# Quantum Many-Body Simulations of Double Dot System

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# Contents

# Introduction

# Quantum-Dot

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

# Quantum-Dot Model

- Schrödinger equation
  - $H\,|\psi\rangle = E\,|\psi\rangle$

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  - $H\left|\psi\right\rangle = E\left|\psi\right\rangle$
- Hamiltonian
  - $H = -\frac{1}{2}\sum_{i}\nabla_i^2 + \sum_{i<j} f\left(\boldsymbol{r}_j, \boldsymbol{r}_j\right) - \frac{1}{2}\sum_{k}\frac{\nabla_k^2}{M_k} + \sum_{k<l} g\left(\boldsymbol{R}_k, \boldsymbol{R}_l\right) + V\left(\boldsymbol{R}, \boldsymbol{r}\right)$

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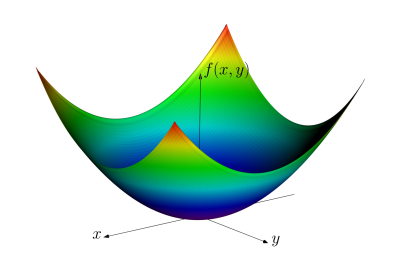
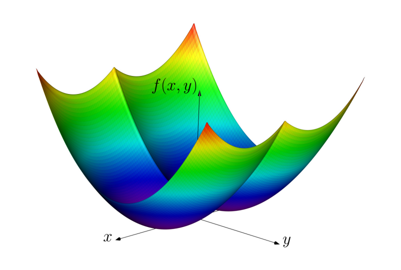
- Interaction: Coulomb repulsion
  - $f\left(\boldsymbol{r}_i, \boldsymbol{r}_j\right) = \frac{1}{\left|\boldsymbol{r}_i - \boldsymbol{r}_j\right|}$
- Confinement: Harmonic Oscillator[1], Double-Well[2]

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




[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.

# Methods

**Hartree-Fock**

**Variational Monte-Carlo**

# Methods: Variational Principle

$$E_0 \leq \frac{\langle \Psi \mid H \mid \Psi \rangle}{\langle \Psi \mid \Psi \rangle}$$

# Methods: Slater Determinant and Energy Functional

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- Slater Determinant
  - $\Psi_T^{\mathrm{AS}} = \frac{1}{\sqrt{N!}} \sum_P (-1)^p P_P \prod_i \psi_i$
  - $\Psi_T^{\mathrm{S}} = \sqrt{\frac{\prod_{i=1}^{N} n_i!}{N!}} \sum_P P_P \prod_i \psi_i$

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- $E[\Psi] = \frac{\langle \Psi \mid H \mid \Psi \rangle}{\langle \Psi \mid \Psi \rangle} = \sum_p \langle p| H_0 |p\rangle + \frac{1}{2} \sum_{p,q} [\langle pq| f_{12} |pq\rangle \pm \langle pq| f_{12} |qp\rangle]$
- $H_0 = -\frac{1}{2} \sum_i \nabla_i^2 + V(r)$

# Methods: Hartree-Fock

- Assumptions
  - The Born-Oppenheimer approximation holds.
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  - The wavefunction can be described by a single *Slater determinant*.
  - The Mean Field Approximation holds.

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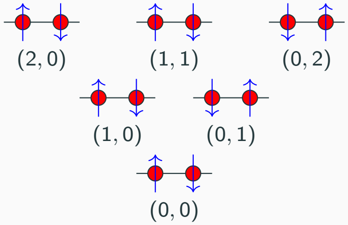

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  - Fock-operator: $F \equiv H_0 + J \pm K$
    - $J \equiv \left\langle \psi_k^* \right| f_{12} \left| \psi_k \right\rangle = \int \psi_k^*(\boldsymbol{r}) f_{12} \psi_k(\boldsymbol{r}) dr$
    - $K \equiv \left\langle \psi_k^* \right| f_{12} \left| \psi \right\rangle = \int \psi_k^*(\boldsymbol{r}) f_{12} \psi(\boldsymbol{r}) dr$
    - $F \left| \psi \right\rangle = \boldsymbol{\varepsilon} \left| \psi \right\rangle, \boldsymbol{\varepsilon} = (\varepsilon_0, \dots, \varepsilon_N)$

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    - $F\left|\psi\right\rangle = \boldsymbol{\varepsilon}\left|\psi\right\rangle, \boldsymbol{\varepsilon} = (\varepsilon_0, \ldots, \varepsilon_N)$
  - $N + 1$ 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: $\boldsymbol{F}\boldsymbol{C}_i = \varepsilon S \boldsymbol{C}_i$
  - $F_{pq} = h_{pq} + \sum_{pq} \rho_{pq} \left(2D_{prqs} \pm D_{prsq}\right)$
  - $h_{pq} \equiv \langle p \,|\, h \,|\, q \rangle$
  - $\rho_{pq} \equiv \sum_{i=1}^{\frac{N}{2}} C_{pi} C_{qi}^*$
  - $D_{pqrs} \equiv \langle pq \,|\, f_{12} \,|\, rs \rangle$
  - $S_{pq} \equiv \langle p \,|\, q \rangle$
- Poople-Nesbet: $\boldsymbol{F}^+\boldsymbol{C}^+ = \varepsilon \boldsymbol{S}\boldsymbol{C}^+$, $\boldsymbol{F}^-\boldsymbol{C}^- = \varepsilon^- \boldsymbol{S}\boldsymbol{C}^-$
  - $F_{pq}^{\pm} = h_{pq} + \sum_{k_\pm} \sum_{rs} C_{rk_\pm}^{\pm\dagger} C_{sk_\pm}^{\pm\dagger} \left[D_{prqs} - D_{prsq}\right] + \sum_{k_\mp} \sum_{rs} C_{rk_\mp}^{\mp\dagger} C_{sk_\mp}^{\mp\dagger} D_{prqs}$

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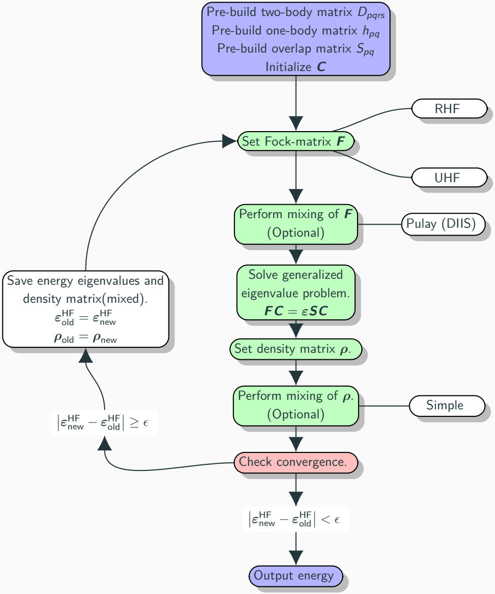

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    - $r^{\text{new}} = r^{\text{old}} + \Delta t \xi$
    - $A_{i \to j} = \min\left( \frac{P_{i \to j}}{P_{j \to i}} \frac{T_{i \to j}}{T_{j \to i}}, 1 \right)$

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

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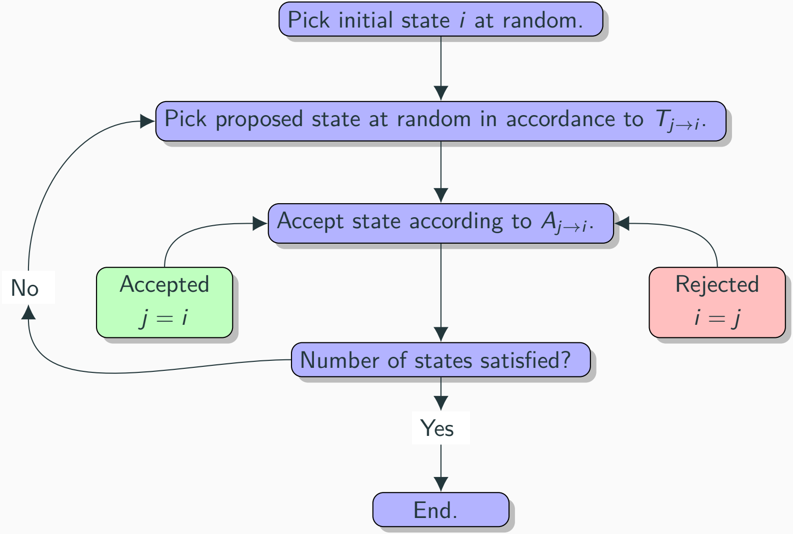

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# Wavefunction: Integral Elements

$$\langle \phi_i(\boldsymbol{r}) \,|\, \phi_j(\boldsymbol{r}) \rangle$$

$$\left\langle \phi_i(\boldsymbol{r}) \,\middle|\, x_d^k \,\middle|\, \phi_j(\boldsymbol{r}) \right\rangle$$

$$\left\langle \phi_i(\boldsymbol{r}) \,\middle|\, \nabla^2 \,\middle|\, \phi_j(\boldsymbol{r}) \right\rangle$$

$$\langle \phi_i(\boldsymbol{r}_1)\phi_j(\boldsymbol{r}_2) \,|\, f_{12} \,|\, \phi_k(\boldsymbol{r}_1)\phi_l(\boldsymbol{r}_2) \rangle$$

# Wavefunction: Single-Well

- Hermite Function: $\psi_n(\boldsymbol{r}) \equiv \prod_d N_d H_{n_d}(\sqrt{\omega}x_d)\exp\left(-\frac{\omega}{2}x_d^2\right)$

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- $\psi_n(\boldsymbol{r}) = \prod_d N_d \sum_{l=1}^{n_d} C_{n_d l}^{\text{Hermite}} g_l\left(\frac{\omega}{2}, \boldsymbol{r}, \boldsymbol{0}\right)$

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- Solution in Cartesian[6]

$$\langle g_i(\boldsymbol{r}) \,|\, g_j(\boldsymbol{r})\rangle$$

$$\left\langle g_i(\boldsymbol{r}) \,\middle|\, x_d^k \,\middle|\, g_j(\boldsymbol{r})\right\rangle$$

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[5] E. Anisimovas and A. Matulis. "Energy spectra of few-electron quantum dots". In: *Journal of Physics: Condensed Matter* (1998).

[6] J. Olsen T. Helgaker P. Jørgensen. *Molecular Electronic-Structure Theory*. Wiley, 2014. isbn: 978-0-47-196755-2. doi: 10.1002/9781119019572.

# Wavefunction: Single-Well Integral Elements

$$\left\langle \psi_i^{\mathrm{HO}} \middle| \psi_j^{\mathrm{HO}} \right\rangle = N_i \delta_{ij}$$

$$\left\langle \psi_i^{\mathrm{HO}} \middle| h^{\mathrm{HO}} \middle| \psi_j^{\mathrm{HO}} \right\rangle = N_i \varepsilon_i^{\mathrm{HO}} \delta_{ij}$$

$$\left\langle \psi_i^{\mathrm{HO}} \psi_j^{\mathrm{HO}} \middle| \tfrac{1}{r_{12}} \middle| \psi_k^{\mathrm{HO}} \psi_l^{\mathrm{HO}} \right\rangle = \tfrac{a N_{ijkl}}{\sqrt{2\omega}} \sum_{tuvw}^{ijkl} H_{tuvw}^{ijkl} \sum_{pq}^{t+v,u+w} E_p^{tv} E_q^{uw} (-1)^q \xi_{p+q} \left( \tfrac{\omega}{2}, \mathbf{0} \right)$$

$$E_t^{i+1,j} = \frac{1}{2(\alpha+\beta)} E_{t-1}^{ij} - \frac{\beta}{\alpha+\beta}(A_x - B_x) E_t^{ij} + (t+1) E_{t+1}^{ij}$$

$$E_t^{i,j+1} = \frac{1}{2(\alpha+\beta)} E_{t-1}^{ij} - \frac{\alpha}{\alpha+\beta}(A_y - B_y) E_t^{ij} + (t+1) E_{t+1}^{ij}$$

$$E_0^{00} = K_{AB}$$

$$\xi_{t+1,u}^n = t\xi_{t-1,u}^{n+1} + X_{AB}\xi_{t,u}^{n+1}$$

$$\xi_{t,u+1}^n = u\xi_{t,u-1}^{n+1} + Y_{AB}\xi_{t,u}^{n+1}$$

$$\xi_{00}^n = \left( \frac{-2\alpha\beta}{\alpha+\beta} \right)^n \zeta_n \left( \frac{\alpha\beta}{\alpha+\beta} R_{AB}^2 \right)$$

$$\zeta_n(x) = \int_{-1}^{1} \frac{u^{2n}}{\sqrt{1-u^2}} e^{-u^2 x} du$$

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# Wavefunction: Double-Well

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- Eigenvalue equation: $\boldsymbol{H}^{\mathrm{DW}} \boldsymbol{C}^{\mathrm{DW}} = \boldsymbol{\varepsilon}^{\mathrm{DW}} \boldsymbol{C}^{\mathrm{DW}}$
    - $H_{ij}^{\mathrm{DW}} = \varepsilon_i^{\mathrm{HO}} \delta_{ij} + \left\langle \psi_i^{\mathrm{HO}} \middle| V_n^{\mathrm{DW}} \middle| \psi_j^{\mathrm{HO}} \right\rangle$

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$$\left\langle \psi_p^{\mathrm{DW}} \middle| \psi_q^{\mathrm{DW}} \right\rangle = \delta_{pq}$$

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- NQS: $J_{\text{NQS}} = e^{-\sum_{i=1}^{N}\frac{(r_i-a_i)^2}{2\sigma^2}}\prod_j^M\left(1+e^{b_j+\sum_{i=1}^{N}\sum_{d=1}^{D}\frac{x_i^{(d)}w_{i+d,j}}{\sigma^2}}\right)$

# Wavefunction: Slater-Jastrow

- Slater determinant: $\psi_T = \det(\boldsymbol{\Phi}(\boldsymbol{R};\boldsymbol{\alpha}))\xi(s)$
- Modified Hermite: $\Phi_{ij} = \psi^{\text{HO}}_{n_j}(\sqrt{\alpha\omega}r_i) = \prod_d N_d H_{n_d}(\sqrt{\alpha\omega}x_d)e^{-\frac{\alpha\omega}{2}x_d^2}$
- Hartree-Fock: $\Phi_{ij} = \sum_l C_{jl}\psi^{\text{HO}}_{n_l}(\sqrt{\omega}r_i)$
- Modified Hartree-Fock: $\Phi_{ij} = \sum_l C_{jl}\psi^{\text{HO}}_{n_l}(\sqrt{\alpha\omega}r_i)$
- Padé-Jastrow: $J_{\text{Padé}} = \prod_{i<j} e^{\frac{a_{ij}r_{ij}}{1+\beta r_{ij}}}$
- NQS: $J_{\text{NQS}} = e^{-\sum_{i=1}^{N}\frac{(r_i-a_i)^2}{2\sigma^2}}\prod_j^M\left(1+e^{b_j+\sum_{i=1}^{N}\sum_{d=1}^{D}\frac{x_i^{(d)}w_{i+d,j}}{\sigma^2}}\right)$
- Padé-NQS: $J = J_{\text{Padé}}J_{\text{NQS}}$

# Implementation

# Summary and Conclusion

**Questions?**

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