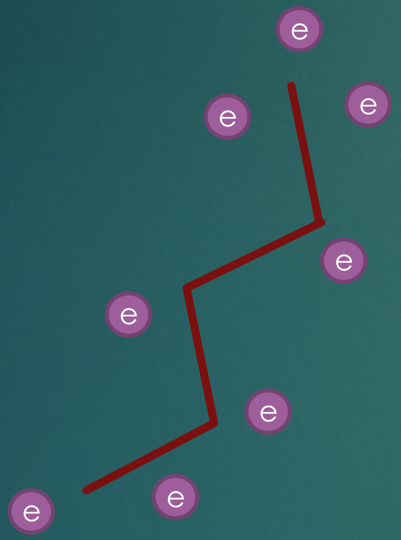
Fermions on a quantum ring

Joshua Cesca, Cedric Simenel, Alexander Bray

ANU, Fundamental and Theoretical Physics

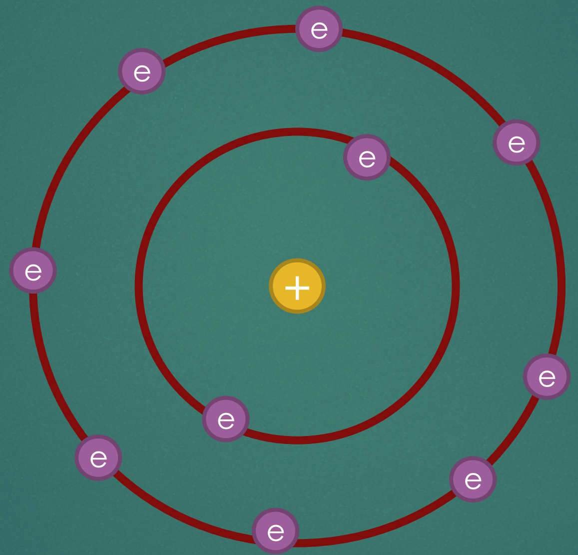
The quantum many-body problem

Many-body Schrodinger equation: $$i\,\hbar\frac{\partial}{\partial t}|\Psi\rangle = \left(\sum_i \hat{T}_i + \sum_{i<j}\hat{V}_{ij}\right)|\Psi\rangle$$



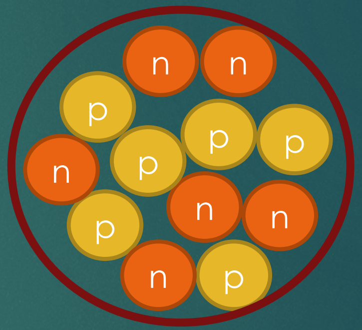
~10^{-9} m

Molecules



~10^{-10} m

Atoms



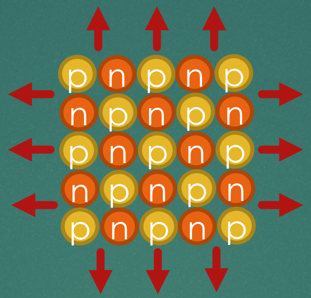
~10^{-15} m

Nuclei

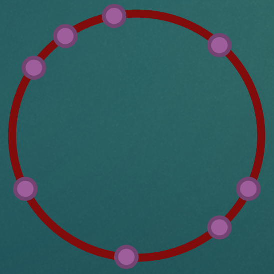
Simplified systems

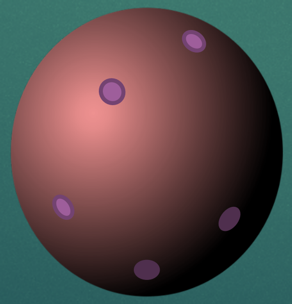
Benchmark many-body approaches with exact solutions

- Homogenous matter



- Quantum rings (ringiums), 2D spheriums…

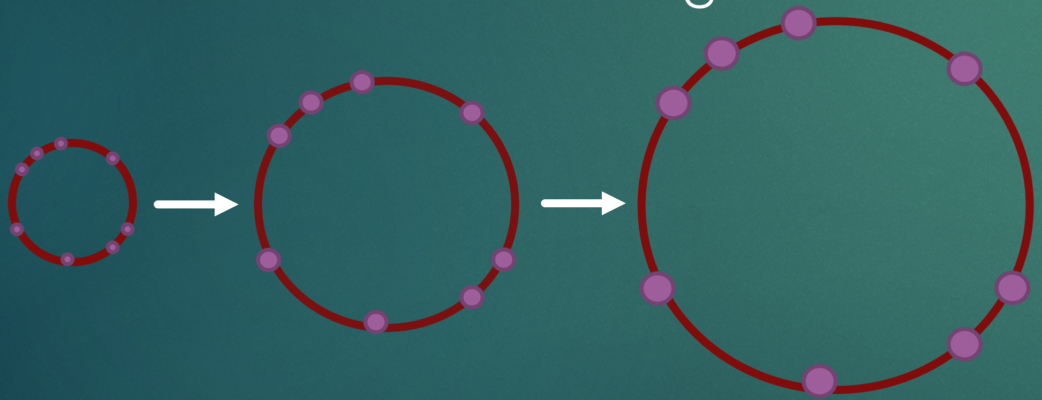




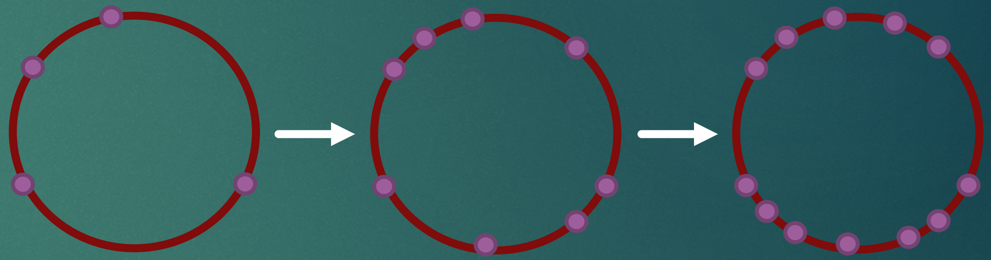
Why a quantum ring?

- Non-homogeneity
- Exact analytical solutions for 2 electrons - *Loos & Gill, Phys. Rev. Lett. 108, 083002 (2012)*
- Generalision to higher dimensions - *Loos & Gill, Phys. Rev. Lett. 103, 123008 (2009)*

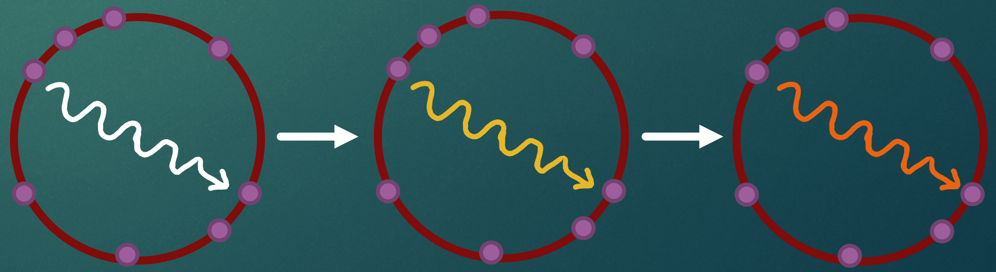
Radius of the ring



Number of fermions



Interaction between fermions



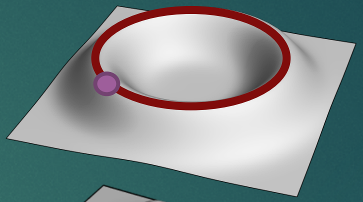
$$H = -\frac{1}{2R^2}\sum_{\alpha=1}^{N}\frac{\partial^2}{\partial\theta_\alpha^2} + \sum_{\alpha<\beta}^{N} V_{\text{int}}(r_{\alpha\beta})$$

Mean-field based methods with ringium

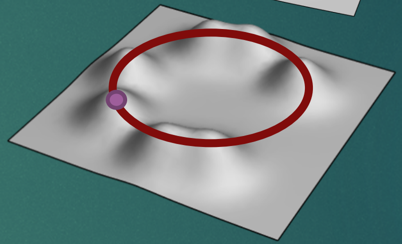
Ground state energy

MF based approaches

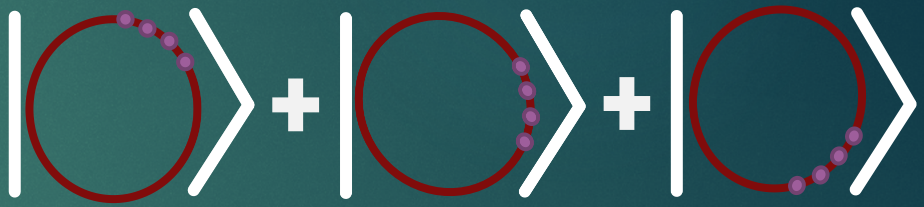
Unbroken symmetry Hartree-Fock



Broken Symmetry Hartree-Fock

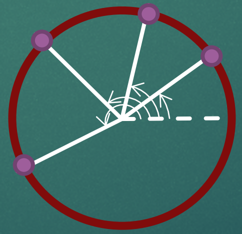


Restored Symmetry Hartree-Fock

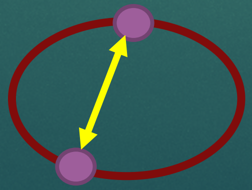


Potentially exact

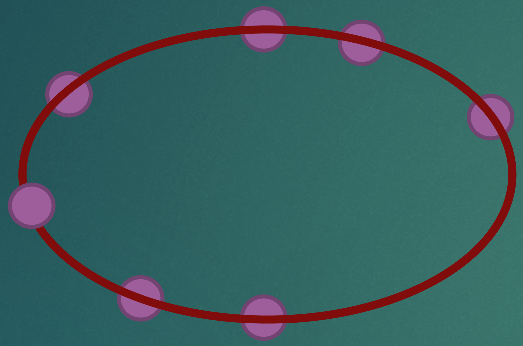
Variational Monte Carlo

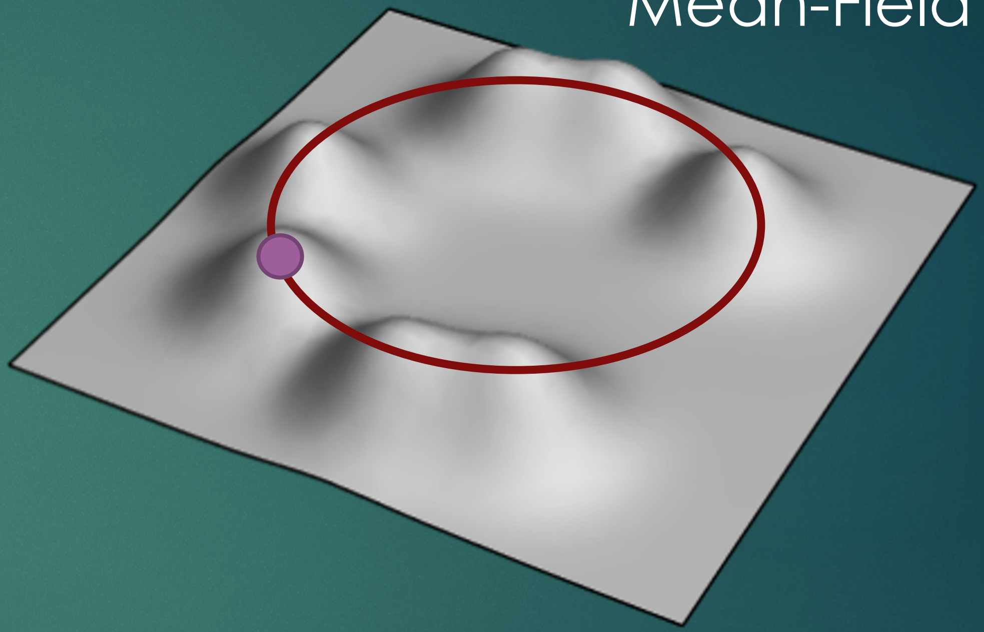


True ground state



The Hartree-Fock approach



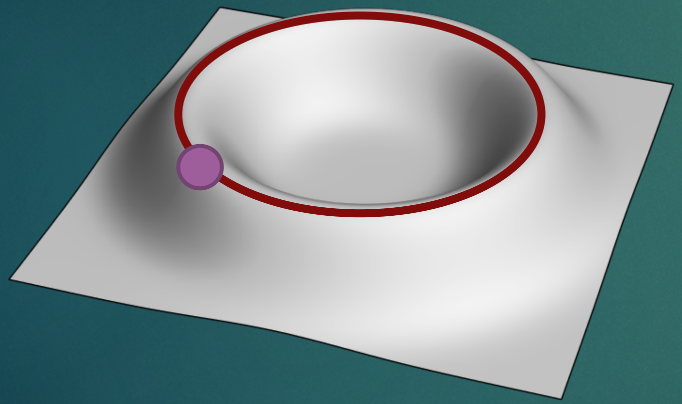


1 x N-body problem → N x 1-body problems

Hartree-Fock state = antisymmetrised product of single-particle wave-functions

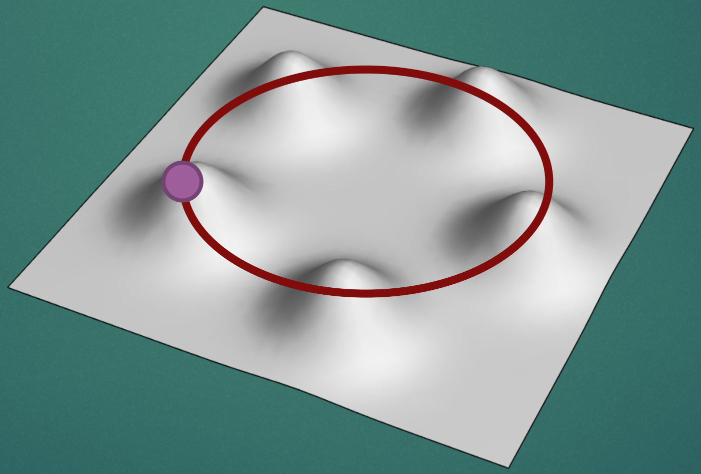
Correlations through symmetry Breaking

Unbroken Symmetry
Hartree-Fock



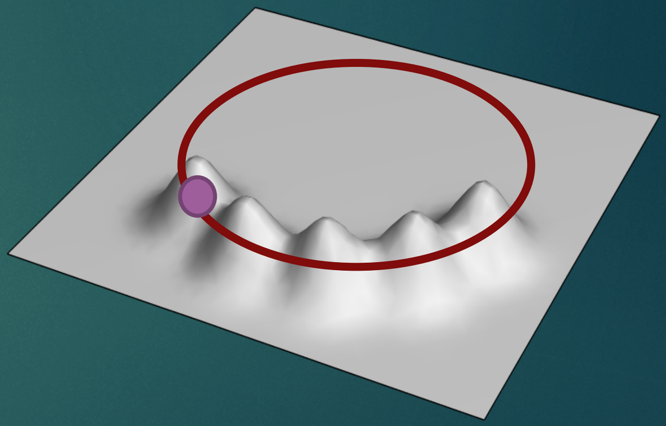
Broken Symmetry
Hartree-Fock

(repulsive interaction)



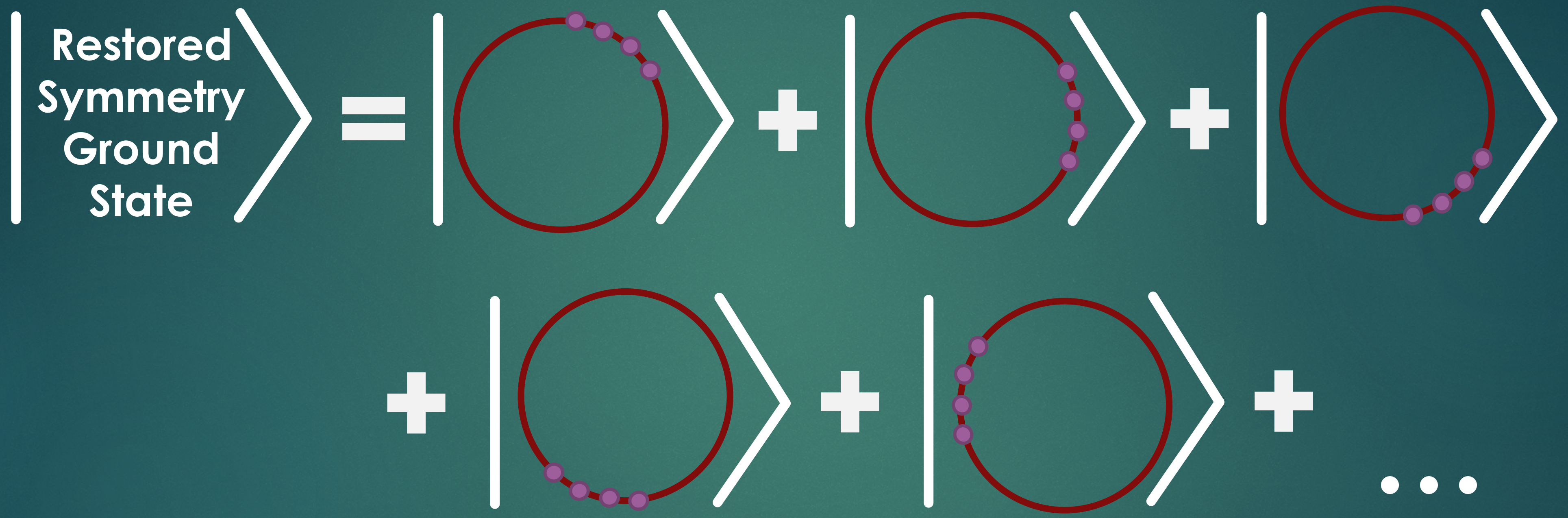
Broken Symmetry
Hartree-Fock

(attractive interaction)



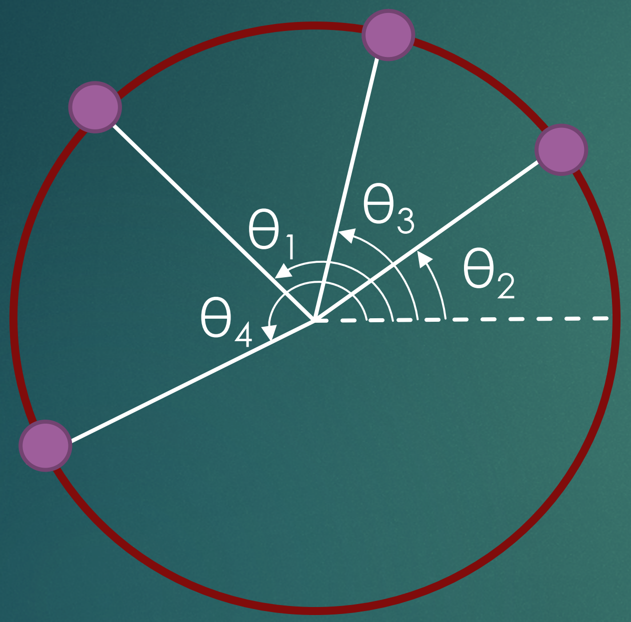
Restoring broken symmetry

True ground state should be symmetric under rotation.



$$|\Psi_{RS}\rangle = \frac{1}{2\pi}\int_0^{2\pi} d\theta \left(e^{-i\theta(J_z - M)}|\Psi_{BS}\rangle\right)$$

Variational Monte Carlo

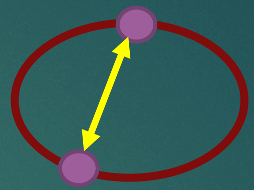


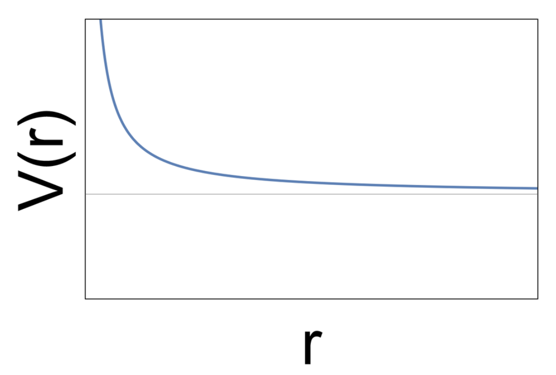
Flexible trial wave function:

$\Psi(\theta_1, \theta_2, \ldots, \theta_n;\ a_1, a_2, \ldots a_m)$

Energy minimisation with respect to the parameters $\{a_1, a_2, \ldots a_m\}$

Comparison with exact results





Exact analytical solutions for 2 electrons

Loos & Gill, Phys. Rev. Lett. 108, 083002 (2012)

Ring Radius (arb. units)	Exact energy (arb. units)	Variational Monte Carlo energy (arb. units)	Hartree-Fock energy (arb. units)
$1/2$	2.25	2.2503 ± 0.0008	2.2732
$\sqrt{3/2}$	0.66667	0.66661 ± 0.00016	0.68646
$\sqrt{\frac{3}{8}(7+\sqrt{33})}$	0.32694	0.32695 ± 0.00006	0.34352
$\sqrt{23/2}$	0.19565	0.19562 ± 0.00003	0.20947

Further VMC comparisons (various interactions and particle numbers) with CASINO solver

Bray & Simenel, Phys. Rev. C, 103, 014302 (2021)

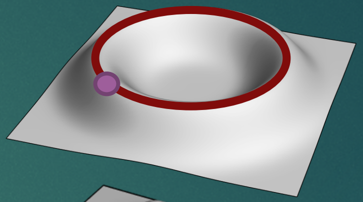
Mean-field based methods with ringium

Ground state energy

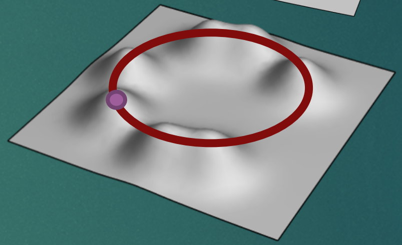
MF based approaches

Numerically "exact"

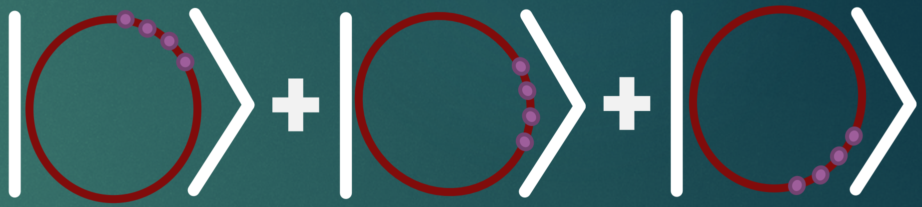
Unbroken symmetry Hartree-Fock



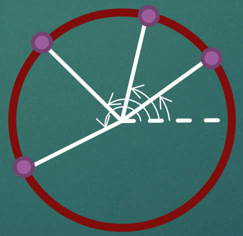
Broken Symmetry Hartree-Fock



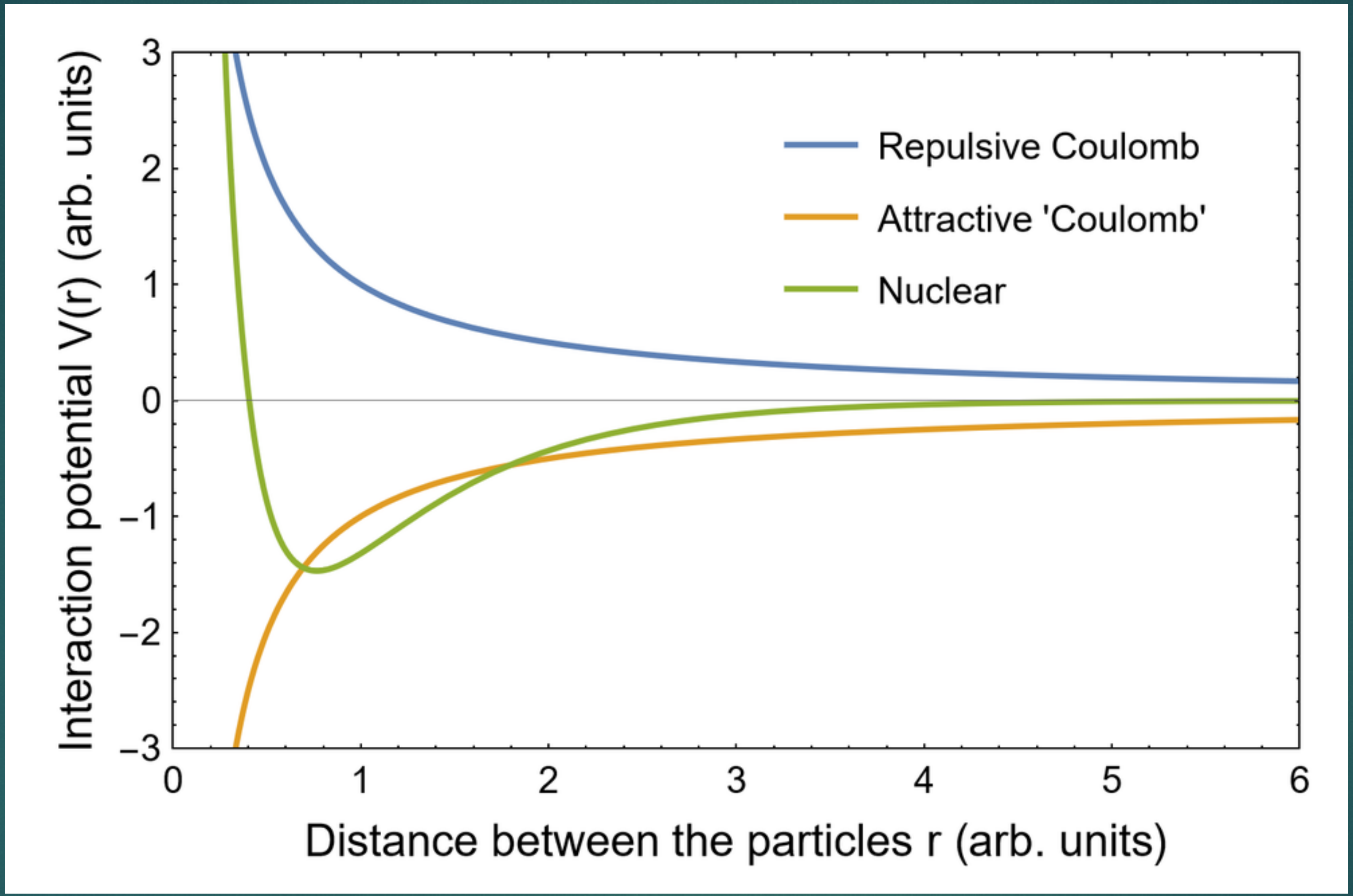
Restored Symmetry Hartree-Fock



Variational Monte Carlo

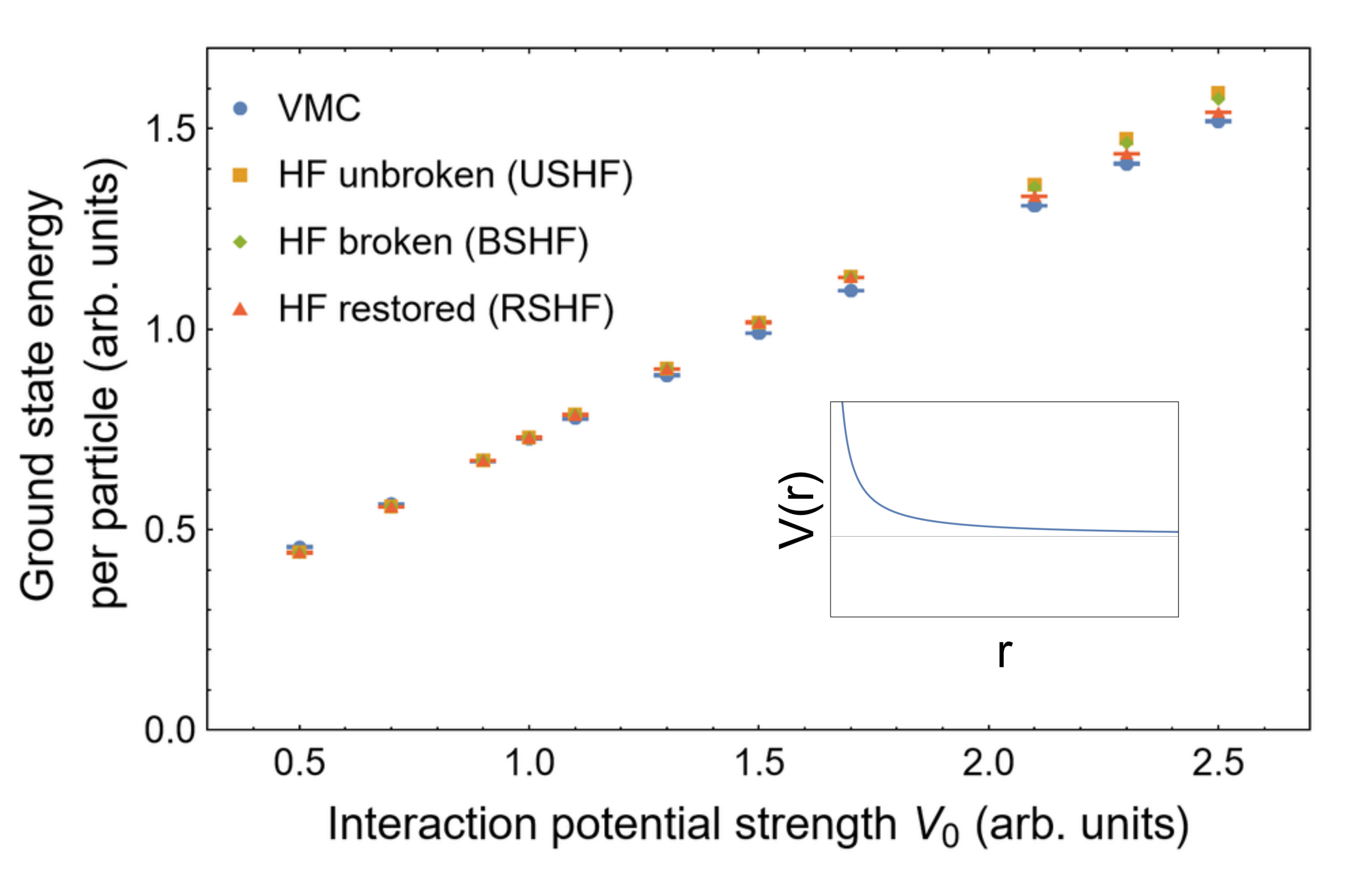


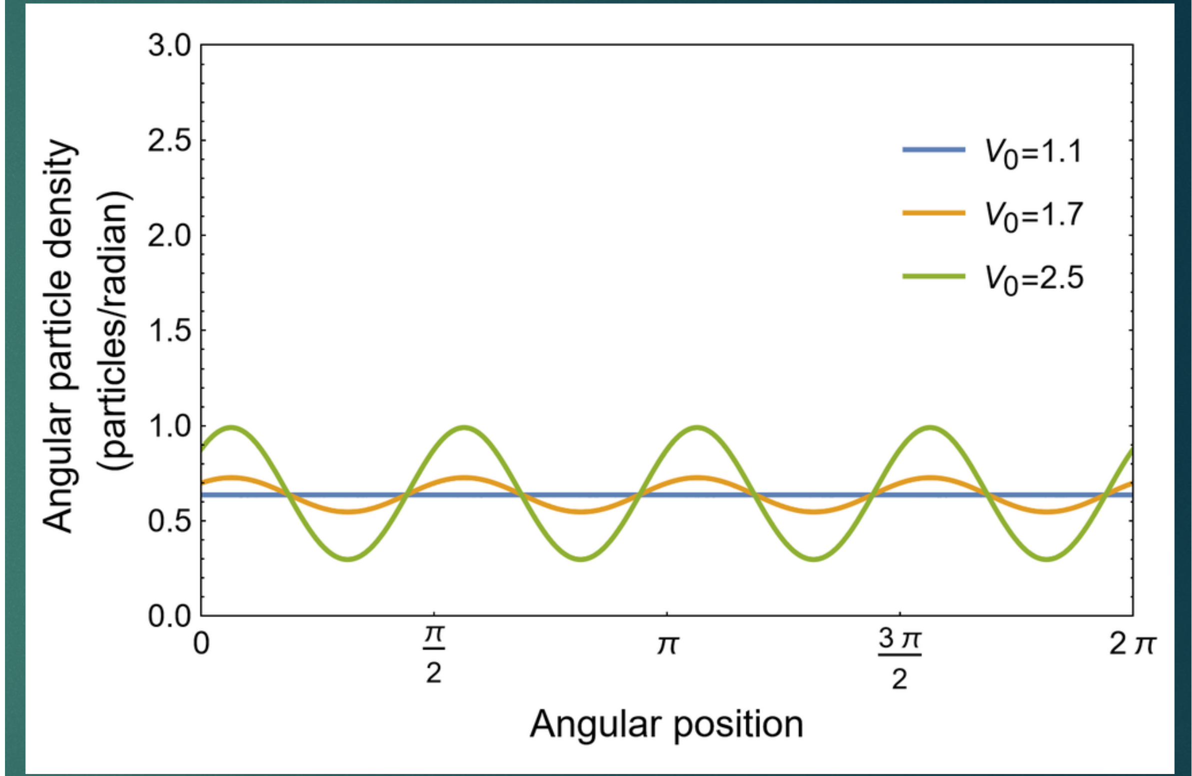
Interactions



Repulsive Interaction:

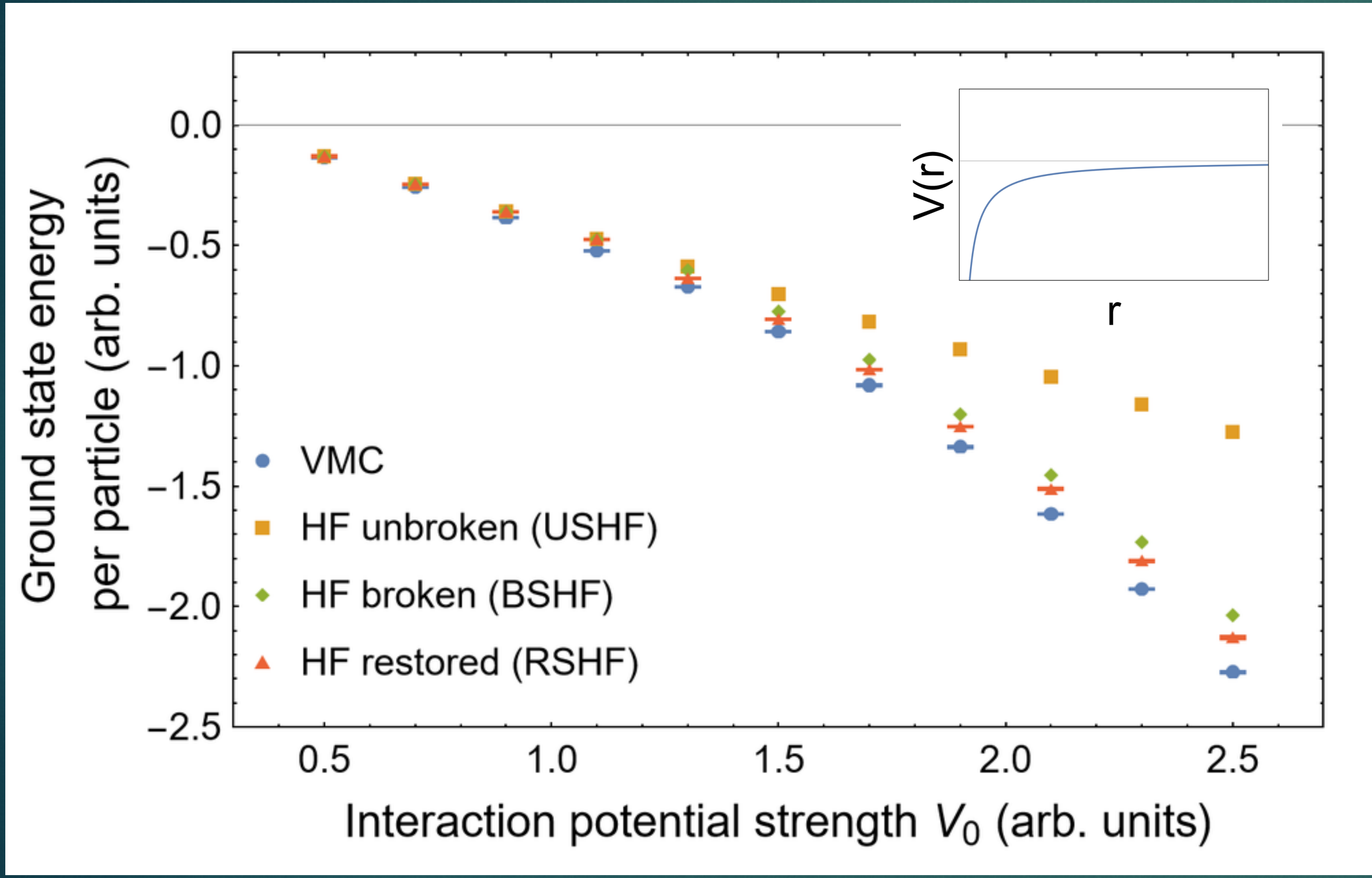
4 particles

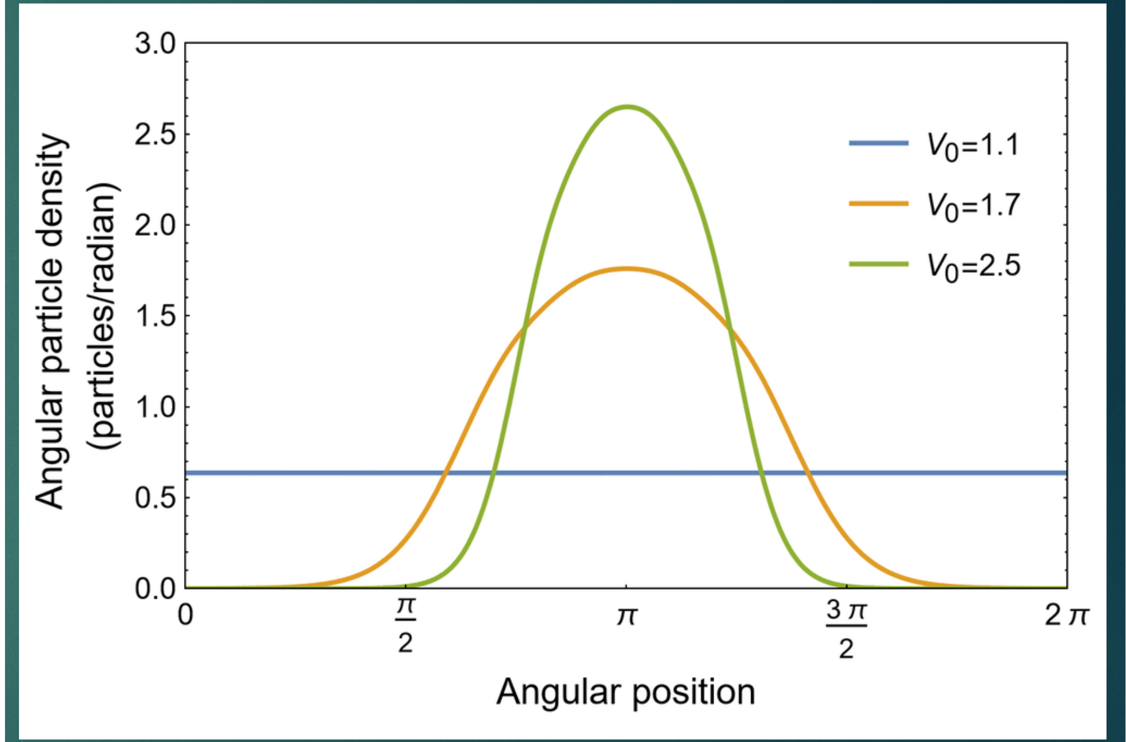




Attractive Interaction:

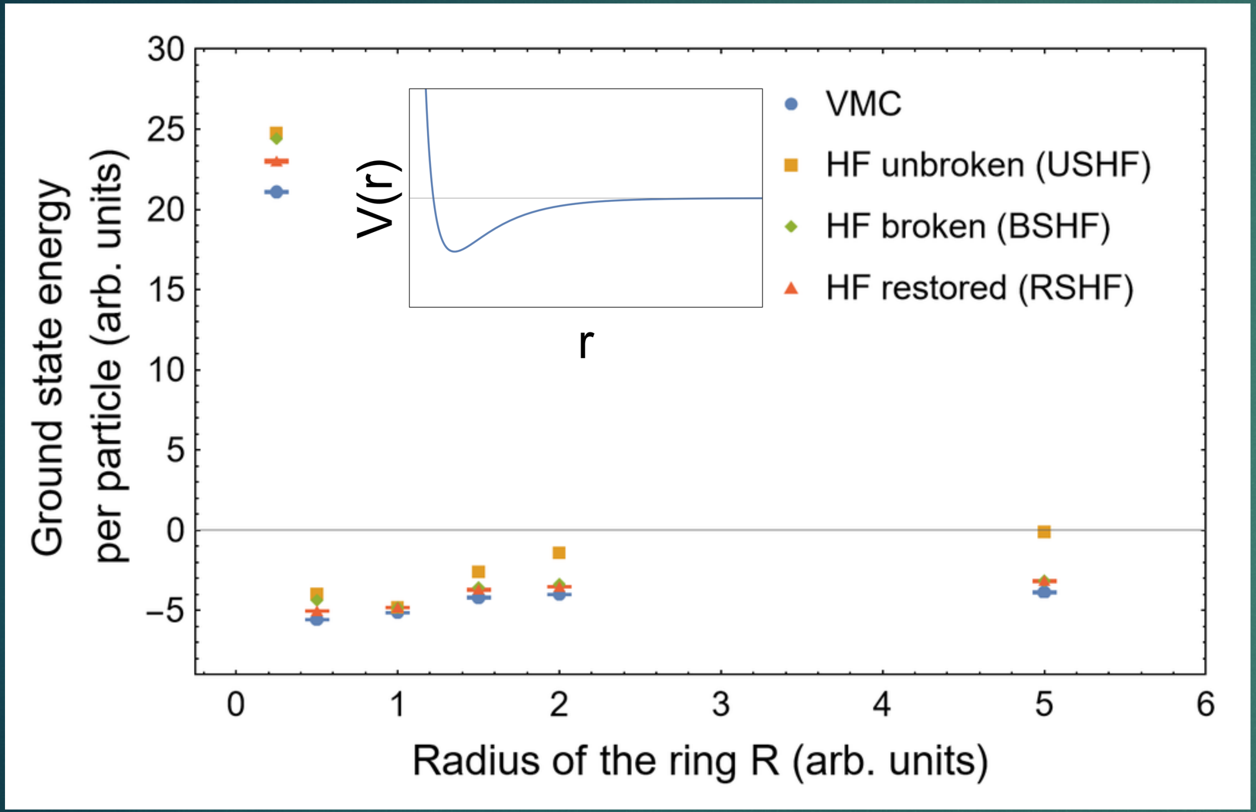
4 particles

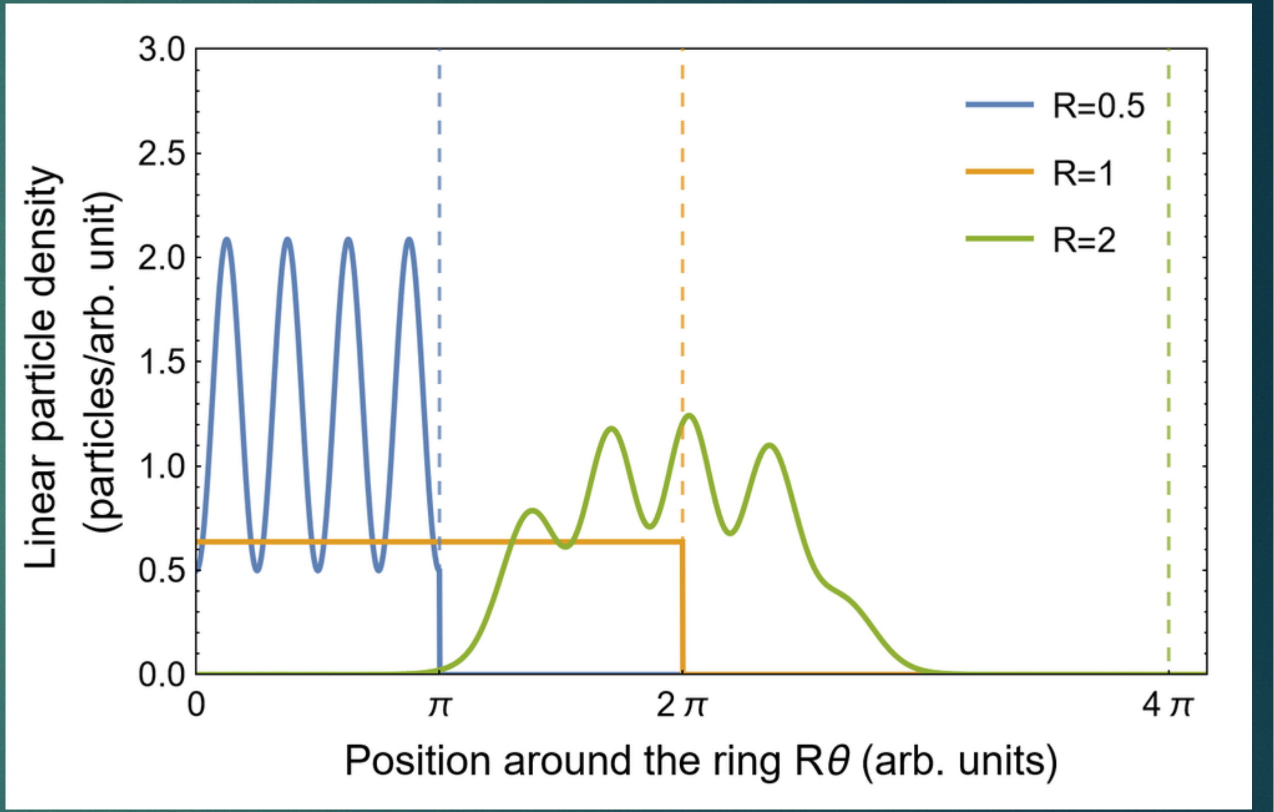




Nuclear interaction:

4 particles





Conclusions and future work

- Numerical solutions for N fermions on a ring MF based methods and VMC
- Symmetry breaking is able to partially account for correlations through localisation
- Restoring the symmetry brings further improvement

- Investigate higher dimensions (2D-spherium)
- Benchmark other approximate methods (e.g. generator coordinate method)
- Break other symmetries (e.g. U(1) gauge invariance ⇒ pairing correlations & superfluidity)

VMC

Energy $\langle\Psi_{\text{vmc}}(\boldsymbol{a})|\hat{H}|\Psi_{\text{vmc}}(\boldsymbol{a})\rangle = \frac{\int d\boldsymbol{\theta}\,\Psi^*_{\text{vmc}}(\boldsymbol{\theta},\boldsymbol{a})H\Psi_{\text{vmc}}(\boldsymbol{\theta},\boldsymbol{a})}{\int d\boldsymbol{\theta}\,\Psi^*_{\text{vmc}}(\boldsymbol{\theta},\boldsymbol{a})\Psi_{\text{vmc}}(\boldsymbol{\theta},\boldsymbol{a})}$

calculated as $\langle\Psi_{\text{vmc}}(\boldsymbol{a})|\hat{H}|\Psi_{\text{vmc}}(\boldsymbol{a})\rangle = \int d\boldsymbol{\theta} P(\boldsymbol{\theta},\boldsymbol{a})E_L(\boldsymbol{\theta},\boldsymbol{a})$ where $P(\boldsymbol{\theta},\boldsymbol{a}) = \frac{|\Psi_{\text{vmc}}(\boldsymbol{\theta},\boldsymbol{a})|^2}{\int d\boldsymbol{\theta}|\Psi_{\text{vmc}}(\boldsymbol{\theta},\boldsymbol{a})|^2}$ and $E_L(\boldsymbol{\theta},\boldsymbol{a}) = \frac{H\Psi_{\text{vmc}}(\boldsymbol{\theta},\boldsymbol{a})}{\Psi_{\text{vmc}}(\boldsymbol{\theta},\boldsymbol{a})}$

treated as a probability — *Energy of the configuration*

using Metropolis algorithm

Uncertainty $\sigma_{E_L} = \sqrt{\frac{\sum_{i=1}^{n_s}(E_L(\boldsymbol{\theta}_i,\boldsymbol{a}) - \langle E_L(\boldsymbol{a})\rangle)^2}{n_s(n_s-1)}}$

Condition for continuity $\left.\frac{\partial^2\Psi}{\partial r^2_{\alpha\beta}}\right|_{r_{\alpha\beta}\to 0} = \left.\frac{V_1}{r_{\alpha\beta}}\Psi\right|_{r_{\alpha\beta}\to 0}$ (equiv. Kato cusp condition)

Wave function

$$\Psi_{\text{vmc}}(\theta_1,\theta_2,...,\theta_n,\boldsymbol{a}) = \begin{vmatrix} \phi_1(\theta_1) & \phi_1(\theta_2) & \cdots & \phi_1(\theta_n) \\ \phi_2(\theta_1) & \phi_2(\theta_2) & \cdots & \phi_2(\theta_n) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_n(\theta_1) & \phi_n(\theta_2) & \cdots & \phi_n(\theta_n) \end{vmatrix} \prod_{\alpha<\beta}^{N} f(r_{\alpha\beta},\boldsymbol{a})$$

$$\propto \prod_{\alpha<\beta}^{N}\sin\left(\frac{\theta_i-\theta_j}{2}\right) \propto \prod_{\alpha<\beta}^{N} r^*_{\alpha\beta}$$

Vandermonde determinant

Jastrow function

$$= \exp\left(\sum_{\alpha<\beta}^{N}\sum_{k=1}^{4} a_k r^k_{\alpha\beta}\right)$$

Single particles for N odd

$$\frac{1}{\sqrt{2\pi}}, \frac{\sin(\theta)}{\sqrt{\pi}}, \frac{\cos(\theta)}{\sqrt{\pi}}, \frac{\sin(2\theta)}{\sqrt{\pi}}, \frac{\cos(2\theta)}{\sqrt{\pi}}, ..., \frac{\sin((N-1)\theta/2)}{\sqrt{\pi}}, \frac{\cos((N-1)\theta/2)}{\sqrt{\pi}}$$

and for Neven

$$\frac{\sin(\theta/2)}{\sqrt{\pi}}, \frac{\cos(\theta/2)}{\sqrt{\pi}}, \frac{\sin(3\theta/2)}{\sqrt{\pi}}, \frac{\cos(3\theta/2)}{\sqrt{\pi}}, ..., \frac{\sin((N-1)\theta/2)}{\sqrt{\pi}}, \frac{\cos((N-1)\theta/2)}{\sqrt{\pi}}$$

R. J. Needs, M. D. Towler, N. D. Drummond, and P. L. Ríos. "Continuum variational and diffusion quantum Monte Carlo calculations". *Journal of Physics: Condensed Matter* 22.2 (2010), p. 023201.