Quantum Many-Body Simulations of Double Dot System

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Introduction

Quantum-Dot

- Small semiconductor nanostructures
- 2-10 nanometers with $10-50$ particles

Quantum-Dot Model

- Schrödinger equation
    - $\mathscr{H}\left|\psi\right\rangle = E\left|\psi\right\rangle$

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Quantum-Dot Model

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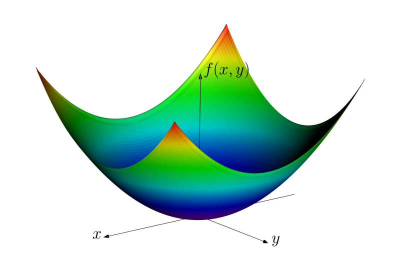
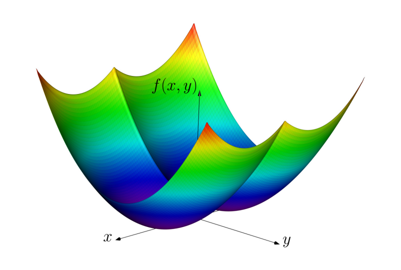
Quantum-Dot Model

- Interaction: Coulomb repulsion
  - $f\left(\boldsymbol{r}_i, \boldsymbol{r}_j\right) = \frac{1}{|\boldsymbol{r}_i - \boldsymbol{r}_j|}$
- Confinement: Harmonic Oscillator[1], Double-Well[2]

$$V(\boldsymbol{r}) = \frac{1}{2}\omega m r^2 \qquad V(\boldsymbol{R}, \boldsymbol{r}) = \frac{1}{2} m\omega^2 \left(r^2 - \delta R|x| + R^2\right)$$





[1] S. Kvaal. "Harmonic Oscillator Eigenfunction Expansions, Quantum dots, and Effective Interactions". In: *Phys. Rev. B* 80 (4 2009), p. 045321.

[2] M. J. A. Schuetz et al. "Nuclear Spin Dynamics in Double Quantum Dots: Multistability, Dynamical Polarization, Criticality, and Entanglement". In: *Phys. Rev. B* 89 (19 2014), p. 195310.

Quantum-Dot Model

#NucleiHaveFeelingsTo

Methods

Methods

Hartree-Fock

Variational Monte-Carlo

Methods: Variational Principle

$$E_0 \leq \frac{\langle \Psi | \mathscr{H} | \Psi \rangle}{\langle \Psi | \Psi \rangle}$$

Methods: Slater Determinant and Energy Functional

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  - $\Psi_T^{\mathsf{AS}} = \frac{1}{\sqrt{N!}} \sum_P (-1)^p \mathscr{P}_P \prod_i \psi_i$
  - $\Psi_T^{\mathsf{S}} = \sqrt{\frac{\prod_{i=1}^{N} n_i!}{N!}} \sum_P \mathscr{P}_P \prod_i \psi_i$

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- $E[\Psi] = \frac{\langle\Psi|\mathscr{H}|\Psi\rangle}{\langle\Psi|\Psi\rangle} = \sum_p \langle p|\mathscr{H}_0|p\rangle + \frac{1}{2}\sum_{p,q}\left[\langle pq|f_{12}|pq\rangle \pm \langle pq|f_{12}|qp\rangle\right]$
- $\mathscr{H}_0 = -\frac{1}{2}\sum_i \nabla_i^2 + V(r)$

Methods: Hartree-Fock

- Assumptions
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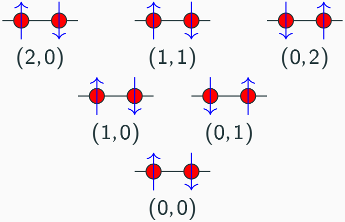

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  - Fock-operator: $\mathscr{F} \equiv \mathscr{H}_0 + \mathscr{J} \pm \mathscr{K}$
    - $\mathscr{J} \equiv \sum_k \langle \psi_k^* | f_{12} | \psi_k \rangle = \int \psi_k^*(\boldsymbol{r}) f_{12} \psi_k(\boldsymbol{r}) dr$
    - $\mathscr{K} \equiv \sum_k \langle \psi_k^* | f_{12} | \psi \rangle = \int \psi_k^*(\boldsymbol{r}) f_{12} \psi(\boldsymbol{r}) dr$
    - $\mathscr{F} | \psi \rangle = \boldsymbol{\varepsilon} | \psi \rangle, \boldsymbol{\varepsilon} = (\varepsilon_0, \ldots, \varepsilon_N)$

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    - $\mathscr{F} | \psi \rangle = \boldsymbol{\varepsilon} | \psi \rangle, \boldsymbol{\varepsilon} = (\varepsilon_0, \ldots, \varepsilon_N)$
  - $N + 1$ equations to be solved.

Methods: Hartree-Fock

- Integrate out spin
- Pair spins as: $\{\psi_{2l-1}, \psi_{2l}\} = \{\phi_l(\boldsymbol{r})\alpha(s), \phi_l(\boldsymbol{r})\beta(s)\}$

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- Expand: $\phi_i(\boldsymbol{r}) = \sum_{p=1}^{L} C_{pi}\chi_p(\boldsymbol{r})$
- Roothan-Hall: $\boldsymbol{F}\boldsymbol{C}_i = \boldsymbol{\varepsilon} S \boldsymbol{C}_i$
  - $F_{pq} = h_{pq} + \sum_{pq} \rho_{pq}\left(2D_{prqs} \pm D_{prsq}\right)$
  - $h_{pq} \equiv \langle p | h | q \rangle$
  - $\rho_{pq} \equiv \sum_{i=1}^{\frac{N}{2}} C_{pi} C_{qi}^{*}$
  - $D_{pqrs} \equiv \langle pq | f_{12} | rs \rangle$
  - $S_{pq} \equiv \langle p | q \rangle$
- Poople-Nesbet: $\boldsymbol{F}^{+}\boldsymbol{C}^{+} = \boldsymbol{\varepsilon}\boldsymbol{S}\boldsymbol{C}^{+}$, $\boldsymbol{F}^{-}\boldsymbol{C}^{-} = \boldsymbol{\varepsilon}^{-}\boldsymbol{S}\boldsymbol{C}^{-}$
  - $F_{pq}^{\pm} = h_{pq} + \sum_{k_{\pm}}\sum_{rs} C_{rk_{\pm}}^{\pm\dagger} C_{sk_{\pm}}^{\pm\dagger}\left[D_{prqs} - D_{prsq}\right] + \sum_{k_{\mp}}\sum_{rs} C_{rk_{\mp}}^{\mp\dagger} C_{sk_{\mp}}^{\mp\dagger} D_{prqs}$

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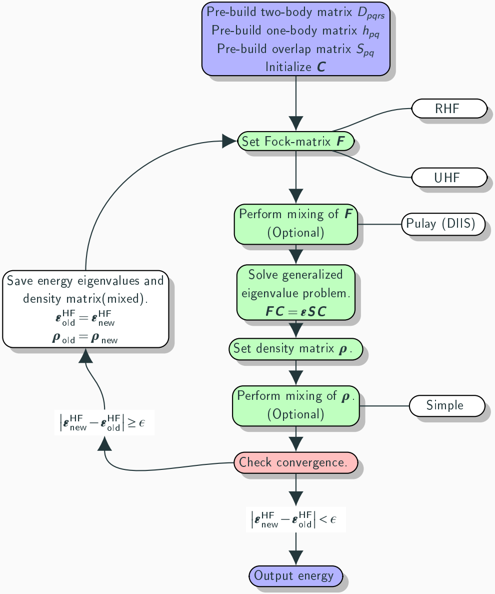

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- Rewrite expectation value: $\frac{\langle\Psi|\mathscr{H}|\Psi\rangle}{\langle\Psi|\Psi\rangle} = \int \frac{\Psi^*\mathscr{H}\Psi}{\int \Psi^*\Psi dr} dr = \int \frac{|\Psi|^2 E_L}{\int \Psi^*\Psi dr} dr$
  - $E_L(\boldsymbol{R};\boldsymbol{\alpha}) \equiv \frac{1}{\Psi}\mathscr{H}\Psi$
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  - $r^{\text{new}} = r^{\text{old}} + \Delta t\xi$
  - $A_{i\to j} = \min\left(\frac{P_{i\to j}}{P_{j\to i}}\frac{T_{i\to j}}{T_{j\to i}}, 1\right)$

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    - Importance Sampling
        - $r^{\text{new}} = r^{\text{old}} + D\Delta t F^{\text{old}} + \sqrt{\Delta t}\xi$
        - $F = \frac{2}{\Psi}\nabla\Psi$
        - $\frac{T(b,a,\Delta t)}{T(a,b,\Delta t)} = \sum_i \exp\left(-\frac{\left(\boldsymbol{r}_i^{(b)}-\boldsymbol{r}_i^{(a)}-D\Delta t\boldsymbol{F}_i^{(a)}\right)^2}{4D\Delta t} + \frac{\left(\boldsymbol{r}_i^{(a)}-\boldsymbol{r}_i^{(b)}-D\Delta t\boldsymbol{F}_i^{(b)}\right)^2}{4D\Delta t}\right)$

Implementation

Summary and Conclusion

Questions?

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