Exchange Interaction Calculation in Si-DQD

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Objective:

- Using NEMO 3-D, implement and investigate exchange splitting of 2-electron system of double dot system used for qubits
- Find out relationship between inter-dot distance and exchange splitting

Approaches:

- Use the spds* tight binding (TB) band model
- Potential is modeled as a quadratic function
- For initial cut, use Heitler-London approximation assuming that the coupling of the electron wavefunction is small
- Compare with other analytical result, such as HL and Hund-Mulliken(HM) approximation

Results and Impacts:

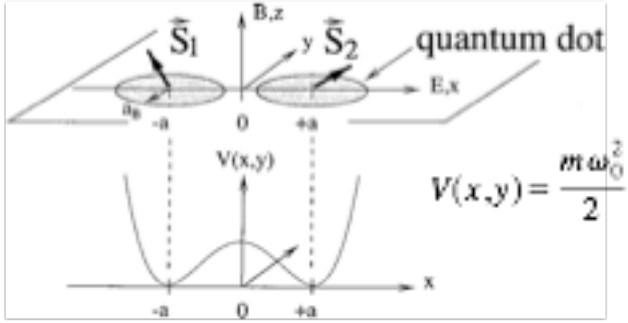
- Depending on the inter-dot distance, the exchange splitting exponentially decays
- Reasonable agreement with analytical solutions

Ongoing work:

- Scaling measurement on Jaguar
- Self-consistent simulation with Configuration Interaction (CI) calculation

Device geometry for simulation:

- Assumed 104.3x104.3x3.3nm3 Si structure (1.7MA) from (arxiv:0906.4793v2)



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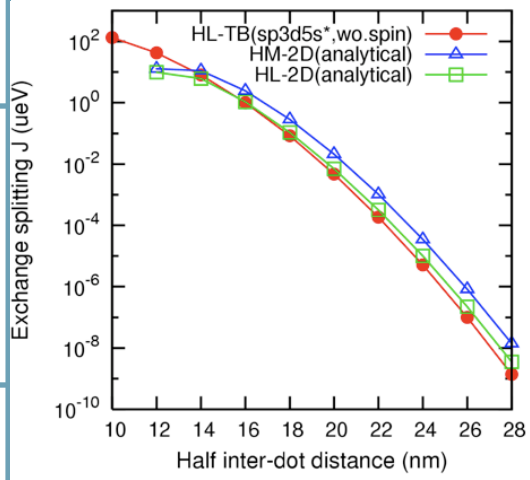
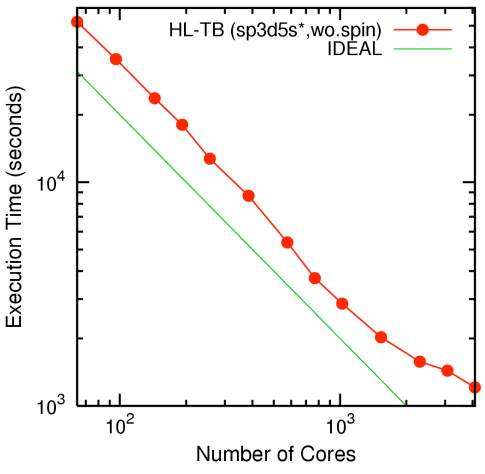
Results



Comparison with analytical results



Scaling test on Ranger@TACC

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