Using the Coupled Cluster Singles and Doubles method to calculate many electron effects in 2D semiconductor structures

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The coupled cluster (CC) method has been shown to be a powerful tool when calculating many-body effects in nuclear, atomic and molecular physics. As other methods used in these areas of physics, the CC method can also be applied to atom-like 2D semiconductor structures. We have implemented the Coupled Cluster Singles and Double (CCSD) method and applied it to a 2D harmonic oscillator quantum dot to investigate the electronic many-body properties [1]. The implementation has proven to be accurate in comparison to previous Full Configuration Interaction and Quantum Monte Carlo calculations for up to twelve electrons and relative interaction strengths of up to at least $\lambda = 2$. Methods for extrapolating onto larger basis-sets have also been presented to enable more accurate results at a low cost.

We are capable of modeling systems of cylindrical symmetry, such as 2D dots, rings and concentric rings using a numerical B-spline basis. The exact shape of the radial potential can be chosen freely, so that hard walls, harmonic oscillators and Gaussian curves are all viable options to match the required system properties. In our early atempts, the program has been used to study concentric rings such as those conceived experimentally by Mano *et al.* [2]. For this we have used the material parameters for GaAs with the radial potential modeled using two superposed Gaussian curves. In Figure 1 the probability density of such a system, containing four electrons, can be seen. This configuration is completely spin polarized and contains one single electron in the outer ring, and the others in the inner. The program is currently being used to further study several interesting properties of this system, including correlation effect when shifting the inner/outer ring placements and interactions with external magnetic fields.

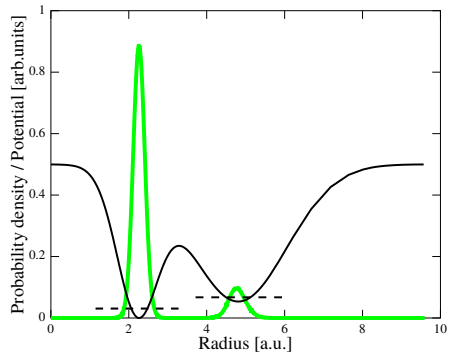

Figure 1: The probability density for concentric quantum rings. The black solid line indicates the shape of the potential in the radial dimension. The two dashed lines represent the energy levels of the states in the inner and outer ring in scale with the potential. Finally the green line is the normalized electron density for the four electrons.

[1] E. Waltersson, C. J. Wesslén, E. Lindroth, Phys. Rev. B **87**, 035112 (2013).
[2] T. Mano *et al.*, Nano Letters **5**, 425 (2005).