Quantum Many-Body Simulations of Double Dot System

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Contents

Introduction

Quantum-Dot Model

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

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- Confinement: Harmonic Oscillator[1], Double-Well[2]

[1] S. Kvaal. "Harmonic Oscillator Eigenfunction Expansions, Quantum dots, and Effective Interactions". In: *Phys. Rev. B* (2009).
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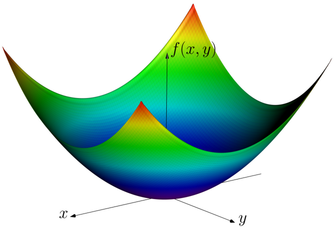
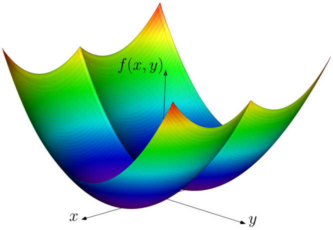
$$V(\boldsymbol{r}) = \frac{1}{2} m\omega^2 r^2 \qquad V(\boldsymbol{r}) = \frac{1}{2} m\omega^2 \left(r^2 - \delta R|x| + R^2\right)$$





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Methods

Hartree-Fock

Variational Monte-Carlo

Methods: Variational Principle

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

Slater Determinant and Energy Functional

Methods: Slater Determinant and Energy Functional

- Pauli Principle

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

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    - $\mathscr{J} \equiv \langle \psi_k^* | f_{12} | \psi_k \rangle = \int \psi_k^*(\boldsymbol{r}) f_{12} \psi_k(\boldsymbol{r}) dr$
    - $\mathscr{K} \equiv \langle \psi_k^* | f_{12} | \psi \rangle = \int \psi_k^*(\boldsymbol{r}) f_{12} \psi(\boldsymbol{r}) dr$

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Methods: Hartree-Fock

- Pair spins as: $\{\psi_{2I-1}, \psi_{2I}\} = \{\phi_I(\boldsymbol{r})\alpha(s), \phi_I(\boldsymbol{r})\beta(s)\}$
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- Expand: $\phi_i(\boldsymbol{r}) = \sum_{p=1}^{L} C_{pi}\chi_p(\boldsymbol{r})$
- Roothan-Hall: $\boldsymbol{F}\boldsymbol{C}_i = \boldsymbol{\varepsilon}\boldsymbol{S}\boldsymbol{C}_i$
  - $F_{pq} = h_{pq} + \sum_{pq}\rho_{pq}\left(2\langle pq|f_{12}|rs\rangle - \langle pq|f_{12}|sr\rangle\right)$
  - $h_{pq} \equiv \langle p|h|q\rangle$
  - $\rho_{pq} \equiv \sum_{i=1}^{\frac{N}{2}} C_{pi}C_{qi}^*$
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- Poople-Nesbet: $\boldsymbol{F}^+\boldsymbol{C}^+ = \boldsymbol{\varepsilon}\boldsymbol{S}\boldsymbol{C}^+$, $\boldsymbol{F}^-\boldsymbol{C}^- = \boldsymbol{\varepsilon}^-\boldsymbol{S}\boldsymbol{C}^-$

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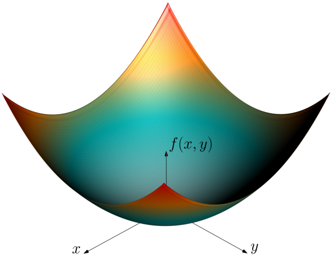
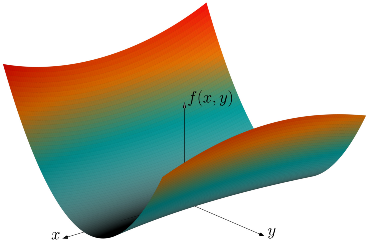
  - Importance Sampling
    - Focker-Planck equation and Langevin equation
    - $r^{(b)} = r^{(a)} + D\Delta t F^{(a)} + \sqrt{\Delta t}\xi$
    - Quantum force: $F = \frac{2}{\Psi}\nabla\Psi$
    - $\frac{T(b,a,\Delta t)}{T(a,b,\Delta t)}$ = Greensfunction ratio

Minimization

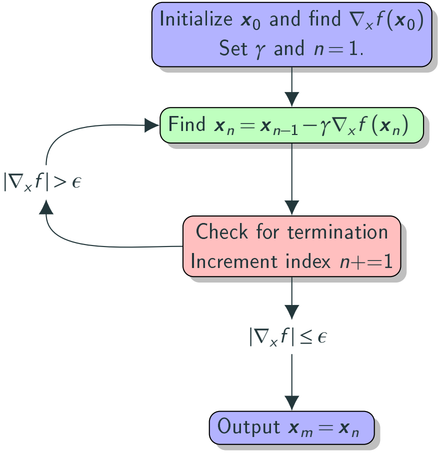
Single-Well



Rosenbrock



Minimization: Gradient Descent



Minimization: Gradient Descent

$\mathbf{x}_0$	γ	Iterations	$\mathbf{x}_m$	$f(\mathbf{x}_m)$
(5,5)	0.9	20	$(-0.072, -0.072)$	0.010
(5,5)	0.9	50	$(-8.920 \times 10^{-5}, -8.920 \times 10^{-5})$	1.591×10^{-8}
(5,5)	0.9	100	$(-1.273 \times 10^{-9}, -1.273 \times 10^{-9})$	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
(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	$(8.920 \times 10^{-5}, 8.920 \times 10^{-5})$	1.591×10^{-8}
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(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
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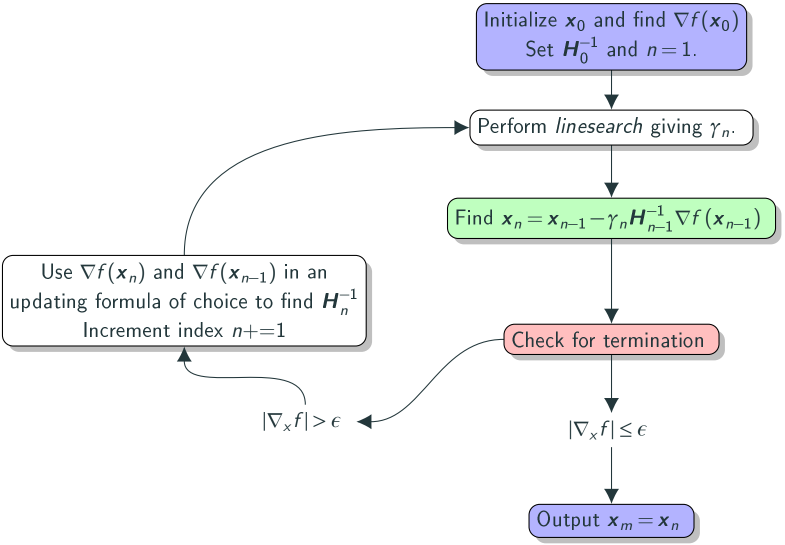
Minimization: Quasi-Newton BFGS



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
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$\boldsymbol{x}_0$	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
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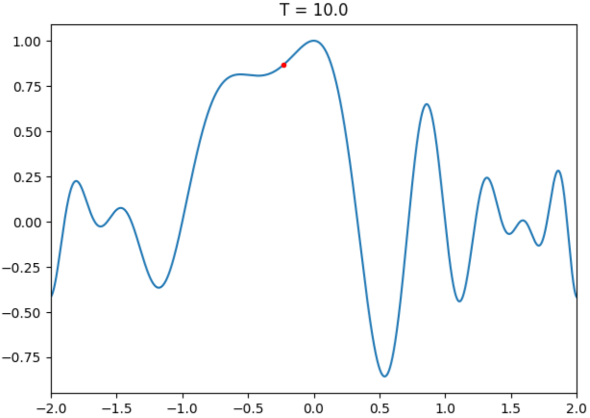
Minimization: Simulated Annealing



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[3]
- $\psi_n(\boldsymbol{r}) = \prod_d N_d \sum_{l=1}^{n_d} C_{n_d l}^{\text{Hermite}} g_l\left(\frac{\omega}{2}, \boldsymbol{r}, \boldsymbol{0}\right), \quad g_l\left(\frac{\omega}{2}, \boldsymbol{r}, \boldsymbol{0}\right) = x_d^{(l)} \exp\left(-\frac{\omega^2}{2} x_d^2\right)$

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- Solution in Cartesian[4]

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

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[4] 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

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

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

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

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

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

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

$$b = \begin{cases} \dfrac{\omega}{2}, & \mathrm{2D} \\ \omega, & \mathrm{3D} \end{cases}$$

Wavefunction: Double-Well

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

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

Wavefunction: Slater-Jastrow

- Slater determinant: $\psi_T = \det(\boldsymbol{\Phi}(\boldsymbol{R};\boldsymbol{\alpha}))\xi(s)$

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

Implementation

Implementation

- C++ and Eigen

Implementation

- C++ and Eigen
    - Performance

Implementation

- C++ and Eigen
    - Performance
    - Generalization

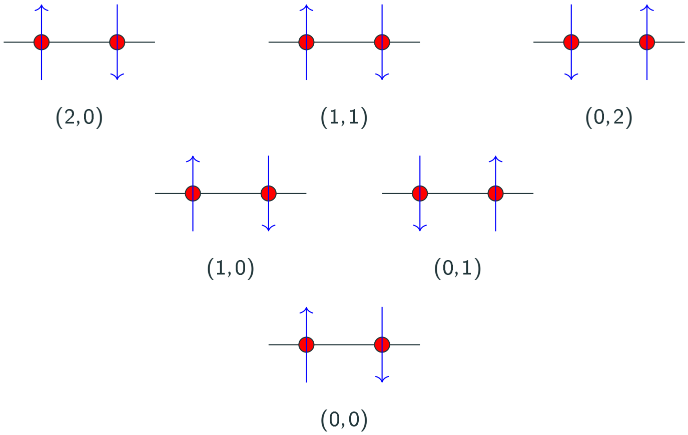
Implementation

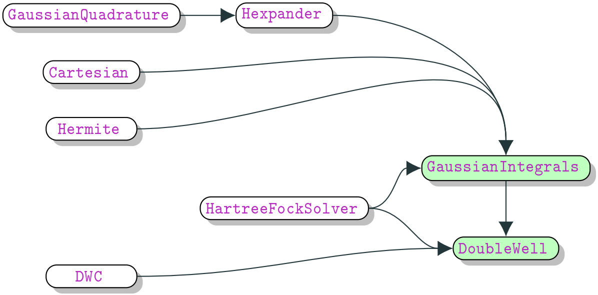
- C++ and Eigen
  - Performance
  - Generalization
- Python

Implementation

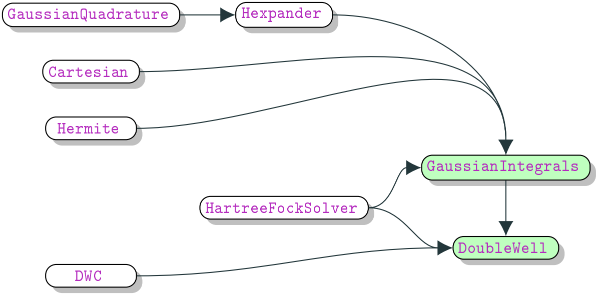
- C++ and Eigen
  - Performance
  - Generalization
- Python
  - Generate C++ code

Implementation: Cartesian



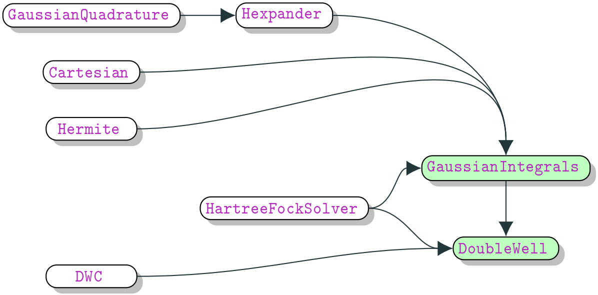

GaussianQuadrature
Hexpander
Cartesian
Hermite
GaussianIntegrals
HartreeFockSolver
DoubleWell
DWC

Implementation: Hartree-Fock



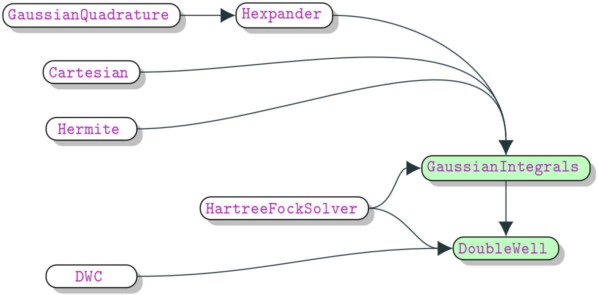
- Parallelization

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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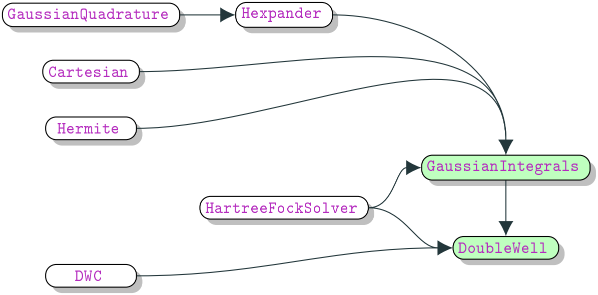

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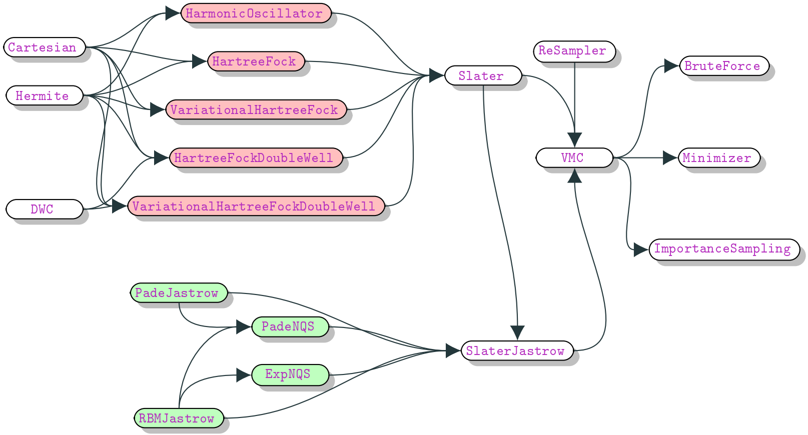
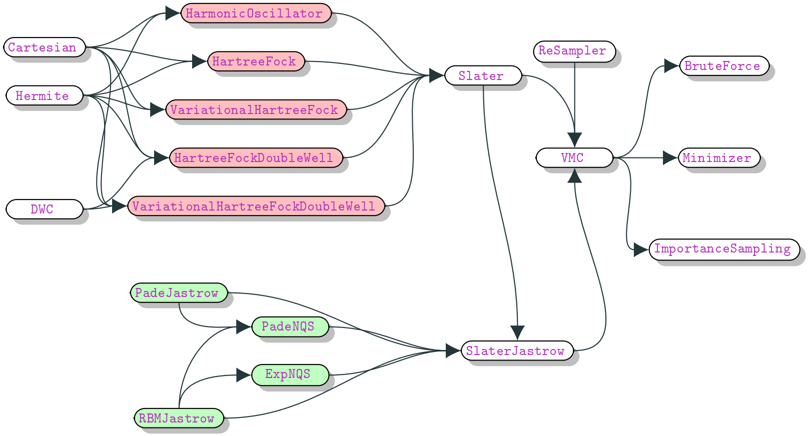
- Tabulation of Two-Body matrix

Implementation: Variational Monte-Carlo

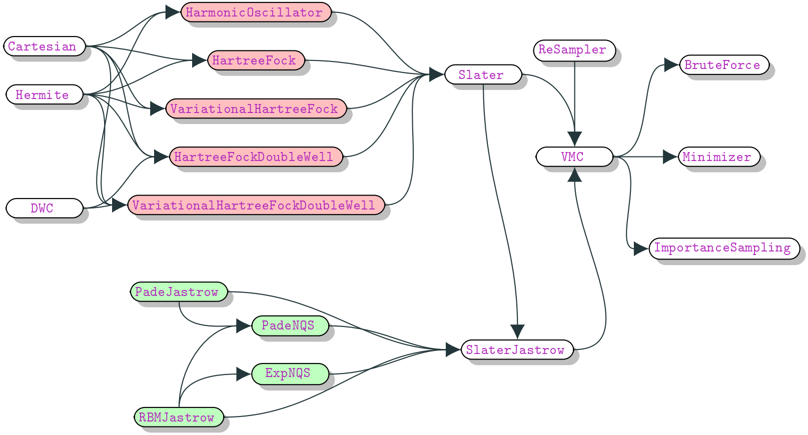


Implementation: Variational Monte-Carlo



- `Hermite` generated with Python and SymPy

Implementation: Variational Monte-Carlo

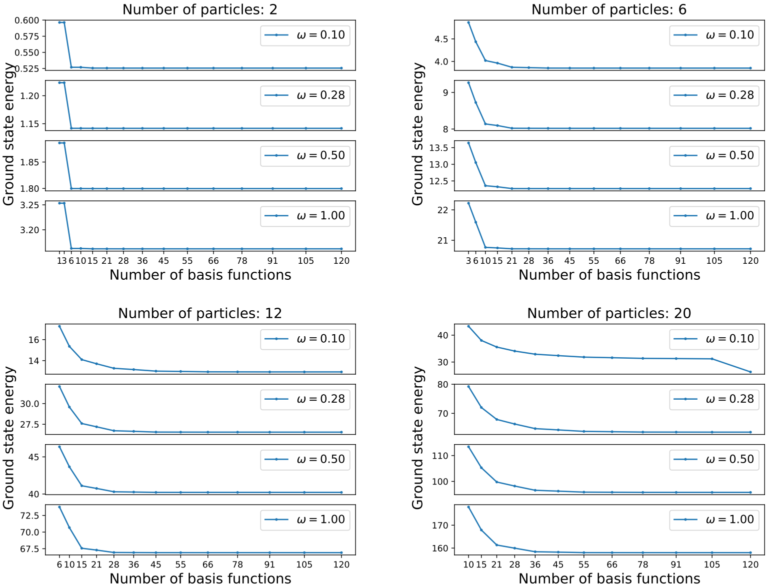


- `Hermite` generated with Python and SymPy
- Wavefunction class generated with Python

Results

Benchmark

Results: Benchmark



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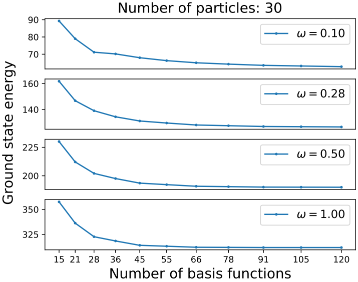

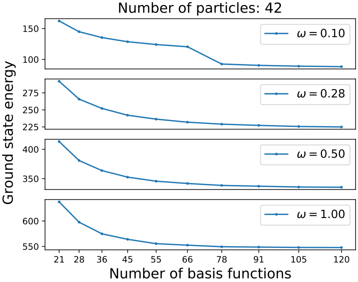

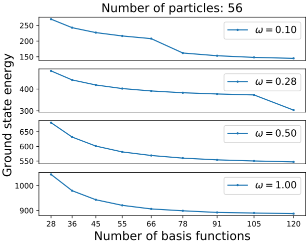

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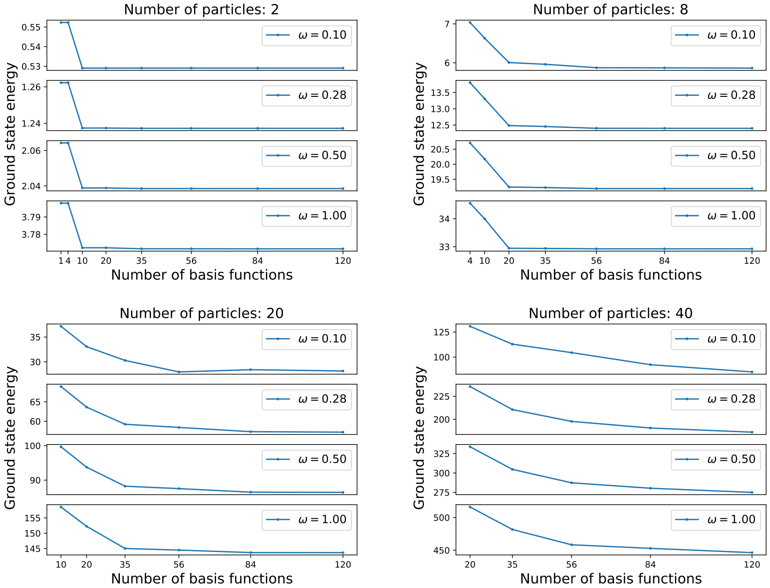


Results: Benchmark

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

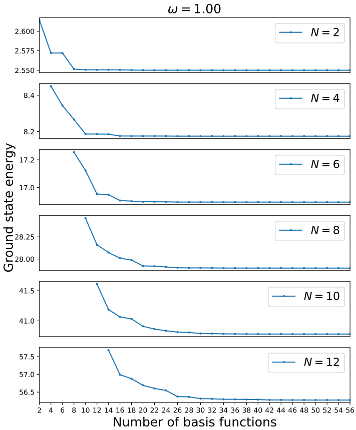
ω	N	
	2	8
0.1	0.51122(5){70}	5.87372(4){120}
0.28	1.21844(5){70}	12.36177(4){168}
0.5	2.02030(4){20}	19.15006(4){112}
1.0	3.72918(5){20}	33.58046(4){168}

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}

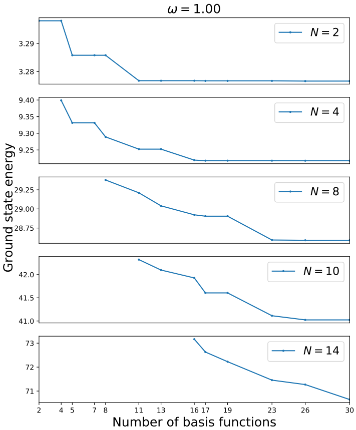
$$\psi_p = \sum_l C_{lp} \psi_l^{\mathrm{HO}}\left(\sqrt{\omega} r\right) J_{\text{Padé}}, \qquad \psi_p = \sum_l C_{lp} \psi_l^{\mathrm{HO}}\left(\sqrt{\alpha\omega} r\right) J_{\text{Padé}}$$

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}

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

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}

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

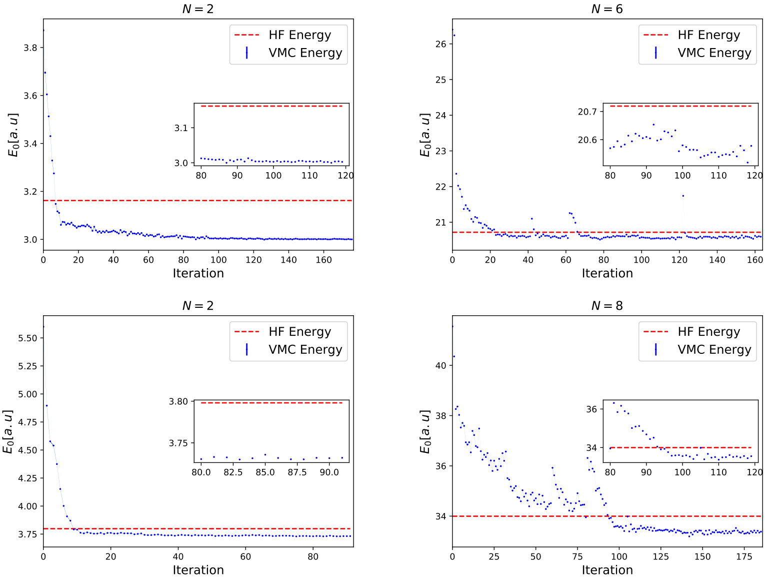
ω	N		
	2	4	8
1.0	3.22226(4){11}	9.17013(4){17}	28.62826(4){26}

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

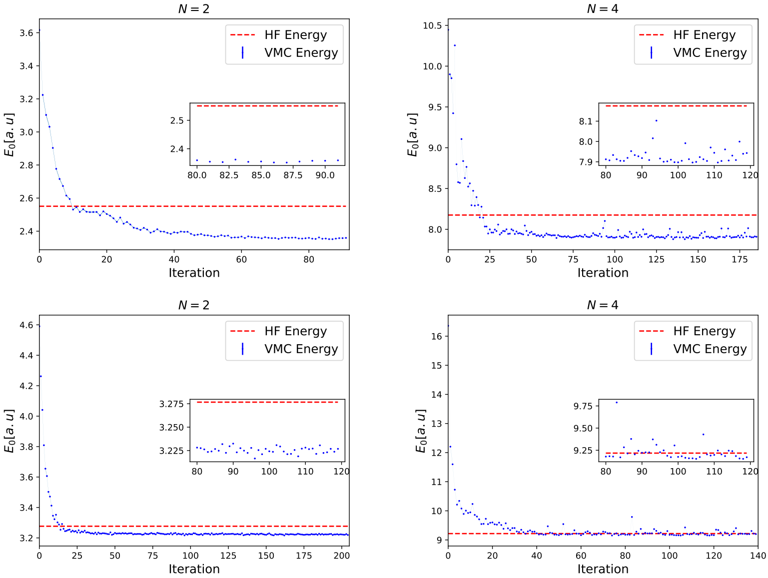
Results: NQS-Jastrow

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

Results: NQS-Jastrow Harmonic Oscillator



Results: NQS-Jastrow Double-Well

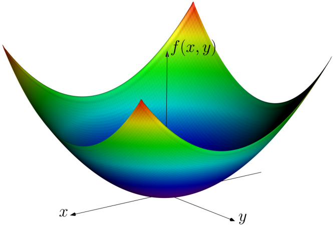


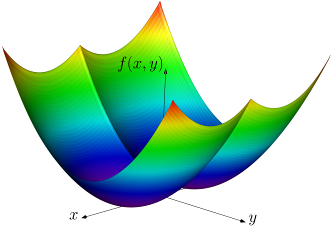
Summary and Conclusion

Summary

- Schrödinger equation: $\mathscr{H}\left|\psi\right\rangle = E\left|\psi\right\rangle$, $\mathscr{H} = -\sum_i \frac{\nabla_i^2}{2} + f(\boldsymbol{r}) + V(\boldsymbol{R},\boldsymbol{r})$
- Interaction: $f(\boldsymbol{r}) = \sum_{i<j} \frac{1}{|r_i - r_j|}$
- Confinement: Harmonic Oscillator, Double-Well

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





Summary

Hartree-Fock

Variational Monte-Carlo

Summary

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

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

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

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

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

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

Summary

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

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

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

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

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Further Work

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End

Questions?

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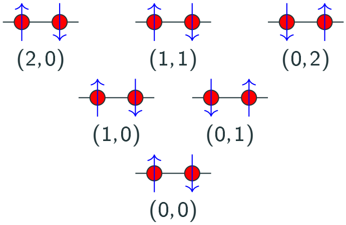

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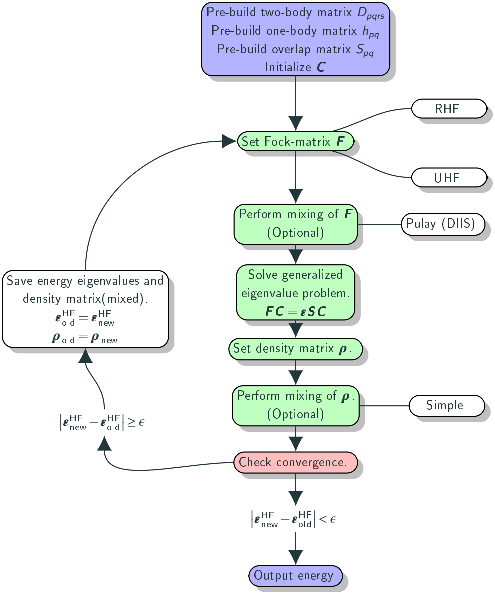

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