Quantum Many-Body Simulations of Double Dot System

Alocias Mariadason

Contents

Introduction

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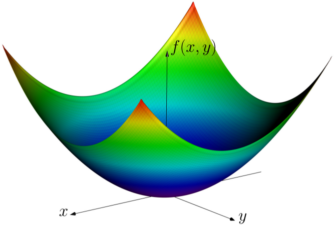
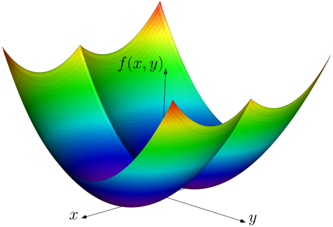
- Interaction:
  - $f(\boldsymbol{r}_i, \boldsymbol{r}_j) = \frac{1}{|\boldsymbol{r}_i - \boldsymbol{r}_j|}$, Coulomb Repulsion
- Confinement: Harmonic Oscillator[1], Double-Well[2]

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





[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

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

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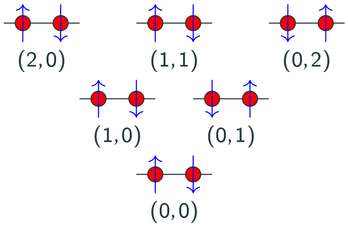

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  - Fock-operator: $\mathscr{F} \equiv \mathscr{H}_0 + \mathscr{J} \pm \mathscr{K}$
    - $\mathscr{J} \equiv \langle\psi_k^*|\, f_{12}\, |\psi_k\rangle = \int \psi_k^*(\boldsymbol{r}) f_{12} \psi_k(\boldsymbol{r}) dr$
    - $\mathscr{K} \equiv \langle\psi_k^*|\,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

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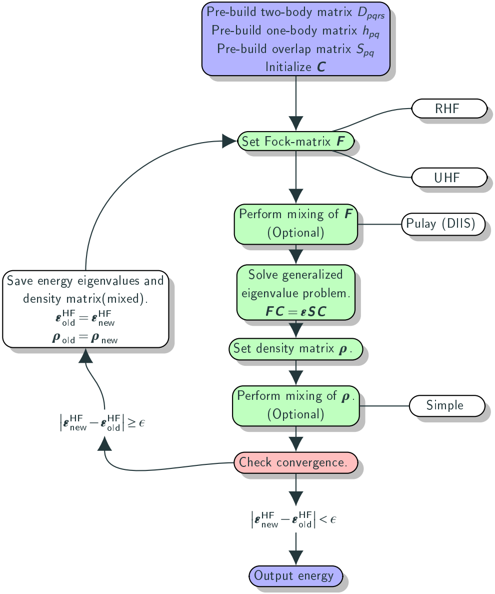
- Poople-Nesbet: $\boldsymbol{F}^+\boldsymbol{C}^+ = \boldsymbol{\varepsilon}\boldsymbol{S}\boldsymbol{C}^+$, $\boldsymbol{F}^-\boldsymbol{C}^- = \boldsymbol{\varepsilon}^-\boldsymbol{S}\boldsymbol{C}^-$
  - $F_{pq}^{\pm} = h_{pq} + \sum_{k_\pm}\sum_{rs} C_{rk_\pm}^{\pm\dagger} C_{sk_\pm}^{\pm\dagger}\left[D_{prqs}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


Pre-build two-body matrix D_{pqrs}
Pre-build one-body matrix h_{pq}
Pre-build overlap matrix S_{pq}
Initialize $\boldsymbol{C}$
Set Fock-matrix $\boldsymbol{F}$
RHF
UHF
Perform mixing of $\boldsymbol{F}$ (Optional)
Pulay (DIIS)
Solve generalized eigenvalue problem. $\boldsymbol{FC} = \boldsymbol{\varepsilon SC}$
Set density matrix $\boldsymbol{\rho}$.
Perform mixing of $\boldsymbol{\rho}$. (Optional)
Simple
Check convergence.
$\left|\boldsymbol{\varepsilon}^{\mathrm{HF}}_{\mathrm{new}} - \boldsymbol{\varepsilon}^{\mathrm{HF}}_{\mathrm{old}}\right| < \epsilon$
Output energy
$\left|\boldsymbol{\varepsilon}^{\mathrm{HF}}_{\mathrm{new}} - \boldsymbol{\varepsilon}^{\mathrm{HF}}_{\mathrm{old}}\right| \geq \epsilon$
Save energy eigenvalues and density matrix(mixed). $\boldsymbol{\varepsilon}^{\mathrm{HF}}_{\mathrm{old}} = \boldsymbol{\varepsilon}^{\mathrm{HF}}_{\mathrm{new}}$ $\boldsymbol{\rho}_{\mathrm{old}} = \boldsymbol{\rho}_{\mathrm{new}}$

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  - $E_L(\boldsymbol{R};\boldsymbol{\alpha}) \equiv \frac{1}{\Psi}\mathscr{H}\Psi$
  - $P(\boldsymbol{R}) \equiv \frac{|\Psi|^2}{\langle\Psi|\Psi\rangle}$

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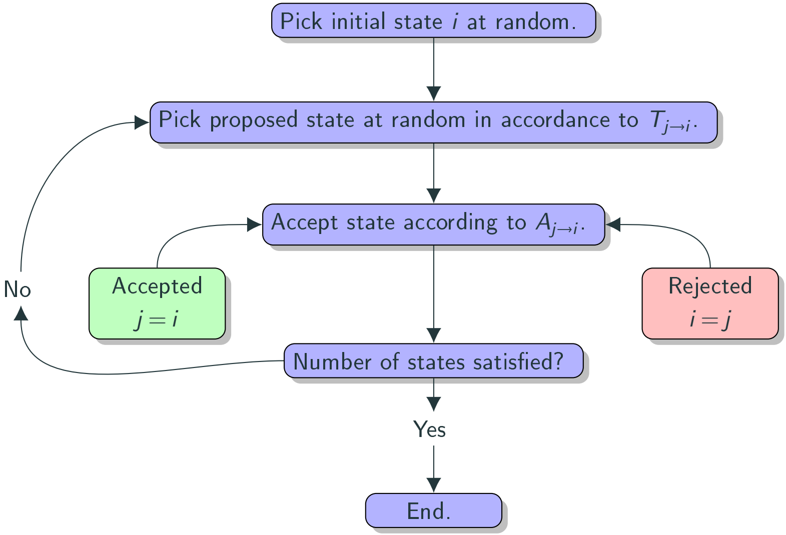
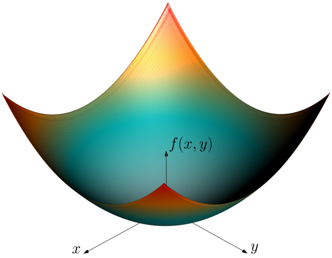
  - Importance Sampling
    - $r^{\text{new}} = r^{\text{old}} + D\Delta t F^{\text{old}} + \sqrt{\Delta t}\xi$
    - $F = \frac{2}{\Psi}\nabla\Psi$
    - $\frac{T(b,a,\Delta t)}{T(a,b,\Delta t)} = \sum_i \exp\left(-\frac{\left(\boldsymbol{r}_i^{(b)}-\boldsymbol{r}_i^{(a)}-D\Delta t\boldsymbol{F}_i^{(a)}\right)^2}{4D\Delta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

Methods: Variational Monte-Carlo

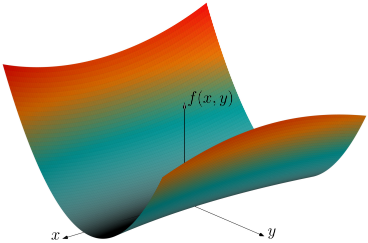


Minimization

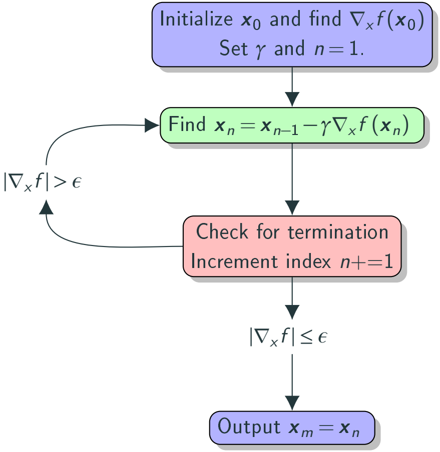
Single-Well



Rosenbrock



Minimization: Gradient Descent

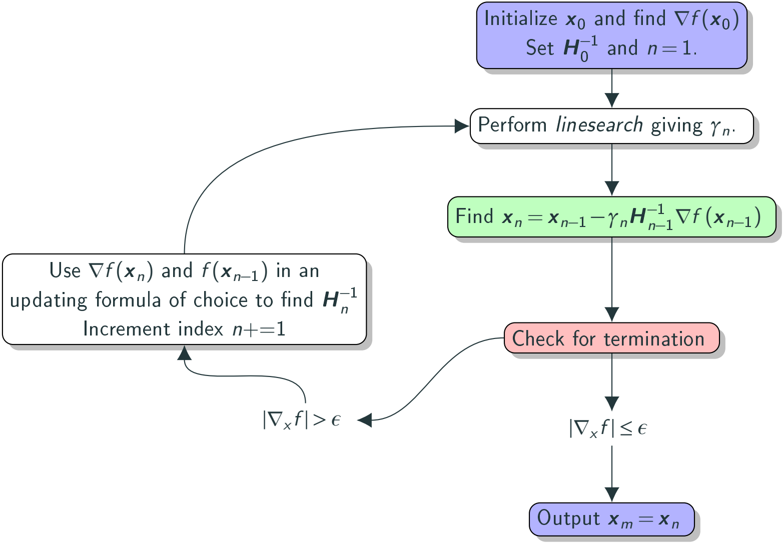


Minimization: Gradient Descent

x_0	γ	Iterations	x_m	$f(x_m)$
$(5,5)$	0.9	20	$(-0.072,-0.072)$	0.010
$(5,5)$	0.9	50	$(-8.920\times10^{-5},-8.920\times10^{-5})$	1.591×10^{-8}
$(5,5)$	0.9	100	$(-1.273\times10^{-9},-1.273\times10^{-9})$	3.242×10^{-18}
$(5,5)$	0.5	20	$(0.0,0.0)$	0.0
$(5,5)$	0.5	50	$(0.0,0.0)$	0.0
$(5,5)$	0.5	100	$(0.0,0.0)$	0.0
$(5,5)$	0.1	20	$(0.072,0.072)$	0.010
$(5,5)$	0.1	50	$(8.920\times10^{-5},8.920\times10^{-5})$	1.591×10^{-8}
$(5,5)$	0.1	100	$(1.273\times10^{-9},1.273\times10^{-9})$	3.242×10^{-18}

x_0	γ	Iterations	x_m	$f(x_m)$
$(0,0.5)$	0.001	100	$(0.181,0.030)$	0.034
$(0,0.5)$	0.001	500	$(0.512,0.258)$	0.327
$(0,0.5)$	0.001	1000	$(0.675,0.454)$	0.106
$(0,0.5)$	0.001	100000	$(1.000,1.000)$	0.0
$(0,0.5)$	0.0001	100	$(0.027,0.068)$	1.399
$(0,0.5)$	0.0001	500	$(0.105,0.009)$	0.801
$(0,0.5)$	0.0001	1000	$(0.184,0.031)$	0.666
$(0,0.5)$	0.0001	100000	$(0.994,0.989)$	3.131×10^{-5}

Minimization: Quasi-Newton BFGS



Minimization: Quasi-Newton BFGS

$\boldsymbol{x}_0$	Iterations	$\boldsymbol{x}_m$	$f(\boldsymbol{x}_m)$
$(1,1)$	1	$(-0.071,-0.071)$	1.000
$(-1,2)$	1	$(0.447,-0.894)$	1.000
$(1,1)$	2	$(0.000,0.000)$	0.000
$(-1,2)$	2	$(0.000,0.000)$	0.000
$(10,10)$	1	$(-0.071,-0.071)$	1.000
$(10,10)$	2	$(0.000,0.000)$	0.000
$(100,100)$	1	$(-0.071,-0.071)$	1.000
$(100,100)$	2	$(0.000,0.000)$	0.000

$\boldsymbol{x}_0$	Iterations	$\boldsymbol{x}_m$	$f(\boldsymbol{x}_m)$
$(-0.5,2.0)$	1	$(-0.706,0.708)$	7.280
$(-0.5,2.0)$	2	$(-0.780,0.649)$	3.342
$(-0.5,2.0)$	10	$(0.238,0.051)$	0.584
$(-0.5,2.0)$	30	$(1.000,1,000)$	0.000
$(5.5,-10.0)$	1	$(-0.996,0.091)$	85.214
$(5.5,-10.0)$	2	$(-0.908,1.087)$	10.549
$(5.5,-10.0)$	10	$(0.027,0.012)$	0.9613
$(5.5,-10.0)$	30	$(1.000,1,000)$	0.000

Wavefunction

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

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- Solution in polar[5]
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- 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

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

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

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

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

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

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

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

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

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

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

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

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Implementation

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- C++ and Eigen

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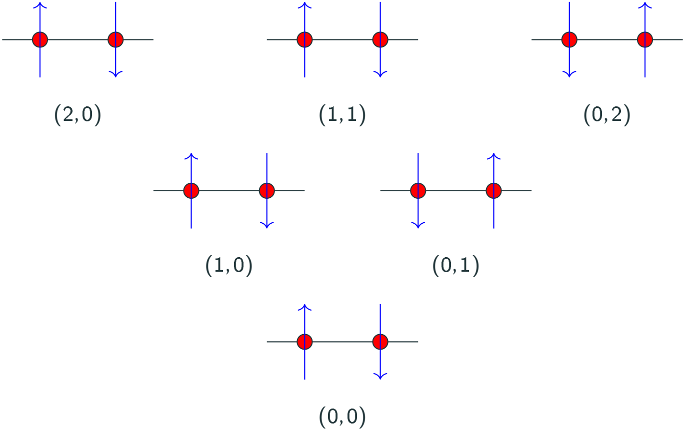
- Python

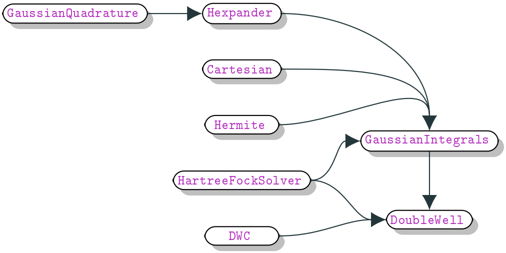
Implementation

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

Implementation: Cartesian



Implementation: Hartree-Fock



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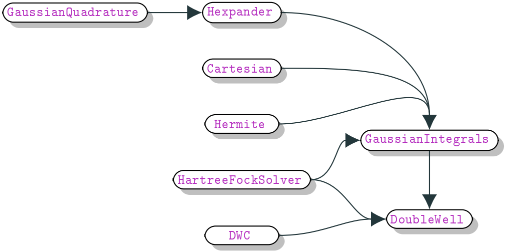
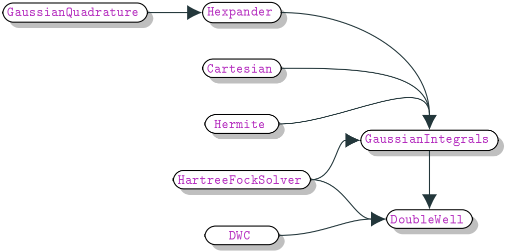


- Parallelization
  - Two-body element is computationally expensive
  - $S_i = \sum_{j=0}^{P_i} \prod_d (n_{j_d} + 1)$

Implementation: Hartree-Fock



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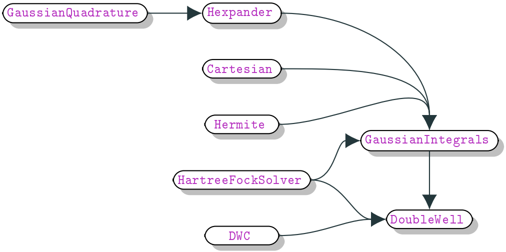
Implementation: Hartree-Fock



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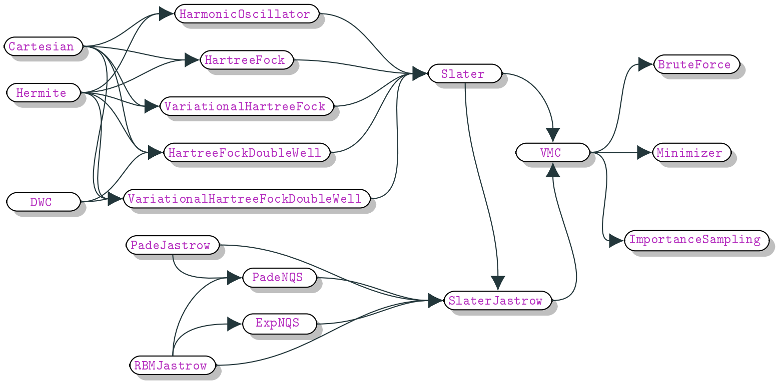
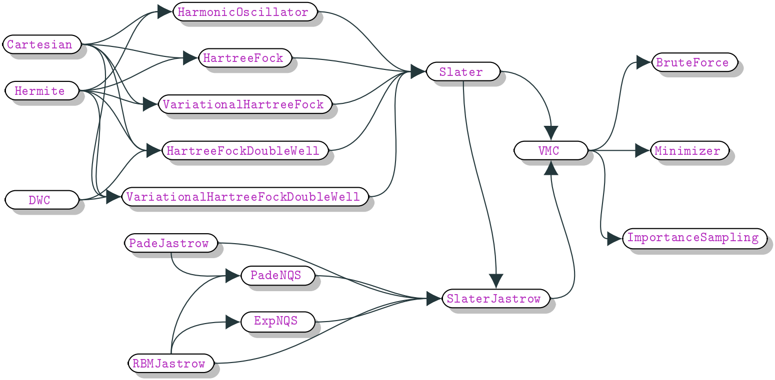
- Tabulation of Two-Body matrix

Implementation: Variational Monte-Carlo



Implementation: Variational Monte-Carlo

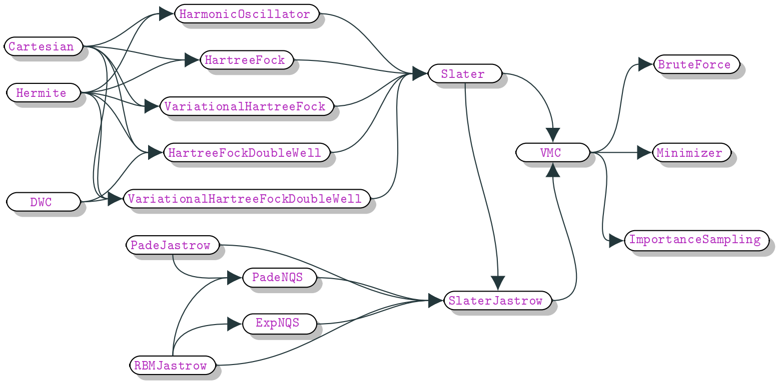


- `Hermite` generated with Python and SymPy

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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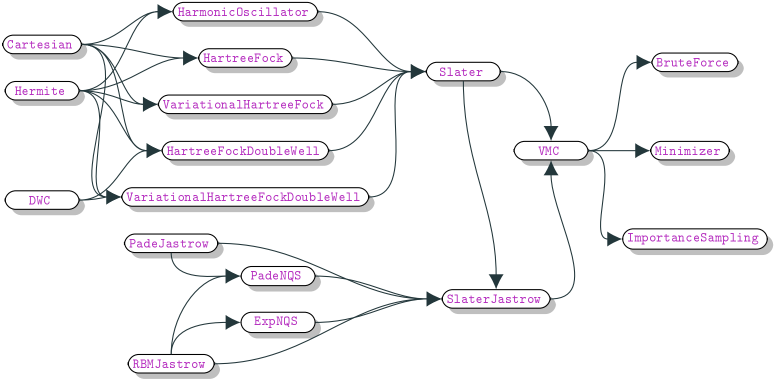

- `Hermite` generated with Python and SymPy
- Wavefunction class can be created with Python

Results

Results: Benchmark

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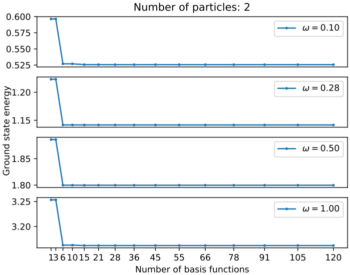

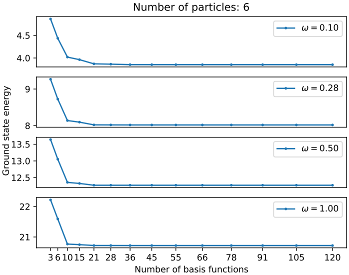

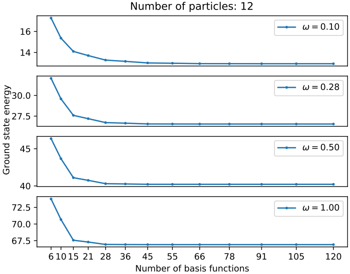

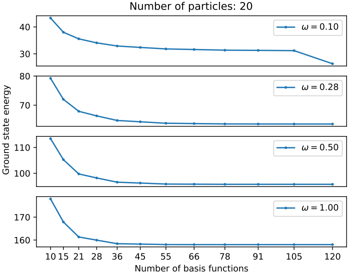

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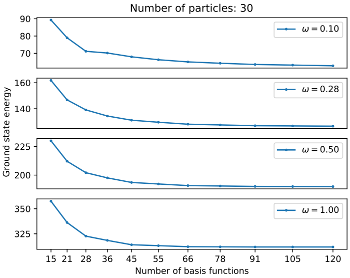

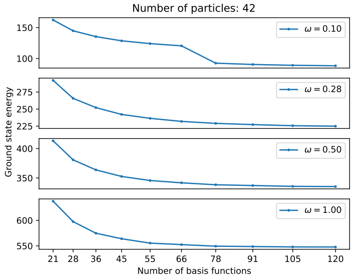

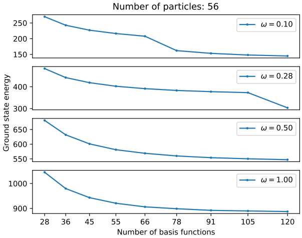

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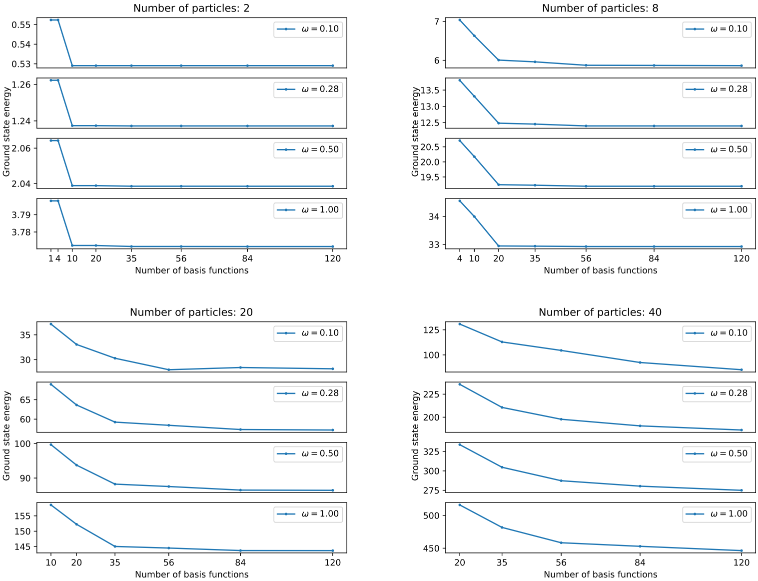


Results: Benchmark

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}

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

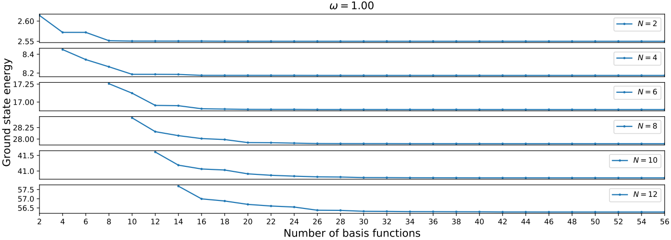
Results: Benchmark

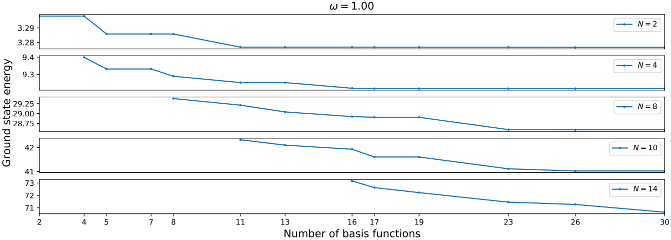
ω	N	
	2	8
0.1	0.51122(5){70}	5.87372(4){120}
0.28	1.21844(5){70}	12.36177(4){168}
0.5	2.02030(4){20}	19.15006(4){112}
1.0	3.72918(5){20}	33.58046(4){168}

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}

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

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

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

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}

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

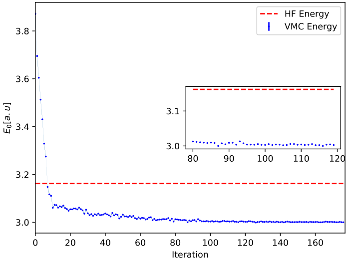
ω	N		
	2	4	8
1.0	3.22226(4){11}	9.17013(4){17}	28.62826(4){26}

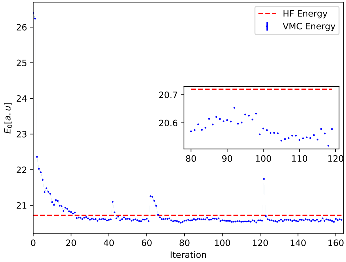
$$\psi_p = \sum_l C^{\mathrm{HF}}_{lp} \sum_k C^{\mathrm{DW}}_{kl} \psi^{\mathrm{HO}}_k \left(\sqrt{\alpha\omega} r\right) J_{\mathrm{Padé}}$$

Results: NQS-Jastrow

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

Results: NQS-Jastrow Harmonic Oscillator





Summary and Conclusion

Questions?

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