

Quantum Many-Body Simulations of Double Dot System

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Contents

1. Introduction
2. Methods
3. Wavefunction
4. Implementation
5. Results
6. Summary and Conclusion

Introduction

Quantum-Dot Model

- Schrödinger equation: $\mathcal{H}|\psi\rangle = E|\psi\rangle$, $\mathcal{H} = -\sum_i \frac{\nabla_i^2}{2} + f(\mathbf{r}) + V(R, \mathbf{r})$

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Quantum-Dot Model

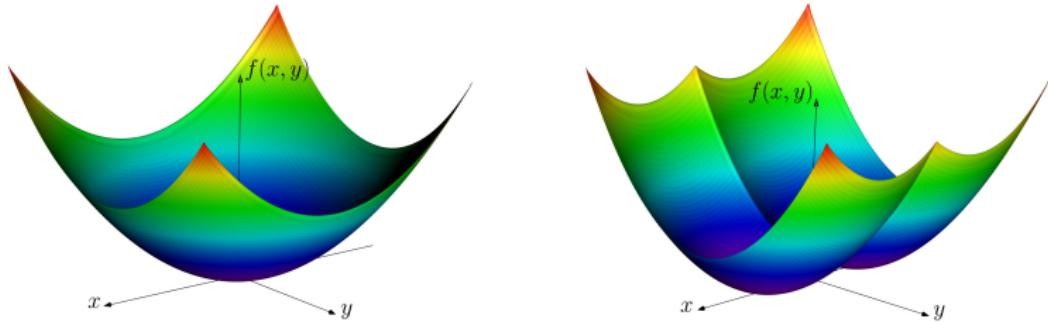
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¹S. Kvaal. "Harmonic Oscillator Eigenfunction Expansions, Quantum dots, and Effective Interactions". In: *Phys. Rev. B* (2009).

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 $V(\mathbf{r}) = \frac{1}{2}m\omega^2 r^2$ $V(\mathbf{r}) = \frac{1}{2}m\omega^2(r^2 - \delta R|x| + R^2)$



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Methods

**Hartree-Fock
Variational Monte-Carlo**

Methods: Variational Principle

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

Slater Determinant and Energy Functional

Methods: Slater Determinant and Energy Functional

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$$\bullet E[\Psi] = \frac{\langle \Psi | \mathcal{H} | \Psi \rangle}{\langle \Psi | \Psi \rangle} = \sum_p \langle p | \mathcal{H}_0 | p \rangle + \frac{1}{2} \sum_{p,q} [\langle pq | f_{12} | pq \rangle \pm \langle pq | f_{12} | qp \rangle]$$



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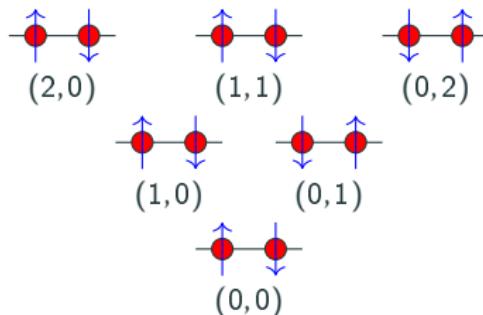
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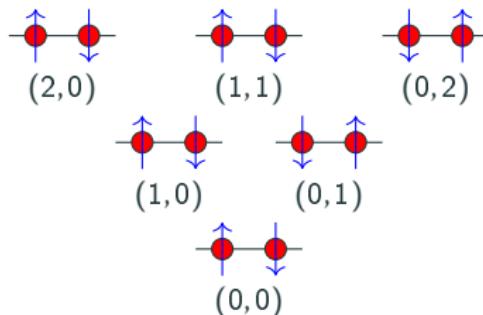
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 - $\mathcal{K} \equiv \langle \psi_k^* | f_{12} | \psi \rangle = \int \psi_k^*(\mathbf{r}) f_{12} \psi(\mathbf{r}) d\mathbf{r}$

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- Roothan-Hall: $\mathbf{F}\mathbf{C}_i = \boldsymbol{\epsilon} S \mathbf{C}_i$
 - $F_{pq} = h_{pq} + \sum_{pq} \rho_{pq} (2\langle pq|f_{12}|rs\rangle - \langle pq|f_{12}|sr\rangle)$
 - $h_{pq} \equiv \langle p|h|q\rangle$
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- Poople-Nesbet: $\mathbf{F}^+ \mathbf{C}^+ = \boldsymbol{\varepsilon} \mathbf{S} \mathbf{C}^+, \mathbf{F}^- \mathbf{C}^- = \boldsymbol{\varepsilon}^- \mathbf{S} \mathbf{C}^-$

Variational Monte-Carlo

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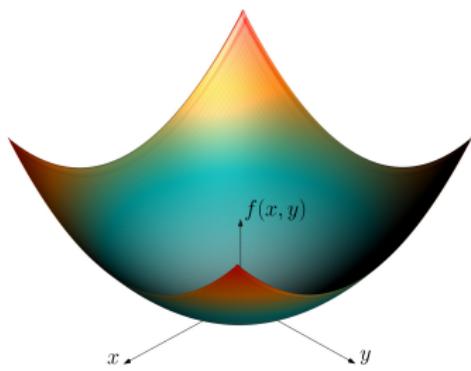
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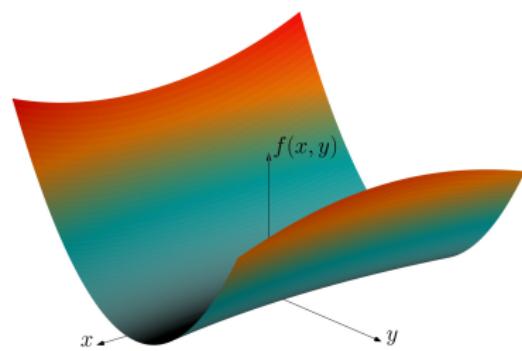
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 - Importance Sampling
 - Focker-Planck equation and Langevin equation
 - $r^{(b)} = r^{(a)} + D \Delta t F^{(a)} + \sqrt{\Delta t} \xi$
 - Quantum force: $F = \frac{2}{\Psi} \nabla \Psi$
 - $\frac{T(b, a, \Delta t)}{T(a, b, \Delta t)} = \text{Greensfunction ratio}$

Minimization

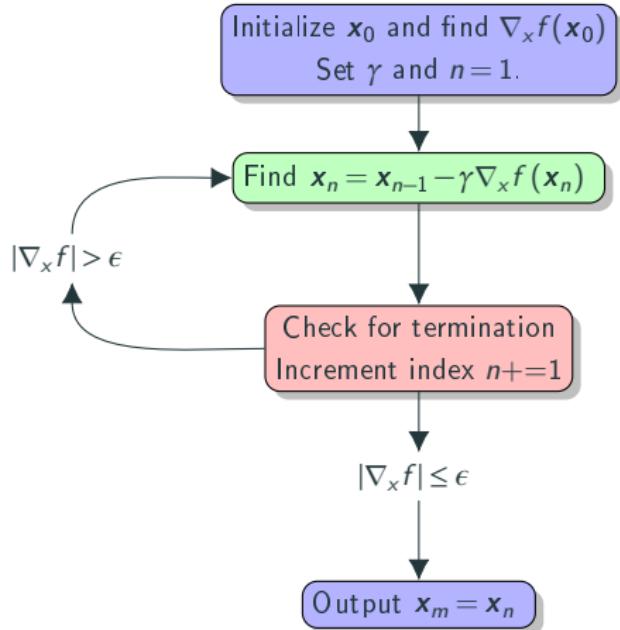
Single-Well



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	(-8.920×10^{-5} , -8.920×10^{-5})	1.591×10^{-8}
(5, 5)	0.9	100	(-1.273×10^{-9} , -1.273×10^{-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
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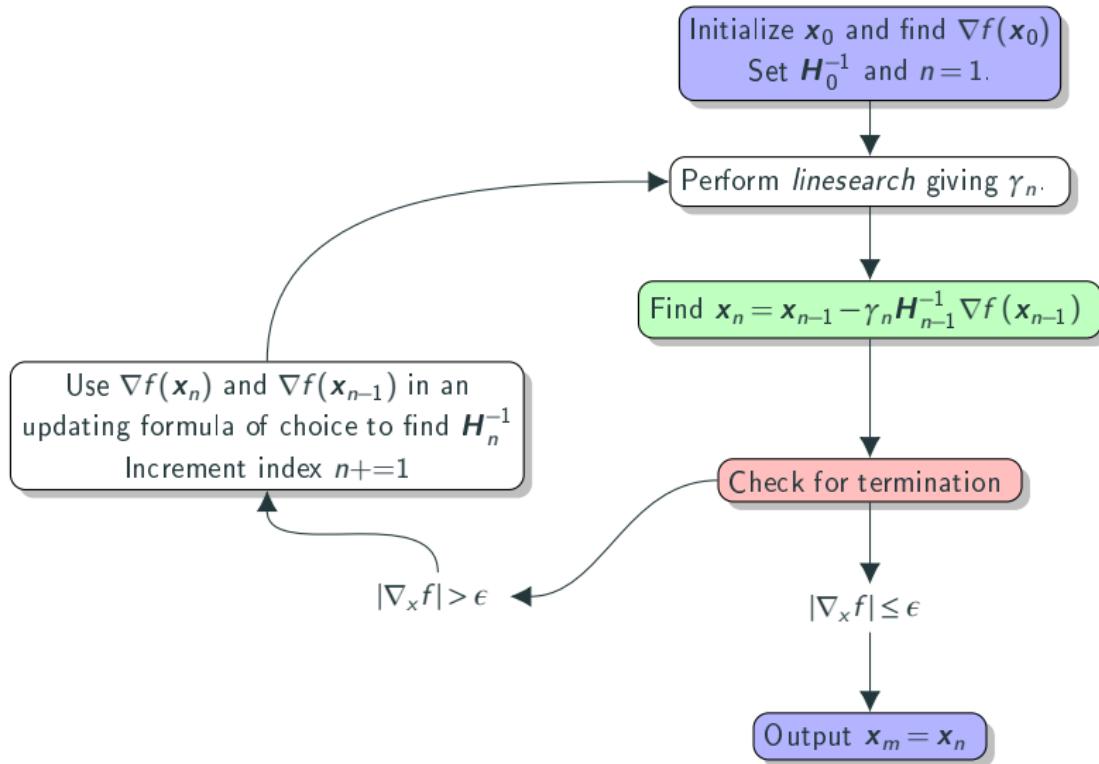
x_0	γ	Iterations	x_m	$f(x_m)$
(0, 0.5)	0.001	100	(0.181, 0.030)	0.034
(0, 0.5)	0.001	500	(0.512, 0.258)	0.327
(0, 0.5)	0.001	1000	(0.675, 0.454)	0.106
(0, 0.5)	0.001	100000	(1.000, 1.000)	0.0
(0, 0.5)	0.0001	100	(0.027, 0.068)	1.399
(0, 0.5)	0.0001	500	(0.105, 0.009)	0.801
(0, 0.5)	0.0001	1000	(0.184, 0.031)	0.666
(0, 0.5)	0.0001	100000	(0.994, 0.989)	3.131×10^{-5}

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Minimization: Quasi-Newton BFGS



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x_0	Iterations	x_m	$f(x_m)$
(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
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(-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
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Minimization: Simulated Annealing

Wavefunction

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Wavefunction: Integral Elements

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

$$\langle \phi_i(\mathbf{r}) | x_d^k | \phi_j(\mathbf{r}) \rangle$$

$$\langle \phi_i(\mathbf{r}) | \nabla^2 | \phi_j(\mathbf{r}) \rangle$$

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

Wavefunction: Single-Well

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

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- Solution in polar³

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- Solution in polar³
- $\psi_n(\mathbf{r}) = \prod_d N_d \sum_{l=1}^{n_d} C_{n_d l}^{\text{Hermite}} g_l\left(\frac{\omega}{2}, \mathbf{r}, \mathbf{0}\right), \quad g_l\left(\frac{\omega}{2}, \mathbf{r}, \mathbf{0}\right) = x_d^{(l)} \exp\left(-\frac{\omega^2}{2}x_d^2\right)$

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- Solution in Cartesian⁴

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

$$\langle g_i(\mathbf{r}) | x_d^k | g_j(\mathbf{r}) \rangle$$

$$\langle g_i(\mathbf{r}) | \nabla^2 | g_j(\mathbf{r}) \rangle$$

$$\langle g_i(\mathbf{r}_1) g_j(\mathbf{r}_2) | f_{12} | g_k(\mathbf{r}_1) g_l(\mathbf{r}_2) \rangle$$

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⁴J. 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

$$\langle \psi_i^{\text{HO}} | \psi_j^{\text{HO}} \rangle = N_i \delta_{ij}$$

$$\langle \psi_i^{\text{HO}} | h^{\text{HO}} | \psi_j^{\text{HO}} \rangle = N_i \epsilon_i^{\text{HO}} \delta_{ij}$$

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

$$E_t^{i_d+1} = \frac{1}{2\omega} E_{t-1}^i \quad \xi_{t_d+1}^n = t_d \xi_{t_d-1}^{n+1}$$

$$E_0^0 = K_{AB} \quad \xi_0^n = (-b)^n \zeta_n(0)$$

$$\zeta_n^{\text{2D}}(x) = \int_{-1}^1 \frac{u^{2n}}{\sqrt{1-u^2}} e^{-u^2} du \quad \zeta_n^{\text{3D}}(x) = \int_{-1}^1 u^{2n} e^{-u^2} du$$

$$b = \begin{cases} \frac{\omega}{2}, & \text{2D} \\ \omega, & \text{3D} \end{cases}$$

Wavefunction: Double-Well

- Perturbation of harmonic oscillator: $U^{\text{DW}}(r) = V^{\text{HO}}(r) + V_n^{\text{DW}}(r)$

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- Eigenvalue equation: $H^{\text{DW}} C^{\text{DW}} = \epsilon^{\text{DW}} C^{\text{DW}}$
 - $H_{ij}^{\text{DW}} = \epsilon_i^{\text{HO}} \delta_{ij} + \langle \psi_i^{\text{HO}} \left| V_n^{\text{DW}} \right| \psi_j^{\text{HO}} \rangle$

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- Integral-Elements

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

$$\left\langle \psi_p^{\text{DW}} \left| h^{\text{DW}} \right| \psi_q^{\text{DW}} \right\rangle = \varepsilon_p^{\text{DW}} \delta_{pq}$$

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

Wavefunction: Slater-Jastrow

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- Padé-NQS: $J = J_{\text{Padé}} J_{\text{NQS}}$

Implementation

Implementation

- C++ and Eigen

Implementation

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 - Performance

Implementation

- C++ and Eigen
 - Performance
 - Generalization

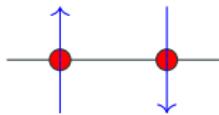
Implementation

- C++ and Eigen
 - Performance
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- Python

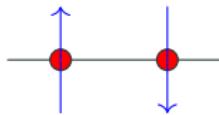
Implementation

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

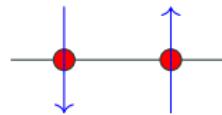
Implementation: Cartesian



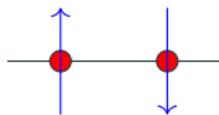
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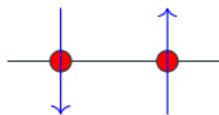
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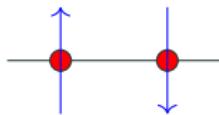
(0,2)



(1,0)

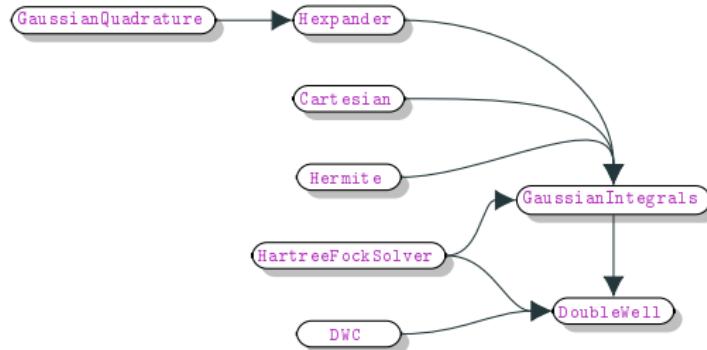


(0,1)

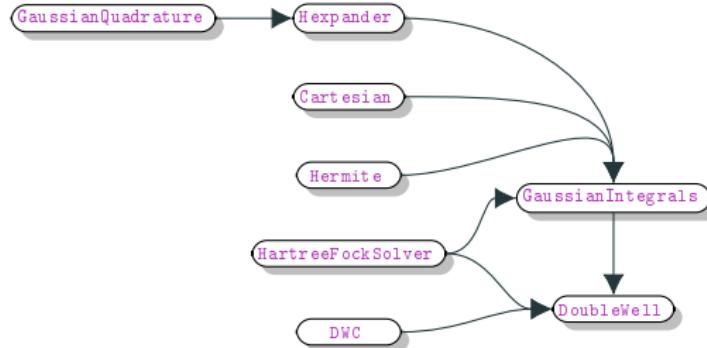


(0,0)

Implementation: Hartree-Fock

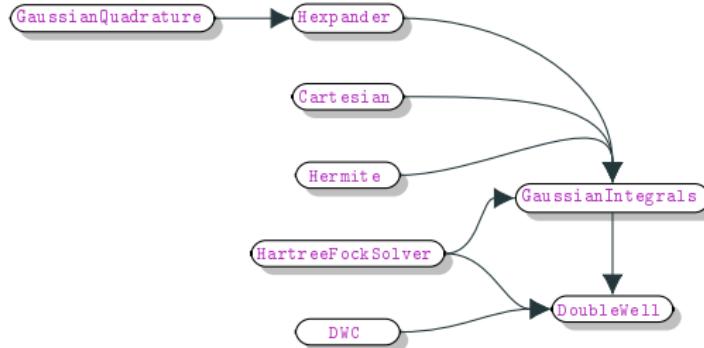


Implementation: Hartree-Fock



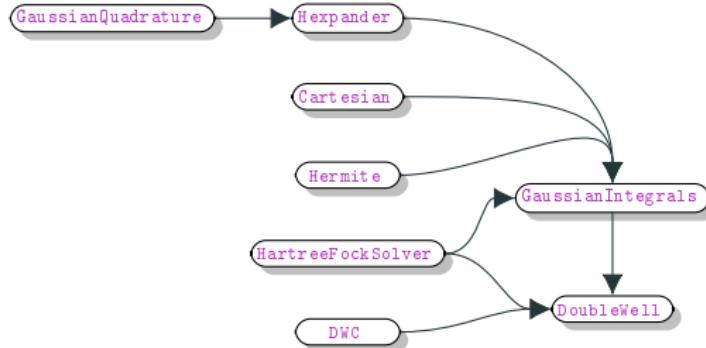
- Parallelization

Implementation: Hartree-Fock



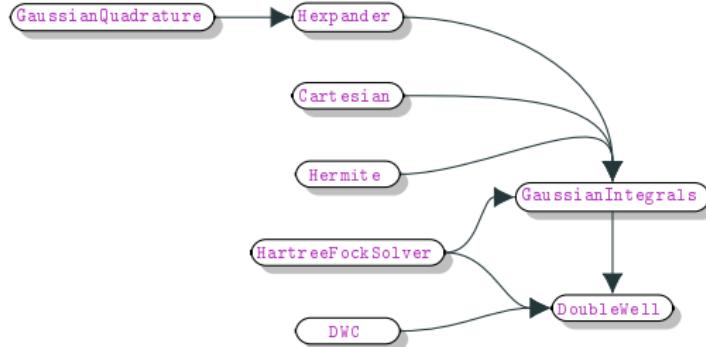
- Parallelization
 - Two-body element is computationally expensive
 - $S_i = \sum_{j=0}^{P_i} \prod_d (n_{j_d} + 1)$

Implementation: Hartree-Fock



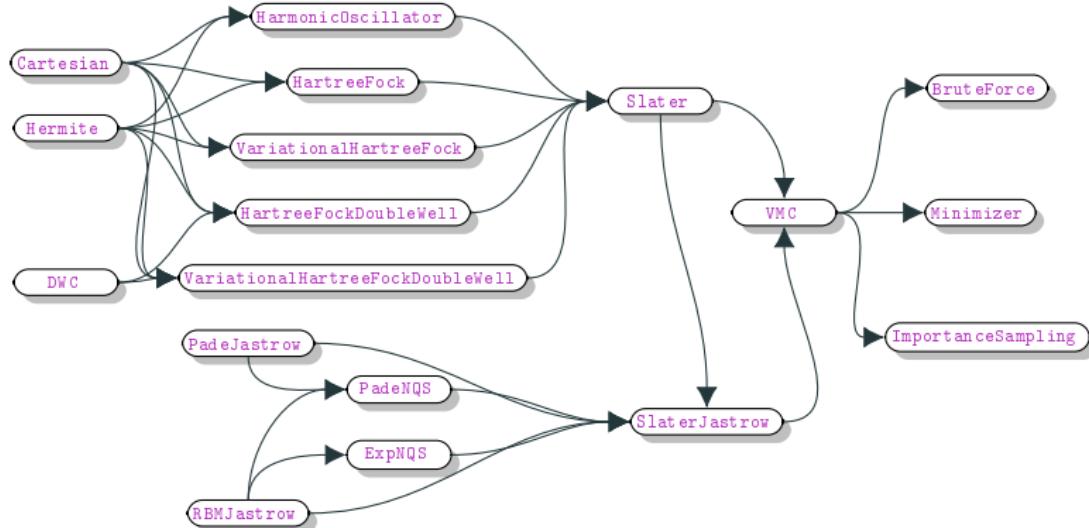
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Implementation: Hartree-Fock

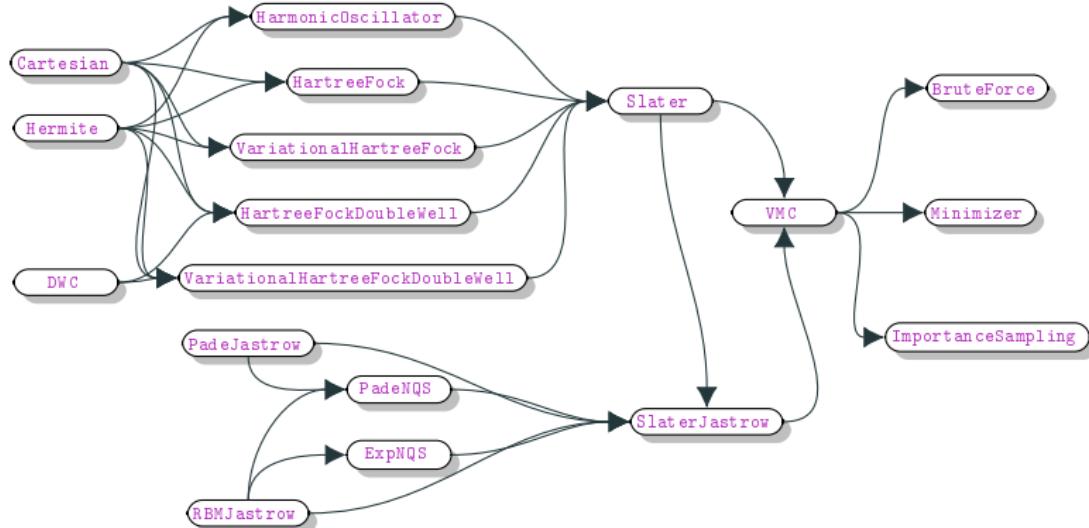


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- Hartree-Fock algorithm only run on one process
- Tabulation of Two-Body matrix

Implementation: Variational Monte-Carlo

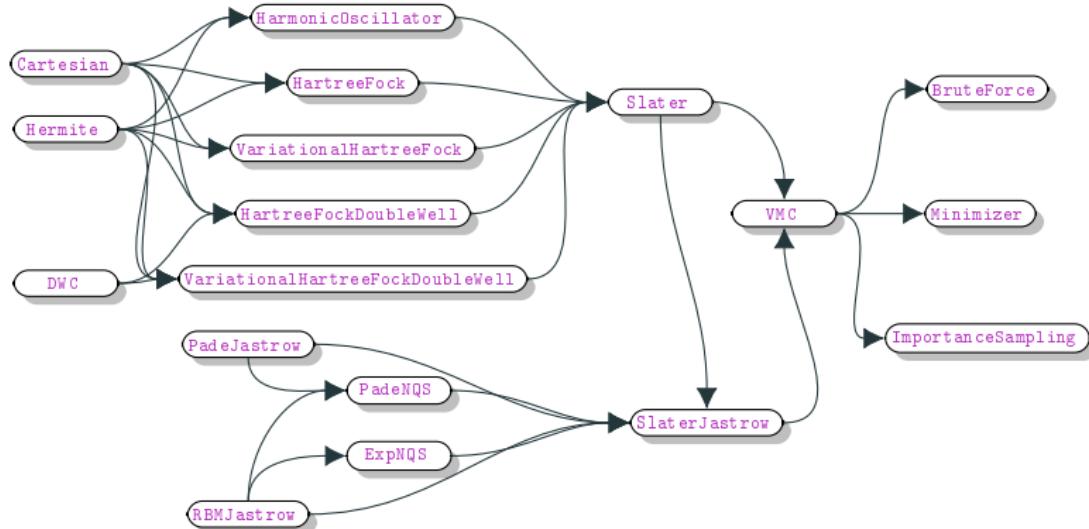


Implementation: Variational Monte-Carlo



- Hermite generated with Python and SymPy

Implementation: Variational Monte-Carlo

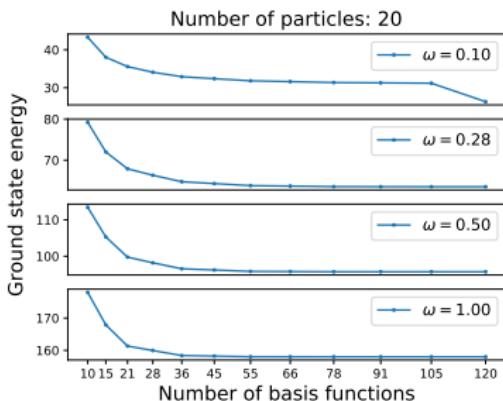
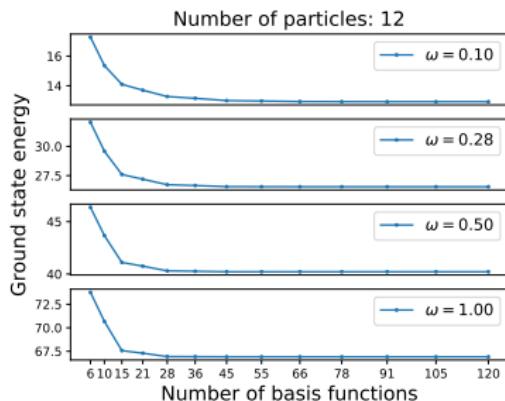
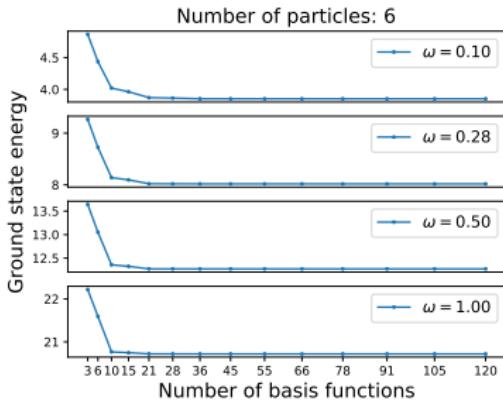
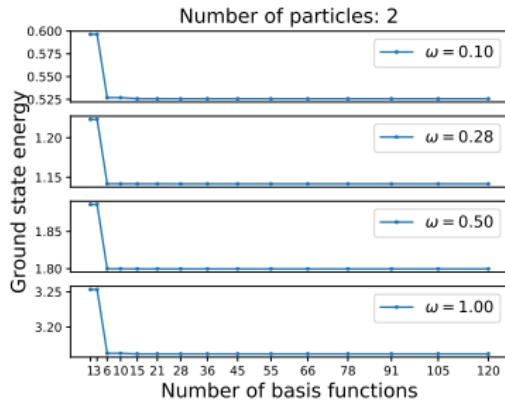


- Hermite generated with Python and SymPy
- Wavefunction class generated with Python

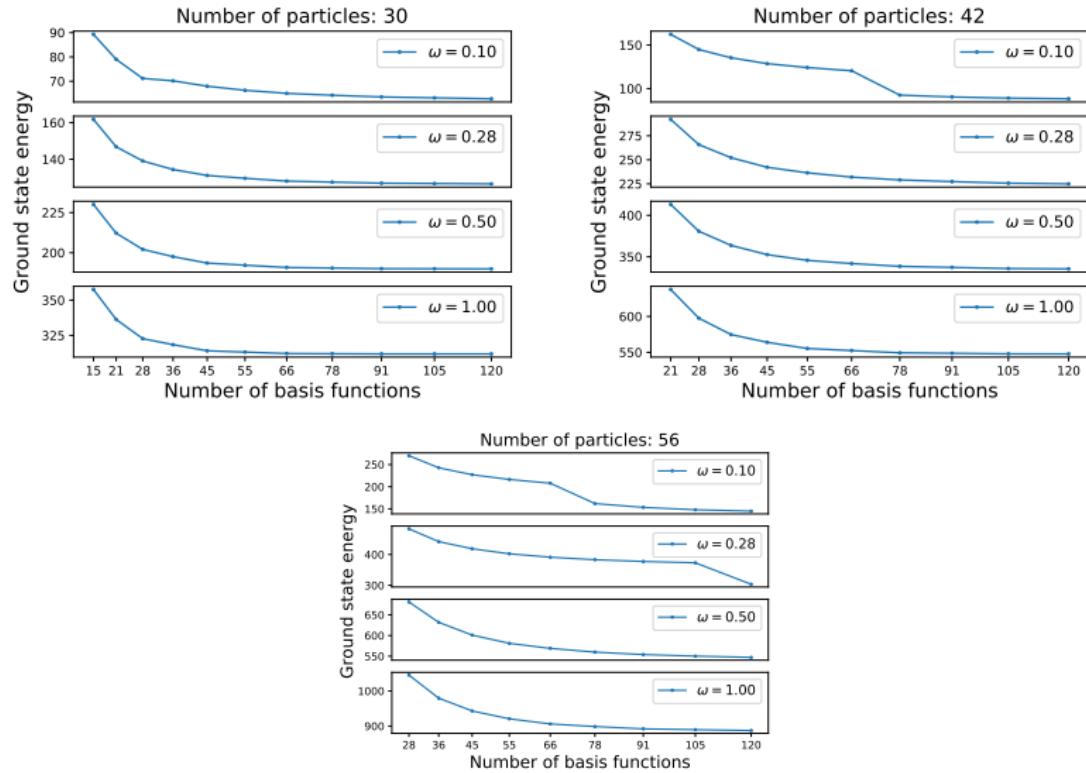
Results

Benchmark

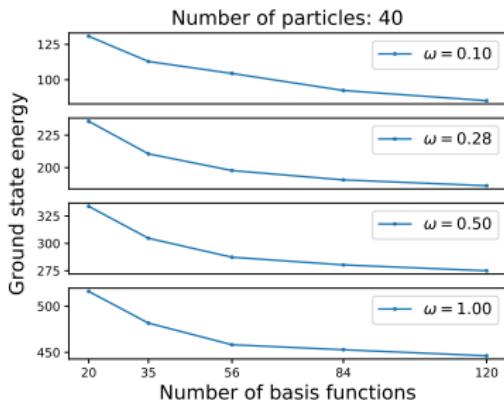
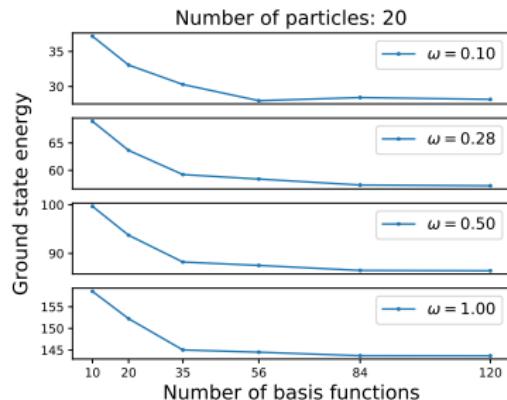
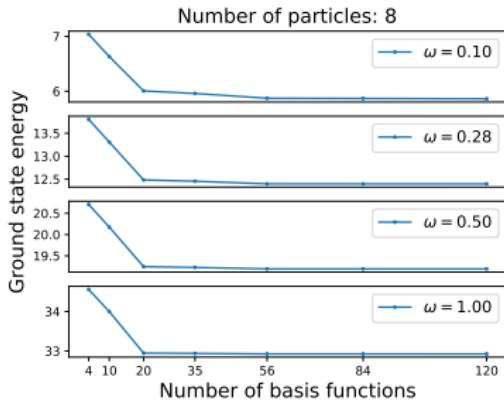
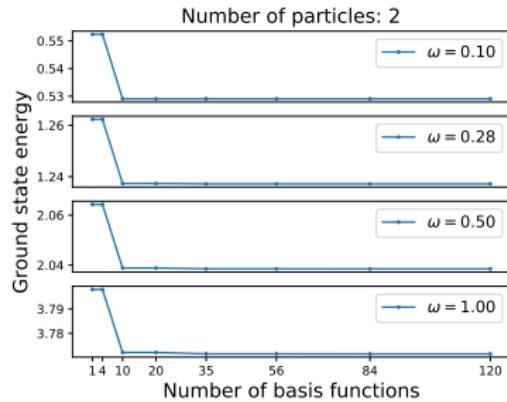
Results: Benchmark



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)

$$\psi = \psi^{\text{HO}}(\sqrt{\alpha\omega}) J_{\text{Pad\'e}}$$

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}

$$\psi_p = \sum_l C_{lp} \psi_l^{\text{HO}}(\sqrt{\omega} r) J_{\text{Pad\'e}}, \quad \psi_p = \sum_l C_{lp} \psi_l^{\text{HO}}(\sqrt{\alpha\omega} r) J_{\text{Pad\'e}}$$

Results: Benchmark

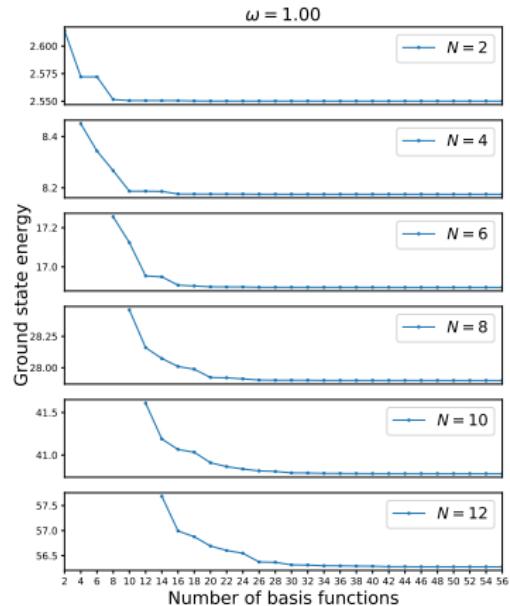
ω	N	
	2	8
0.1	0.51122(5){70}	5.87372(4){120}
0.28	1.21844(5){70}	12.36177(4){168}
0.5	2.02030(4){20}	19.15006(4){112}
1.0	3.72918(5){20}	33.58046(4){168}

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}

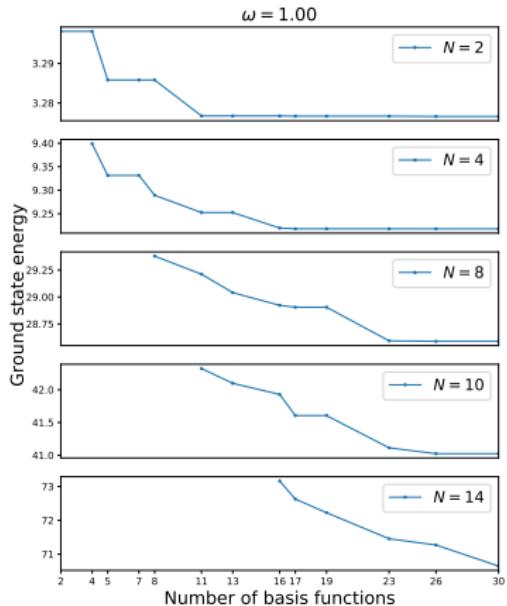
$$\psi_p = \sum_l C_{lp} \psi_l^{\text{HO}}(\sqrt{\omega} r) J_{\text{Pad\'e}}, \quad \psi_p = \sum_l C_{lp} \psi_l^{\text{HO}}(\sqrt{\alpha\omega} r) J_{\text{Pad\'e}}$$

Results: Double-Well Hartree-Fock

2D



3D



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}

$$\psi_p = \sum_l C_{lp}^{\text{HF}} \sum_k C_{kl}^{\text{DW}} \psi_k^{\text{HO}} (\sqrt{\omega} r) J_{\text{Pad\'e}}$$

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

$$\psi_p = \sum_l C_{lp}^{\text{HF}} \sum_k C_{kl}^{\text{DW}} \psi_k^{\text{HO}} (\sqrt{\alpha \omega} r) J_{\text{Pad\'e}}$$

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}

$$\psi_p = \sum_l C_{lp}^{\text{HF}} \sum_k C_{kl}^{\text{DW}} \psi_k^{\text{HO}} (\sqrt{\omega} r) J_{\text{Pad\'e}}$$

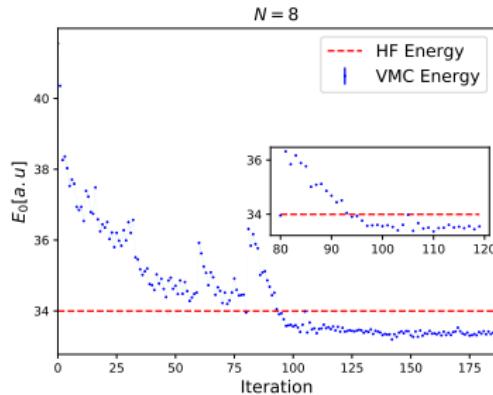
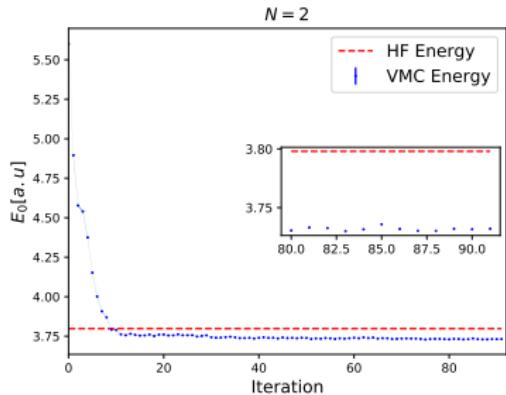
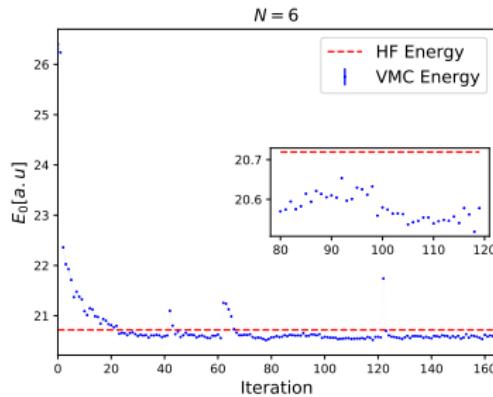
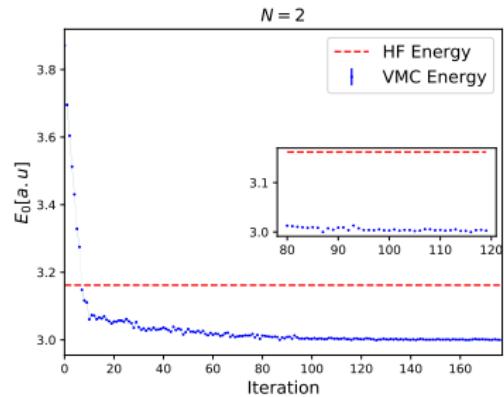
ω	N		
	2	4	8
1.0	3.22226(4){11}	9.17013(4){17}	28.62826(4){26}

$$\psi_p = \sum_l C_{lp}^{\text{HF}} \sum_k C_{kl}^{\text{DW}} \psi_k^{\text{HO}} (\sqrt{\alpha\omega} r) J_{\text{Pad\'e}}$$

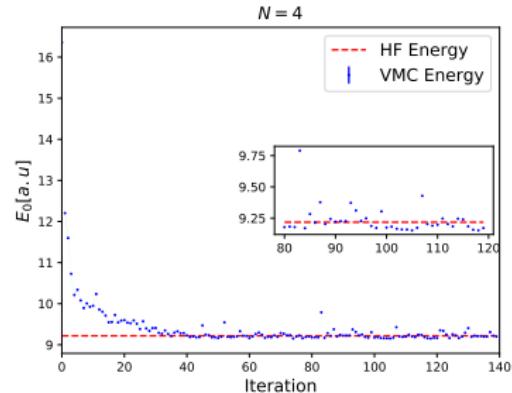
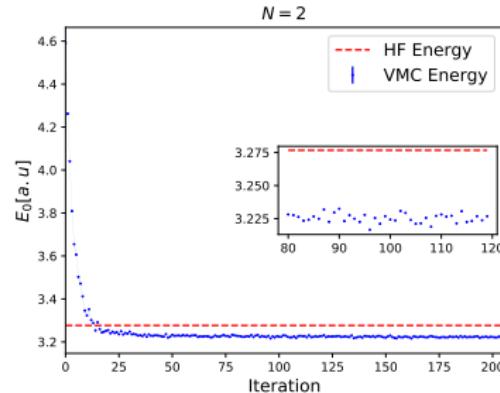
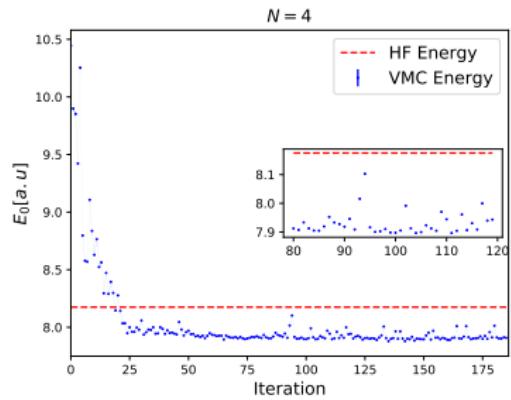
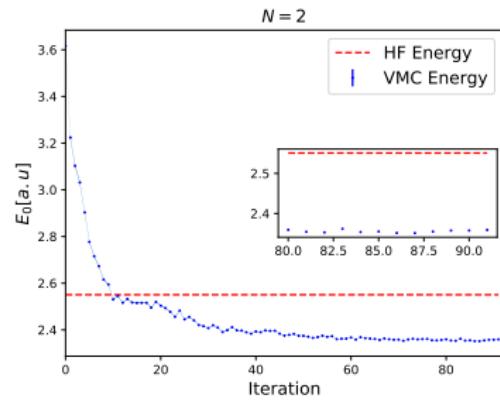
Results: NQS-Jastrow

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

Results: NQS-Jastrow Harmonic Oscillator



Results: NQS-Jastrow Double-Well



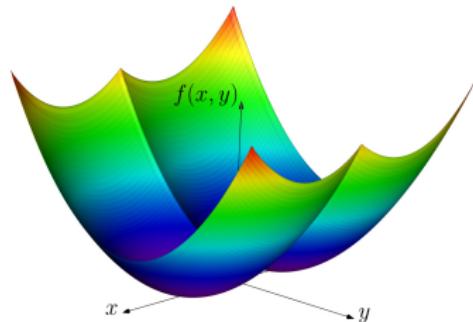
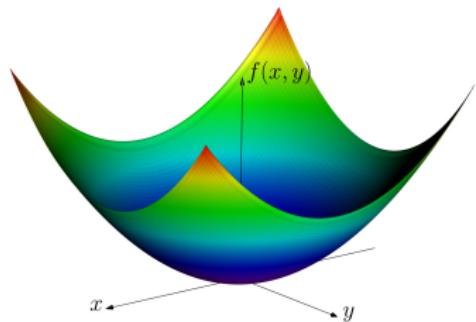
Summary and Conclusion

Summary

- Schrödinger equation: $\mathcal{H}|\psi\rangle = E|\psi\rangle$, $\mathcal{H} = -\sum_i \frac{\nabla_i^2}{2} + f(\mathbf{r}) + V(\mathbf{R}, \mathbf{r})$
- Interaction: $f(\mathbf{r}) = \sum_{i < j} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}$
- Confinement: Harmonic Oscillator, Double-Well

$$V(\mathbf{r}) = \frac{1}{2} m \omega^2 r^2$$

$$V(\mathbf{r}) = \frac{1}{2} m \omega^2 (r^2 - \delta R |x| + R^2)$$



**Hartree-Fock
Variational Monte-Carlo**

Summary

$$\begin{aligned}\left\langle \psi_i^{\text{HO}} \middle| \psi_j^{\text{HO}} \right\rangle &= N_i \delta_{ij} \\ \left\langle \psi_i^{\text{HO}} \middle| h^{\text{HO}} \right\rangle &= N_i \varepsilon_i^{\text{HO}} \delta_{ij}\end{aligned}$$

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

$$\begin{aligned}E_t^{i_d+1} &= \frac{1}{2\omega} E_{t-1}^i & \xi_{t_d+1}^n &= t_d \xi_{t_d-1}^{n+1} \\ E_0^0 &= K_{AB} & \xi_0^n &= (-b)^n \zeta_n(0)\end{aligned}$$

$$\zeta_n^{\text{2D}}(x) = \int_{-1}^1 \frac{u^{2n}}{\sqrt{1-u^2}} e^{-u^2 x} du \quad \zeta_n^{\text{3D}}(x) = \int_{-1}^1 u^{2n} e^{-u^2 x} du$$

$$b = \begin{cases} \frac{\omega}{2}, & \text{2D} \\ \omega, & \text{3D} \end{cases}$$

Summary

- Perturbation of harmonic oscillator: $U^{\text{DW}}(r) = V^{\text{HO}}(r) + V_n^{\text{DW}}(r)$
- Expand in HO-functions: $\left| \psi_p^{\text{DW}} \right\rangle = \sum_l C_{lp}^{\text{DW}} \left| \psi_l^{\text{HO}} \right\rangle$
- Eigenvalue equation: $H^{\text{DW}} C^{\text{DW}} = \epsilon^{\text{DW}} C^{\text{DW}}$
 - $H_{ij}^{\text{DW}} = \epsilon_i^{\text{HO}} \delta_{ij} + \langle \psi_i^{\text{HO}} \left| V_n^{\text{DW}} \right| \psi_j^{\text{HO}} \rangle$
- Integral-Elements

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

$$\langle \psi_p^{\text{DW}} \left| h^{\text{DW}} \right| \psi_q^{\text{DW}} \rangle = \epsilon_p^{\text{DW}} \delta_{pq}$$

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

Conclusion

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- Hartree-Fock energies improved with Variational Monte-Carlo
- Stable minimization with NQS-Jastrow

Further Work

- Binding with Python

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- Rewrite with sparse matrices in Hartree-Fock

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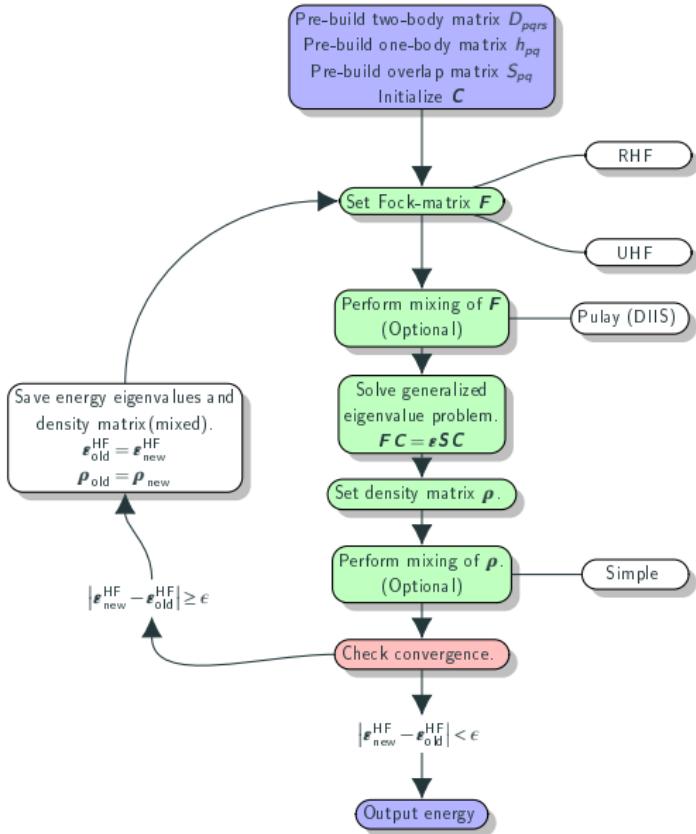
- Binding with Python
- Optimize and clean-up code
- Rewrite with sparse matrices in Hartree-Fock
- Extend to non-isotropic gaussians

Questions?

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Methods: Hartree-Fock



Methods: Variational Monte-Carlo

