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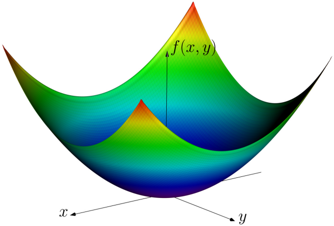
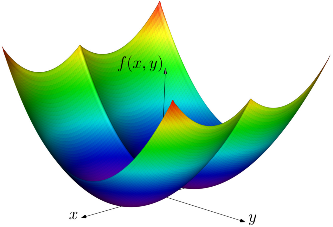
$$V(\boldsymbol{r}) = \frac{1}{2} m\omega^2 r^2 \qquad V(\boldsymbol{r}) = \frac{1}{2} m\omega^2 \left(r^2 - \delta R|x| + R^2\right)$$





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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

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

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    - $\mathscr{J} \equiv \langle \psi_k^* | f_{12} | \psi_k \rangle = \int \psi_k^*(\boldsymbol{r}) f_{12} \psi_k(\boldsymbol{r}) dr$
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- Roothan-Hall: $\boldsymbol{F}\boldsymbol{C}_i = \boldsymbol{\varepsilon}\boldsymbol{S}\boldsymbol{C}_i$
  - $F_{pq} = h_{pq} + \sum_{pq}\rho_{pq}\left(2\langle pq|f_{12}|rs\rangle - \langle pq|f_{12}|sr\rangle\right)$
  - $h_{pq} \equiv \langle p|h|q\rangle$
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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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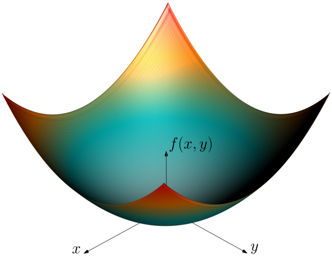
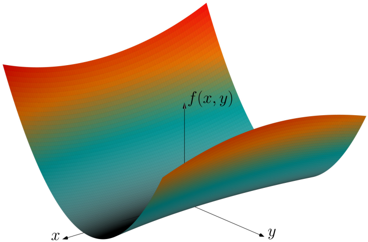
  - Importance Sampling
    - Focker-Planck equation and Langevin equation
    - $r^{(b)} = r^{(a)} + D\Delta t F^{(a)} + \sqrt{\Delta t}\xi$
    - Quantum force: $F = \frac{2}{\Psi}\nabla\Psi$
    - $\frac{T(b,a,\Delta t)}{T(a,b,\Delta t)} =$ Greensfunction ratio

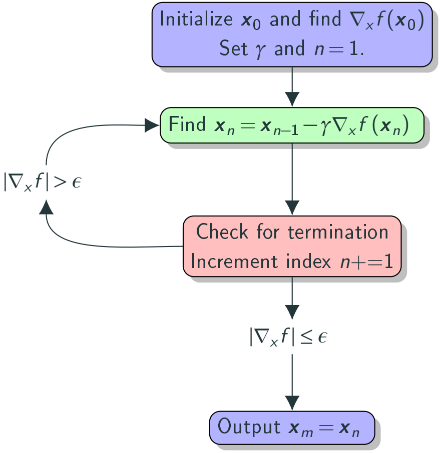
Minimization

Single-Well



Rosenbrock




Initialize $\boldsymbol{x}_0$ and find $\nabla_x f(\boldsymbol{x}_0)$
Set γ and $n = 1$.
Find $\boldsymbol{x}_n = \boldsymbol{x}_{n-1} - \gamma \nabla_x f(\boldsymbol{x}_n)$
$|\nabla_x f| > \epsilon$
Check for termination
Increment index $n{+}{=}1$
$|\nabla_x f| \leq \epsilon$
Output $\boldsymbol{x}_m = \boldsymbol{x}_n$

Minimization: Gradient Descent

$\boldsymbol{x}_0$	γ	Iterations	$\boldsymbol{x}_m$	$f(\boldsymbol{x}_m)$
$(5,5)$	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}
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$\boldsymbol{x}_0$	γ	Iterations	$\boldsymbol{x}_m$	$f(\boldsymbol{x}_m)$
$(0,0.5)$	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
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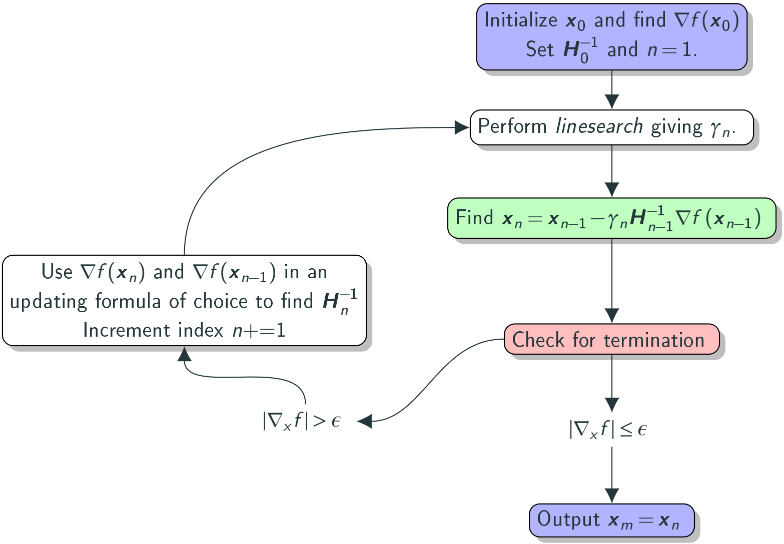

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$\boldsymbol{x}_0$	Iterations	$\boldsymbol{x}_m$	$f(\boldsymbol{x}_m)$
$(1,1)$	1	$(-0.071,-0.071)$	1.000
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$(-0.5,2.0)$	1	$(-0.706,0.708)$	7.280
$(-0.5,2.0)$	2	$(-0.780,0.649)$	3.342
$(-0.5,2.0)$	10	$(0.238,0.051)$	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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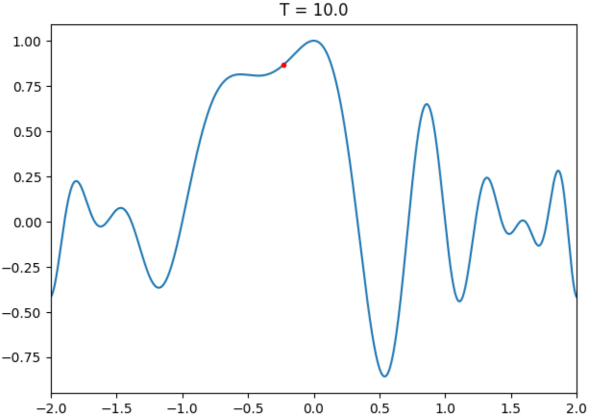
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0.50
0.25
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−0.25
−0.50
−0.75
−2.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0

Wavefunction

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$$\phi_i(\boldsymbol{r}) = \sum_{p=1}^{L} C_{pi}\chi_p(\boldsymbol{r})$$

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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 Cartesian[4]

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

[3] E. Anisimovas and A. Matulis. "Energy spectra of few-electron quantum dots". In: *Journal of Physics: Condensed Matter* (1998), p. 601.
[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

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

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

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

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

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

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

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

Wavefunction: Double-Well

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- Integral-Elements

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

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

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

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

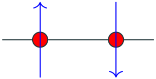
Implementation

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

Implementation

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

Implementation: Cartesian



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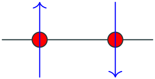

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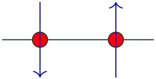

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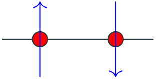

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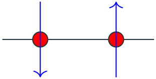

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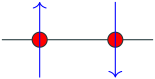

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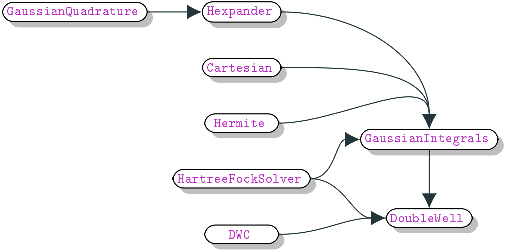
Implementation: Hartree-Fock



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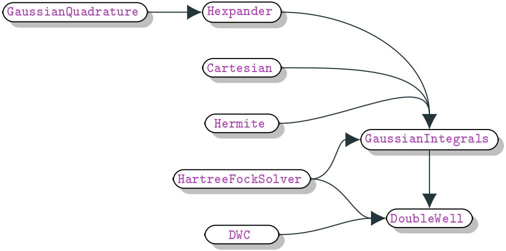
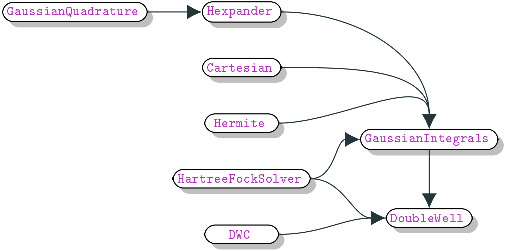


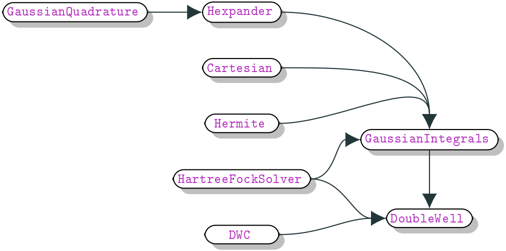
- Parallelization

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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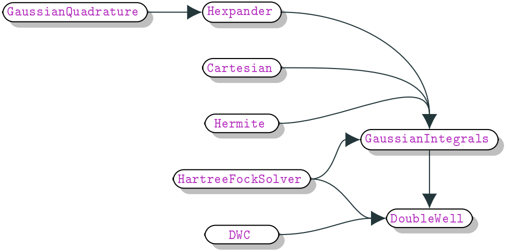

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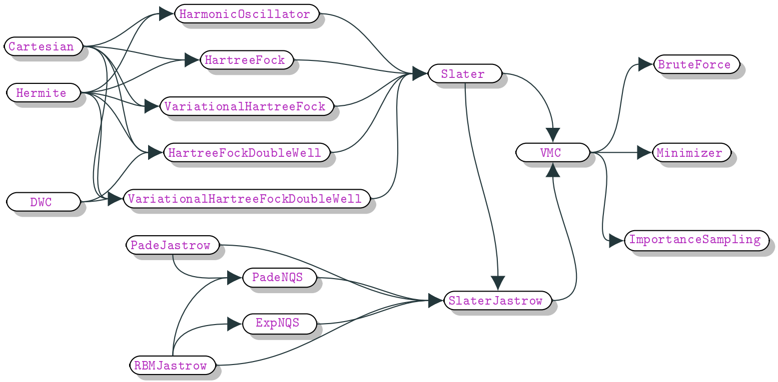
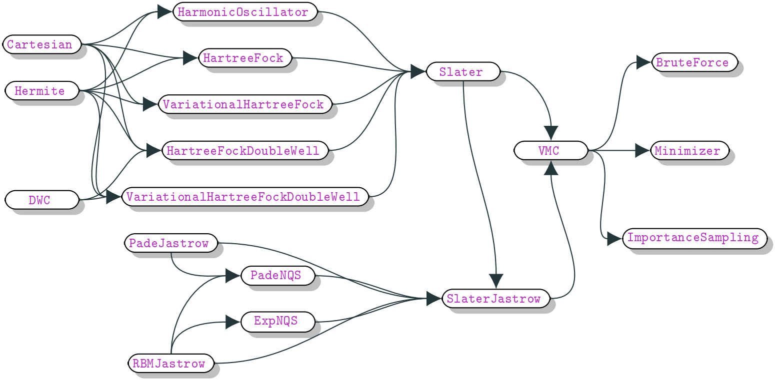
- Tabulation of Two-Body matrix

Implementation: Variational Monte-Carlo

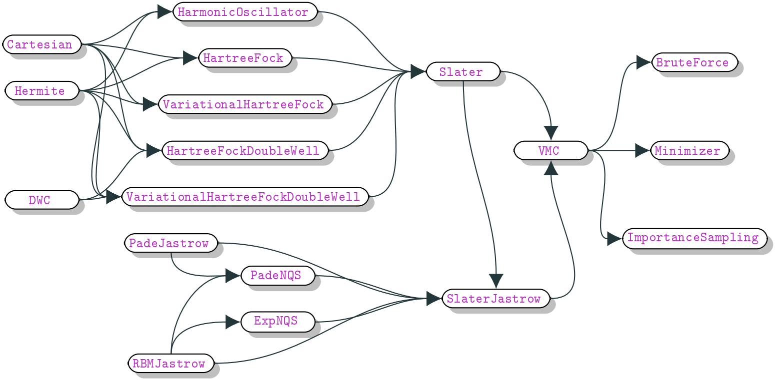


Implementation: Variational Monte-Carlo



- `Hermite` generated with Python and SymPy

Implementation: Variational Monte-Carlo

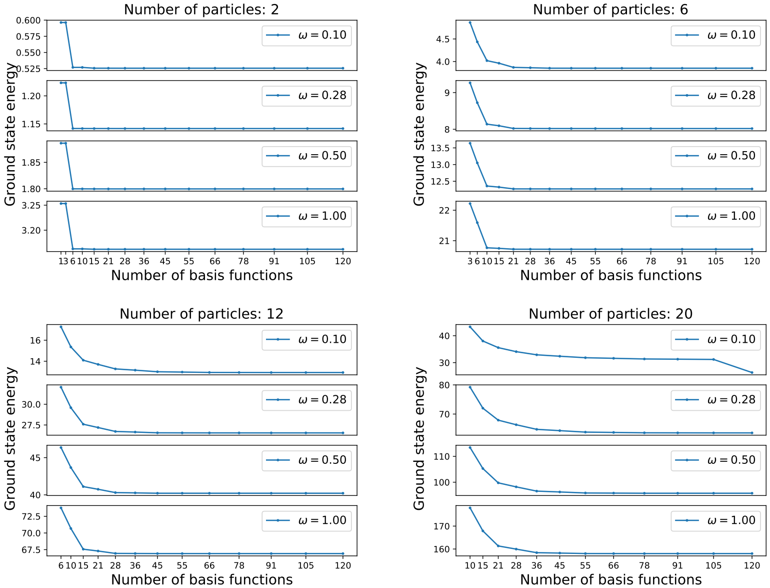


- `Hermite` generated with Python and SymPy
- Wavefunction class generated with Python

Results

Benchmark

Results: Benchmark



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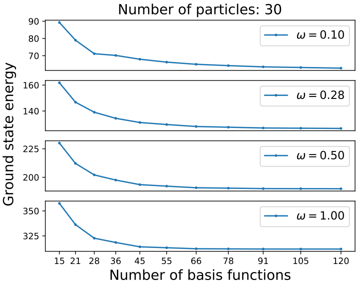
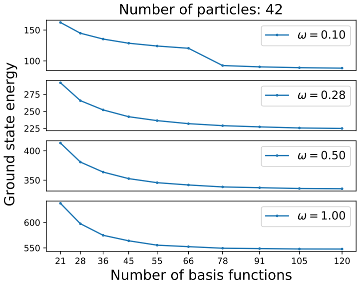
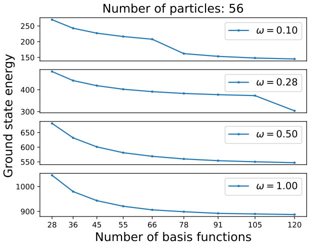
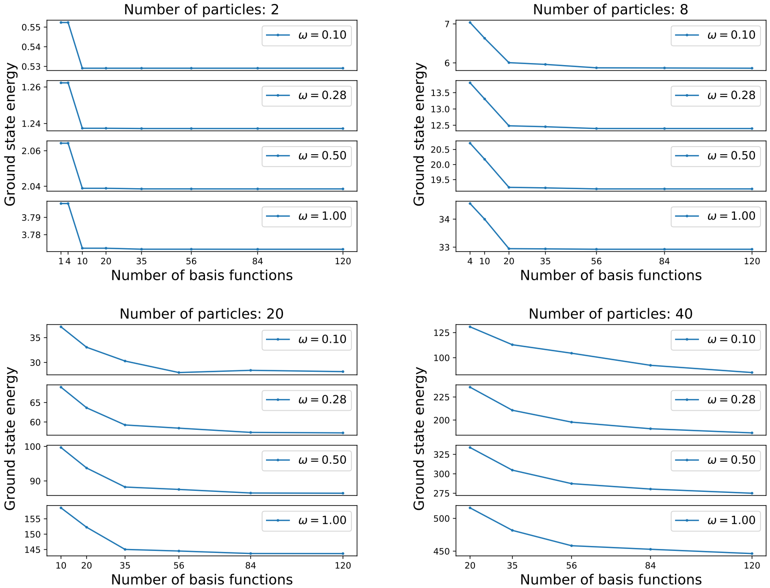






Results: Benchmark



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}

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

Results: Benchmark

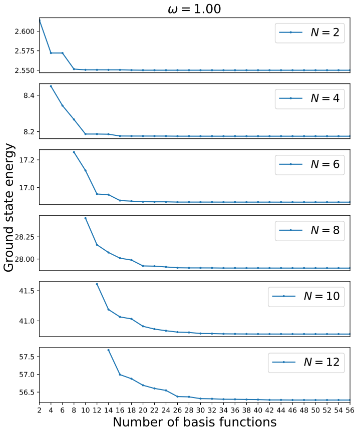
ω	N	
	2	8
0.1	0.51122(5){70}	5.87372(4){120}
0.28	1.21844(5){70}	12.36177(4){168}
0.5	2.02030(4){20}	19.15006(4){112}
1.0	3.72918(5){20}	33.58046(4){168}

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}

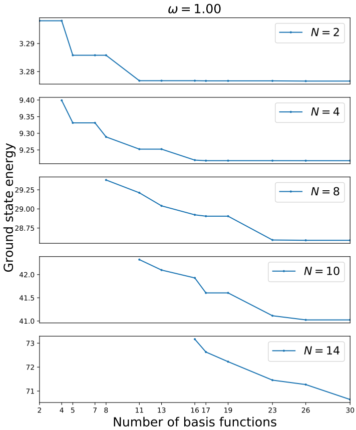
$$\psi_p = \sum_l C_{lp} \psi_l^{\mathrm{HO}}\left(\sqrt{\omega} r\right) J_{\mathrm{Padé}}, \qquad \psi_p = \sum_l C_{lp} \psi_l^{\mathrm{HO}}\left(\sqrt{\alpha\omega} r\right) J_{\mathrm{Padé}}$$

Results: Double-Well Hartree-Fock

2D



3D



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}

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

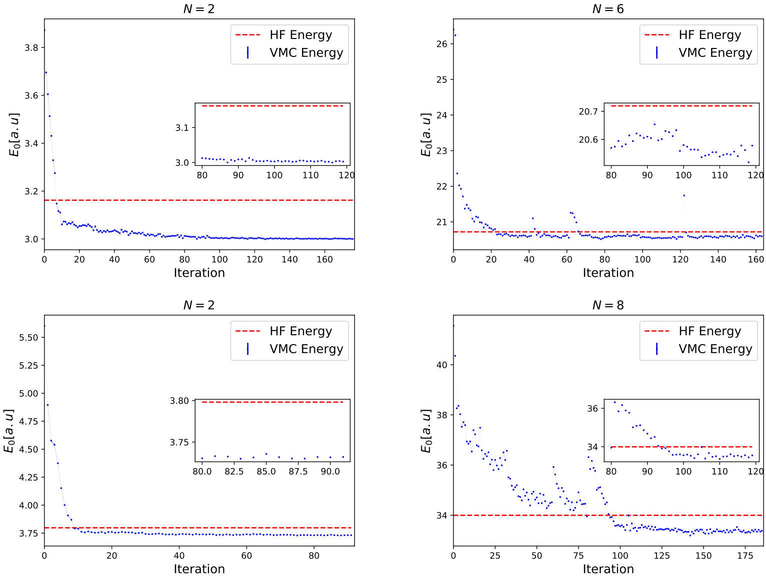
ω	N		
	2	4	8
1.0	3.22226(4){11}	9.17013(4){17}	28.62826(4){26}

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

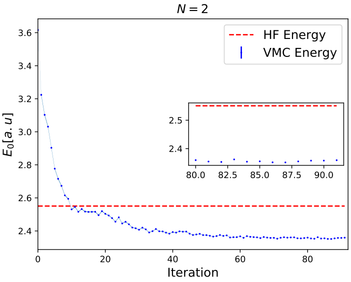
Results: NQS-Jastrow

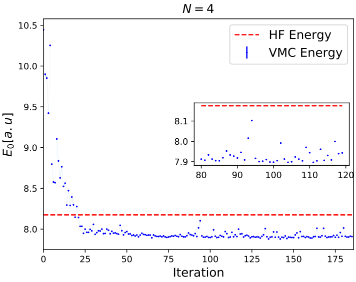
$$J_{\mathbf{NQS}} = e^{-\sum_{i=1}^{N} \frac{\left(r_i - a_i\right)^2}{2\sigma^2}} \prod_{j}^{M} \left(1 + e^{b_j + \sum_{i=1}^{N} \sum_{d=1}^{D} \frac{x_i^{(d)} w_{i+d,j}}{\sigma^2}} \right)$$

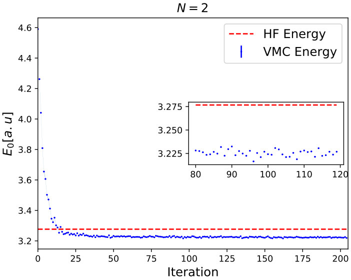
Results: NQS-Jastrow Harmonic Oscillator

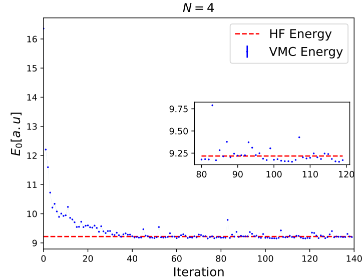


Results: NQS-Jastrow Double-Well







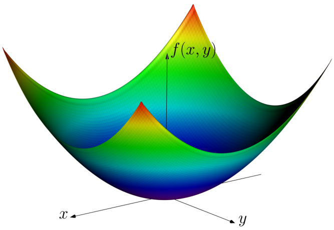


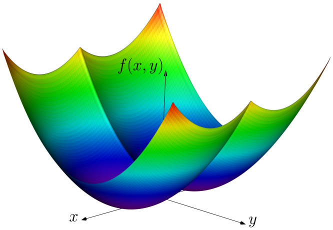
Summary and Conclusion

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

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

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

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

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

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

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

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

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

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

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

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

Conclusion

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Further Work

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- Rewrite with sparse matrices in Hartree-Fock

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- Rewrite with sparse matrices in Hartree-Fock
- Extend to non-isotropic gaussians

End

Questions?

Methods: Hartree-Fock

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

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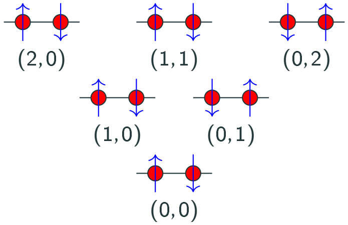

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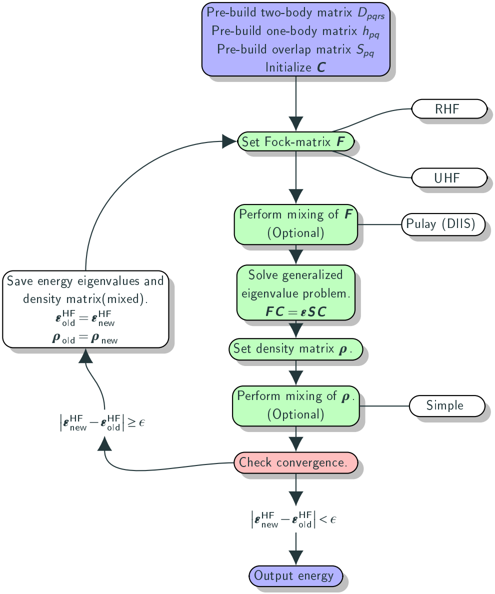

Methods: Variational Monte-Carlo