Universität Augsburg
Mathematisch-Naturwissenschaftlich-Technische Fakultät

Classical networks for the Hubbard model with a tilted potential

- Master Thesis Colloquium -

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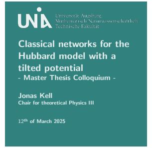
Chair for theoretical Physics III

12^{th} of March 2025



1. Thank you for coming
2. Title: Classical networks for the Hubbard model with a tilted potential
3. Quickly what this will be about

Outline

1.
   - Introduction to the physical theory
   - In depth: Time evolution - why and how
   - Quickly: Sampling Strategy and simplifications
   - To give the title justice: Variational classical networks - what is is all about
   - End (if there is time or if questions lead into that direction): Implementation and experiments
   - Outlook

Outline
1 Introduction of the Physical Problem

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2 Time Evolution

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3 Sampling & Simplifications

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4 Variational Classical Networks

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1 Introduction of the Physical Problem
2 Time Evolution
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4 Variational Classical Networks
5 Implementation & Experiments

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Particle Types

Introduction of the Physical Problem

- Bosonic operators

$$\left[\hat{\mathrm{b}}_l, \hat{\mathrm{b}}_m\right] = 0$$
$$\left[\hat{\mathrm{b}}_l^\dagger, \hat{\mathrm{b}}_m^\dagger\right] = 0$$
$$\left[\hat{\mathrm{b}}_l, \hat{\mathrm{b}}_m^\dagger\right] = \delta_{l,m}$$

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1. Wanna discuss, because during the writing of the thesis quite new insight in what in fact the differences of behavior are in between the particle types
2. First of all wanna point out how we have lattice operators, so fixed sites where there can be particles
3. Occupation number from 0 to infinity
4. Nice to handle because they commute

Particle Types

Introduction of the Physical Problem

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  - Commutation relations

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- Bosonic operators
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- Fermionic operators

$$\left\{\hat{c}_l, \hat{c}_m\right\} = 0$$

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1. Occupation number only 0 and one: nice for computational handling
2. Anti-commute: not so nice to handle in the preparation

Particle Types
Introduction of the Physical Problem
Bosonic operators
Commutation relations
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Particle Types

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Bosonic operators
Commutation relations
Fermionic operators
Anti-commutation relations

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Particle Types

Introduction of the Physical Problem

- Bosonic operators
  - Commutation relations
- Fermionic operators
  - Anti-commutation relations
- Hard-core bosonic operators

$$\left[\hat{h}_l, \hat{h}_m\right] = 0$$

$$\left[\hat{h}_l^\dagger, \hat{h}_m^\dagger\right] = 0$$

$$\left[\hat{h}_l, \hat{h}_m^\dagger\right] = \left(1 - 2 \cdot \hat{h}_m^\dagger \hat{h}_m\right) \cdot \delta_{l,m}$$

$$\left(\hat{h}_l^\dagger \hat{h}_l\right)^n = \hat{h}_l^\dagger \hat{h}_l \qquad \forall n \in \mathbb{N}$$

1. Hard-core bosons: best fo both worlds
2. Like the fermions nice because only occupation number 0 and 1
3. but COMMUTATION relations, because of that we will be able to generate an important mapping
4. Finally: number operator is *idempotent* (power = potenz in english) which we need for one mathematical step later

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- Spins (Pauli operators/matrices)

$$\hat{\sigma}^0 = \mathbb{1} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$\hat{\sigma}^2 = \hat{\sigma}^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

$$\hat{\sigma}^1 = \hat{\sigma}^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$\hat{\sigma}^3 = \hat{\sigma}^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

1. Final particle type: spins - watch the 1/2 if it is a pauli or spin operator
2. Has also mostly commutative properties (also mainly *angular momentum* relations), but also one anti-commutation relation because of the properties of the Pauli matrices
3. Will be necessary for one mathematical re-formulation

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- Bosonic operators
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- Hard-core bosonic operators
  - Commutation relations
  - Occupation number limited to 0 and 1
  - Number operator is idempotent
- Spins (Pauli operators/matrices)
  - Particles from different sites commute
  - Different spin directions on the same site anti-commute
  - They obey angular momentum commutation relations

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$$\left\{\hat{\sigma}_l^\alpha, \hat{\sigma}_l^\beta\right\} = 2 \cdot \delta_{\alpha,\beta}$$

$$\left[\hat{\sigma}_l^\alpha, \hat{\sigma}_m^\beta\right] = 2 \cdot i \cdot \varepsilon_{\alpha,\beta,\gamma} \cdot \delta_{l,m} \cdot \hat{\sigma}_l^\gamma$$

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Particle Types - Mappings

Introduction of the Physical Problem

- Properties of Pauli matrices

Particle Types - Mappings
Introduction of the Physical Problem
Properties of Pauli matrices

1. Pauli matrices are a base for the complex 2x2 matrices
2. Kronecker product of two pauli matrices therefore base for complex 4x4 matrices
3. Simple transformation that can be verified for its commutation relations or derived from two *Jordan-Wigner Transformations*
4. Important to watch the order of base states and keep convention or -1 will be introduced unexpectedly

Particle Types - Mappings

Introduction of the Physical Problem

- Properties of Pauli matrices
  - Base of the complex 2x2 matrices

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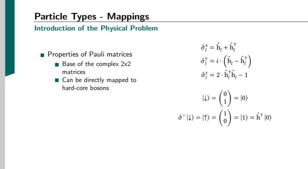
Particle Types - Mappings

Introduction of the Physical Problem

- Properties of Pauli matrices
  - Base of the complex 2x2 matrices
  - Can be directly mapped to hard-core bosons

$$\hat{\sigma}_l^{\mathrm{x}} = \hat{\mathrm{h}}_l + \hat{\mathrm{h}}_l^\dagger$$
$$\hat{\sigma}_l^{\mathrm{y}} = i \cdot \left(\hat{\mathrm{h}}_l - \hat{\mathrm{h}}_l^\dagger\right)$$
$$\hat{\sigma}_l^{\mathrm{z}} = 2 \cdot \hat{\mathrm{h}}_l^\dagger \hat{\mathrm{h}}_l - 1$$

$$|\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} = |0\rangle$$
$$\hat{\sigma}^+ |\downarrow\rangle = |\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = |1\rangle = \hat{\mathrm{h}}^\dagger |0\rangle$$



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Hamiltonian of the system

Introduction of the Physical Problem

- Hubbard model Hamiltonian

$$\mathcal{H} = \mathcal{H}_0 + \hat{\mathrm{V}}$$

$$\mathcal{H}_0 = U \cdot \sum_{l} \hat{\mathrm{n}}_{l,\uparrow} \hat{\mathrm{n}}_{l,\downarrow} + \sum_{l,\sigma} \underbrace{\left(\vec{E} \cdot \vec{r}_l\right)}_{\varepsilon_l} \hat{\mathrm{n}}_{l,\sigma}$$

$$\hat{\mathrm{V}} = -J \cdot \sum_{\langle l,m \rangle,\sigma} \left(\hat{\mathrm{h}}^{\dagger}_{l,\sigma} \hat{\mathrm{h}}_{m,\sigma} + \hat{\mathrm{h}}^{\dagger}_{m,\sigma} \hat{\mathrm{h}}_{l,\sigma} \right)$$

Hamiltonian of the system
Introduction of the Physical Problem
Hubbard model Hamiltonian

1. Hubbard model:
   - Double occupation term
   - Two particle degrees of freedom (= spin but not same spin as before: so also written as h and d)
   - Here: electrical field that acts symmetrical on both spin directions
   - Hopping term that is here treated as a perturbation

Hamiltonian of the system

Introduction of the Physical Problem

- Hubbard model Hamiltonian
- Constant external electric field

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Hamiltonian of the system

Introduction of the Physical Problem

- Hubbard model Hamiltonian
- Constant external electric field
- Two particle types (spin degrees)

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Hamiltonian of the system

Introduction of the Physical Problem

- Hubbard model Hamiltonian
- Constant external electric field
- Two particle types (spin degrees)
  - Different *spins* than for Pauli spin operators

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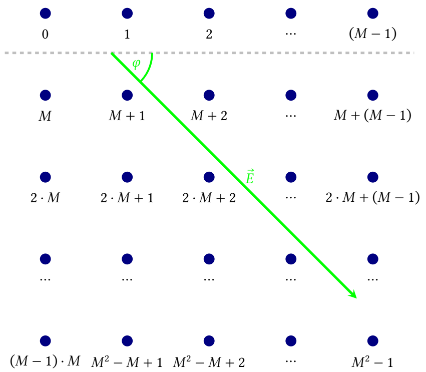
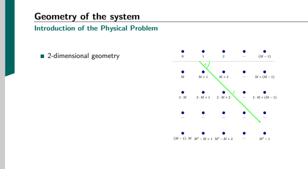
Geometry of the system

Introduction of the Physical Problem

- 2-dimensional geometry



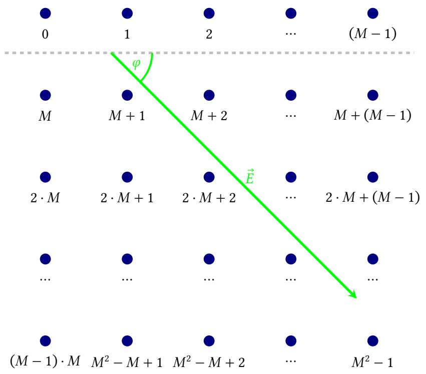


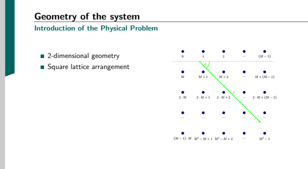
1. two-dimensional
2. square
3. Electrical field and we want to calculate generally for angle, field strength and number of sites

Geometry of the system

Introduction of the Physical Problem

- 2-dimensional geometry
- Square lattice arrangement





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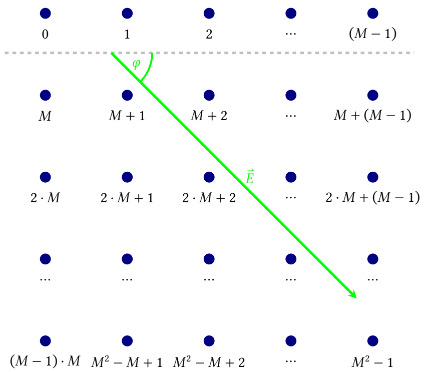
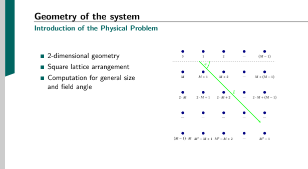
Geometry of the system

Introduction of the Physical Problem

- 2-dimensional geometry
- Square lattice arrangement
- Computation for general size and field angle





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Goal of the Calculation

Time Evolution

- Evaluate the time-evolution of the system for various observables

Goal of the Calculation
Time Evolution
- Evaluate the time-evolution of the system for various observables

1. Goal: evaluate the time-evolution for different observables (effectively)
2. Brute-force calculation is at least NP-hard, definitely exponential and one of the hardest problems to solve computationally generally
3. Strategy: perform a controlled expansion in the perturbation V and re-express the formulas as a dependency on a operator-free "effective Hamiltonian"
   - Can be re-ordered without concern as no operators
   - For the re-formulation we will use the interaction picture
4. Particle-type dependency is stored in this formula in the BASE STATES. Because in this re-formulation, the Heff is a pure number (no operator) and the initial state is a number (not operator dependent at all). But the base-state contains different info for fermions than for bosons, as the operators for hc-bosons commute and so the base-states are uniquely defined. But there are multiple possibilities for teh fermions, because swaps introduce minus signs. (State is not just 0s and 1s, but vacuum that is pre-set with operators and they have an order!!!!!)

Goal of the Calculation

Time Evolution

- Evaluate the time-evolution of the system for various observables
  - Uses calculation in the *Interaction Picture*

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Time Evolution

- Evaluate the time-evolution of the system for various observables
  - Uses calculation in the *Interaction Picture*
  - Introduce operator-less *effective Hamiltonian*

$$\left|\Psi^{S}(t)\right\rangle = \sum_{N} e^{\mathcal{H}_{\text{eff}}(N,t)}\Psi_{N}\left|N\right\rangle$$

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The effective Hamiltonian

Time Evolution

$$\mathcal{H}_{\text{eff}}(N,t) = -iE_0(N)t + \mathcal{H}_N(t)$$

1. Comprised of two parts:
   - Simple, quickly stated term that depends on the base energy
   - Complicated one that will be expanded in the perturbation

The effective Hamiltonian
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The effective Hamiltonian

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$$\mathcal{H}_{\text{eff}}(N,t) = -iE_0(N)t + \mathcal{H}_N(t)$$

- Constructed from the contributions of the base energy and the perturbation

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Constructed from the contributions of the base energy and the perturbation

The effective Hamiltonian

Time Evolution

$$\mathcal{H}_{\text{eff}}(N,t) \;=\; -iE_0(N)t \,+\, \mathcal{H}_N(t)$$

- Constructed from the contributions of the base energy and the perturbation
- Base energy contribution:

$$\begin{aligned} E_0(N) &= \frac{\langle N|\mathcal{H}_0|N\rangle}{\langle N|N\rangle} \\ &= \langle N|U\cdot\sum_l \hat{\mathrm{n}}_{l,\uparrow}\hat{\mathrm{n}}_{l,\downarrow}|N\rangle + \langle N|\sum_{l,\sigma}\varepsilon_l\hat{\mathrm{n}}_{l,\sigma}|N\rangle \\ &= U\cdot\sum_l n_{l,\uparrow}n_{l,\downarrow} + \sum_{l,\sigma}\varepsilon_l n_{l,\sigma} \end{aligned}$$

The effective Hamiltonian
Time Evolution
$\mathcal{H}_{\text{eff}}(N,t) = -iE_0(N)t + \mathcal{H}_N(t)$
Constructed from the contributions of the base energy and the perturbation
Base energy contribution:

1. Comprised of two parts:
   - Simple, quickly stated term that depends on the base energy
   - Complicated one that will be expanded in the perturbation

The effective Hamiltonian

Time Evolution

- To evaluate the time-evolution of the perturbation

$$\hat{V} = -J \cdot \sum_{\langle l,m \rangle} \left(\hat{h}_l^\dagger \hat{h}_m + \hat{h}_m^\dagger \hat{h}_l + \hat{d}_l^\dagger \hat{d}_m + \hat{d}_m^\dagger \hat{d}_l \right)$$

The effective Hamiltonian
Time Evolution
To evaluate the time-evolution of the perturbation
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1. Need: V-Operator in the Interaction picture
2. For that: first solve the equations of motion for the ladder operators and the plug in
3. Solving the equations of motions in the interaction picture requires their number operator being *idempotent*

The effective Hamiltonian

Time Evolution

- To evaluate the time-evolution of the perturbation

$$\hat{\mathrm{V}} = -J \cdot \sum_{\langle l,m \rangle} \left(\hat{\mathrm{h}}_l^\dagger \hat{\mathrm{h}}_m + \hat{\mathrm{h}}_m^\dagger \hat{\mathrm{h}}_l + \hat{\mathrm{d}}_l^\dagger \hat{\mathrm{d}}_m + \hat{\mathrm{d}}_m^\dagger \hat{\mathrm{d}}_l \right)$$

- Solve the equation of motion for the ladder operators

$$\hat{\mathrm{h}}_m^{\dagger\mathrm{I}}(t) = e^{i\cdot\varepsilon_m\cdot t} \left(1 + \left(e^{i\cdot U\cdot t} - 1 \right) \hat{\mathrm{d}}_m^{\dagger\mathrm{S}} \hat{\mathrm{d}}_m^{\mathrm{S}} \right) \hat{\mathrm{h}}_m^{\dagger\mathrm{S}}$$

$$\hat{\mathrm{h}}_m^{\mathrm{I}}(t) = e^{-i\cdot\varepsilon_m\cdot t} \left(1 + \left(e^{-i\cdot U\cdot t} - 1 \right) \hat{\mathrm{d}}_m^{\dagger\mathrm{S}} \hat{\mathrm{d}}_m^{\mathrm{S}} \right) \hat{\mathrm{h}}_m^{\mathrm{S}}$$

$$\hat{\mathrm{d}}_m^{\dagger\mathrm{I}}(t) = e^{i\cdot\varepsilon_m\cdot t} \left(1 + \left(e^{i\cdot U\cdot t} - 1 \right) \hat{\mathrm{h}}_m^{\dagger\mathrm{S}} \hat{\mathrm{h}}_m^{\mathrm{S}} \right) \hat{\mathrm{d}}_m^{\dagger\mathrm{S}}$$

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The effective Hamiltonian

Time Evolution

- Insert and reorder the operators

$$\begin{aligned}\hat{\mathrm{V}}^{\mathrm{I}}(t) &= \left\{\hat{\mathrm{V}}^{\mathrm{S}}\right\}^{\mathrm{I}}(t) = -J \cdot \sum_{[l,m]} \left\{ \left(\hat{\mathrm{h}}_l^{\dagger\mathrm{S}} \hat{\mathrm{h}}_m^{\mathrm{S}} + \hat{\mathrm{d}}_l^{\dagger\mathrm{S}} \hat{\mathrm{d}}_m^{\mathrm{S}} \right) \right\}^{\mathrm{I}}(t) \\ &= -J \cdot \sum_{[l,m]} \left(\hat{\mathrm{h}}_l^{\dagger\mathrm{I}}(t) \hat{\mathrm{h}}_m^{\mathrm{I}}(t) + \hat{\mathrm{d}}_l^{\dagger\mathrm{I}}(t) \hat{\mathrm{d}}_m^{\mathrm{I}}(t) \right) \\ &= -J \cdot \sum_{[l,m]} \left[\Lambda_{\mathrm{A}}(l,m,t) \cdot \hat{\mathrm{F}}_{\mathrm{A}}(l,m) + \Lambda_{\mathrm{B}}(l,m,t) \cdot \hat{\mathrm{F}}_{\mathrm{B}}(l,m) + \Lambda_{\mathrm{C}}(l,m,t) \cdot \hat{\mathrm{F}}_{\mathrm{C}}(l,m) \right]\end{aligned}$$

1. Inserting yields TWO kinds of terms
   - time-dependent analytical pre-factors (or their integral as one sees later)
   - dressed hopping terms, basically only depending on the occupation of the state N

The effective Hamiltonian

Time Evolution

- Insert and reorder the operators

$$
\begin{aligned}
\hat{V}^{I}(t) &= \left\{\hat{V}^{S}\right\}^{I}(t) = -J\cdot\sum_{[l,m]}\left\{\left(\hat{h}_{l}^{\dagger S}\hat{h}_{m}^{S}+\hat{d}_{l}^{\dagger S}\hat{d}_{m}^{S}\right)\right\}^{I}(t)\\
&= -J\cdot\sum_{[l,m]}\left(\hat{h}_{l}^{\dagger I}(t)\hat{h}_{m}^{I}(t)+\hat{d}_{l}^{\dagger I}(t)\hat{d}_{m}^{I}(t)\right)\\
&= -J\cdot\sum_{[l,m]}\left[\Lambda_{A}(l,m,t)\cdot\hat{F}_{A}(l,m)+\Lambda_{B}(l,m,t)\cdot\hat{F}_{B}(l,m)+\Lambda_{C}(l,m,t)\cdot\hat{F}_{C}(l,m)\right]
\end{aligned}
$$

$$
\begin{aligned}
\Lambda_{A}(l,m,t) &= e^{i\cdot(\varepsilon_l-\varepsilon_m)\cdot t} & \hat{F}_{A}(l,m) &= \sum_{\sigma\in\{\uparrow,\downarrow\}}\hat{h}_{l,\sigma}^{\dagger S}\hat{h}_{m,\sigma}^{S}\left(1+2\cdot\hat{n}_{l,\bar{\sigma}}^{S}\hat{n}_{m,\bar{\sigma}}^{S}-\hat{n}_{l,\bar{\sigma}}^{S}-\hat{n}_{m,\bar{\sigma}}^{S}\right)\\
\Lambda_{B}(l,m,t) &= e^{i\cdot(\varepsilon_l-\varepsilon_m+U)\cdot t} & \hat{F}_{B}(l,m) &= \sum_{\sigma\in\{\uparrow,\downarrow\}}\hat{h}_{l,\sigma}^{\dagger S}\hat{h}_{m,\sigma}^{S}\left(\hat{n}_{l,\bar{\sigma}}^{S}-\hat{n}_{l,\bar{\sigma}}^{S}\hat{n}_{m,\bar{\sigma}}^{S}\right)\\
\Lambda_{C}(l,m,t) &= e^{i\cdot(\varepsilon_l-\varepsilon_m-U)\cdot t} & \hat{F}_{C}(l,m) &= \sum_{\sigma\in\{\uparrow,\downarrow\}}\hat{h}_{l,\sigma}^{\dagger S}\hat{h}_{m,\sigma}^{S}\left(\hat{n}_{m,\bar{\sigma}}^{S}-\hat{n}_{m,\bar{\sigma}}^{S}\hat{n}_{l,\bar{\sigma}}^{S}\right)
\end{aligned}
$$

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   - time-dependent analytical pre-factors (or their integral as one sees later)
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The effective Hamiltonian

Time Evolution

- Evaluate the contribution to the effective Hamiltonian

The effective Hamiltonian
Time Evolution
Evaluate the contribution to the effective Hamiltonian

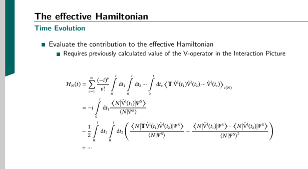
1. Generally any expansion possible, but here we expand the *argument of the exponential* - cumulant
2. first order easily derivable with the info from the previous slide (integrate)
3. second and higher orders very complicated occupation terms and the pre-factors require quite a lot of edge-cases to integrate with the time-ordering operator
   - Hint onto the thesis for this exact derivation

The effective Hamiltonian

Time Evolution

- Evaluate the contribution to the effective Hamiltonian
  - Requires previously calculated value of the V-operator in the Interaction Picture

$$
\begin{aligned}
\mathcal{H}_N(t) &= \sum_{v=1}^{\infty} \frac{(-i)^v}{v!} \int_0^t \mathrm{d}t_1 \int_0^t \mathrm{d}t_2 \cdots \int_0^t \mathrm{d}t_v \left\langle \mathbb{T}\, \hat{\mathrm{V}}^{\mathrm{I}}(t_1) \hat{\mathrm{V}}^{\mathrm{I}}(t_2) \cdots \hat{\mathrm{V}}^{\mathrm{I}}(t_v) \right\rangle_{c(N)} \\
&= -i \int_0^t \mathrm{d}t_1 \frac{\left\langle N \middle| \hat{\mathrm{V}}^{\mathrm{I}}(t_1) \middle| \Psi^{\mathrm{S}} \right\rangle}{\langle N | \Psi^{\mathrm{S}} \rangle} \\
&- \frac{1}{2} \int_0^t \mathrm{d}t_1 \int_0^t \mathrm{d}t_2 \left(\frac{\left\langle N \middle| \mathbb{T} \hat{\mathrm{V}}^{\mathrm{I}}(t_1) \hat{\mathrm{V}}^{\mathrm{I}}(t_2) \middle| \Psi^{\mathrm{S}} \right\rangle}{\langle N | \Psi^{\mathrm{S}} \rangle} - \frac{\left\langle N \middle| \hat{\mathrm{V}}^{\mathrm{I}}(t_1) \middle| \Psi^{\mathrm{S}} \right\rangle \cdot \left\langle N \middle| \hat{\mathrm{V}}^{\mathrm{I}}(t_2) \middle| \Psi^{\mathrm{S}} \right\rangle}{\langle N | \Psi^{\mathrm{S}} \rangle^2} \right) \\
&+ \cdots
\end{aligned}
$$



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The effective Hamiltonian

Time Evolution

- Evaluate the contribution to the effective Hamiltonian
  - Requires previously calculated value of the V-operator in the Interaction Picture
  - Controllable *cumulant expansion*

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\mathcal{H}_N(t) &= \sum_{v=1}^{\infty} \frac{(-i)^v}{v!} \int_0^t \mathrm{d}t_1 \int_0^t \mathrm{d}t_2 \cdots \int_0^t \mathrm{d}t_v \, \left\langle \mathbb{T}\, \hat{\mathrm{V}}^{\mathrm{I}}(t_1)\hat{\mathrm{V}}^{\mathrm{I}}(t_2) \cdots \hat{\mathrm{V}}^{\mathrm{I}}(t_v) \right\rangle_{\mathrm{c}(N)} \\
&= -i \int_0^t \mathrm{d}t_1 \frac{\left\langle N \middle| \hat{\mathrm{V}}^{\mathrm{I}}(t_1) \middle| \Psi^{\mathrm{S}} \right\rangle}{\langle N | \Psi^{\mathrm{S}} \rangle} \\
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Handling of Observables

Time Evolution

- This allows for general evaluation of expectation values

$$\frac{\left\langle \Psi^S(t) \middle| \hat{\mathcal{O}} \middle| \Psi^S(t) \right\rangle}{\langle \Psi^S(t) | \Psi^S(t) \rangle} =$$

Handling of Observables
Time Evolution
This allows for general evaluation of expectation values

1. Why? General evaluation of an expectation value for an observable.
   - Probability for state
   - Local observable (can be swapped for many different ones)
2. Does ONLY require difference of effective Hamiltonian for evaluation (notice for later)

Handling of Observables

Time Evolution

- This allows for general evaluation of expectation values
  - Requires a probability for the state
  - Requires a local observable

$$\frac{\left\langle \Psi^{S}(t) \middle| \hat{\mathcal{O}} \middle| \Psi^{S}(t) \right\rangle}{\langle \Psi^{S}(t) | \Psi^{S}(t) \rangle} =$$

$$\sum_{N} \mathrm{P}(N,t) \underbrace{\sum_{K} \langle N|\hat{\mathcal{O}}|K\rangle \, e^{\mathcal{H}_{\mathrm{eff}}(K,t)-\mathcal{H}_{\mathrm{eff}}(N,t)} \frac{\Psi_K}{\Psi_N}}_{\hat{\mathcal{O}}_{\mathrm{loc}}(N,t)} = \sum_{N} \mathrm{P}(N,t) \hat{\mathcal{O}}_{\mathrm{loc}}(N,t)$$

Handling of Observables
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Time Evolution

- Local observable for double occupation measurement

Simple Observables
Time Evolution
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1. Complex valued observable, make sure this cancels in the case of approximations
2. *SHOULD MENTION:* Energy and variance (most expensive ones, are assumed to keep constant, can be used to gauge the quality of the expansion)

Simple Observables

Time Evolution

- Local observable for double occupation measurement
  - Observables generally are very sparse matrices
  - Reduces to pure occupation measurement

$$\hat{\mathcal{O}}_{\text{loc}}(N,t) = \sum_K \langle N|\hat{\mathcal{O}}_{\text{do}}(l)|K\rangle\, e^{\mathcal{H}_{\text{eff}}(K,t)-\mathcal{H}_{\text{eff}}(N,t)}\frac{\Psi_K}{\Psi_N} = n_{l,\uparrow}\cdot n_{l,\downarrow}$$

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Time Evolution
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- Local observable for particle current measurement
  - Requires evaluation of the difference of two effective Hamiltonians

$$\hat{\mathcal{O}}_{\mathrm{loc}}(N,t) = i \cdot \left[n_{m,\sigma} \cdot (1-n_{l,\sigma}) - n_{l,\sigma} \cdot (1-n_{m,\sigma})\right] \cdot \frac{\Psi_{\tilde{N}}}{\Psi_N} \cdot e^{\mathcal{H}_{\mathrm{eff}}(\tilde{N},t)-\mathcal{H}_{\mathrm{eff}}(N,t)}$$

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Access to Density-Matrics

Time Evolution

- Non-classical (*quantum*) measurements depend on the (reduced) density matrix

Access to Density-Matrics
Time Evolution
- Non-classical (*quantum*) measurements depend on the (reduced) density matrix

1. Quite interesting, because of this extra mentioned the Pauli operators
2. No access to the full density matrix, can not trace out, because too many states to trace out
3. BUT: as the complex 4x4 matrix can be written in the base of the kronecker product of two pauli matrices, can be expressed (because the pauli operators can be translated into hard-core bosonic ones again and for these we have the general fromula for expectation values)

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Access to Density-Matrics

Time Evolution

- Non-classical (*quantum*) measurements depend on the (reduced) density matrix
  - Access to *purity*, *concurrence* and other entanglement measures/monotones
- Direct calculation not possible

$$\rho_A = \mathrm{Tr}_B\left(\rho_{AB}\right) = \sum_{k=0}^{M} \left(\mathbb{1}_A \otimes \langle \chi_k|\right) \rho_{AB} \left(\mathbb{1}_A \otimes |\chi_k\rangle\right)$$

Access to Density-Matrics
Time Evolution
Non-classical (quantum) measurements depend on the (reduced) density matrix
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- Use Pauli matrices to expand the complex 4x4 matrix

$$\rho_A(t) = \rho_{l,\sigma,m,\mu}(t) = \frac{1}{4} \sum_{\alpha,\beta\in\{0,x,y,z\}} \left\langle \hat{\sigma}^{\alpha}_{l,\sigma} \hat{\sigma}^{\beta}_{m,\mu} \right\rangle_{(t)} \left(\hat{\sigma}^{\alpha} \otimes \hat{\sigma}^{\beta}\right)$$

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Access to Density-Matrics

Time Evolution

$$\hat{\mathcal{O}} = \hat{\sigma}^{\mathrm{x}}_{l,\sigma}\hat{\sigma}^{0}_{m,\mu} \quad : \quad \hat{\mathcal{O}}_{\mathrm{loc}}(N,t) = \frac{\Psi_{\tilde{N}}}{\Psi_N} \cdot e^{\mathcal{H}_{\mathrm{eff}}(\tilde{N},t)-\mathcal{H}_{\mathrm{eff}}(N,t)}$$

$$\hat{\mathcal{O}} = \hat{\sigma}^{\mathrm{y}}_{l,\sigma}\hat{\sigma}^{0}_{m,\mu} \quad : \quad \hat{\mathcal{O}}_{\mathrm{loc}}(N,t) = \frac{\Psi_{\tilde{N}}}{\Psi_N} \cdot e^{\mathcal{H}_{\mathrm{eff}}(\tilde{N},t)-\mathcal{H}_{\mathrm{eff}}(N,t)} \cdot i \cdot (1 - 2 \cdot n_{l,\sigma})$$

$$\hat{\mathcal{O}} = \hat{\sigma}^{\mathrm{z}}_{l,\sigma}\hat{\sigma}^{0}_{m,\mu} \quad : \quad \hat{\mathcal{O}}_{\mathrm{loc}}(N,t) = \frac{\Psi_{\tilde{N}}}{\Psi_N} \cdot e^{\mathcal{H}_{\mathrm{eff}}(\tilde{N},t)-\mathcal{H}_{\mathrm{eff}}(N,t)} \cdot (2 \cdot n_{l,\sigma} - 1)$$

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$$\hat{\mathcal{O}} = \hat{\sigma}^{\mathrm{x}}_{l,\sigma}\hat{\sigma}^{\mathrm{y}}_{m,\mu} \quad : \quad \hat{\mathcal{O}}_{\mathrm{loc}}(N,t) = \frac{\Psi_{\tilde{\tilde{N}}}}{\Psi_N} \cdot e^{\mathcal{H}_{\mathrm{eff}}(\tilde{\tilde{N}},t)-\mathcal{H}_{\mathrm{eff}}(N,t)} \cdot i \cdot (1 - 2 \cdot n_{m,\mu})$$

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Access to Density-Matrics
Time Evolution

1. Sixteen terms (with missing cases trivially derived from the ones that are given)
2. Again all depend on the difference of effective hamiltonians between two states ith local modifications

Probability Calculations

Sampling & Simplifications

- Full probability still requires normalization

Probability Calculations
Sampling & Simplifications
Full probability still requires normalization

1. Normalization requires knowing exponential amount of states and we need to sample an exponential amount to get all
2. switch to METROPOLIS HASTINGS algorithm
   - only fixed number of samples required (depends on the desired precision)
   - No normalization needed, because it cancels in the division

Probability Calculations

Sampling & Simplifications

- Full probability still requires normalization
- Switch to the Metropolis *Hastings* algorithm
  - Non-exponential number of samples

$$\frac{\langle \Psi^S(t)|\hat{\mathcal{O}}|\Psi^S(t)\rangle}{\langle \Psi^S(t)|\Psi^S(t)\rangle} = \sum_N \mathrm{P}(N,t)\cdot\hat{\mathcal{O}}_{\mathrm{loc}}(N,t) \approx \frac{1}{|\{N\}_{\mathrm{MC}}|}\sum_{\{N\}_{\mathrm{MC}}}\hat{\mathcal{O}}_{\mathrm{loc}}(N,t)$$

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Probability Calculations

Sampling & Simplifications

- Full probability still requires normalization
- Switch to the Metropolis *Hastings* algorithm
  - Non-exponential number of samples
  - Depends only on a transition probability
  - Does not need normalization because it cancels

$$\alpha = \frac{\mathrm{P}(\widetilde{N},t)}{\mathrm{P}(N,t)} = \frac{f(\widetilde{N},t)}{f(N,t)} = \frac{\left|e^{\mathcal{H}_{\mathrm{eff}}(\widetilde{N},t)}\right|^2 |\Psi_{\widetilde{N}}|^2}{\left|e^{\mathcal{H}_{\mathrm{eff}}(N,t)}\right|^2 |\Psi_N|^2}$$

$$= \frac{|\Psi_{\widetilde{N}}|^2}{|\Psi_N|^2} \frac{e^{\Re(\mathcal{H}_{\mathrm{eff}}(\widetilde{N},t))+i\Im(\mathcal{H}_{\mathrm{eff}}(\widetilde{N},t))+\Re(\mathcal{H}_{\mathrm{eff}}(\widetilde{N},t))-i\Im(\mathcal{H}_{\mathrm{eff}}(\widetilde{N},t))}}{e^{\Re(\mathcal{H}_{\mathrm{eff}}(N,t))+i\Im(\mathcal{H}_{\mathrm{eff}}(N,t))+\Re(\mathcal{H}_{\mathrm{eff}}(N,t))-i\Im(\mathcal{H}_{\mathrm{eff}}(N,t))}}$$

$$= \frac{|\Psi_{\widetilde{N}}|^2}{|\Psi_N|^2} e^{2\cdot\Re(\mathcal{H}_{\mathrm{eff}}(\widetilde{N},t))-2\cdot\Re(\mathcal{H}_{\mathrm{eff}}(N,t))}$$

$$= \frac{|\Psi_{\widetilde{N}}|^2}{|\Psi_N|^2} e^{2\cdot\Re(\mathcal{H}_{\mathrm{eff}}(\widetilde{N},t)-\mathcal{H}_{\mathrm{eff}}(N,t))}$$

$$\frac{\left\langle \Psi^S(t) \middle| \hat{\mathcal{O}} \middle| \Psi^S(t) \right\rangle}{\left\langle \Psi^S(t) \middle| \Psi^S(t) \right\rangle} = \sum_N \mathrm{P}(N,t) \cdot \hat{\mathcal{O}}_{\mathrm{loc}}(N,t) \approx \frac{1}{|\{N\}_{\mathrm{MC}}|} \sum_{\{N\}_{\mathrm{MC}}} \hat{\mathcal{O}}_{\mathrm{loc}}(N,t)$$

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Analytical Simplifications

Sampling & Simplifications

- Choose a helpful initial state

Analytical Simplifications
Sampling & Simplifications
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1. Choose the helpful *initial state* with all base states having the same probability
2. because of this the divisions of Psi-N over Psi-K everywhere give 1 and many terms cancel (outside of the local interaction ragne of the modificaiton)

Analytical Simplifications

Sampling & Simplifications

- Choose a helpful initial state

$$\Psi_N = \frac{1}{\sqrt{\#(\text{states})}} = \frac{1}{\sqrt{2^{\#(\text{sites})\cdot 2}}} = \frac{1}{2^{\#(\text{sites})}}$$

$$\left|\Psi^{S}(t=0)\right\rangle = \bigotimes_{l=1}^{\#(\text{states})} \frac{1}{2}\left(1 + \hat{\mathrm{h}}_{l,\uparrow}^{\dagger S} + \hat{\mathrm{h}}_{l,\downarrow}^{\dagger S} + \hat{\mathrm{h}}_{l,\uparrow}^{\dagger S}\hat{\mathrm{h}}_{l,\downarrow}^{\dagger S}\right)|0\rangle$$

- Now *almost all* terms cancel in *differences* of the effective Hamiltonian

1. Choose the helpful *initial state* with all base states having the same probability
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- Choose a helpful initial state

$$\Psi_N = \frac{1}{\sqrt{\#(\text{states})}} = \frac{1}{\sqrt{2^{\#(\text{sites})\cdot 2}}} = \frac{1}{2^{\#(\text{sites})}}$$

$$\left|\Psi^S(t=0)\right\rangle = \bigotimes_{l=1}^{\#(\text{states})} \frac{1}{2}\left(1 + \hat{\mathrm{h}}^{\dagger S}_{l,\uparrow} + \hat{\mathrm{h}}^{\dagger S}_{l,\downarrow} + \hat{\mathrm{h}}^{\dagger S}_{l,\uparrow}\hat{\mathrm{h}}^{\dagger S}_{l,\downarrow}\right)|0\rangle$$

- Now *almost all* terms cancel in *differences* of the effective Hamiltonian
  - Exemplary for single flip on base energy term

$$\begin{aligned} E_0(N) - E_0(\widetilde{N}) &= U\sum_l n_{l,\downarrow}n_{l,\uparrow} - U\sum_l \widetilde{n}_{l,\downarrow}\widetilde{n}_{l,\uparrow} + \sum_{l,\sigma}\varepsilon_l n_{l,\sigma} - \sum_{l,\sigma}\varepsilon_l\widetilde{n}_{l,\sigma} \\ &= \varepsilon_i\left(2n_{i,\sigma_i}-1\right) + U\cdot\begin{cases}\sigma_i=\uparrow: & n_{i,\downarrow}(2n_{i,\uparrow}-1)\\ \sigma_i=\downarrow: & n_{i,\uparrow}(2n_{i,\downarrow}-1)\end{cases}\end{aligned}$$

1. Choose the helpful *initial state* with all base states having the same probability
2. because of this the divisions of Psi-N over Psi-K everywhere give 1 and many terms cancel (outside of the local interaction ragne of the modificaiton)

Why and How should Parameters be variational?

Variational Classical Networks

- Theoretically: always better approximation through higher order terms

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   - Find a parametrized *wavefunction*
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4. *time DERIVATIVE*

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$$\sum_{k'} \overleftrightarrow{S}_{k,k'}\dot{\vec{\eta}}_{k'} = -i\vec{F}_k$$

$$\dot{\vec{\eta}} = -i\overleftrightarrow{S}^{-1}\vec{F}$$

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First Try: Cumulant Expansion Prefactors

Variational Classical Networks

- Idea: generate a variational Hamiltonian by replacing the analytical prefactors

$$\mathcal{H}_N(t) = \sum_i C_i(t) \cdot \Phi_i(N) \quad \leftrightarrow \quad \mathcal{H}_{\mathrm{VCN}}(N, \vec{\eta}) = \sum_i \eta_i \cdot \Phi_i(N)$$

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$$\begin{aligned}
C_1(t) &= \varPi_{\mathrm{A}}(0,1,t) & \varPhi_1(N) &= J \sum_l \sum_{\langle l \overset{+(\mathrm{x})}{<} m\rangle} \sum_K \frac{\Psi_K}{\Psi_N} \langle N|\hat{\mathrm{F}}_{\mathrm{A}}(l,m)|K\rangle & C_5(t) &= \varPi_{\mathrm{B}}(1,0,t) & \varPhi_5(N) &= J \sum_l \sum_{\langle l \overset{+(\mathrm{x})}{>} m\rangle} \sum_K \frac{\Psi_K}{\Psi_N} \langle N|\hat{\mathrm{F}}_{\mathrm{B}}(l,m)|K\rangle \\
C_2(t) &= \varPi_{\mathrm{B}}(0,1,t) & \varPhi_2(N) &= J \sum_l \sum_{\langle l \overset{+(\mathrm{x})}{<} m\rangle} \sum_K \frac{\Psi_K}{\Psi_N} \langle N|\hat{\mathrm{F}}_{\mathrm{B}}(l,m)|K\rangle & C_6(t) &= \varPi_{\mathrm{C}}(1,0,t) & \varPhi_6(N) &= J \sum_l \sum_{\langle l \overset{+(\mathrm{x})}{>} m\rangle} \sum_K \frac{\Psi_K}{\Psi_N} \langle N|\hat{\mathrm{F}}_{\mathrm{C}}(l,m)|K\rangle \\
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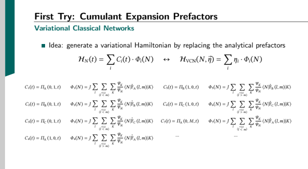
C_4(t) &= \varPi_{\mathrm{A}}(1,0,t) & \varPhi_4(N) &= J \sum_l \sum_{\langle l \overset{+(\mathrm{x})}{>} m\rangle} \sum_K \frac{\Psi_K}{\Psi_N} \langle N|\hat{\mathrm{F}}_{\mathrm{A}}(l,m)|K\rangle & &\cdots & &\cdots
\end{aligned}$$



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Correction: Watch Explicit Time-Dependency

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- First strategy is not suitable
  - Energy- and variance is not conserved

1. Fails because not taken the explicit time-dependency into account as it was *differentiated away* wrongfully
2. As a solution: introduce variational base-energy factors - which is a successful strategy

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$$\frac{\partial \mathcal{H}_{\text{eff}}(N,\vec{\eta},t)}{\partial \vec{\eta}_k} = \frac{\partial\left(-iE_0(N)t + \mathcal{H}_{\text{VCN}}(N,\vec{\eta})\right)}{\partial \vec{\eta}_k}$$

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- Solution: Replace base energy factors with variational parameters

$$E_0(N) = U\cdot\sum_m n_{m,\uparrow}n_{m,\downarrow} + \sum_{l,\sigma}\varepsilon_l n_{l,\sigma}$$

$$\eta_l^{\text{b.e.}} = \begin{cases} l=0: & -i\cdot U\cdot t \\ l>0: & -i\cdot\varepsilon_l\cdot t \end{cases}$$

$$\Phi_l^{\text{b.e.}}(N) = \begin{cases} l=0: & \sum_m n_{m,\uparrow}n_{m,\downarrow} \\ l>0: & \sum_\sigma n_{l,\sigma} \end{cases}$$

$$\mathcal{H}_{\text{eff}}^{\text{VCN}}(N,\vec{\eta}) = \sum_{n=1}^{\#(\text{var.})}\eta_n^{\text{var.}}\cdot\Phi_n^{\text{var.}}(N) + \sum_{l=0}^{L}\eta_l^{\text{b.e.}}\cdot\Phi_l^{\text{b.e.}}(N) = \sum_l \eta_l\cdot\Phi_l(N)$$

$$\vec{\eta} = \left(\eta_1^{\text{var.}},\eta_2^{\text{var.}},\ldots,\eta_{\#(\text{var.})}^{\text{var.}},\eta_0^{\text{b.e.}},\eta_1^{\text{b.e.}},\ldots,\eta_L^{\text{b.e.}}\right)^{\text{T}}$$

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Implementation

Implementation & Experiments

- Too much code to properly show
  - Look at repository for overview

1. While nothing is looked at in detail maybe interesting for some
2. Testing: validation and assertion based programming
3. Optimization: code style runtime experiments

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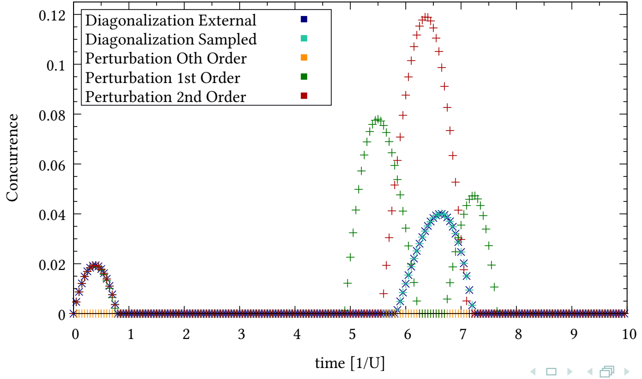
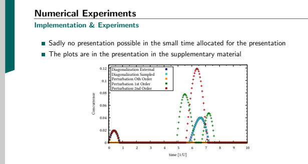
Numerical Experiments

Implementation & Experiments

- Sadly no presentation possible in the small time allocated for the presentation
- The plots are in the presentation in the supplementary material





1. See supplementary material for more plots and stuff

Conclusion & Outlook

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Conclusion:

- Successfully transferred and validated the theory
- Working implementation
  - Extensively tested
  - Configurable and extensible
- Started validating expectations with measurements on the compute cluster

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1. Conclusion:
   - Managed to Solve all problems
   - Provide heavily *tested* and *extensible* library of code AND theoretical summary
   - Started to validate expectations with computations on the cluster
2. Future plans:
   - re-write in performant language after testing is successful
   - Go through the parameters to start investigating the behavior of the systems

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Outlook:

- Re-write in lower level language to gain performance over Python
- Start more real experiments now that the theory is validated to work

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Thank you for your kind attention

Universität Augsburg
Mathematisch-Naturwissenschaftlich-Technische Fakultät

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University of Augsburg
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www.uni-augsburg.de

1. Thank you for your kind attention
2. All tools and other resources are referenced in the presentation
3. You can also find everything on my Github

References I

Summary & Conclusion

[1] J. Kell, *Latex sources for this presentation and the main thesis*, (2025) https://github.com/jonas-kell/master-thesis-documents.

[2] J. Kell, *Thesis code implementation and reference*, (2025) https://github.com/jonas-kell/master-thesis-code.

[3] J. Kell, *Https://github.com/jonas-kell/beamer-theme-unia-mntf*, (2024) https://github.com/jonas-kell/math-manipulator.

Master Colloquium Presentation
└Summary & Conclusion
└References

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Extra Plots: Overview

Extra slides

- Exact comparison density matrix
- First orders: energy and variance comparison
- J parameter sweep
- Monte Carlo sampling convergence
- Runtime validation
- VCN: parametrization failiure
- VCN: energy conservation can be controlled
- VCN: minimal square reference system
- VCN: larger square reference system in direct comparison
- VCN: system size dependency

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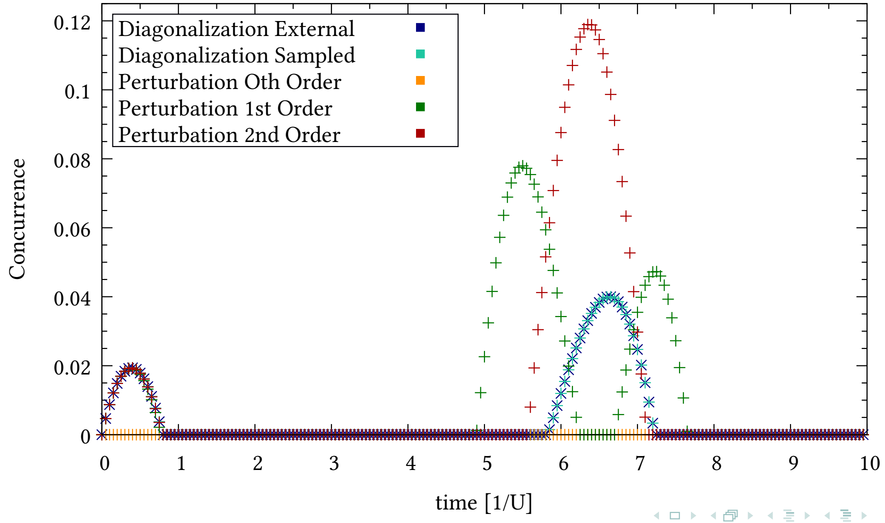
Exact Comparison: Concurrence

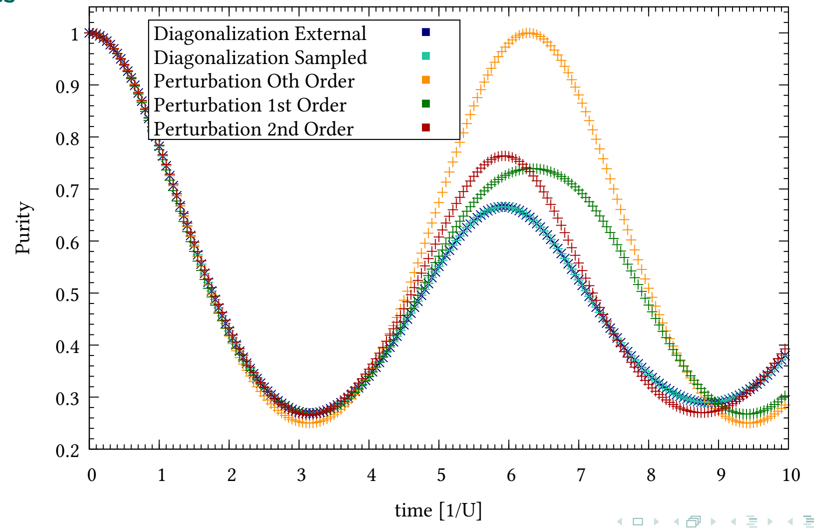
Extra slides

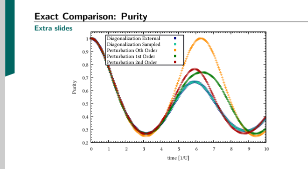


1. Concurrence comparison of small system with exact calculations and comparison thereof
2. See extreme boost of second order
3. NOTICE: how the External calculation is done COMPLETELY on density matrices and diagonalization, so prooves we can sample the reduced density matrix out

Exact Comparison: Purity

Extra slides

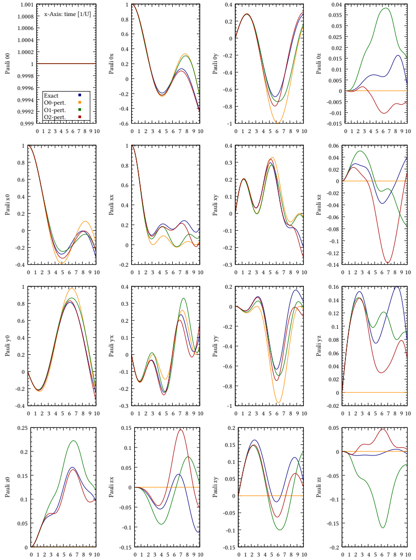


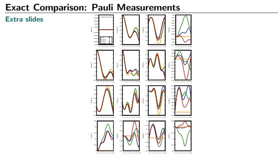


1. Purity measurements for the graph of the measurement from one page before

Exact Comparison: Pauli Measurements

Extra slides

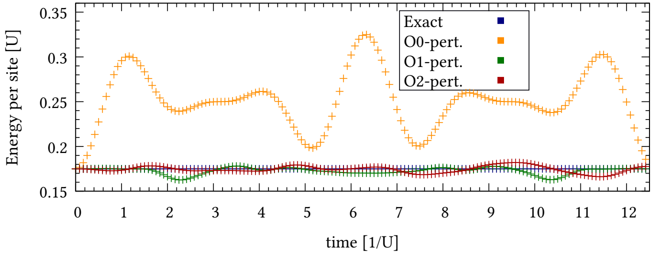


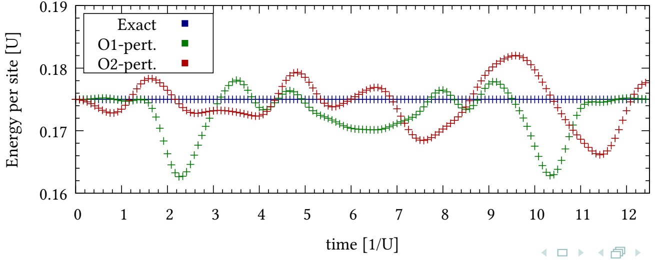


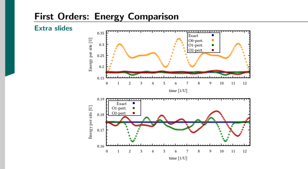
1. Portrait mode format, because extracted from the thesis.
2. You can see what a problem the z-contributions are

First Orders: Energy Comparison

Extra slides



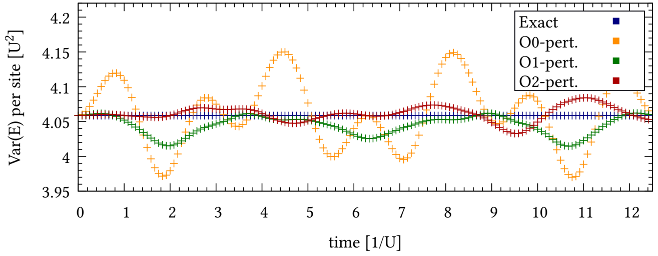


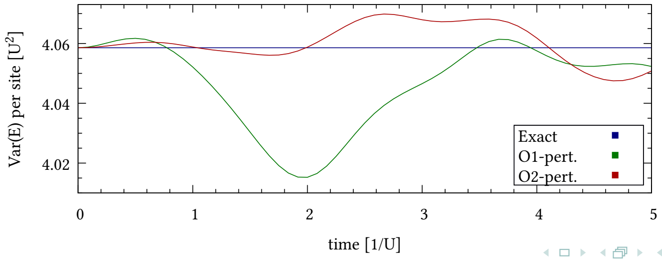


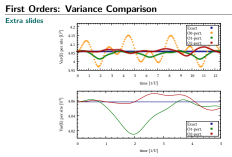
1. Second picture zoomed in

First Orders: Variance Comparison

Extra slides



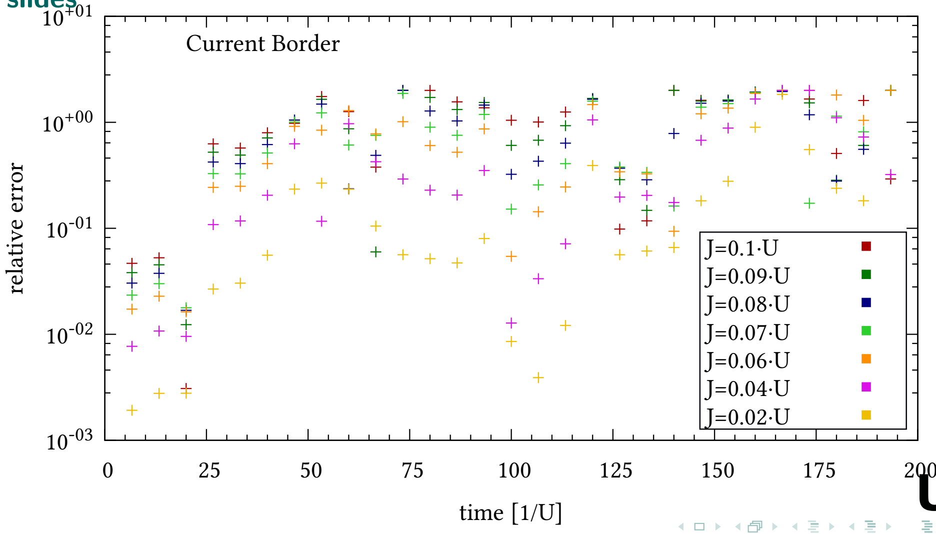


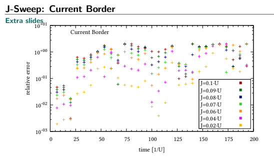


1. Second picture zoomed in

J-Sweep: Current Border

Extra slides

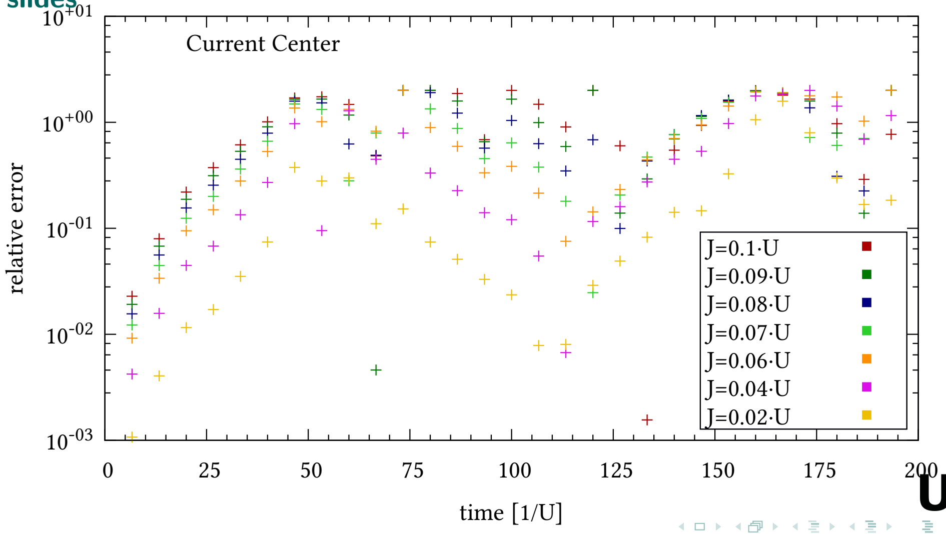


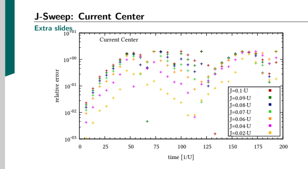


1. Logarithmic plot
2. Measurements show the trend of the convergence of the relative error for small perturbations
3. Depends on the observable though, still

J-Sweep: Current Center

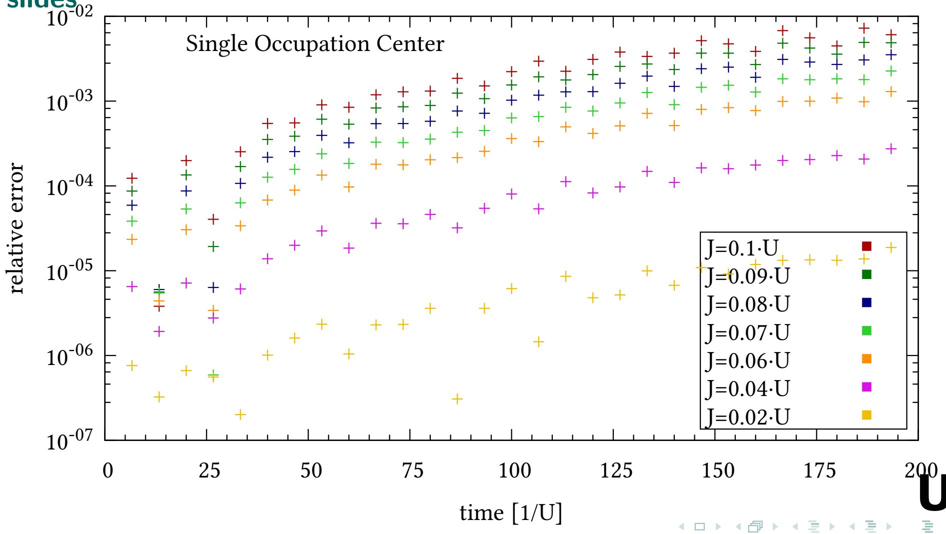
Extra slides

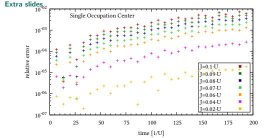




J-Sweep: Single Occupation Center

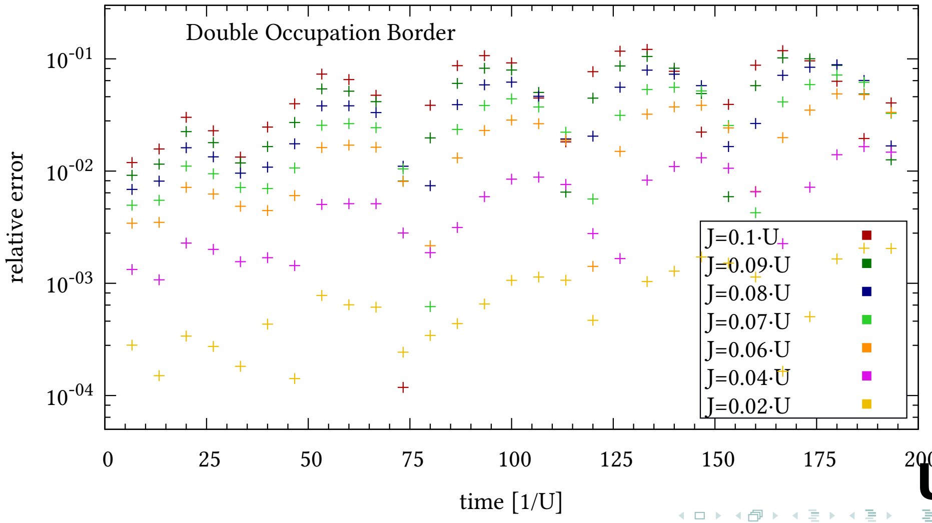
Extra slides





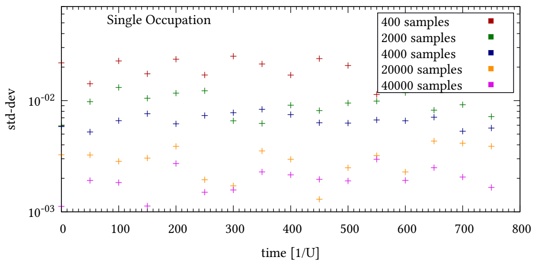
J-Sweep: Double Occupation Border

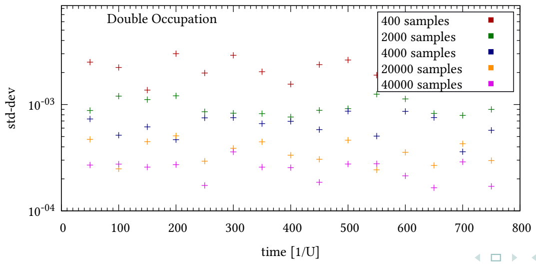
Extra slides

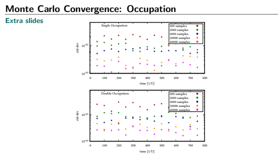


Monte Carlo Convergence: Occupation

Extra slides



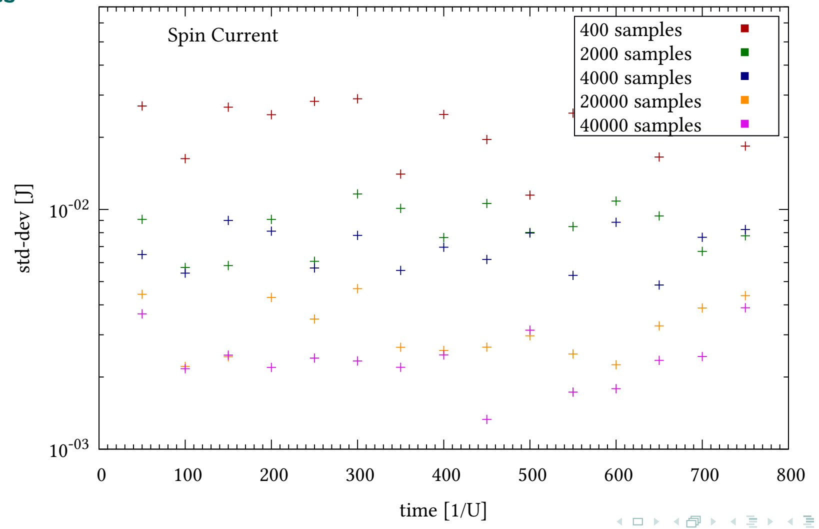


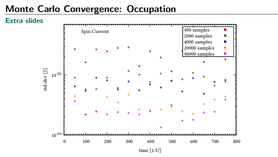


1. Well as we can see, the apprixmination converges as the variance gos to zero

Monte Carlo Convergence: Occupation

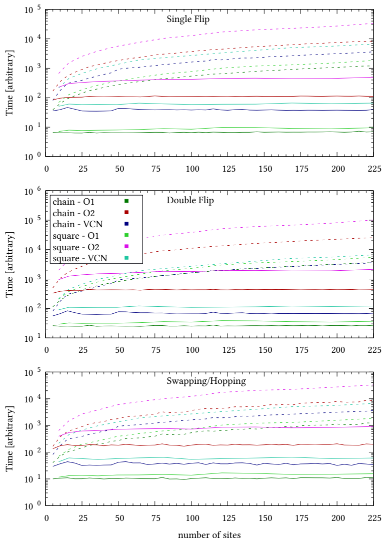
Extra slides

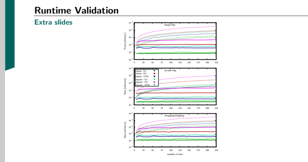




Runtime Validation

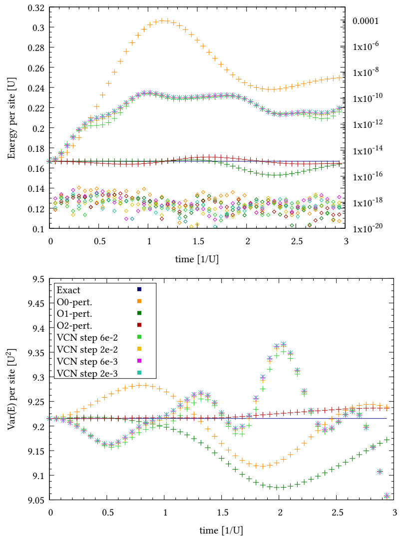
Extra slides

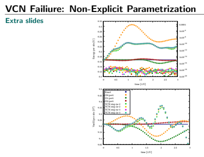




VCN Failiure: Non-Explicit Parametrization

Extra slides

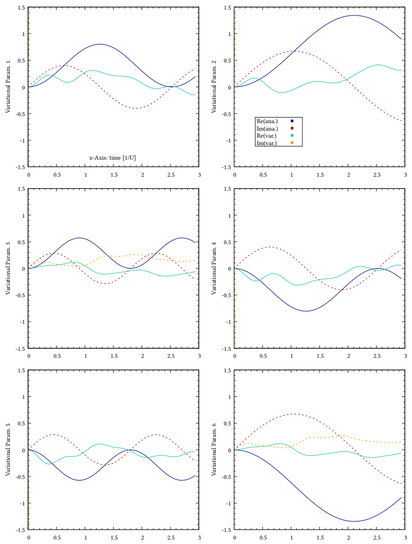


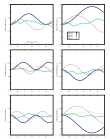


1. Complex part now properly vanishes (was long a problem)
2. See how the vcn goes like the base energy curve only in the beginning (suspiciously)

VCN Failiure: Non-Explicit Parametrization

Extra slides

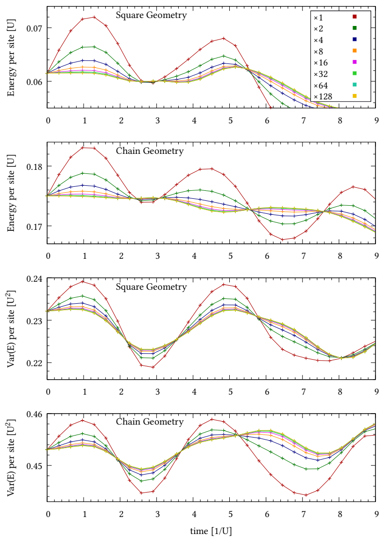


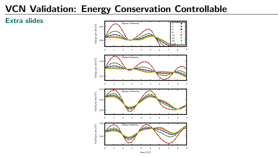


1. See complex part jetting off to infinity because it doesn't knwo how to compensate

VCN Validation: Energy Conservation Controllable

Extra slides

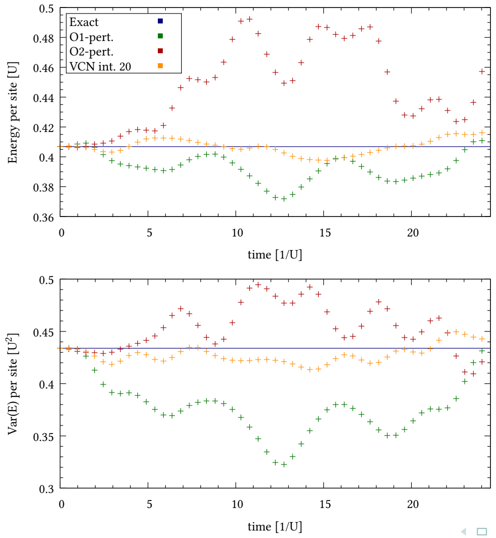


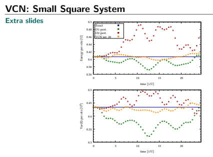


1. Still no perfect conservation for infinite steps, but this is probably due to first order integration only

VCN: Small Square System

Extra slides

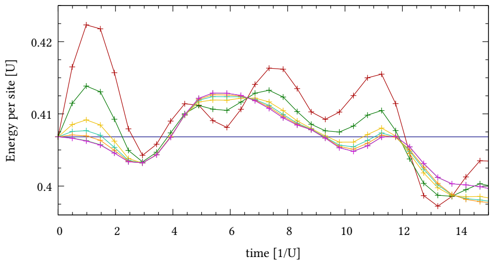


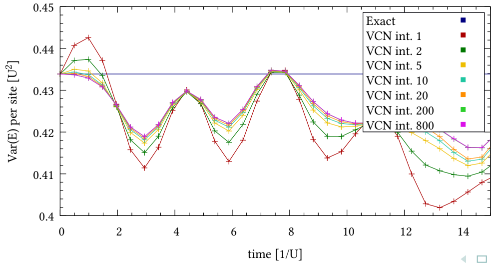


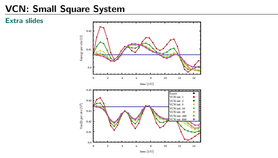
1. Notice how VCN now is MUCH better

VCN: Small Square System

Extra slides



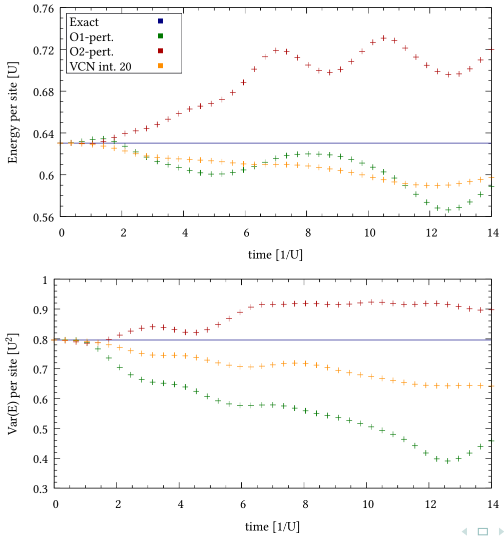


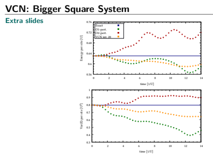


1. Step size dependent version of previous slide

VCN: Bigger Square System

Extra slides

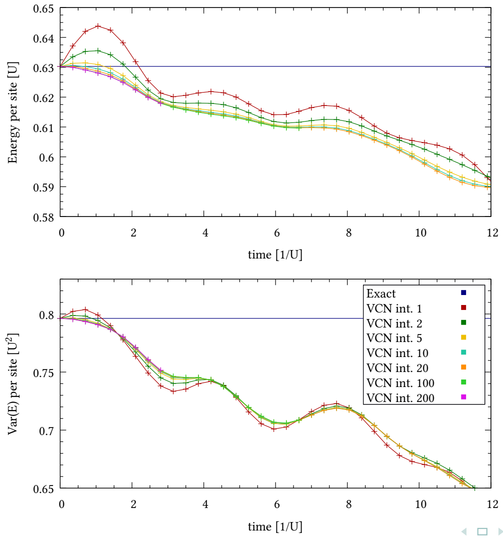


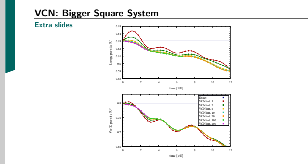


1. Now not a guarantee for immediately better results, but very promising

VCN: Bigger Square System

Extra slides

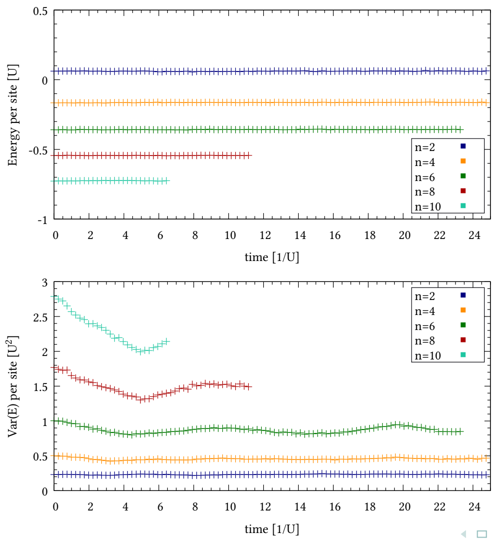


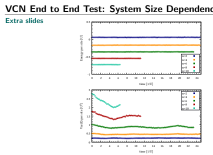


1. Here one can see very quickly more steps doesn't only make it better

VCN End to End Test: System Size Dependency

Extra slides

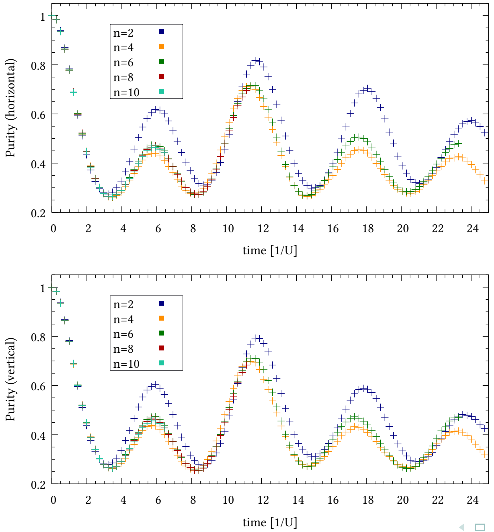


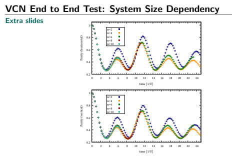


1. This is the energy for validation

VCN End to End Test: System Size Dependency

Extra slides

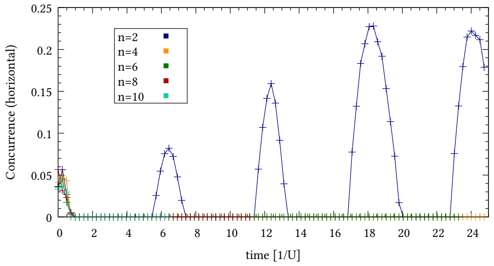


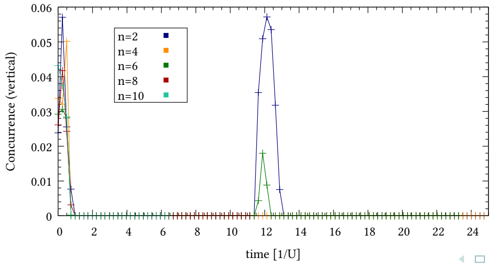


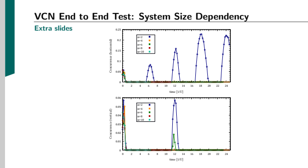
1. This is the purity
2. Does not seem to have a huge variation

VCN End to End Test: System Size Dependency

Extra slides



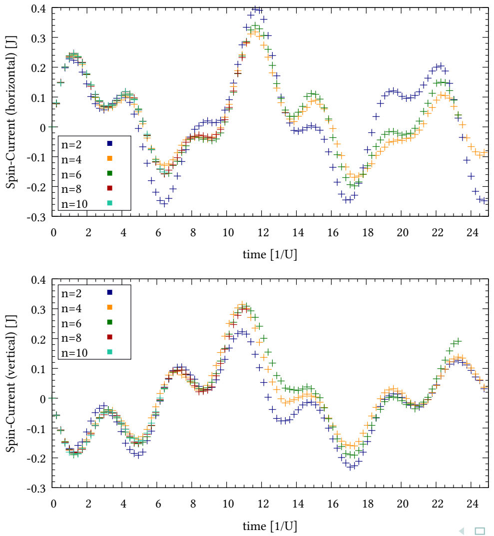




1. This is the concurrence
2. Poorly resolved, this should be looked into possibly in the future

VCN End to End Test: System Size Dependency

Extra slides



1. This is the current
2. Most obvious effect, but still extremely stable over a order of magnitude of sites
3. See assymmetric behavior, because electrical field is set to not be symmetric