Modeling of Atoms; Comparing the Hubbard Model with Variational Monte Carlo for insight into N-body problems

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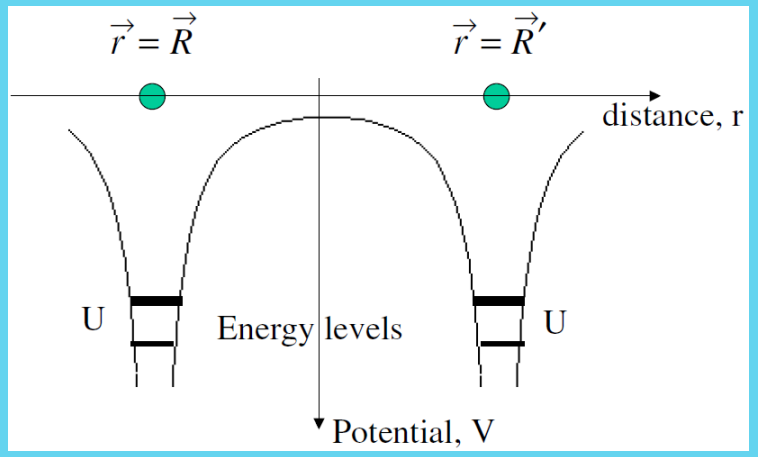
Outline

- The Hamiltonian
- The Hubbard Model
- Variational Monte Carlo
- Results
- Conclusion

Modeling Molecular Hydrogen



$$\hbar = m_e = e = 1$$

$$H = -\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 + \frac{1}{|R_1 - R_2|} + \frac{1}{|r_1 - R_1|} + \frac{1}{|r_1 - R_2|} + \frac{1}{|r_2 - R_1|} + \frac{1}{|r_2 - R_2|} + \frac{1}{|r_1 - r_2|}$$

$$h_1 = -\frac{1}{2}\nabla_1^2 + \frac{1}{|r_1 - R_1|} + \frac{1}{|r_1 - R_2|} \qquad h_2 = -\frac{1}{2}\nabla_2^2 + \frac{1}{|r_2 - R_1|} + \frac{1}{|r_2 - R_2|} \qquad V_{12} = \frac{1}{|r_1 - r_2|} \qquad R_{12} = |r_1 - r_2|$$

$$\boxed{H = h_1 + h_2 + V_{12} + \frac{1}{R_{12}}}$$

Hubbard Model

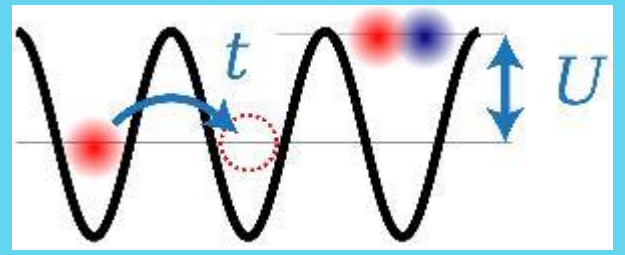
Second Quantization

$$\Psi^\dagger = \sum_{\alpha k} \varphi_{\alpha k}^*(x) c_{\alpha k}^\dagger$$

Variational Monte Carlo

$$E_v = \frac{\langle \Psi_T | H | \Psi_T \rangle}{\langle \Psi_T | \Psi_T \rangle} \geq E_0$$

One Band Hubbard Model PBC



$$H = -t\sum_{j}^{L}\left(c_{j\uparrow}^{\dagger}c_{(j+1)\uparrow} + c_{(j+1)\downarrow}^{\dagger}c_{j\downarrow}\right) + U\sum_{j}^{L} n_{j\uparrow}n_{j\downarrow}$$

$$t_{j,j+1} = \int \varphi_j^*(r)\left[-\frac{1}{2}\nabla^2 + V(r)\right]\varphi_{j+1}(r)d^3r$$

$$U_{jj} = \int \varphi_j^*(r)\varphi_i^*(r')\frac{1}{|r-r'|}\varphi_j(r)\varphi_j(r')d^3rd^3r'$$

$\|0\rangle$	No electron on site j
$c_{j\uparrow}^{\dagger}\|0\rangle$	Spin up electron on site j
$c_{j\downarrow}^{\dagger}\|0\rangle$	Spin down electron on site j
$c_{j\uparrow}^{\dagger}c_{j\downarrow}^{\dagger}\|0\rangle$	Spin up and down on electron on site j
$c_{2\uparrow}^{\dagger}c_{1\downarrow}^{\dagger}c_{3\downarrow}^{\dagger}\|0\rangle$	All electron states can be expressed in terms of the vacuum state and creation/annihilation operators

$$c_{2\uparrow}^{\dagger}c_{1\downarrow}^{\dagger}c_{3\downarrow}^{\dagger}c_{3\uparrow}^{\dagger}|0\rangle = |\updownarrow\uparrow\downarrow 0\rangle = |\downarrow 0\downarrow 0\rangle_{\downarrow}|\uparrow\uparrow 0\ 0\rangle_{\uparrow} = |1010\rangle_{\downarrow}|1100\rangle_{\uparrow}$$

The Code: Building the basis and applying the ladder operators

$L = 4 \qquad N_\uparrow = 3 \qquad N_\downarrow = 2$

0. $\|0111\rangle$	0. $\|0011\rangle$
1. $\|1011\rangle$	1. $\|0101\rangle$
2. $\|1101\rangle$	2. $\|0110\rangle$
3. $\|1110\rangle$	3. $\|1001\rangle$
	4. $\|1010\rangle$
	5. $\|1100\rangle$

$\binom{4}{3} * \binom{4}{2} = 24\ possible\ combinations$

Indexing: Row-major order

$$index = index_\uparrow * 6 + index_\downarrow$$

Hopping Term

$$-t \sum_{j=1}^{4} \left(c_{j\uparrow}^\dagger c_{(j+1)\uparrow} + c_{(j+1)\downarrow}^\dagger c_{j\downarrow} \right)$$

$$\sum_{j=1}^{4} \left(c_{j\uparrow}^\dagger c_{(j+1)\uparrow} \right) |1011\rangle_\uparrow |0110\rangle_\downarrow = (|1101\rangle_\uparrow + |0111\rangle_\uparrow)|0110\rangle_\downarrow$$

$$\sum_{j=1}^{4} \left(c_{(j+1)\downarrow}^\dagger c_{j\downarrow} \right) |1011\rangle_\uparrow |0110\rangle_\downarrow = |1011\rangle_\uparrow (|1010\rangle_\downarrow + |0101\rangle_\downarrow)$$

Memory Limitations: integer → 4 bytes double → 8 bytes

10 choose 5 = 252 252*2 = 63,504 $63{,}504^2$ = 4,032,758,016 4,032,758,016*8 bytes = 32.3 Gbytes

Variational Monte Carlo Method

Variational Principle

(Total energy) $E_v = \frac{\langle \Psi_T | H | \Psi_T \rangle}{\langle \Psi_T | \Psi_T \rangle} \geq E_0$

Monte Carlo Integration

$$E_v = \frac{\langle \Psi_T | H | \Psi_T \rangle}{\langle \Psi_T | \Psi_T \rangle} = \frac{\int dR \Psi_T(R)^2 E_L(R)}{\int dR \Psi_T(R)^2} = \int dR \rho(R) E_L(R)$$

Local energy $E_L(R) = \frac{H\Psi_T(R)}{\Psi_T(R)}$

Normalized Probability Density $\rho(R) = \frac{\Psi_T(R)^2}{\int dR \Psi_T(R)^2}$

Variational energy is the average of the local energy on a sample of M points, R_k sampled from the probability density

$$E_v \cong \langle E_L \rangle = \frac{1}{M} \sum_{k=1}^{M} E_L(R_k)$$

Variational Monte Carlo Method

The wave function $\Psi_T(R) = J(R)\Phi(R)$

$\Phi(R)$ Slater Determinant

$J(R)$ Jastow Factor

<u>Helium</u>

$$\Psi_T(r_1, r_2) = e^{-2r_1} e^{-2r_2} e^{\frac{r_{12}}{2(1+\alpha r_{12})}}$$

$$E_L(R) = \frac{H\Psi_T(R)}{\Psi_T(R)}$$

$$E_L(r_1, r_2) = -4 + \frac{\alpha}{(1+\alpha r_{12})} + \frac{\alpha}{(1+\alpha r_{12})^2} + \frac{\alpha}{(1+\alpha r_{12})^3} + \frac{1}{4(1+\alpha r_{12})^4} + \frac{\hat{r}_{12}\cdot(\hat{r}_1 - \hat{r}_2)}{(1+\alpha r_{12})^2}$$

Variational Monte Carlo Method

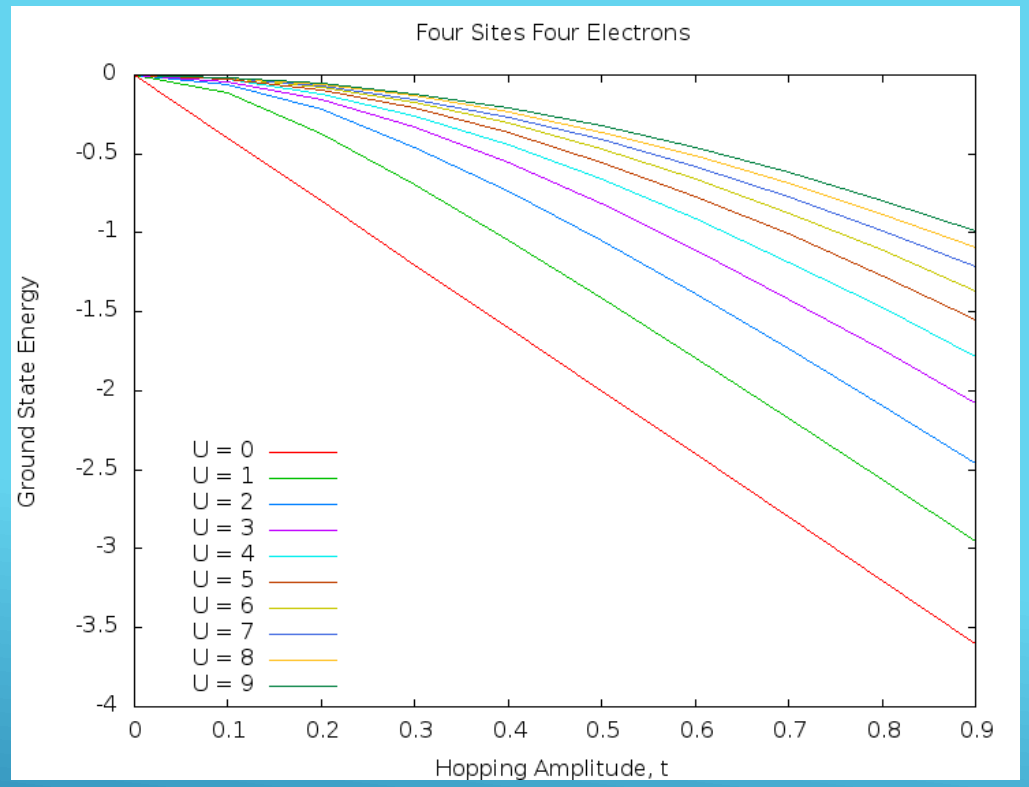
Algorithm

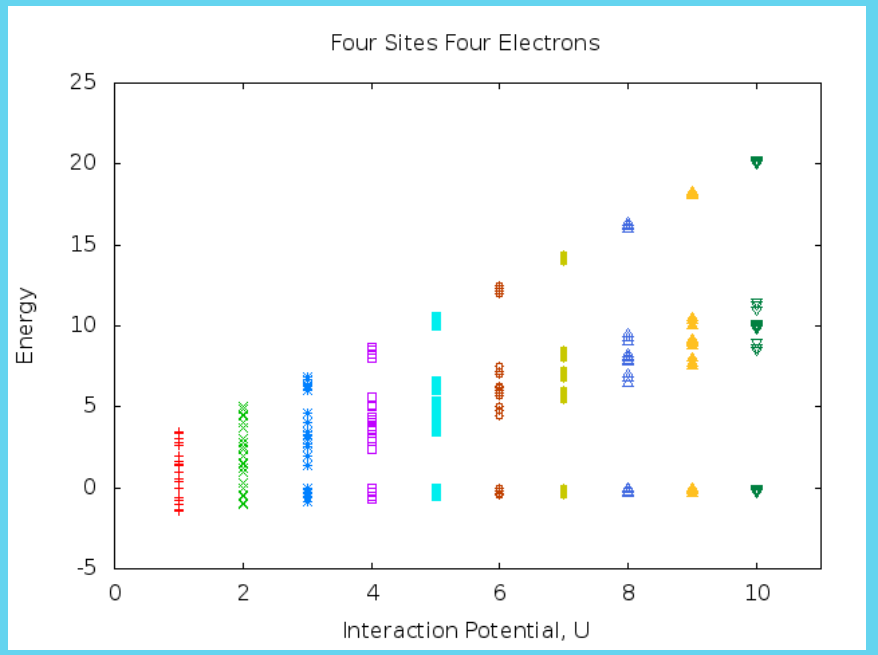
1) Initialize random positions for electrons
2) Calculate a new random position for the electrons
3) Calculate wave function for initial positions and trial positions
4) Calculate probability ratio of the two wave functions.
5) If ratio is greater than one; accept move, else only accept if ratio is larger than a random value between 0 and 1
6) Calculate local energy of accepted wave function
7) Repeat

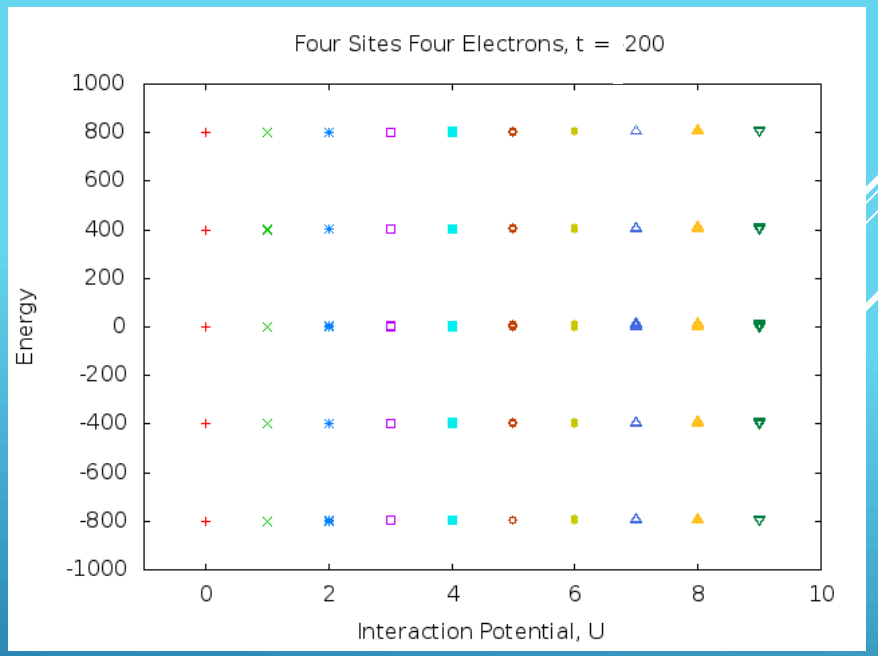
Acceptance Ratio

$$\frac{\rho(R_{trial})}{\rho(R)}$$

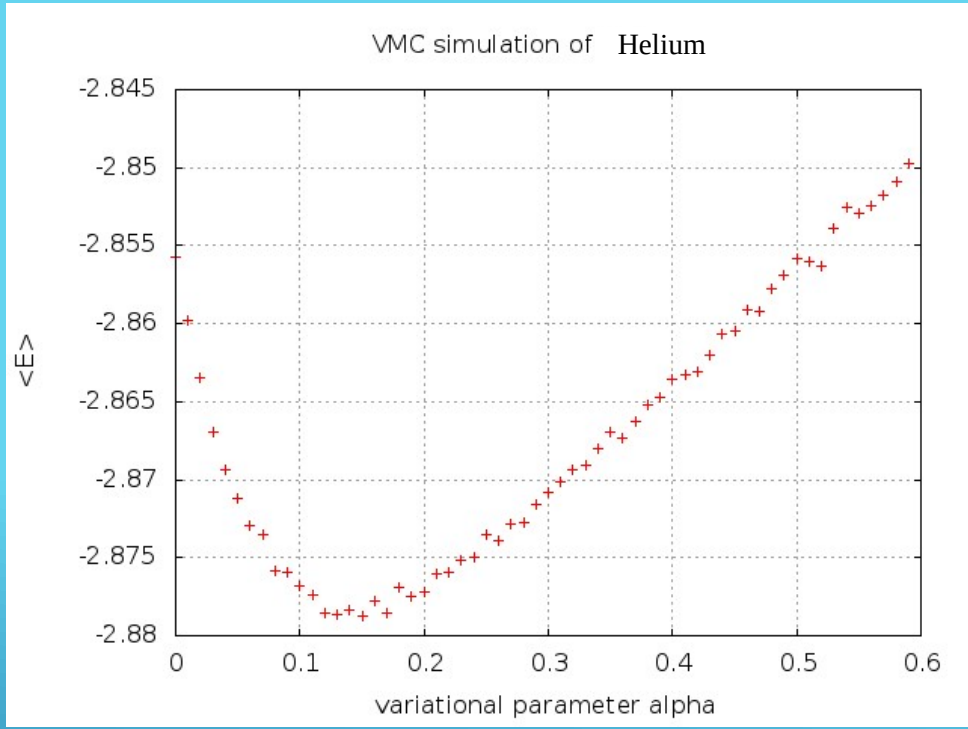
Results – The Hubbard Model

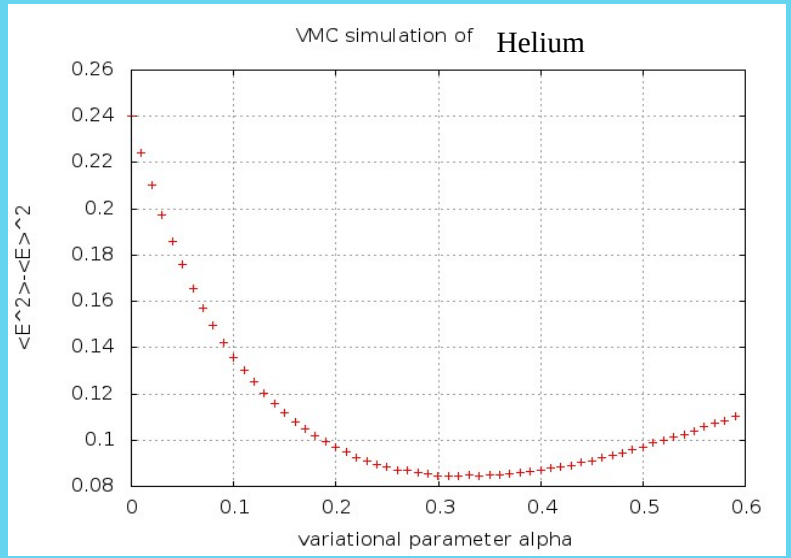


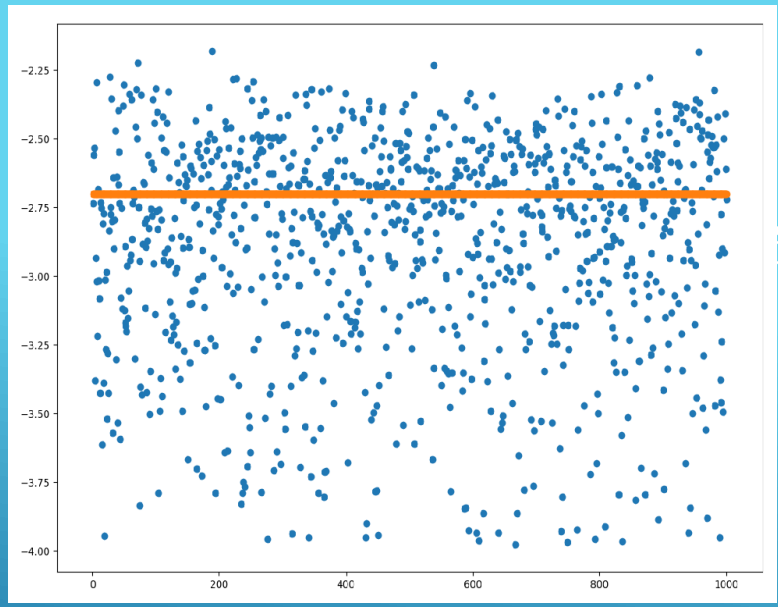




Results – Variational Monte Carlo







Conclusion

Hubbard Model

- Encapsulate lots of physics, complex strongly correlated electron systems
- Limited in system size due to memory limitations
- Complexity of code matches complexity of system

Variational Monte Carlo

- Large systems
- Time limitations, computation time
- Complexity of code doesn’t change with complexity of system