Quantum Many-Body Simulations of Double Dot System

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Contents

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Quantum-Dot

- Small semiconductor nanostructures

Quantum-Dot Model

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

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

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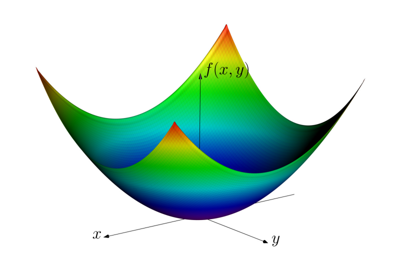
Quantum-Dot Model

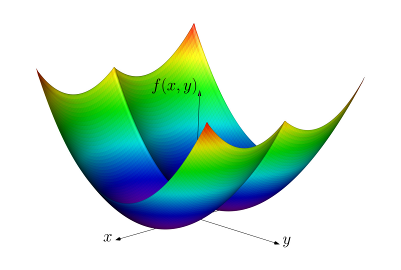
- Interaction
  - $f\left(\boldsymbol{r}_i, \boldsymbol{r}_j\right) = \frac{1}{\left|\boldsymbol{r}_i - \boldsymbol{r}_j\right|}$

Quantum-Dot Model

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

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





[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

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

Methods: Slater Determinant and Energy Functional

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

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

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  - The Born-Oppenheimer approximation holds.
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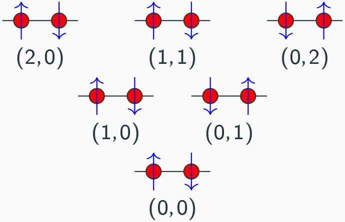

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  - Fock-operator: $\mathscr{F} \equiv \mathscr{H}_0 + \mathscr{J} \pm \mathscr{K}$
    - $\mathscr{J} \equiv \langle \psi_k^* | f_{12} | \psi_k \rangle = \int \psi_k^*(\boldsymbol{r}) f_{12} \psi_k(\boldsymbol{r}) dr$
    - $\mathscr{K} \equiv \langle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

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- Roothan-Hall: $\boldsymbol{F}\boldsymbol{C}_i = \boldsymbol{\varepsilon}S\boldsymbol{C}_i$
    - $F_{pq} = h_{pq} + \sum_{pq} \rho_{pq}\left(2D_{prqs} \pm D_{prsq}\right)$
    - $h_{pq} \equiv \langle p|h|q\rangle$
    - $\rho_{pq} \equiv \sum_{i=1}^{\frac{N}{2}} C_{pi}C^*_{qi}$
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  - $S_{pq} \equiv \langle p|q\rangle$
- 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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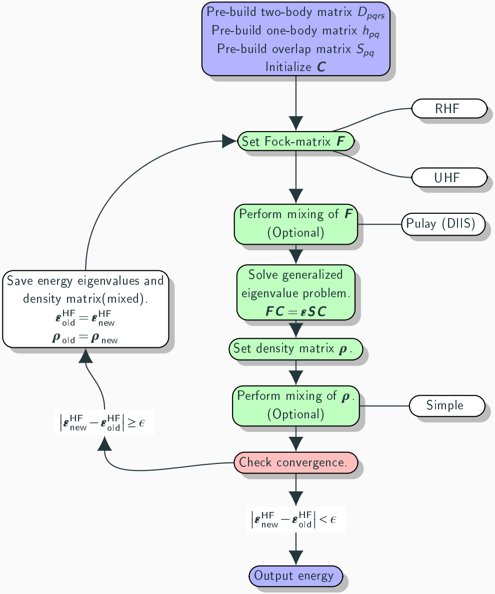

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  - $E_L(\boldsymbol{R}; \boldsymbol{\alpha}) \equiv \frac{1}{\Psi} \mathscr{H} \Psi$
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    - $E_L(\boldsymbol{R};\boldsymbol{\alpha}) \equiv \frac{1}{\Psi}\mathscr{H}\Psi$
    - $P(\boldsymbol{R}) \equiv \frac{|\psi_T|^2}{\langle\Psi_T|\Psi_T\rangle}$
- Metropolis-Hastings Algorithm
    - $r^{\text{new}} = r^{\text{old}} + \Delta t\xi$
    - $A_{i\to j} = \min\left(\frac{P_{i\to j}}{P_{j\to i}}\frac{T_{i\to j}}{T_{j\to i}}, 1\right)$

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

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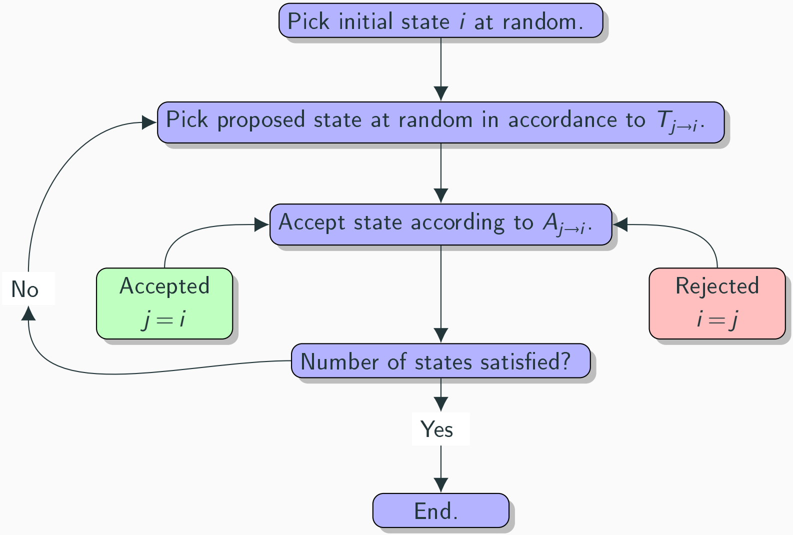

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Wavefunction: Integral Elements

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

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

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

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

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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- Solution in polar[3]

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- Solution in polar[4]
- $\psi_n(\boldsymbol{r}) = \prod_d N_d \sum_{l=1}^{n_d} C_{n_d l}^{\text{Hermite}} g_l\left(\frac{\omega}{2}, \boldsymbol{r}, \mathbf{0}\right)$

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- Hermite Function: $\psi_n(\boldsymbol{r}) \equiv \prod_d N_d H_{n_d}(\sqrt{\omega} x_d) \exp\left(-\frac{\omega}{2} x_d^2\right)$
- Solution in polar[5]
- $\psi_n(\boldsymbol{r}) = \prod_d N_d \sum_{l=1}^{n_d} C_{n_d l}^{\text{Hermite}} g_l\left(\frac{\omega}{2}, \boldsymbol{r}, \boldsymbol{0}\right)$
- Solution in Cartesian[6]

$$\left\langle g_i(\boldsymbol{r}) \middle| g_j(\boldsymbol{r}) \right\rangle$$
$$\left\langle g_i(\boldsymbol{r}) \middle| x_d^k \middle| g_j(\boldsymbol{r}) \right\rangle$$
$$\left\langle g_i(\boldsymbol{r}) \middle| \nabla^2 \middle| g_j(\boldsymbol{r}) \right\rangle$$
$$\left\langle g_i(\boldsymbol{r}_1) g_j(\boldsymbol{r}_2) \middle| f_{12} \middle| g_k(\boldsymbol{r}_1) g_l(\boldsymbol{r}_2) \right\rangle$$

[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

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

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

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

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

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

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

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

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

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

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

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

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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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- Integral-Elements

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

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$$\left\langle \psi_p^{\mathrm{DW}} \psi_q^{\mathrm{DW}} \middle| \frac{1}{r_{12}} \middle| \psi_r^{\mathrm{DW}} \psi_s^{\mathrm{DW}} \right\rangle = \sum_{tuvw}^{ijkl} C_{tp}^{\mathrm{DW}} C_{uq}^{\mathrm{DW}} C_{vr}^{\mathrm{DW}} C_{ws}^{\mathrm{DW}} \left\langle \psi_t^{\mathrm{HO}} \psi_u^{\mathrm{HO}} \middle| \frac{1}{r_{12}} \middle| \psi_v^{\mathrm{HO}} \psi_w^{\mathrm{HO}} \right\rangle$$

Wavefunction: Slater-Jastrow

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- Padé-Jastrow: $J_{\text{Padé}} = \prod_{i<j} e^{\frac{a_{ij}r_{ij}}{1+\beta r_{ij}}}$

Wavefunction: Slater-Jastrow

- Slater determinant: $\psi_T = \det(\mathbf{\Phi}(\boldsymbol{R};\boldsymbol{\alpha}))\xi(s)$
- 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: $\Phi_{ij} = \sum_l C_{jl} \psi^{\text{HO}}_{n_l}(\sqrt{\omega} r_i)$
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- Padé-Jastrow: $J_{\text{Padé}} = \prod_{i<j} e^{\frac{a_{ij} r_{ij}}{1+\beta r_{ij}}}$
- NQS: $J_{\text{NQS}} = e^{-\sum_{i=1}^{N} \frac{(\boldsymbol{r}_i - \boldsymbol{a}_i)^2}{2\sigma^2}} \prod_j^M \left(1 + e^{b_j + \sum_{i=1}^{N} \sum_{d=1}^{D} \frac{x_i^{(d)} w_{i+d,j}}{\sigma^2}}\right)$

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Implementation

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- C++ and Eigen

Implementation

- C++ and Eigen
  - Performance

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  - Performance
  - Generalization

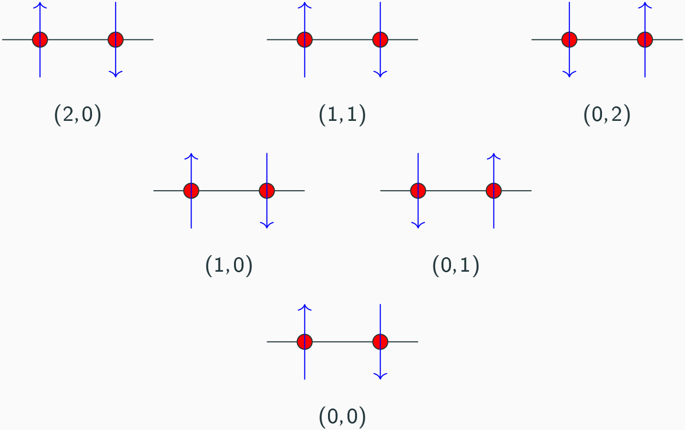
Implementation

- C++ and Eigen
    - Performance
    - Generalization
- Python

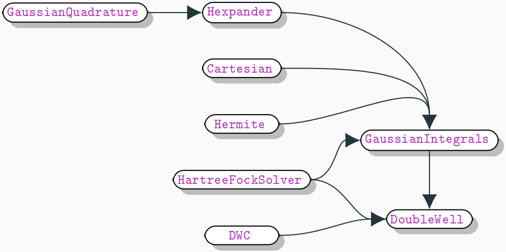
Implementation

- C++ and Eigen
  - Performance
  - Generalization
- Python
  - Generate C++ code

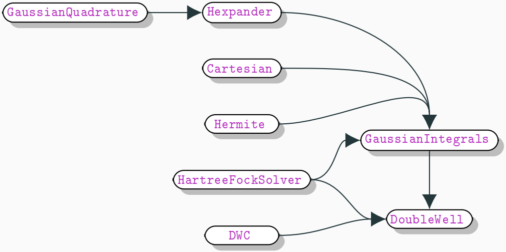
Implementation: Cartesian



Implementation: Hartree-Fock

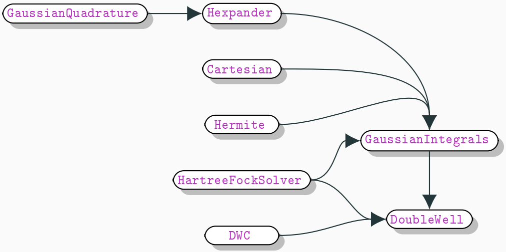


Implementation: Hartree-Fock



- Parallelization
    - Two-body element is computationally expensive
    - $S_i = \sum_{j=0}^{P_i} \prod_d (n_{j_d} + 1)$

Implementation: Hartree-Fock



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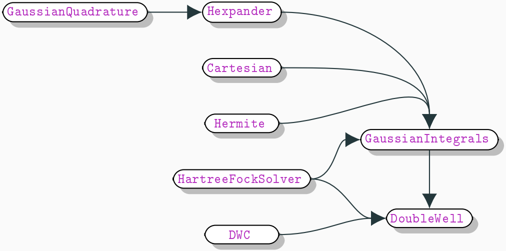
Implementation: Hartree-Fock



- Parallelization
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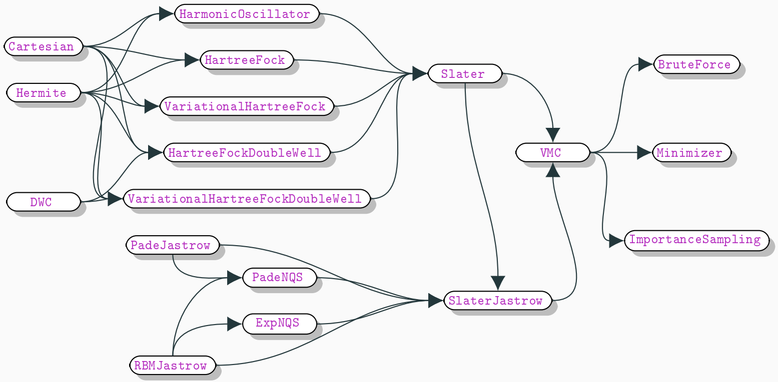
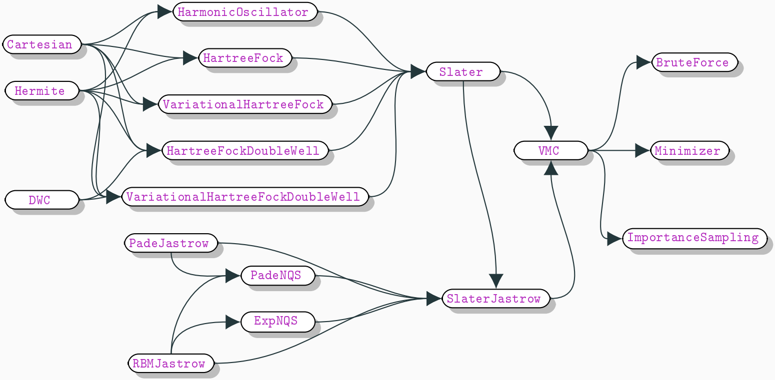
    - $S_i = \sum_{j=0}^{P_i} \prod_{d} (n_{j_d} + 1)$
- Hartree-Fock algorithm only run on one process
- Tabulation of Two-Body matrix

Implementation: Variational Monte-Carlo



Implementation: Variational Monte-Carlo

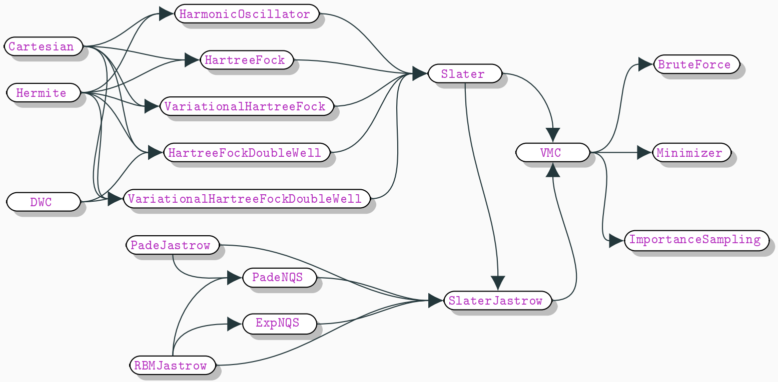


- `Hermite` generated with Python and SymPy

Implementation: Variational Monte-Carlo

- `set`: Called during initialization (before each sampling)
- `reSetAll`: Sets all matrices to zero (used in testing)
- `initializeMatrices`: Allocate memory
- `update`: Update positions and wavefunction
- `reset`: Revert to previous positions and wavefunction
- `resetGradient`: Revert to previous gradient
- `acceptState`: Update previous positions and wavefunction to current
- `acceptGradient`: Update previous gradient to current one

Implementation: Variational Monte-Carlo



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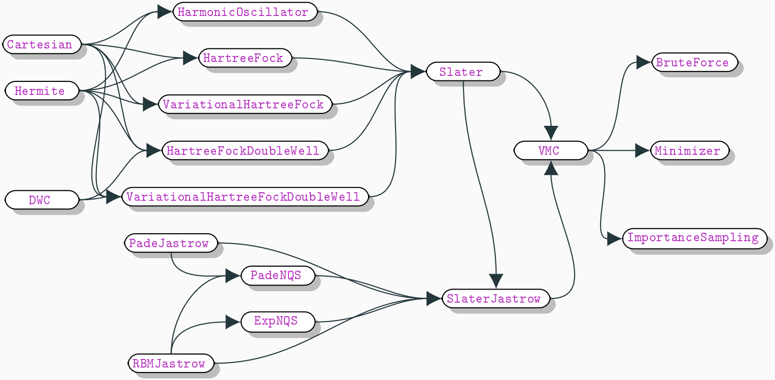

- Hermite generated with Python and SymPy
- Wavefunction class can be created with Python

Results

Results: Benchmark

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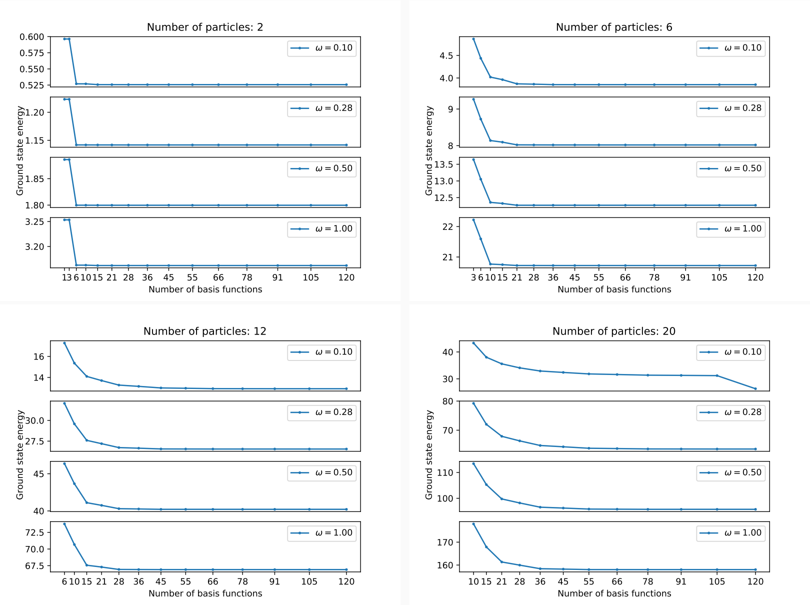
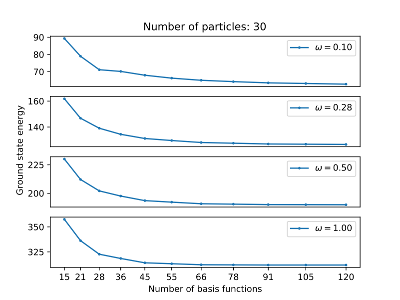
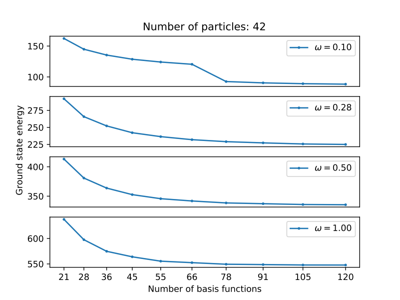
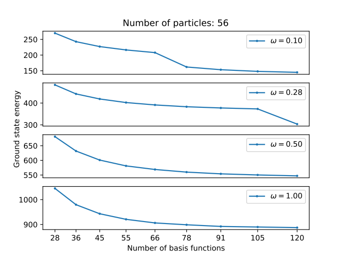


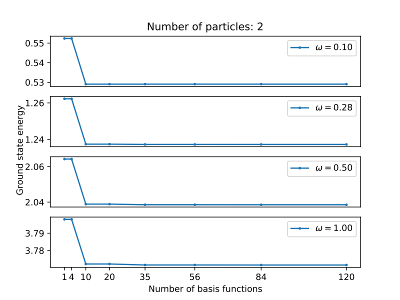
Results: Benchmark

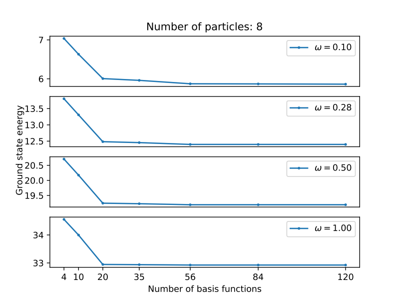


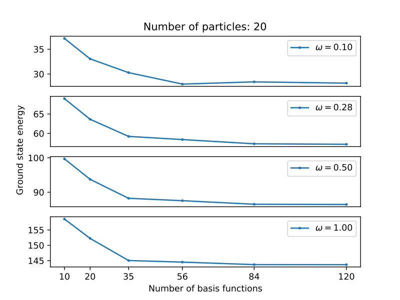


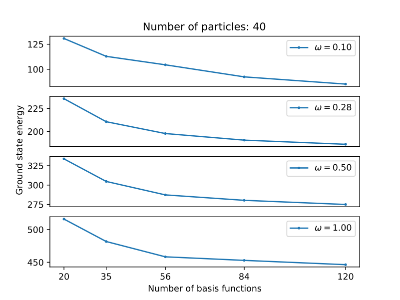


Results: Benchmark









Results: Benchmark

ω[a.u]	N			
	2	6	12	20
0.1	0.4407(4)	3.5650(4)	12.3164(4)	30.0480(4)
0.28	1.0020(4)	7.6198(4)	25.5948(3)	61.8090(3)
0.5	1.6650(4)	11.8017(4)	39.3166(3)	93.9240(2)
1.0	3.0000(5)	20.2863(3)	68.1465(3)	156.2778(2)

ω[a.u]	N	
	2	8
0.1	0.50006(5)	5.80479(4)
0.28	1.20156(5)	12.48178(4)
0.5	2.00027(5)	19.33356(4)
1.0	3.72985(5)	33.30958(4)

$$\psi = \psi^{\mathrm{HO}}\left(\sqrt{\alpha\omega}\right) J_{\mathrm{Padé}}$$

Results: Benchmark

ω[a.u]	N			
	2	6	12	20
0.1	0.46552(5){15}	3.70137(4){36}	12.64342(4){91}	-
0.28	1.04939(4){6}	7.89627(4){36}	26.21301(4){66}	62.93503(5){120}
0.5	1.70130(4){6}	12.02776(4){21}	39.76442(3){45}	95.21976(3){91}
1.0	3.05625(4){6}	20.45876(3){36}	66.37115(3){45}	157.41119(3){78}

ω[a.u]	N			
	2	6	12	20
0.10	0.44473(5){15}	3.63897(4){36}	12.46408(4){91}	—
0.28	1.04978(4){6}	7.72929(4){36}	25.96595(4){66}	62.65652(3){120}
0.50	1.66418(4){6}	11.97781(4){21}	39.57182(3){45}	94.76303(3){91}
1.00	3.00624(4){6}	20.38811(3){36}	66.28996(3){45}	157.46167(3){78}

$$\psi_p = \sum_l C_{lp} \psi_l^{\mathrm{HO}}\left(\sqrt{\omega} r\right) J_{\text{Padé}}, \qquad \psi_p = \sum_l C_{lp} \psi_l^{\mathrm{HO}}\left(\sqrt{\alpha\omega} r\right) J_{\text{Padé}}$$

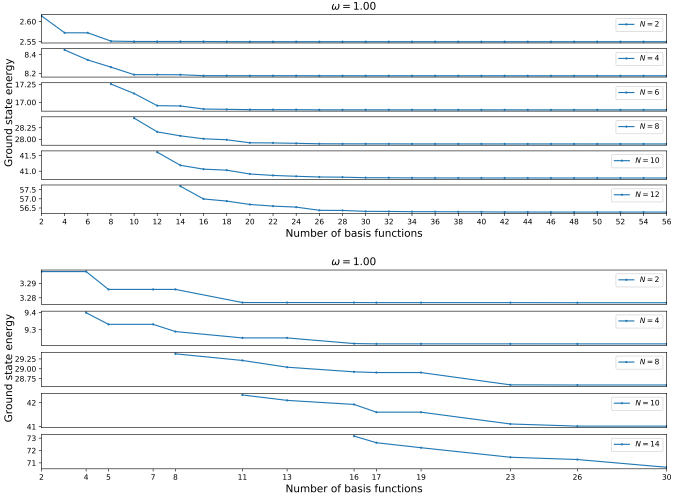
Results: Benchmark

ω	N	
	2	8
0.1	0.51122(5){70}	5.87372(4){120}
0.28	1.21844(5){70}	12.36177(4){168}
0.5	2.02030(4){20}	19.15006(4){112}
1.0	3.72918(5){20}	33.58046(4){168}

ω	N	
	2	8
0.1	0.50751(5){70}	5.84082(4){240}
0.28	1.20320(5){20}	12.37435(4){168}
0.5	2.01439(4){20}	19.09917(4){112}
1.0	3.72959(5){70}	33.04162(4){168}

$$\psi_p = \sum_l C_{lp} \psi_l^{\mathrm{HO}} \left(\sqrt{\omega} r\right) J_{\mathrm{Padé}}, \qquad \psi_p = \sum_l C_{lp} \psi_l^{\mathrm{HO}} \left(\sqrt{\alpha\omega} r\right) J_{\mathrm{Padé}}$$

Results: Double-Well Hartree-Fock



Results: Double-Well Variational Monte-Carlo

ω	N			
	2	4	6	8
1.0	2.42238(4){10}	7.95247(4){42}	16.61419(4){44}	27.54453(3){50}

$$\psi_p = \sum_l C_{lp}^{\mathrm{HF}} \sum_k C_{kl}^{\mathrm{DW}} \psi_k^{\mathrm{HO}} \left(\sqrt{\omega} r\right) J_{\text{Padé}}$$

ω	N			
	2	4	6	8
1.0	2.36618(4){10}	7.90232(4){42}	16.55609(4){44}	27.58524(4){50}

$$\psi_p = \sum_l C_{lp}^{\mathrm{HF}} \sum_k C_{kl}^{\mathrm{DW}} \psi_k^{\mathrm{HO}} \left(\sqrt{\alpha\omega} r\right) J_{\text{Padé}}$$

Results: Double-Well Variational Monte-Carlo

ω	N		
	2	4	8
1.0	3.25118(4){11}	9.17489(4){17}	28.49671(4){26}

$$\psi_p = \sum_l C^{\mathrm{HF}}_{lp} \sum_k C^{\mathrm{DW}}_{kl} \psi^{\mathrm{HO}}_k \left(\sqrt{\omega} r\right) J_{\text{Padé}}$$

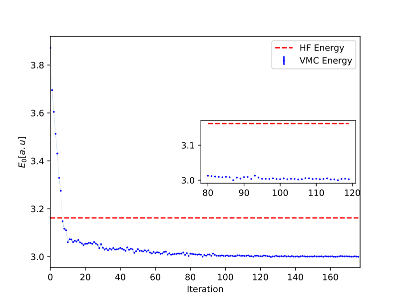
ω	N		
	2	4	8
1.0	3.22226(4){11}	9.17013(4){17}	28.62826(4){26}

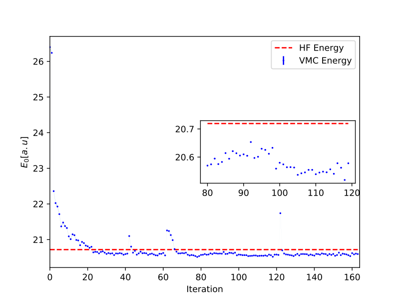
$$\psi_p = \sum_l C^{\mathrm{HF}}_{lp} \sum_k C^{\mathrm{DW}}_{kl} \psi^{\mathrm{HO}}_k \left(\sqrt{\alpha\omega} r\right) J_{\text{Padé}}$$

Results: NQS-Jastrow

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

Results: NQS-Jastrow Harmonic Oscillator





Summary and Conclusion

Questions?

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