0(\beta r) Y_0(\beta r_0)}{J_0(\beta r_0)} + Y_0(\beta r) \right) \cos \left(\frac{\pi z}{L_z} \right),$$

where J_0 and Y_0 are Bessel functions of the first and second kind, $L_z = |z_1 - z_0|$ and A is a normalisation constant.

- β has to be determined numerically for each ring geometry, such that $\phi_h(r = r_1) = 0$.

Hole Orbitals - 3

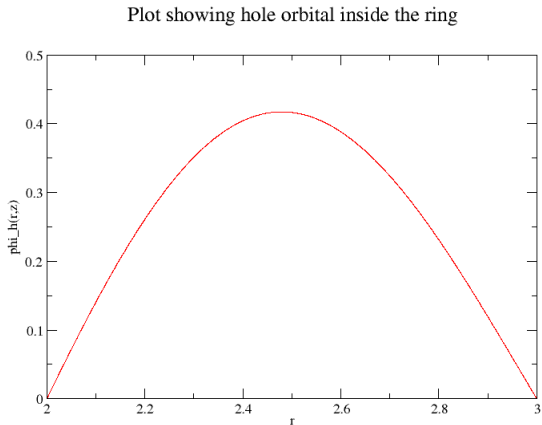


Figure 3: Plot showing hole orbital inside the ring.

Hole Orbitals - 4

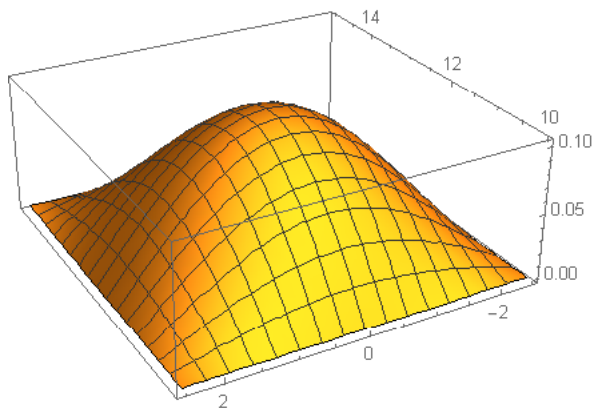


Figure 4: 3D plot of hole orbital inside ring region.

Jastrow Factor - 1

- Needs to describe correlation effects.

$$\Psi = e^J S(\phi_e, \phi_e),$$

where J is a Jastrow factor and S is a Slater determinant of the electron and hole orbitals.

Jastrow Factor - 2

- Jastrow factor takes account of:
 - 1 Electrostatic energy is lower if particles of same charge are not close together.
 - 2 Electrostatic energy is lower if particles of opposite charge are close together.
- Also needed are cusp conditions. These ensure any divergence in the potential energy (such as when one particle passes very close to another) is cancelled by the kinetic energy, so that the local energy does not diverge.

Jastrow Factor - 3

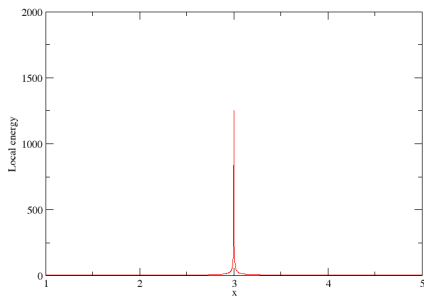
For position trion Jastrow factor is of the form

$$J = \frac{m_h r_{ab}}{2(1 + \alpha r_{ab})} - \frac{\mu_{eh} r_{1a} + \alpha r_{1a}^2}{1 + a' r_{1a}} - \frac{\mu_{eh} r_{1b} + b r_{1b}^2}{1 + b' r_{1b}}.$$

m_h is the effective hole mass, $\mu_{eh} = (m_h + m_e)/m_e m_h$ and m_e is the effective electron mass, r_{ij} is the distance between particles i and j with letters referring to holes and numbers to electrons. a, a', b, b' are variational constants.

Jastrow Factor - 4

Plot of local energy, biexciton, electron at $x=3$, without Jastrow factor



Plot of local energy, biexciton, electron at $x=3$, with Jastrow factor

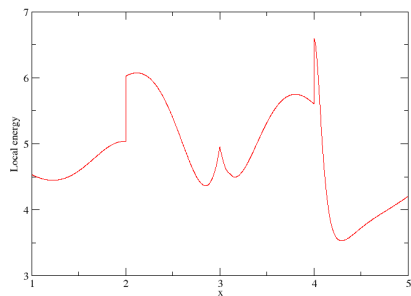


Figure 5: Plots showing local energy in a biexciton: left, without a Jastrow factor and right, with a Jastrow factor.

Implementation

- To create a modified version of CASINO, all the Jastrow factors and orbitals needed to be coded up.
- Gradients and Laplacians of each needed too.
- Numerical tests then carried out to ensure the gradients and Laplacians are accurate.
- Newton-Raphson procedure to evaluate parameter β in hole orbitals.
- These modules then integrated into CASINO².

²Integration into CASINO done by Neil Drummond.

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Testing - 1

- Gradients and Laplacians can also be testing on a long VMC.
- CASINO estimate the kinetic energies in multiple ways, involving the gradient and/or the Laplacians. So running VMC calculations and checking all these different estimations give the same result can also help show the gradient and Laplacians are correct.

Testing - 2

- Example: For biexction we have the different kinetic energy estimates³ as
 - $K = 15.084(7)$ a.u.
 - $T = 15.03(2)$ a.u.
 - $FISQ = 14.99(5)$ a.u.

³Energies in Hartree atomic units $\hbar = |e| = m_e = 4\pi\epsilon_0 = 1$.

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Calculations

- Use VMC and an optimisation algorithm to optimise wave function (lower the energy).
- Then use DMC and extrapolate to zero time step to obtain exact ground-state energy.

Time Step Bias - 1

- For sufficiently small time steps the dependence of the DMC energy is linearly dependent on time step.
- So run calculations in this linear regime then extrapolate to zero time step.
- Find linear regime by running over a wider range of time steps.

Time Step Bias - 2

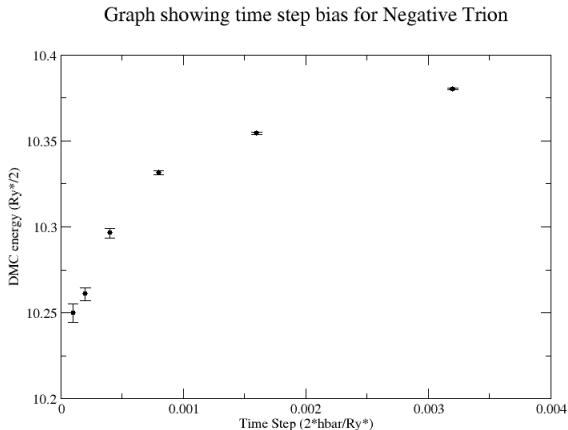


Figure 6: Graph showing time step bias for a negative trion.

DMC Calculations

- Run DMC calculations for all complexes for two different time steps in the linear regime.
- Extrapolate these results to zero time step to obtain exact ground-state energy of each system.

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Binding Energies - 1

- For a biexciton the binding energy E_b is defined to be

$$E_b = 2E_E - E_B,$$

where E_E the exciton energy and E_B is the biexciton energy.

- For our representative choice of ring⁴ the binding energy was found to be

$$E_b = -0.544(6)\text{Ry}^*$$

⁴A ring with inner radius 6nm, width in radial direction 2nm and height in z direction 2.5nm [2,3].

Binding Energies - 2

- For a negative trion in the representative ring geometry, the binding energy was calculated to be

$$E_b = 1.00(7)\text{Ry}^*$$

Dependence on Geometry

- Next step is to investigate these binding energies in a wide variety of different ring dimensions to investigate the dependence of the binding energy on these these parameters.
- Look at rings with the same volume, and vary aspect ratio or inner radius.

References

- [1] Needs R J, Towler M D, Drummond N D, López Riós P, 2010 *J. Phys.: Condens. Matter* **22** 023201
- [2] Young R J, Smakman E P, Sanchez A M, Hodgson P, Koenraad P M, Hayne M, 2012 *App. Phys. Lett.* **100** 082104
- [3] Hodgson P D, Hayne M, Robson A J, Zhuang Q D, Danos L, 2016 *J. Appl. Phys.* **119** 044305