Implementation of the Variational Monte Carlo method for the Hubbard model

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Contents

My Master's thesis

- October '12 – May '13
  Implementation of VMC for the Hubbard model
- June '13 – July '13
  Using VMC to study the bilayer Hubbard model

Not so much physics today, sorry!
(... but there will be a paper about the bilayer model ...)

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The Hubbard model

$$\hat{H} = -t \sum_{\langle ij \rangle} \sum_{\sigma} \left(\hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} + \text{h.c.} \right) + U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

- "simple" model for interacting electrons on a lattice
- competition between kinetic and Coulomb term, consider half filled case:
  - kinetic part favors delocalization of electrons, making the system conducting
  - on-site Coulomb repulsion localizes one electron per site, making the system Mott insulating
  - which tendency wins is determined by U/t
- not solved analytically (except in 1d), but various numerical methods are available

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The Variational Monte Carlo method

... introducting the configuration basis

Define configuration basis, where all particle positions and spins along the z-axis are defined.

$$\text{e.g.} \qquad |x\rangle = |\downarrow, \Updownarrow, 0, \uparrow\rangle = \hat{c}^\dagger_{2\uparrow} \hat{c}^\dagger_{4\uparrow} \hat{c}^\dagger_{1\downarrow} \hat{c}^\dagger_{2\downarrow} |\emptyset\rangle$$

Distinguishable configurations are a basis of the many-particle Hilbert space!

$$|\Psi\rangle = \sum_x |x\rangle \langle x|\Psi\rangle \quad \Leftrightarrow \quad \mathbb{1} = \sum_x |x\rangle \langle x|$$

The Variational Monte Carlo method

... rewriting the expectation value as a sum over configuration space

Brute force method

Insert the $\mathbb{1} = \sum_x |x\rangle \langle x|$ into the expectation value.

$$\langle \hat{O} \rangle = \frac{\langle \Psi | \hat{O} | \Psi \rangle}{\langle \Psi | \Psi \rangle} = \frac{\sum_x \langle \Psi | x \rangle \langle x | \hat{O} | \Psi \rangle}{\sum_x \langle \Psi | x \rangle \langle x | \Psi \rangle} = \frac{\sum_x \frac{\langle x | \hat{O} | \Psi \rangle}{\langle x | \Psi \rangle} |\langle x | \Psi \rangle|^2}{\sum_x |\langle x | \Psi \rangle|^2}$$

Let us define $O_{\mathrm{loc}}(x) = \frac{\langle x | \hat{O} | \Psi \rangle}{\langle x | \Psi \rangle}$ as the local value of the observable.

Problem: Number of configurations is *huge* for any reasonably sized system! Straightforward summation takes forever! e.g.:

$$\underbrace{4^{100}}_{100 \text{ sites}} / \underbrace{(34 \cdot 10^{15} \mathrm{s}^{-1})}_{\text{Tianhe-2 flops}} \approx 10^{26} \times \text{ age of the universe}$$

The Variational Monte Carlo method

... stochastic sampling of configuration space

Monte Carlo simple sampling

Idea: Restrict sum to random multisubset $\mathcal{S}_1 = \{ x_1, \ldots, x_N \}$.

$$\langle \hat{O} \rangle \approx \frac{\sum_{x \in \mathcal{S}_1} O_{\mathrm{loc}}(x) \left| \langle x | \Psi \rangle \right|^2}{\sum_{x \in \mathcal{S}_1} \left| \langle x | \Psi \rangle \right|^2}$$

Exact for $N \to \infty$, but a bad approximation nevertheless ...

Failing example: Large Coulomb repulsion U discourages double occupancies, but randomly generated configuration x has 1/4 of the sites doubly occupied.
$\Rightarrow$ We would mostly sample states with a very small $\left| \langle x | \Psi \rangle \right|^2$ ...

The Variational Monte Carlo method

... importance sampling of configuration space

Monte Carlo importance sampling

Idea: generate randomly and weigh with probabilities
$\Longrightarrow$ generate according to probabilities and weigh evenly

$$\langle \hat{O} \rangle \approx \frac{1}{N} \sum_{x \in \mathcal{S}_\rho} O_{\mathrm{loc}}(x)$$

With a multisubset $\mathcal{S}_\rho$ containing N configurations distributed according to $\rho \propto |\langle x|\Psi\rangle|^2$.

Question: How to generate configurations according to some probability distribution ρ?

We'll get to that later, let's just assume we can ...

Open questions:

- How to generate configurations according to $\rho(x)$?

The Variational Monte Carlo method

... properties of the Hamiltonian

The Hamiltonian itself is just an ordinary observable.

$$\langle \hat{H} \rangle \approx \frac{1}{N} \sum_{x \in \mathcal{S}_\rho} E_{\mathrm{loc}}(x) \quad \text{with} \quad E_{\mathrm{loc}}(x) = \frac{\langle x | \hat{H} | \Psi \rangle}{\langle x | \Psi \rangle}$$

There is the Rayleigh-Ritz principle for its expectation value.

$$\langle \hat{H} \rangle = \frac{\sum_{n=0}^{N} E_n \langle \Psi | n \rangle \langle n | \Psi \rangle}{\langle \Psi | \Psi \rangle} \geq \frac{\sum_{n=0}^{N} E_0 \langle \Psi | n \rangle \langle n | \Psi \rangle}{\langle \Psi | \Psi \rangle} = E_0$$

(In words: Its expectation value is bounded from below by the ground state energy.)

The Variational Monte Carlo method

... exploiting the Rayleigh-Ritz principle

Let us make a variational ansatz for the ground state wavefunction:

$$|\Psi\rangle = |\Psi(\alpha_1, \ldots, \alpha_p)\rangle$$

This wavefunction is closest to the true ground state of the system if the variational parameters $\{\alpha\}$ are chosen such that the expectation value of the energy is minimized!

$\Rightarrow$ Approximation of the ground state within a variational ansatz!

The Variational Monte Carlo method

... putting things together

1. Find the variational parameters that minimize the energy expectation value of the trial wavefunction. Any expectation values needed to do this can be evaluated using:

$$\langle \hat{O} \rangle \approx \frac{1}{N} \sum_{x \in \mathcal{S}_\rho} O_{\mathrm{loc}}(x)$$

2. Use this equation again with the optimized wavefunction to calculate the desired observables.

Contents

Open questions:

- How to generate configurations according to $\rho(x)$?
- How to find the energy minimizing variational parameters?
- What is a reasonable variational wavefunction?

VMC for the Hubbard model

... using a Markov chain to implement the importance sampling in configuration space

We need to find the configurations with a large overlap $|\langle x|\Psi\rangle|^2$, because they are the most important ones!

The Markov chain Monte Carlo idea

1. Find one of the "important configurations".
2. Randomly modify it a litte bit to get another important one.

Question:
Which Markov process produces the right distribution?

VMC for the Hubbard model

... choosing a suitable Markov process

The Metropolis algorithm (no derivation here)

1. Pick a random spin-σ electron and propose to hop it to a random site in its vicinity.
2. If the target site not occupied by another spin-σ electron, accept the hop with the probability $\min\left(1, \left|\frac{\langle x'|\Psi\rangle}{\langle x|\Psi\rangle}\right|^2\right)$, otherwise reject.
3. Repeat until enough configuration have been generated.

Question: How to calculate these overlap ratios $\langle x'|\Psi\rangle \,/\, \langle x|\Psi\rangle$, where x and x' only differ by one particle?

Open questions:

- ~~How to generate configurations according to $\rho(x)$?~~ ✓
- How to find the energy minimizing variational parameters?
- What is a reasonable variational wavefunction?
- How to calculate the overlap ratios $\langle x'|\Psi\rangle \,/\, \langle x|\Psi\rangle$?

VMC for the Hubbard model

... deriving the Stochastic Reconfiguration optimization

Expand the wavefunction in the variational parameters:

$$|\Psi'\rangle = \delta\alpha_0 |\Psi\rangle + \sum_{k'=1}^{p} \delta\alpha_{k'} \frac{\partial}{\partial\alpha_{k'}} |\Psi\rangle$$

Insert $\mathbb{1} = \sum_x |x\rangle \langle x|$ into the equation.

$$\begin{aligned}
|\Psi'\rangle &= \delta\alpha_0 |\Psi\rangle + \sum_{k'=1}^{p} \delta\alpha_{k'} \frac{\partial}{\partial\alpha_{k'}} \sum_x |x\rangle \langle x|\Psi\rangle \\
&= \delta\alpha_0 |\Psi\rangle + \sum_{k'=1}^{p} \delta\alpha_{k'} \sum_x \frac{\partial \langle x|\Psi\rangle}{\partial\alpha_{k'}} |x\rangle \\
&= \delta\alpha_0 |\Psi\rangle + \sum_{k'=1}^{p} \delta\alpha_{k'} \sum_x \frac{\partial \ln \langle x|\Psi\rangle}{\partial\alpha_{k'}} |x\rangle \langle x|\Psi\rangle
\end{aligned}$$

VMC for the Hubbard model

... deriving the Stochastic Reconfiguration optimization

Define the so called logarithmic derivative operators:

$$|\Psi'\rangle = \sum_{k'=0}^{p} \delta\alpha_{k'} \hat{\Delta}_{\Psi k'} |\Psi\rangle \quad \text{with} \quad \hat{\Delta}_{\Psi k} = \begin{cases} \mathbb{1} & \text{for } k = 0 \\ \sum_x \frac{\partial \ln\langle x|\Psi\rangle}{\partial \alpha_k} |x\rangle \langle x| & \text{for } k \neq 0 \end{cases}$$

Projector based optimization: Successive application of $(\Lambda - \hat{H})$ projects out the ground state since $(\Lambda - E_0) \geq (\Lambda - E_i) \; \forall \; i > 0$.

$$|\Psi\rangle = \sum_{n=0}^{\infty} \langle n|\Psi\rangle |n\rangle \quad \Rightarrow \quad \left(\Lambda - \hat{H}\right)^N |\Psi\rangle = \sum_{n=0}^{\infty} (\Lambda - E_n)^N \langle n|\Psi\rangle |n\rangle$$

Inserting into ansatz: $\Rightarrow \quad (\Lambda - \hat{H}) |\Psi\rangle = \sum_{k'=0}^{p} \delta\alpha_{k'} \hat{\Delta}_{\Psi k'} |\Psi\rangle$

Can be rewritten as a linear system of equations ...

VMC for the Hubbard model

... deriving the Stochastic Reconfiguration optimization

The Stochastic Reconfiguration method

$$(\boldsymbol{S} + \epsilon \mathbb{1})\, \delta\vec{\alpha} = \vec{f} \qquad \text{with} \qquad S_{kk'} = \langle \hat{\Delta}_{\Psi k} \hat{\Delta}_{\Psi k'} \rangle - \langle \hat{\Delta}_{\Psi k} \rangle \langle \hat{\Delta}_{\Psi k'} \rangle$$

$$f_k = \langle \hat{\Delta}_{\Psi k} \rangle \langle \hat{H} \rangle - \langle \hat{\Delta}_{\Psi k} \hat{H} \rangle$$

- Is applied iteratively until convergence.
- Expectation values are evaluated using MC integration.
- Convergence detection through Mann-Kendall trend test.

$$\tau = \frac{2\,|\zeta|}{N(N-1)} \quad \text{with} \quad \zeta = \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} \operatorname{sgn}\left(\alpha_k(t_i) - \alpha_k(t_j)\right)$$

Question:

How to calculate the local energy and logarithmic derivatives?

Open questions:

- ~~How to generate configurations according to $\rho(x)$?~~ ✓
- ~~How to find the energy minimizing variational parameters?~~✓
- What is a reasonable variational wavefunction?
- How to calculate the overlap ratios $\langle x'|\Psi\rangle \,/\, \langle x|\Psi\rangle$?
- How to calculate $E_{\mathrm{loc}}(x)$ and $\Delta_{\Psi k,\mathrm{loc}}(x)$?

VMC for the Hubbard model

So far everything has been applicable in general.

Now we specialize things for the Hubbard model!

VMC for the Hubbard model

... the general form of a variational wavefunction

$$|\Psi\rangle = \hat{\mathcal{P}}_J \, |\Phi\rangle$$

- Slater determinant $|\Phi\rangle$ ensures antisymmetry.
  Is built from the eigenstates of a variational
  single particle Hamiltonian $\hat{H}_{\text{var}}$.
- Jastrow factor $\hat{\mathcal{P}}_J$ changes magnitude of the wavefunction
  but leaves its antisymmetry intact.

VMC for the Hubbard model

... the variational single particle Hamiltonian

$$\hat{H} = \hat{H}_t + \hat{H}_U = -\sum_{i<j} t_{ij} \sum_{\sigma} \left(\hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} + \text{h.c.} \right) + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

Throw out interaction, include correlation induced phenomena:

$$\hat{H}_{\text{var}} = \hat{H}_t^{(\text{var})} + \hat{H}_{\Delta} + \hat{H}_{\text{mag}} + \hat{H}_{\mu}$$

with $$\hat{H}_t^{(\text{var})} = -\sum_{i<j} t_{ij}^{(\text{var})} \sum_{\sigma} \left(\hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} + \text{h.c.} \right)$$

$$\hat{H}_{\Delta} = \Delta_0 \sum_i \left(\hat{c}^{\dagger}_{i\uparrow} \hat{c}^{\dagger}_{i\downarrow} + \text{h.c.} \right) + \sum_{i<j} \Delta_{ij} \left(\hat{c}^{\dagger}_{i\uparrow} \hat{c}^{\dagger}_{j\downarrow} + \hat{c}^{\dagger}_{j\uparrow} \hat{c}^{\dagger}_{i\downarrow} + \text{h.c.} \right)$$

$$\hat{H}_{\text{mag}} = \mu_m \sum_i (-1)^{\tau(i)} \hat{S}^z_i = \mu_m \sum_i (-1)^{\tau(i)} \frac{\hat{m}^z_i}{2}$$

$$\hat{H}_{\mu} = -\mu \sum_i \hat{n}_i$$

VMC for the Hubbard model

... the particle-hole transformation

Canonical particle-hole transformation:

$$\hat{c}_{i\uparrow} \to \hat{d}_{i\uparrow} \qquad \text{and} \qquad \hat{c}^\dagger_{i\uparrow} \to \hat{d}^\dagger_{i\uparrow}$$
$$\hat{c}_{i\downarrow} \to \hat{d}^\dagger_{i\downarrow} \qquad \text{and} \qquad \hat{c}^\dagger_{i\downarrow} \to \hat{d}_{i\downarrow}$$

- Brings pairing term into $\hat{d}^\dagger \hat{d}$ form.

$$\hat{H}_\Delta = \Delta_0 \sum_i \left(\hat{d}^\dagger_{i\uparrow} \hat{d}_{i\downarrow} + \text{h.c.} \right) + \sum_{i<j} \Delta_{ij} \left(\hat{d}^\dagger_{i\uparrow} \hat{d}_{j\downarrow} + \hat{d}^\dagger_{j\uparrow} \hat{d}_{i\downarrow} + \text{h.c.} \right)$$

- Switches magnetization and occupation operators.

$$\hat{m}^z_i = \hat{u}_i + 1 \quad \text{with} \quad \hat{u}_i \equiv \hat{u}_{i\uparrow} + \hat{u}_{i\downarrow} = \hat{d}^\dagger_{i\uparrow} \hat{d}_{i\uparrow} + \hat{d}^\dagger_{i\downarrow} \hat{d}_{i\downarrow}$$
$$\hat{n}_i = \hat{n}_{i\uparrow} + \hat{n}_{i\downarrow} = \hat{u}_{i\uparrow} - \hat{u}_{i\downarrow} + 1 = \hat{w}^z_i + 1$$

- New particle number N_p, new vacuum $|\tilde{\emptyset}\rangle$

VMC for the Hubbard model

... diagonalizing the variational Hamiltonian

Written in $\mathcal{B}_d = \left\{ \hat{d}_i^\dagger \left| \tilde{\emptyset} \right\rangle \mid i \in \{1, \ldots, 2L\} \right\}$ basis:

$$\hat{H}_{\text{var}} = \sum_{i,j=1}^{2L} \hat{d}_i^\dagger \left(\boldsymbol{H}_{\text{var}} \right)_{ij} \hat{d}_j$$

Diagonalize matrix $\boldsymbol{H}_{\text{var}}$ with $\boldsymbol{U}^\dagger \boldsymbol{H}_{\text{var}} \boldsymbol{U}$. Build the Slater determinant from the lowest N_p eigenstates.

$$\hat{\gamma}_n^\dagger = \sum_{i=1}^{2L} \boldsymbol{U}_{in} \hat{d}_i^\dagger \qquad \Rightarrow \qquad |\Phi\rangle = \hat{\gamma}_1^\dagger \hat{\gamma}_2^\dagger \ldots \hat{\gamma}_{N_p}^\dagger \left| \tilde{\emptyset} \right\rangle$$

VMC for the Hubbard model

... the Gutzwiller factor

$$\hat{\mathcal{P}}_g = \exp\left(-g \sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}\right)$$

- only one variational parameter g
- reduces the magnitude of the wavefunction depending on the number of double occupancies
- unable to induce Mott insulating behavior for a finite g

VMC for the Hubbard model

... the Jastrow correlator

$$\hat{\mathcal{P}}_J = \exp\left(\frac{1}{2}\sum_{ij} v_{ij}\hat{n}_i\hat{n}_j\right) = \exp\left(\frac{1}{2}\sum_{ij} v_{ij}\left(\hat{n}_{i\uparrow}+\hat{n}_{i\downarrow}\right)\left(\hat{n}_{j\uparrow}+\hat{n}_{j\downarrow}\right)\right)$$

- variational parameters v_{ij} really depend on the distance between site i and $j \Rightarrow$ one variational parameter per distance on the lattice
- written in terms of doublon $\hat{D}_i = \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$ and holon $\hat{H}_i = (1-\hat{n}_{i\uparrow})(1-\hat{n}_{i\downarrow})$ operators:

$$\hat{n}_i\hat{n}_j = \hat{D}_i\hat{D}_j + \hat{H}_i\hat{H}_j - \hat{H}_i\hat{D}_j - \hat{D}_i\hat{H}_j + \hat{n}_i + \hat{n}_j - 1$$

$\Rightarrow$ acts as HD attraction, HH/DD repulsion!

Open questions:

- ~~How to generate configurations according to $\rho(x)$?~~ ✓
- ~~How to find the energy minimizing variational parameters?~~✓
- ~~What is a reasonable variational wavefunction?~~ ✓
- How to calculate the overlap ratios $\langle x'|\Psi\rangle \,/\, \langle x|\Psi\rangle$?
- How to calculate $E_{\mathrm{loc}}(x)$ and $\Delta_{\Psi k,\mathrm{loc}}(x)$?

VMC for the Hubbard model

... calculating the local energy

The particle-hole transformed Hamiltonian:

$$\hat{H} = -\sum_{i<j} t_{ij} \left(\hat{d}^\dagger_{i\uparrow} \hat{d}_{j\uparrow} - \hat{d}^\dagger_{i\downarrow} \hat{d}_{j\downarrow} + \text{h.c.} \right) + U \sum_i \hat{u}_{i\uparrow}(1 - \hat{u}_{i\downarrow})$$

Its local value:

$$E_{\text{loc}}(x) = \frac{\langle x|\hat{H}|\Psi\rangle}{\langle x|\Psi\rangle} = \sum_{x'} \langle x|\hat{H}|x'\rangle \frac{\langle x'|\Psi\rangle}{\langle x|\Psi\rangle}$$

$$= -\sum_{x \curvearrowright x'} t_{ij}(-1)^{\delta_{\sigma\downarrow}} \frac{\langle x'|\Psi\rangle}{\langle x|\Psi\rangle} + U \sum_i u_{i\uparrow}(x)(1 - u_{i\downarrow}(x))$$

x and x' differ only by a single particle position!
(same overlap ratio as needed for the Metropolis algorithm)

Open questions:

- ~~How to generate configurations according to $\rho(x)$?~~ ✓
- ~~How to find the energy minimizing variational parameters?~~✓
- ~~What is a reasonable variational wavefunction?~~ ✓
- How to calculate the overlap ratios $\langle x'|\Psi\rangle \,/\, \langle x|\Psi\rangle$?
- How to calculate ~~$E_{\mathrm{loc}}(x)$ and~~ $\Delta_{\Psi k,\mathrm{loc}}(x)$?

VMC for the Hubbard model

... logarithmic derivatives of the Jastrow parameters

$$\Delta_{\Psi k,\mathrm{loc}}(x) = \frac{\langle x|\hat{\Delta}_{\Psi k}|\Psi\rangle}{\langle x|\Psi\rangle} = \frac{\left\langle x \left| \sum_{x'} \frac{\partial \ln\langle x'|\Psi\rangle}{\partial\alpha_k} \right| x' \right\rangle \langle x'|\Psi\rangle}{\langle x|\Psi\rangle} = \frac{\partial \ln\langle x|\Psi\rangle}{\partial\alpha_k}$$

$$\begin{aligned}
\frac{\partial \ln\langle x|\Psi\rangle}{\partial v_{lm}} &= \frac{\partial}{\partial v_{lm}} \ln\langle x|\hat{\mathcal{P}}_J|\Phi\rangle = \frac{\partial}{\partial v_{lm}} \ln\langle \Phi|\hat{\mathcal{P}}_J|x\rangle^* \\
&= \frac{\partial}{\partial v_{lm}} \ln\left\langle \Phi \left| \exp\left(\frac{1}{2}\sum_{ij} v_{ij}\hat{w}_i^z\hat{w}_j^z\right) \right| x \right\rangle^* \\
&= \frac{\partial}{\partial v_{lm}} \left(\frac{1}{2}\sum_{ij} v_{ij} w_i^z(x) w_j^z(x) + \ln\langle \Phi \,|\, x\rangle^*\right) \\
&= \frac{1}{2}\sum_{ij} \delta_{r_{ij},r_{lm}} w_i^z(x) w_j^z(x)
\end{aligned}$$

VMC for the Hubbard model

... logarithmic derivatives of the determinantal parameters

Treat the term that is proportional to the variational parameter as a perturbation of the variational Hamiltonian.

$$\hat{H}'_{\mathrm{var}} = \hat{H}_{\mathrm{var}} + \sum_{k=1}^{p} \delta\alpha_k \, \hat{V}_k$$

First order correction to the Slater determinant:

$$|\Phi'\rangle = |\Phi\rangle + \left(\sum_{k=1}^{p} \delta\alpha_k \sum_{\eta,\nu=1}^{2L} (\boldsymbol{Q}_k)_{\eta\nu} \hat{\gamma}_\eta^\dagger \hat{\gamma}_\nu \right) |\Phi\rangle + \mathcal{O}(\delta\alpha_k^2)$$

$$\text{with} \quad \boldsymbol{Q}_k = \begin{cases} \frac{\left(\boldsymbol{U}^\dagger \boldsymbol{V}_k \boldsymbol{U}\right)_{\eta\nu}}{\epsilon_\nu - \epsilon_\eta} & \text{if } \eta > N_p \text{ and } \nu \leq N_p \\ 0 & \text{otherwise} \end{cases}$$

VMC for the Hubbard model

... logarithmic derivatives of the determinantal parameters

Compare this equation with the one from the beginning (where we introduced the log. derivative operators):

$$|\Psi'\rangle = \sum_{k=0}^{p} \delta\alpha_k \hat{\Delta}_{\Psi k} |\Psi\rangle \quad \Rightarrow \quad \hat{\Delta}_{\Psi k} = \sum_{\eta,\nu=1}^{2L} (\boldsymbol{Q}_k)_{\eta\nu} \hat{\gamma}_\eta^\dagger \hat{\gamma}_\nu$$

Switch back to $\mathcal{B}_d = \left\{ \hat{d}_i^\dagger |\tilde{\emptyset}\rangle \mid i \in \{1, \ldots, 2L\} \right\}$ basis:

$$\hat{\Delta}_{\Phi k} = \sum_{i,j=1}^{2L} (\boldsymbol{A}_k)_{ij} \hat{d}_i^\dagger \hat{d}_j \quad \text{with} \quad \boldsymbol{A}_k = \boldsymbol{U} \boldsymbol{Q}_k \boldsymbol{U}^\dagger$$

$$\Delta_{\Psi k,\mathrm{loc}}(x) = \frac{\langle x|\hat{\Delta}_{\Phi k}|\Phi\rangle}{\langle x|\Phi\rangle} = \sum_{i,j=1}^{2L} (\boldsymbol{A}_k)_{ij} \frac{\langle x|\hat{d}_i^\dagger \hat{d}_j |\Phi\rangle}{\langle x|\Phi\rangle}$$

Open questions:

- ~~How to generate configurations according to $\rho(x)$?~~ ✓
- ~~How to find the energy minimizing variational parameters?~~✓
- ~~What is a reasonable variational wavefunction?~~ ✓
- How to calculate the overlap ratios $\langle x'|\Psi\rangle \,/\, \langle x|\Psi\rangle$?
- ~~How to calculate $E_{\mathrm{loc}}(x)$ and $\Delta_{\Psi k,\mathrm{loc}}(x)$?~~ ✓

VMC for the Hubbard model

... separating the overlap ratios

$$\frac{\langle x'|\Psi\rangle}{\langle x|\Psi\rangle} = \frac{\langle x'|\hat{P}_J|\Phi\rangle}{\langle x|\hat{P}_J|\Phi\rangle} = \frac{P_J(x')}{P_J(x)}\frac{\langle x'|\Phi\rangle}{\langle x|\Phi\rangle}$$

Can be calculated separately for determinant and Jastrow!

VMC for the Hubbard model

... overlap ratios of the determinantal part

Let $|\phi_n\rangle = \hat{\gamma}_n^\dagger |\tilde{\emptyset}\rangle$ be the n-th lowest eigenstate of $\hat{H}_{\text{var}}$.
Let x_α be the position of the α-th particle.

$$\langle x|\Phi\rangle = \det \boldsymbol{D} \quad \text{with} \quad \boldsymbol{D} = \begin{pmatrix} \langle x_1|\phi_1\rangle & \langle x_1|\phi_2\rangle & \cdots & \langle x_1|\phi_{N_p}\rangle \\ \langle x_2|\phi_1\rangle & \langle x_2|\phi_2\rangle & \cdots & \langle x_2|\phi_{N_p}\rangle \\ \vdots & \vdots & \ddots & \vdots \\ \langle x_{N_p}|\phi_1\rangle & \langle x_{N_p}|\phi_2\rangle & \cdots & \langle x_{N_p}|\phi_{N_p}\rangle \end{pmatrix}$$

- would in principle work, but determinant is $\mathcal{O}(N_p^3)$!
  (even for rejected Metropolis steps!)
- prone to underflow

Question: Better solution that exploits that we only need ratios $\langle x'|\Phi\rangle \,/\, \langle x|\Phi\rangle$ where x and x' are almost the same?

VMC for the Hubbard model

... overlap ratios of the determinantal part

The matrix $\boldsymbol{U}$ (that diagonalizes the variational Hamiltonian) has the eigenvectors of $\boldsymbol{H}_{\text{var}}$ written in the basis $\mathcal{B}_d = \left\{ \hat{d}_i^\dagger \, |\tilde{\emptyset}\rangle \mid i \in \{1, \ldots, 2L\} \right\}$ as the columns.

Drop unoccupied orbitals to obtain the $2L \times N_p$ matrix $\boldsymbol{M}$.

$$\boldsymbol{U} \quad \Rightarrow \quad \boldsymbol{M} = \begin{pmatrix} \langle 1|\phi_1\rangle & \langle 1|\phi_2\rangle & \cdots & \langle 1|\phi_{N_p}\rangle \\ \langle 2|\phi_1\rangle & \langle 2|\phi_2\rangle & \cdots & \langle 2|\phi_{N_p}\rangle \\ \vdots & \vdots & \ddots & \vdots \\ \langle 2L|\phi_1\rangle & \langle 2L|\phi_2\rangle & \cdots & \langle 2L|\phi_{N_p}\rangle \end{pmatrix}$$

VMC for the Hubbard model

... overlap ratios of the determinantal part

Recalculation of $\boldsymbol{W}$

$$\frac{\langle x'|\Phi\rangle}{\langle x|\Phi\rangle} = \frac{\det \boldsymbol{D}'}{\det \boldsymbol{D}} = W_{l\beta} \quad \text{with} \quad \boldsymbol{W} = \boldsymbol{M}\,\boldsymbol{D}^{-1}$$

- $x \curvearrowright x'$ by hopping the β-th particle from site k to l
- $\mathcal{O}(N_p^3)$ complexity; constant time lookup of overlap ratios
- numerically it is faster to solve $\boldsymbol{D}^T\,\boldsymbol{W}^T = \boldsymbol{M}^T$

Quick update of $\boldsymbol{W}$

$$W'_{i\alpha} = W_{i\alpha} - \frac{W_{i\beta}}{W_{l\beta}}\Big(W_{l\alpha} - \delta_{\alpha\beta}\Big)$$

- $\mathcal{O}(N_p^2)$ complexity; beware floating point errors!

VMC for the Hubbard model

... overlap ratios of the determinantal part

Straightforward evaluation:

$$P_J(x) = \frac{1}{2} \sum_{ij} v_{ij} w_i^z(x) w_j^z(x)$$

Works, but has exactly the same problems as for the determinantal part ...

VMC for the Hubbard model

... overlap ratios of the Jastrow part

Recalculation of $\vec{T}$

$$\frac{\mathcal{P}_J(x')}{\mathcal{P}_J(x)} = \exp\left((-1)^{\delta_{\downarrow\sigma}}\left(T_l(x) - T_k(x)\right) + v_{ll} - v_{lk}\right)$$

with $$T_i(x) = \sum_j v_{ij} w_i^z(x)$$

- $x \curvearrowright x'$ by hopping the β-th particle from site k to l
- $\mathcal{O}(L^2)$ complexity; constant time lookup of overlap ratios

Quick update of $\vec{T}$

$$T_i(x') = T_i(x) + (-1)^{\delta_{\downarrow\sigma}}\left(v_{il} - v_{ik}\right)$$

- $\mathcal{O}(L)$ complexity; beware floating point errors!

Open questions:

- ~~How to generate configurations according to $\rho(x)$?~~ ✓
- ~~How to find the energy minimizing variational parameters?~~✓
- ~~What is a reasonable variational wavefunction?~~ ✓
- ~~How to calculate the overlap ratios $\langle x'|\Psi\rangle \,/\, \langle x|\Psi\rangle$?~~ ✓
- ~~How to calculate $E_{\mathrm{loc}}(x)$ and $\Delta_{\Psi k,\mathrm{loc}}(x)$?~~ ✓

Done!

VMC for the Hubbard model

... a rough summary

1. Diagonalize the variational single particle Hamiltonian to obtain $\boldsymbol{M}$ and the $\boldsymbol{A}_k$.
2. Run Metropolis algorithm and keep the overlap ratios in $\boldsymbol{W}$ and $\vec{T}$ up to date. Recalculate them every once in a while to avoid the accumulation of floating point errors.
3. Measure the local energy and the logarithmic derivatives using the overlap ratios and the $\boldsymbol{A}_k$. Return to [2] until enough data has been gathered.
4. Use the energy and the logarithmic derivatives in the Stochastic Reconfiguration linear system and obtain new variational parameters. Return to [1] until converged according to Mann-Kendall test.

Contents

What I learned about software development

... my implementation of Variational Monte Carlo for the Hubbard model

`github.com/robertrueger/hVMC`

I learned a lot writing this code!

What I learned about software development

... use the Eigen3 linear algebra libraries!

Eigen3 [`http://eigen.tuxfamily.org`]

- linear algebra template library for C++
- header only library, no run-time dependencies!
- Matlab like code with C++ like performance
- works nicely together with BLAS/LAPACK

What I learned about software development

... use the Eigen3 linear algebra libraries!

Calculating the matrix $\boldsymbol{W}$ by solving $\boldsymbol{D}^T \boldsymbol{W}^T = \boldsymbol{M}^T$:

```
W = D.transpose().partialPivLu().solve(
        M.transpose()
    ).transpose();
```

Updating W through $W'_{i\alpha} = W_{i\alpha} - \frac{W_{i\beta}}{W_{l\beta}} \Big(W_{l\alpha} - \delta_{\alpha\beta} \Big)$:

```
tempWrow = W.row( l );
tempWrow( beta ) -= 1.f;
W -= ( W.col( beta ) / W( l, beta ) ) * tempWrow;
```

What I learned about software development

... use the Eigen3 linear algebra libraries!

Updating W with the Eigen3 classes and an external CBLAS:

```
cblas_sger(
  CblasColMajor,
  W.rows(),
  W.cols(),
  - 1.f / W( 1, beta ),
  tempWcol.data(), 1,
  tempWrow.data(), 1,
  W.data(),
  W.rows()
);
```

Could not think of a reason not to use Eigen!

What I learned about software development

... check Boost libraries before writing something yourself!

Boost C++ Libraries [boost.org]

- set of C++ template libraries
- widely available, & cross platform
- often get adopted into C++ standard library

Boost Program Options and Boost Filesystem

Defining the command line options:

```
po::options_description clionly( "command line options" );
clionly.add_options()
  ( "help,h", "print this help message and exit" )
  ( "version,V", "print hVMC's version and exit" )
  ( "verbose,v", "makes hVMC verbose" )
  ( "job-file,J", po::value<fs::path>(), "job file" );
```

Retrieving options:

```
if ( opts.count( "verbose" ) ) {
  fs::remove_all( opts["job-file"].as<fs::path>() );
}
```

Boost Serialization and Boost MPI

Use cases:

- Class → Serialization → MPI → Deserialization → Class
- Class → Serialization → Disk
- Disk → Deserialization → Class

Advantages:

- STL containers can be serialized out of the box.
- Serializing own classes is not too complicated.
- Unified code for disk writing and MPI transfers.

What I learned about software development

... Boost Serialization and Boost MPI

Making a class serializable:

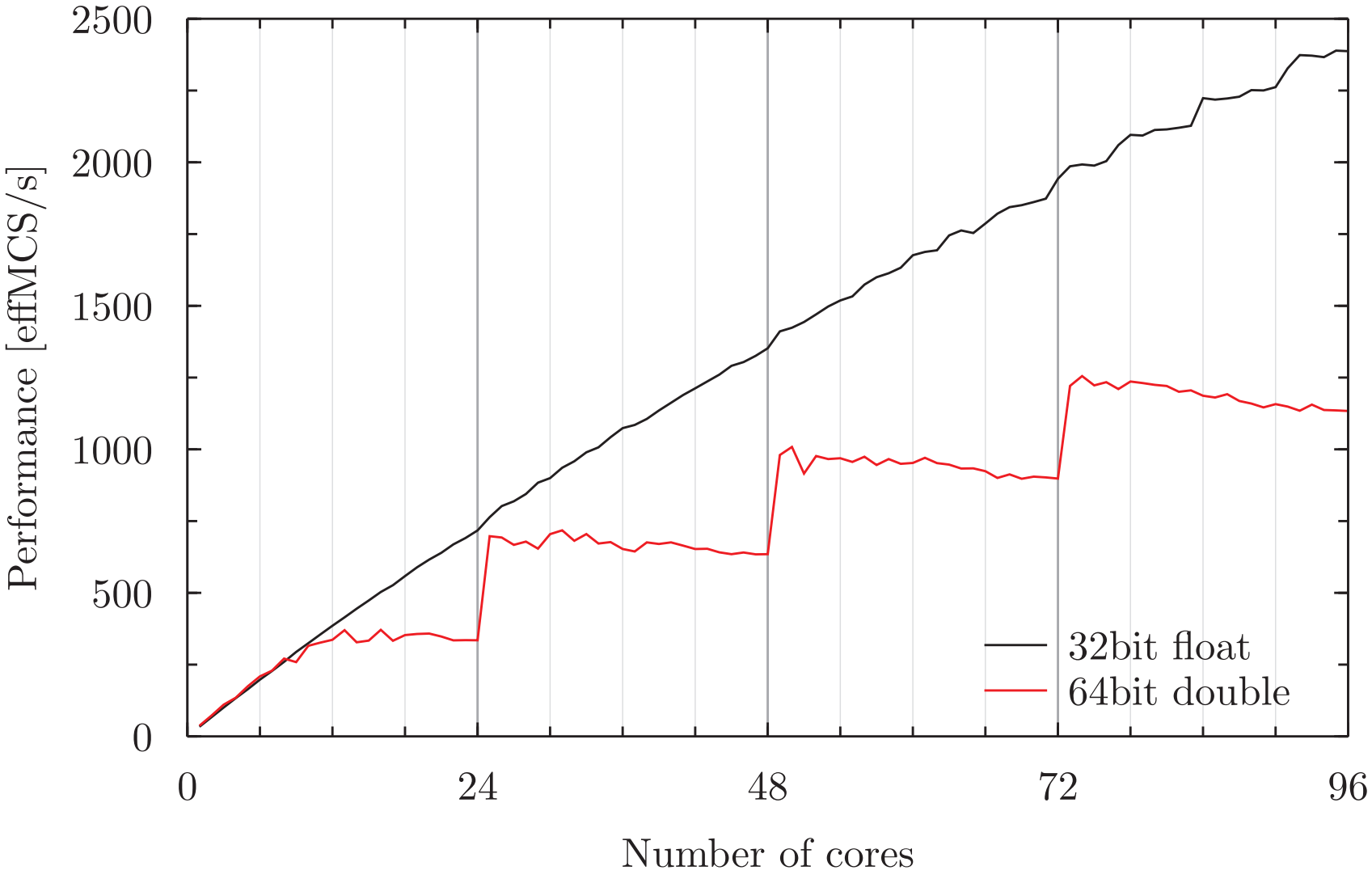
```
friend class boost::serialization::access;
template<class Archive>
void serialize( Archive& ar, const unsigned int ) {
  ar & target;
  ar & recalcs;
  ar & misses;
  ar & hits;
  ar & mag1_misses;
  ar & mag1_hits;
}
```

Gathering it via MPI into a `std::vector` :

```
mpi::gather( mpicomm, model.get_devstat(), devstats, 0 );
```

What I learned about software development

... consider calculating in single precision!



References

Variational Monte Carlo

- W. L. McMillan. Ground State of Liquid He^4. *Phys. Rev.*, 138:A442–A451, Apr 1965.
- D. Ceperley, G. V. Chester, and M. H. Kalos. Monte Carlo simulation of a many-fermion study. *Phys. Rev. B*, 16:3081–3099, Oct 1977.

Stochastic Reconfiguration optimization

- Sandro Sorella. Generalized Lanczos algorithm for variational quantum Monte Carlo. *Phys. Rev. B*, 64:024512, June 2001.
- Michele Casula, Claudio Attaccalite, and Sandro Sorella. Correlated geminal wave function for molecules: An efficient resonating valence bond approach. *The Journal of Chemical Physics*, 121(15):7110–7126, 2004.

References

Mann-Kendall test

- M. G. Kendall. A New Measure of Rank Correlation. *Biometrika*, 30(1/2):81–93, 1938.
- Henry B. Mann. Nonparametric Tests Against Trend. *Econometrica*, 13(3):245–259, 1945.

Metropolis algorithm

- Nicholas Metropolis, Arianna W. Rosenbluth, Marshall N. Rosenbluth, Augusta H. Teller, and Edward Teller. Equation of State Calculations by Fast Computing Machines. *J. Chem. Phys.*, 21(6):1087–1092, 1953.

Jastrow factor and computational tricks

- Manuela Capello. *Variational description of Mott insulators*. PhD thesis, SISSA/ISAS Trieste Italy, 2006.

Thank you for your attention! :-)