Quantum Many-Body Simulations of Double Dot System

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Quantum-Dot

1. Small semiconductor nanostructures

Quantum-Dot Model

- Schrödinger equation

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

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

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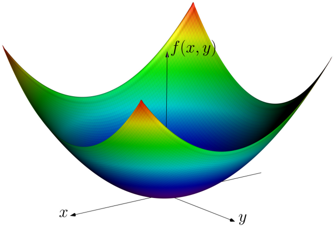
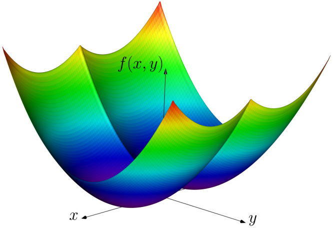
$$V(\boldsymbol{r}) = \frac{1}{2} m\omega^2 r^2 \qquad V(\boldsymbol{r}) = \frac{1}{2} m\omega^2 \left(r^2 - \delta R|x| + R^2\right)$$





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

Slater Determinant and Energy Functional

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

Hartree-Fock

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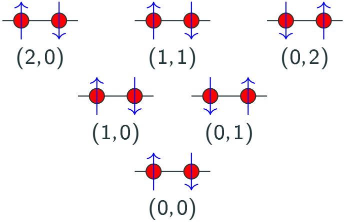

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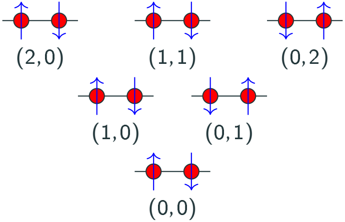
  - The Mean Field Approximation holds.



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    - $\mathscr{F} | \psi \rangle = \boldsymbol{\varepsilon} | \psi \rangle, \boldsymbol{\varepsilon} = (\varepsilon_0, \ldots, \varepsilon_N)$

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- Roothan-Hall: $\boldsymbol{F}\boldsymbol{C}_i = \boldsymbol{\varepsilon}\boldsymbol{S}\boldsymbol{C}_i$
  - $F_{pq} = h_{pq} + \sum_{pq}\rho_{pq}\left(2D_{prqs} \pm D_{prsq}\right)$
  - $h_{pq} \equiv \langle p|h|q\rangle$
  - $\rho_{pq} \equiv \sum_{i=1}^{\frac{N}{2}} C_{pi}C_{qi}^*$
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- 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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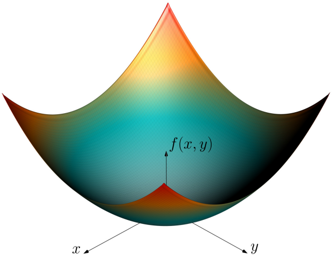
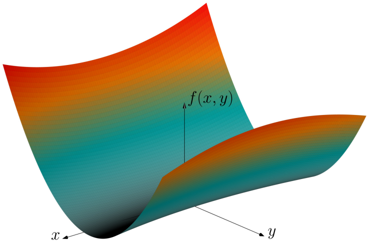
  - Importance Sampling
    - $r^{\text{new}} = r^{\text{old}} + D\Delta t F^{\text{old}} + \sqrt{\Delta t}\xi$
    - $F = \frac{2}{\Psi}\nabla\Psi$
    - $\frac{T(b,a,\Delta t)}{T(a,b,\Delta t)} = \sum_i \exp\left(-\frac{\left(\boldsymbol{r}_i^{(b)} - \boldsymbol{r}_i^{(a)} - D\Delta t\boldsymbol{F}_i^{(a)}\right)^2}{4D\Delta t} + \frac{\left(\boldsymbol{r}_i^{(a)} - \boldsymbol{r}_i^{(b)} - D\Delta t\boldsymbol{F}_i^{(b)}\right)^2}{4D\Delta t}\right)$

Minimization

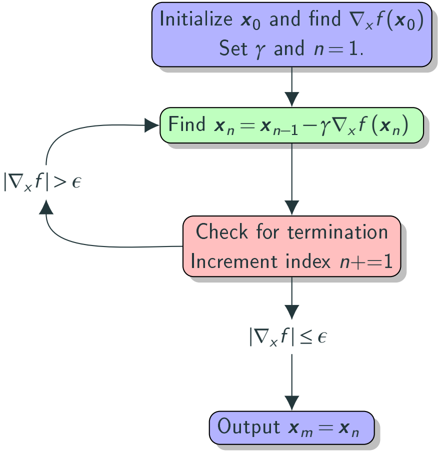
Single-Well



Rosenbrock



Minimization: Gradient Descent



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	$(-8.920 \times 10^{-5}, -8.920 \times 10^{-5})$	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
(0,0.5)	0.0001	100000	(0.994,0.989)	3.131×10^{-5}

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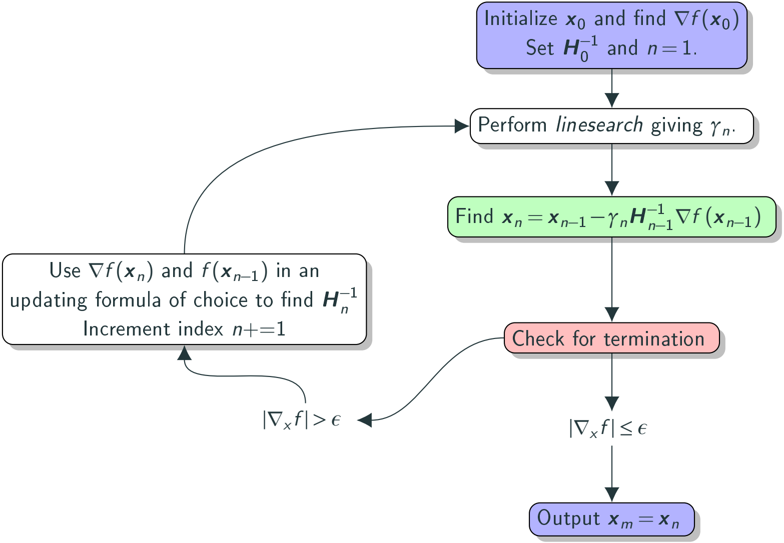

Minimization: Quasi-Newton BFGS

$\boldsymbol{x}_0$	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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$(-0.5,2.0)$	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
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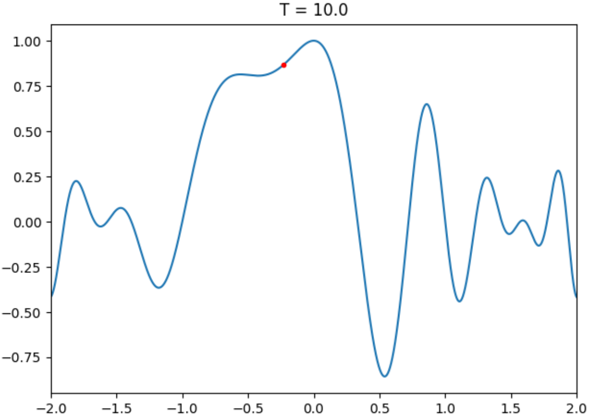
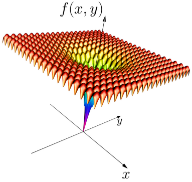
$(5.5,-10.0)$	1	$(-0.996,0.091)$	85.214
$(5.5,-10.0)$	2	$(-0.908,1.087)$	10.549
$(5.5,-10.0)$	10	$(0.027,0.012)$	0.9613
$(5.5,-10.0)$	30	$(1.000,1,000)$	0.000

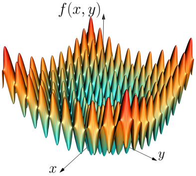
Minimization: Simulated Annealing



Ackley



Rastrigin



Wavefunction

Wavefunction

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

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]

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

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

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- Solution in Cartesian[4]

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

[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

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

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

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

$$E_t^{i+1,j} = \frac{1}{2\omega} E_{t-1}^{ij}$$

$$E_t^{i,j+1} = \frac{1}{2\omega} E_{t-1}^{ij}$$

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

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

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

$$\xi_{00}^n = \left(\frac{-\omega}{2}\right)^n \zeta_n(0)$$

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

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

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Wavefunction: Double-Well

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

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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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Wavefunction: Slater-Jastrow

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

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

Implementation

Implementation

- C++ and Eigen

Implementation

- C++ and Eigen
    - Performance

Implementation

- C++ and Eigen
  - Performance
  - Generalization

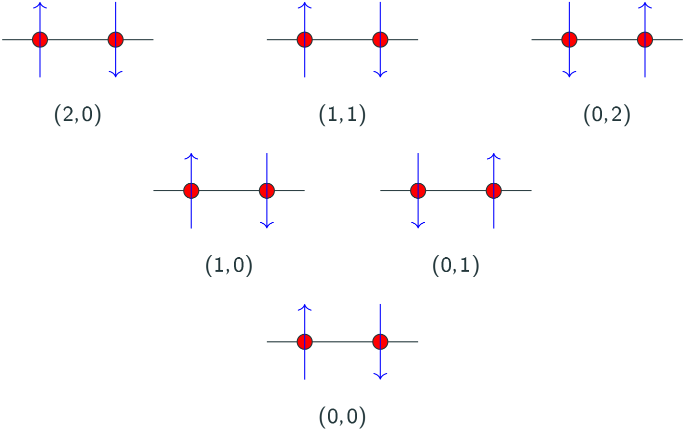
Implementation

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

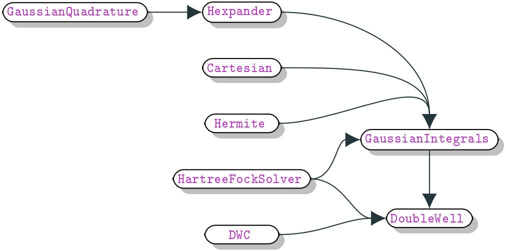
Implementation

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

Implementation: Cartesian



Implementation: Hartree-Fock



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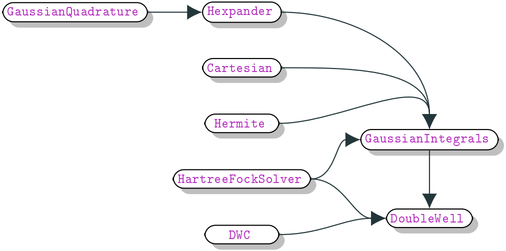
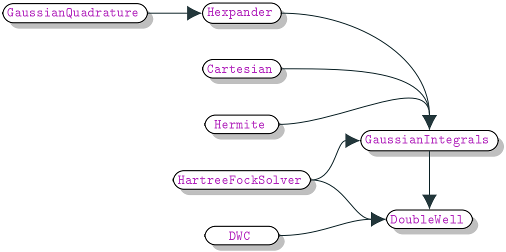


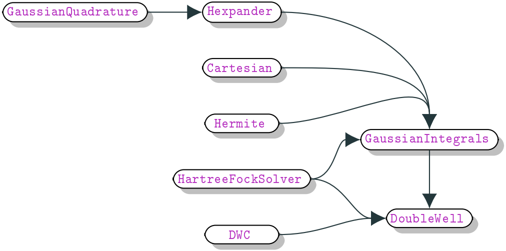
- Parallelization

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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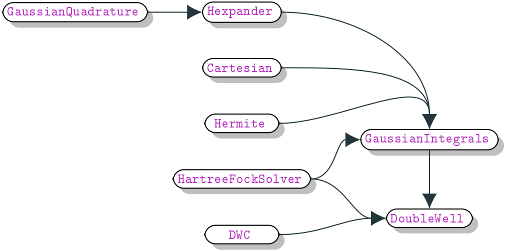
Implementation: Hartree-Fock



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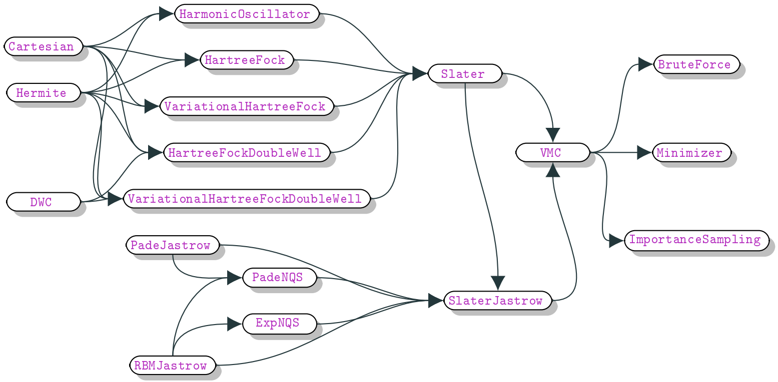
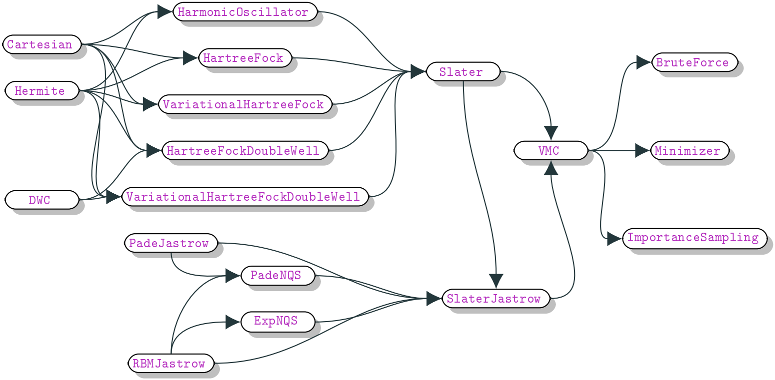
- Hartree-Fock algorithm only run on one process
- Tabulation of Two-Body matrix


HarmonicOscillator
Cartesian
HartreeFock
Hermite
VariationalHartreeFock
HartreeFockDoubleWell
DWC
VariationalHartreeFockDoubleWell
Slater
BruteForce
VMC
Minimizer
ImportanceSampling
PadeJastrow
PadeNQS
ExpNQS
RBMJastrow
SlaterJastrow

Implementation: Variational Monte-Carlo

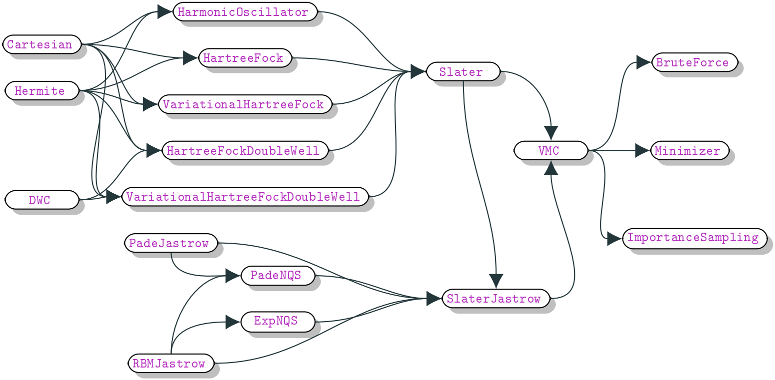


- `Hermite` generated with Python and SymPy

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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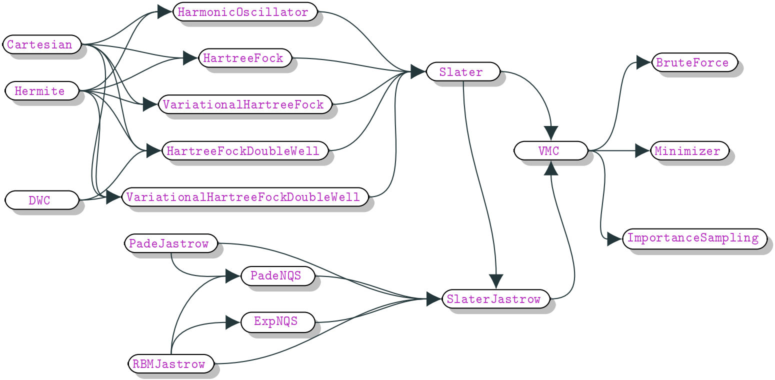
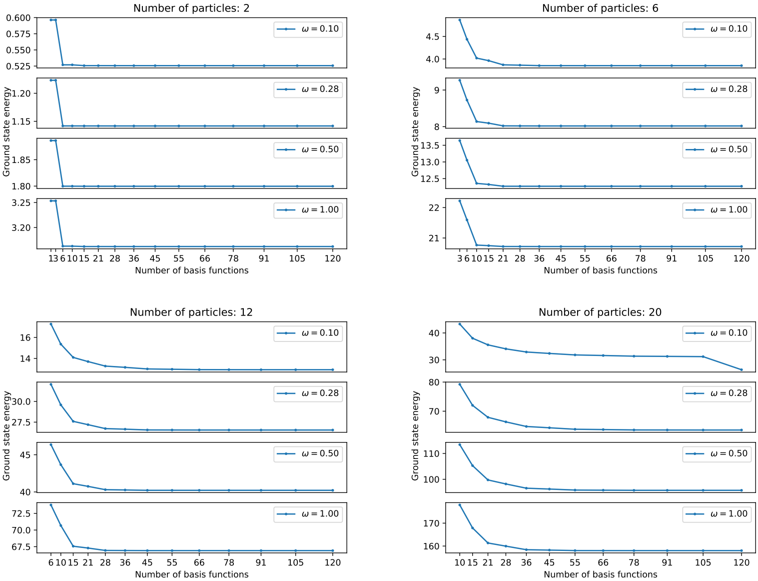


- `Hermite` generated with Python and SymPy
- Wavefunction class can be created with Python

Results

Benchmark

Results: Benchmark



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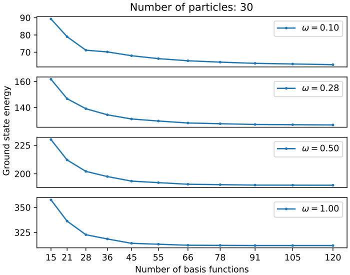
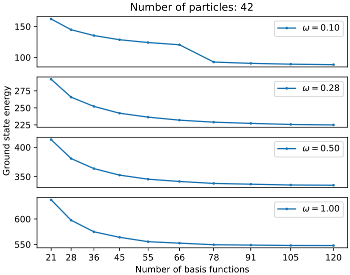
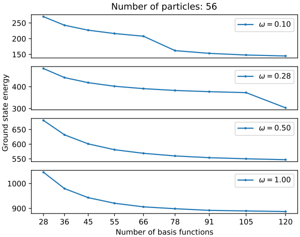
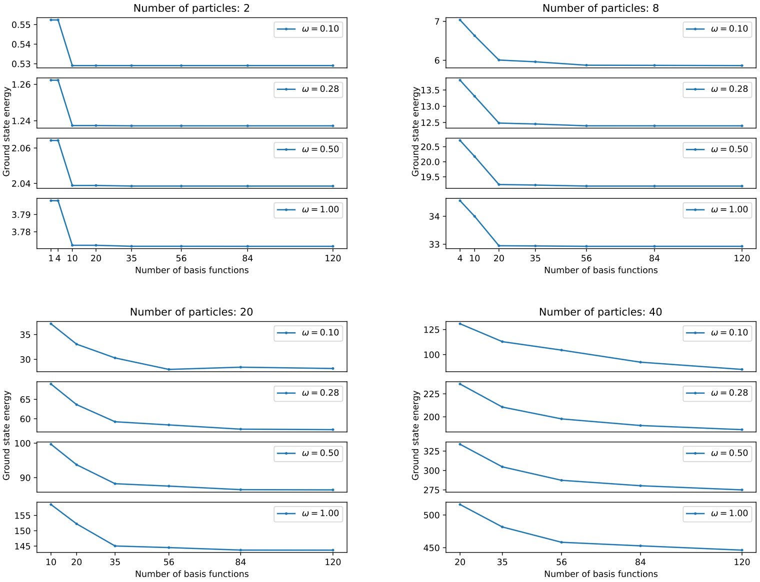






Results: Benchmark



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}

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

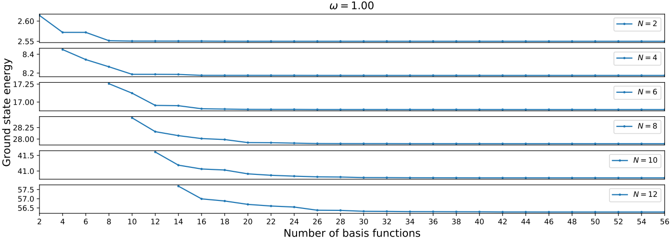
Results: Benchmark

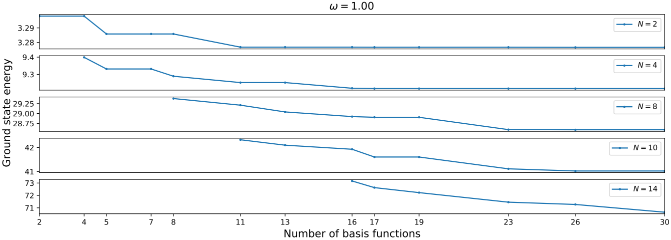
ω	N	
	2	8
0.1	0.51122(5){70}	5.87372(4){120}
0.28	1.21844(5){70}	12.36177(4){168}
0.5	2.02030(4){20}	19.15006(4){112}
1.0	3.72918(5){20}	33.58046(4){168}

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}

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

Results: Double-Well Hartree-Fock





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}

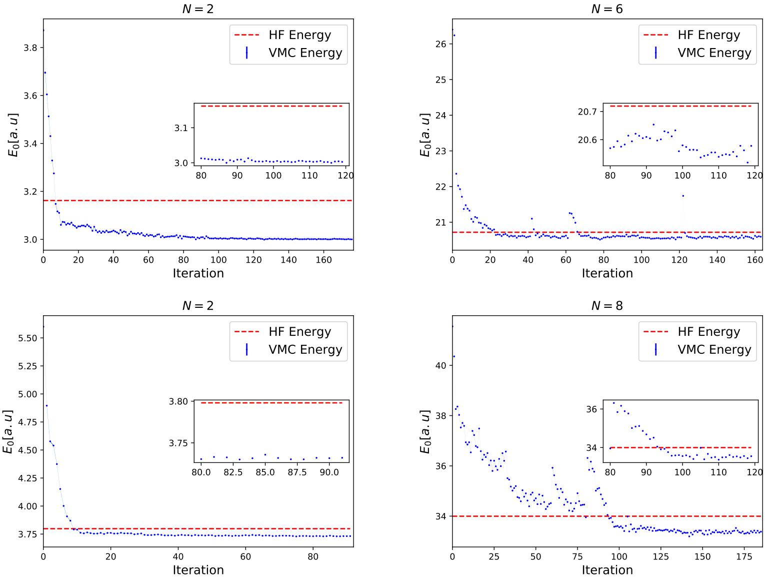
$$\psi_p = \sum_l C_{lp}^{\mathrm{HF}} \sum_k C_{kl}^{\mathrm{DW}} \psi_k^{\mathrm{HO}} \left(\sqrt{\omega} r\right) J_{\text{Padé}}$$

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

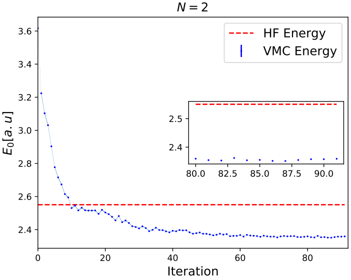
$$\psi_p = \sum_l C_{lp}^{\mathrm{HF}} \sum_k C_{kl}^{\mathrm{DW}} \psi_k^{\mathrm{HO}} \left(\sqrt{\alpha\omega} r\right) J_{\text{Padé}}$$

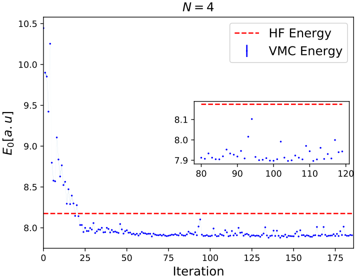
$$J_{\mathbf{NQS}} = e^{-\sum_{i=1}^{N} \frac{\left(r_i - a_i\right)^2}{2\sigma^2}} \prod_{j}^{M} \left(1 + e^{b_j + \sum_{i=1}^{N} \sum_{d=1}^{D} \frac{x_i^{(d)} w_{i+d,j}}{\sigma^2}} \right)$$

Results: NQS-Jastrow Harmonic Oscillator



Results: NQS-Jastrow Double-Well



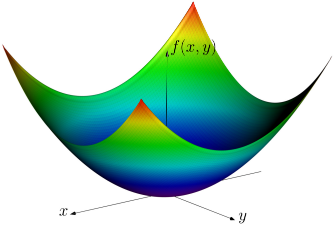


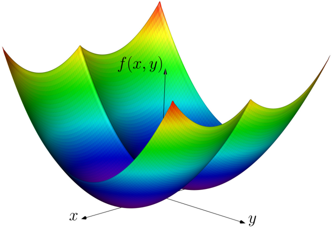
Summary and Conclusion

Summary

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

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





Hartree-Fock

Variational Monte-Carlo

Summary

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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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- General C++ code implemented
- Hartree-Fock limit reached
- Hartree-Fock energies improved with Variational Monte-Carlo
- Stable minimization with NQS-Jastrow

Further Work

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- Extend to non-isotropic gaussians

Questions?

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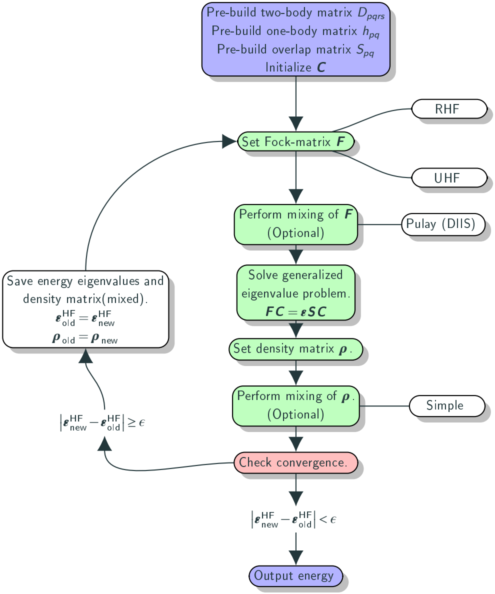
Methods: Hartree-Fock



Methods: Variational Monte-Carlo