Universität Augsburg
Mathematisch-Naturwissenschaftlich-Technische Fakultät

Computer aided Analytical Calculations for Physical Many-Body Problems

- Project Work Presentation -

Jonas Kell
Chair for theoretical Physics III

15th of Mai 2024

Outline

Outline

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Physics of what we calculate

Introduction of the problem

- Content of my Practical Training (Fachpraktikum)

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

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

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

Physics of what we calculate

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- Content of my Practical Training (Fachpraktikum)
- Hubbard Model Hamiltonian

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Physics of what we calculate

Introduction of the problem

- Content of my Practical Training (Fachpraktikum)
- Hubbard Model Hamiltonian
- System under influence of external electric field

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

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

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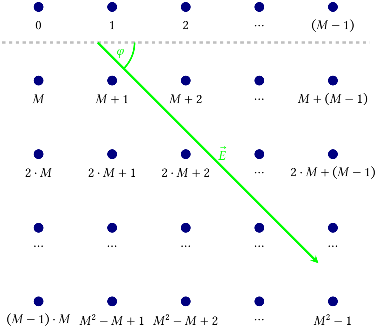
Physics of what we calculate

Introduction of the problem

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

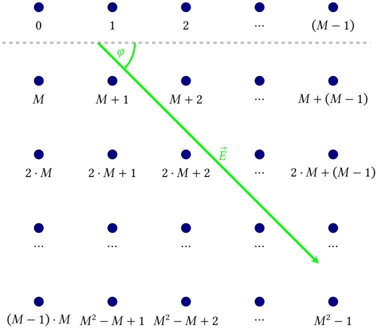


Physics of what we calculate

Introduction of the problem

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

Goal: Approximate evaluation of time-evolution using Monte-Carlo Sampling



Physics of what we calculate

Introduction of the problem

- Hard-Core Bosonic operators

$$\left[\hat{c}_{l,\sigma}, \hat{c}_{l',\sigma'}\right] = \left[\hat{c}^{\dagger}_{l,\sigma}, \hat{c}^{\dagger}_{l',\sigma'}\right] = 0$$
$$\left[\hat{c}_{l,\sigma}, \hat{c}^{\dagger}_{l',\sigma'}\right] = \delta(l,l') \cdot \delta(\sigma,\sigma')$$

Physics of what we calculate

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- Hard-Core Bosonic operators
  - (Would work analogously with Fermionic operators)

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Physics of what we calculate

Introduction of the problem

- Hard-Core Bosonic operators
  - (Would work analogously with Fermionic operators)
- Two spin-degrees of freedom rewritten in alternate notation

$$\left[\hat{c}_{l,\sigma}, \hat{c}_{l',\sigma'}\right] = \left[\hat{c}^\dagger_{l,\sigma}, \hat{c}^\dagger_{l',\sigma'}\right] = 0$$
$$\left[\hat{c}_{l,\sigma}, \hat{c}^\dagger_{l',\sigma'}\right] = \delta(l,l') \cdot \delta(\sigma,\sigma')$$

$$\hat{c}^{(\dagger)}_{l,\uparrow} \leftrightarrow \hat{c}^{(\dagger)}_{l} \qquad \hat{c}^{(\dagger)}_{l,\downarrow} \leftrightarrow \hat{d}^{(\dagger)}_{l}$$

$$\mathcal{H}_0 = U \cdot \sum_l \hat{c}^\dagger_l \hat{c}_l \hat{d}^\dagger_l \hat{d}_l + \sum_l \varepsilon_l \hat{c}^\dagger_l \hat{c}_l \sum_l \varepsilon_l \hat{d}^\dagger_l \hat{d}_l$$

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

Working on paper: A Computer-Scientists view

Introduction of the problem

Doing Theoretical Physics often requires lengthy analytical calculations

Working on paper: A Computer-Scientists view

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Doing Theoretical Physics often requires lengthy analytical calculations

Advantages of working on paper:

- No barrier to entry (required Skill & technology)
- Maximum liberty how to operate
- Fast iteration for high variation workload
- "Offline" available

Working on paper: A Computer-Scientists view

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Doing Theoretical Physics often requires lengthy analytical calculations

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- Fast iteration for high variation workload
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Problems of working on paper:

- Repetitive tasks not automizable
- Error-prone and time-consuming to fix mistakes
- Difficult & non-standard to share/archive
- No version-control
- Need to produce final version anyway

Examples from "Theoretical Solid State Physics"

Introduction of the problem

$$[S, H] = [c_1^\dagger c_2 - c_2^\dagger c_1,\ \varepsilon(c_1^\dagger c_1 + \Delta(c_1^\dagger c_2 + c_2^\dagger c_1))] \qquad \nearrow [c_1^\dagger c_2, c_1^\dagger c_2] = 0, \text{ obvious, usw.}$$

$$= \varepsilon[c_1^\dagger c_2, c_1^\dagger c_1] - \varepsilon[c_2^\dagger c_1, c_1^\dagger c_1] + \Delta[c_1^\dagger c_2, c_2^\dagger c_1] - \Delta[c_2^\dagger c_1, c_1^\dagger c_2]$$

$$\underbrace{c_1^\dagger \underbrace{c_2 c_1^\dagger}_{=-c_1^\dagger c_2}}_{0} c_1 - c_1^\dagger \underbrace{c_1 c_1^\dagger}_{=1-c_1^\dagger c_1} c_2 = c_1^\dagger c_2 \quad \Big| \quad c_2^\dagger c_1 \quad \Big| \quad c_1^\dagger \underbrace{c_2 c_2^\dagger}_{+c_2^\dagger c_2} c_1 - c_2^\dagger \underbrace{c_1 c_1^\dagger}_{1-c_1^\dagger c_1} c_2 =$$

$$= c_1^\dagger c_1 - c_1^\dagger c_2^\dagger \underbrace{c_2 c_1}_{-c_1 c_2} - c_2^\dagger c_2 + \underbrace{c_2^\dagger c_1^\dagger}_{-c_1^\dagger c_2^\dagger} c_1 c_2 =$$

$$= c_1^\dagger c_1 + c_1^\dagger c_2^\dagger c_1 c_2 - c_2^\dagger c_2 - c_1^\dagger c_2^\dagger c_1 c_2 = c_1^\dagger c_1 - c_2^\dagger c_2$$

$$= \varepsilon\, c_1^\dagger c_2 - \varepsilon\, c_2^\dagger c_1 + 2\Delta(c_1^\dagger c_1 - c_2^\dagger c_2)$$

$$= \varepsilon\,(c_1^\dagger c_2 - c_2^\dagger c_1) + 2\Delta\,(c_1^\dagger c_1 - c_2^\dagger c_2)$$

$$= -\frac{\varepsilon}{U} V + 2\Delta\,(c_1^\dagger c_1 - c_2^\dagger c_2)$$

Examples from "Theoretical Solid State Physics"

Introduction of the problem

Find transform

$$c^\dagger_{k\sigma}(t) = e^{iHt} c^\dagger_{k\sigma} e^{-iHt} \quad \to \text{complicated}$$

$$\tilde{c}^\dagger_{k\sigma}(t) = e^{i\tilde{H}t} \tilde{c}^\dagger_{k\sigma} e^{-i\tilde{H}t} \quad \to \text{easier}$$

$$\tilde{c}^\dagger_{k\sigma} = e^S c^\dagger_{k\sigma} e^{-S} \approx c^\dagger_{k\sigma} + [S, c^\dagger_{k\sigma}] + O(U^2)$$

$$[S, c^\dagger_{k\sigma}] = \frac{U}{N} \sum_{k_1 \dots k_4}{}' \frac{\delta(k_1-k_2+k_3-k_4)}{\epsilon_{k_1}-\epsilon_{k_2}+\epsilon_{k_3}-\epsilon_{k_4}} [c^\dagger_{k_1\uparrow} c_{k_2\uparrow} c^\dagger_{k_3\downarrow} c_{k_4\downarrow}, c^\dagger_{k\sigma}] =$$

$$c^\dagger_{k_1\uparrow} c^\dagger_{k_3\downarrow} c_{k_4\downarrow} \delta_{kk_2} \delta_{\sigma\uparrow} + c^\dagger_{k_1\uparrow} c_{k_2\uparrow} c^\dagger_{k_3\downarrow} \delta_{kk_4} \delta_{\sigma\downarrow}$$

$$\tilde{c}^\dagger_{k\sigma} = e^S c^\dagger_{k\sigma} e^{-S} = c^\dagger_{k\sigma} + \frac{U}{N} \sum_{k_1 \dots k_4}{}' \frac{\delta(k_1-k_2+k_3-k_4)}{\epsilon_{k_1}-\epsilon_{k_2}+\epsilon_{k_3}-\epsilon_{k_4}}$$

change index $k_2 \leftrightarrow k_4$, $k_1 \leftrightarrow k_3$

$$= c^\dagger_{k\sigma} + \frac{U}{N} \sum_{k_1 \dots k_4}{}' \frac{\delta(k_1-k_2+k_3-k_4)}{\epsilon_{k_1}-\epsilon_{k_2}+\epsilon_{k_3}-\epsilon_{k_4}} \delta_{kk_2} c^\dagger_{k_1\sigma} c^\dagger_{k_3\bar{\sigma}} c_{k_4\bar{\sigma}}$$

$k_4 \to k_1 - k_2 + k_3$

$$= c^\dagger_{k\sigma} + \frac{U}{N} \sum_{k_1 \dots k_4}{}' \frac{1}{\epsilon_{k_1}-\epsilon_{k}+\epsilon_{k_3}-\epsilon_{k_1-k+k_3}} c^\dagger_{k\sigma} c^\dagger_{k_3\bar{\sigma}} c_{k_1-k+k_3\,\bar{\sigma}}$$

ii)

$$\bar{H} = uHu^\dagger = e^S H e^{-S} = H + [S, H_0] + O(U^2) \qquad [S, V] \to \text{second order}$$

$$[S, H_0] = \frac{U}{N} \sum_{k_1 \dots k_4}{}' \frac{\delta(k_1-k_2+k_3-k_4)}{\epsilon_{k_1}-\epsilon_{k_2}+\epsilon_{k_3}-\epsilon_{k_4}} [c^\dagger_{k_1\uparrow} c_{k_2\uparrow} c^\dagger_{k_3\downarrow} c_{k_4\downarrow}, \sum_{k\sigma} \epsilon_k n_{k\sigma}]$$

$\to$ use $[c^\dagger_{k\sigma}, n_{k'\sigma'}]$

$$-(\epsilon_{k_1}-\epsilon_{k_2}+\epsilon_{k_3}-\epsilon_{k_4}) c^\dagger_{k_1\uparrow} c_{k_2\uparrow} c^\dagger_{k_3\downarrow} c_{k_4\downarrow}$$

$$u = e^S, \quad S = \frac{1}{N} \sum_{k_1 \dots k_4}{}' \delta(k_1-k_2+k_3-k_4) \frac{U}{\epsilon_{k_1}-\epsilon_{k_2}+\epsilon_{k_3}-\epsilon_{k_4}} c^\dagger_{k_1\uparrow} c_{k_2\uparrow} c^\dagger_{k_3\downarrow} c_{k_4\downarrow} \quad (2)$$

we can eliminate to leading order in U the interaction term. Notice that the summation $\sum'_{k_1 \dots k_4}$ only involves those contributions for which $\epsilon_{k_1}-\epsilon_{k_2}+\epsilon_{k_3}-\epsilon_{k_4} \neq 0$.

a) Calculate to the leading order in U the time evolution $c^\dagger_{k\sigma}(t)$ of single fermion operators in Heisenberg picture:

$$c^\dagger_{k\sigma}(t) = e^{iHt} c^\dagger_{k\sigma} e^{-iHt} \quad (3)$$

i) First transform both the Hamiltonian H and $c^\dagger_{k\sigma}$ with u:

$$\tilde{H} = uHu^\dagger, \quad \tilde{c}^\dagger_{k\sigma} = uc^\dagger_{k\sigma}u^\dagger \quad (4)$$

(see previous exercise sheet)

ii) Show that the transformed Hamiltonian has the following form

$$\tilde{H} = uHu^\dagger = \sum_{k,\sigma} \varepsilon_k n_{k\sigma} + \sum_{k,k'} F_{k,k'} n_{k\uparrow} n_{k'\downarrow} + O(U^2) \quad (5)$$

and determine $F_{k,k'}$.

Examples from the Practical Training

Introduction of the problem

- Goal: produce time evolution of operator

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

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Introduction of the problem

- Goal: produce time evolution of operator
- Uses calculation in Interaction Picture

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

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

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

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Examples from the Practical Training

Introduction of the problem

- Goal: produce time evolution of operator
- Uses calculation in Interaction Picture
- Workflow:
  - Inserting Definitions
  - Expanding
  - Ordering
  - Rewriting efficiently

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

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

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Paper-like writing on digital devices

Solutions: Off the shelf

- Can give benefits that paper lacks
  - Copy/Paste
  - Collaborate
  - Convert to text
  - Searching and ordering large amounts of notes

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- HOWEVER
  - Still no proper automatization
  - Easily access is lost when using proprietary technology
  - "Vendor-Locking"

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TIP:

Always export to a standard format (like pdf) for manual backup!

Computer-Algebra Systems

Solutions: Off the shelf

- Proprietary Software (Often payed):

- Standalone Online Calculators

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  - Wolfram-Alpha
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  - ...
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- Standalone Online Calculators
  - Integralrechner.de (Integral-Calculator)
  - Matrix-Calculators
  - ...

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  - ...
- Standalone Online Calculators
  - Integralrechner.de (Integral-Calculator)
  - Matrix-Calculators
  - ...
- ... and many more

What is Math-Manipulator?

Math-Manipulator - What did I do?

```
sum((n = 0); 100; int(-inf; inf; (123+(A*4)/100); x))
```

$$\sum_{n=0}^{100} \int_{-\infty}^{\infty} \left(123 + \boxed{\frac{(A \cdot 4)}{100}}\right) \mathrm{d}x$$

Sel. Parent | Sel. First Child | Sel. Previous Sibling | Sel. Next Sibling

Replace | Replace All Equal | Replace (With Export) | Define Variable | Commute with subsequent | Fold Numbers | Cleanup Terms | Pull Out Minus | Reduce | Rename With Swap | Pack Same Variables | Replace All With

Selected Export to Clipboard | Show Export Structure (UUIDs) | Show Export Structure | Show Latex

```
T
```

$$\sum_{n=0}^{100} \int_{-\infty}^{\infty} (123 + T) \mathrm{d}x$$

Math-Manipulator [1]

In the Browser

Math-Manipulator - How can you use it

- Available open-source on GitHub
- Self-hosting possible
- Hosted version available in every modern browser

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- Hosted version available in every modern browser

Available here

https://jonas-kell.github.io/math-manipulator/

Usage as VS-Code Extension

Math-Manipulator - How can you use it

- Offline-Use after installed once
- Store progress in files
- Directly integrated in powerful IDE, and with that version control

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Note

Do not allow a spellchecker to run on the file, it will break everything performance-wise

Demo Problems from before

Math-Manipulator - Interactive Demonstration

$$= \epsilon [c_1^\dagger c_2, c_1^\dagger c_1] - \epsilon [c_2^\dagger c_1, c_1^\dagger c_1] + \Delta [c_1^\dagger c_2, c_2^\dagger c_1] - \Delta [c_2^\dagger c_1, c_1^\dagger c_2]$$

$$= \epsilon \left(c_1^\dagger c_2 - c_2^\dagger c_1\right) + 2\Delta \left(c_1^\dagger c_1 - c_2^\dagger c_2\right)$$

$$\left[c_{k_1\uparrow}^\dagger c_{k_2\uparrow} c_{k_3\downarrow}^\dagger c_{k_4\downarrow}, \sum_{k\sigma} \epsilon_k n_{k\sigma} \right]$$

$$-\left(\epsilon_{k_1} - \epsilon_{k_2} + \epsilon_{k_3} - \epsilon_{k_4}\right) c_{k_1\uparrow}^\dagger c_{k_2\uparrow} c_{k_3\downarrow}^\dagger c_{k_4\downarrow}$$

Usage for the Practical Training

Math-Manipulator - Interactive Demonstration

$$
\begin{aligned}
\hat{\mathrm{V}}^{\mathrm{I}}(t) &= \left\{\hat{\mathrm{V}}^{\mathrm{S}}\right\}(t) \overset{2.11}{=} -J \cdot \sum_{[l,m]} \left\{\left(\hat{\mathrm{c}}_l^{\dagger\mathrm{S}}\hat{\mathrm{c}}_m^{\mathrm{S}} + \hat{\mathrm{d}}_l^{\dagger\mathrm{S}}\hat{\mathrm{d}}_m^{\mathrm{S}}\right)\right\}(t) \\
&= -J \cdot \sum_{[l,m]} \left(\hat{\mathrm{c}}_l^{\dagger\mathrm{I}}(t)\hat{\mathrm{c}}_m^{\mathrm{I}}(t) + \hat{\mathrm{d}}_l^{\dagger\mathrm{I}}(t)\hat{\mathrm{d}}_m^{\mathrm{I}}(t)\right) \\
&\overset{\mathrm{MM}}{=} -J \cdot \sum_{[l,m]} \Big[e^{i\cdot(\varepsilon_m-\varepsilon_l)\cdot t} \cdot \hat{\mathrm{V}}_{\text{Part A}}(l,m) + \\
&\qquad e^{i\cdot(\varepsilon_m-\varepsilon_l+U)\cdot t} \cdot \hat{\mathrm{V}}_{\text{Part B}}(l,m) + e^{i\cdot(\varepsilon_m-\varepsilon_l-U)\cdot t} \cdot \hat{\mathrm{V}}_{\text{Part C}}(l,m)\Big]
\end{aligned}
$$

Usage for the Practical Training

Math-Manipulator - Interactive Demonstration

$$\begin{aligned}
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&= -J \cdot \sum_{[l,m]} \left(\hat{\mathrm{c}}_l^{\dagger\mathrm{I}}(t)\hat{\mathrm{c}}_m^{\mathrm{I}}(t) + \hat{\mathrm{d}}_l^{\dagger\mathrm{I}}(t)\hat{\mathrm{d}}_m^{\mathrm{I}}(t)\right) \\
&\overset{\mathrm{MM}}{=} -J \cdot \sum_{[l,m]} \Big[e^{i\cdot(\varepsilon_m-\varepsilon_l)\cdot t} \cdot \hat{\mathrm{V}}_{\text{Part A}}(l,m) + \\
&\qquad e^{i\cdot(\varepsilon_m-\varepsilon_l+U)\cdot t} \cdot \hat{\mathrm{V}}_{\text{Part B}}(l,m) + e^{i\cdot(\varepsilon_m-\varepsilon_l-U)\cdot t} \cdot \hat{\mathrm{V}}_{\text{Part C}}(l,m)\Big]
\end{aligned}$$

$$\begin{aligned}
\hat{\mathrm{V}}_{\text{Part A}}(l,m) \overset{\mathrm{MM}}{=}\ & \left(5 \cdot \hat{\mathrm{c}}_l^{\mathrm{S}}\hat{\mathrm{c}}_m^{\dagger\mathrm{S}}\right) + \left(5 \cdot \hat{\mathrm{d}}_l^{\mathrm{S}}\hat{\mathrm{d}}_m^{\dagger\mathrm{S}}\right) + \left(2 \cdot \hat{\mathrm{c}}_l^{\mathrm{S}}\hat{\mathrm{c}}_m^{\mathrm{S}}\hat{\mathrm{c}}_l^{\dagger\mathrm{S}}\hat{\mathrm{c}}_m^{\dagger\mathrm{S}}\hat{\mathrm{d}}_l^{\mathrm{S}}\hat{\mathrm{d}}_m^{\dagger\mathrm{S}}\right) + \left(2 \cdot \hat{\mathrm{c}}_l^{\mathrm{S}}\hat{\mathrm{c}}_m^{\dagger\mathrm{S}}\hat{\mathrm{d}}_l^{\mathrm{S}}\hat{\mathrm{d}}_m^{\mathrm{S}}\hat{\mathrm{d}}_l^{\dagger\mathrm{S}}\hat{\mathrm{d}}_m^{\dagger\mathrm{S}}\right) + \\
& + \left(-3 \cdot \hat{\mathrm{c}}_l^{\mathrm{S}}\hat{\mathrm{c}}_l^{\dagger\mathrm{S}}\hat{\mathrm{d}}_l^{\mathrm{S}}\hat{\mathrm{d}}_m^{\dagger\mathrm{S}}\right) + \left(-3 \cdot \hat{\mathrm{c}}_m^{\mathrm{S}}\hat{\mathrm{c}}_m^{\dagger\mathrm{S}}\hat{\mathrm{d}}_l^{\mathrm{S}}\hat{\mathrm{d}}_m^{\dagger\mathrm{S}}\right) + \left(-3 \cdot \hat{\mathrm{c}}_l^{\mathrm{S}}\hat{\mathrm{c}}_m^{\dagger\mathrm{S}}\hat{\mathrm{d}}_l^{\mathrm{S}}\hat{\mathrm{d}}_l^{\dagger\mathrm{S}}\right) + \left(-3 \cdot \hat{\mathrm{c}}_l^{\mathrm{S}}\hat{\mathrm{c}}_m^{\dagger\mathrm{S}}\hat{\mathrm{d}}_m^{\mathrm{S}}\hat{\mathrm{d}}_m^{\dagger\mathrm{S}}\right) \\
\hat{\mathrm{V}}_{\text{Part B}}(l,m) \overset{\mathrm{MM}}{=}\ & \left(-2 \cdot \hat{\mathrm{c}}_l^{\mathrm{S}}\hat{\mathrm{c}}_m^{\dagger\mathrm{S}}\right) + \left(-2 \cdot \hat{\mathrm{d}}_l^{\mathrm{S}}\hat{\mathrm{d}}_m^{\dagger\mathrm{S}}\right) + \left(-1 \cdot \hat{\mathrm{c}}_l^{\mathrm{S}}\hat{\mathrm{c}}_m^{\mathrm{S}}\hat{\mathrm{c}}_l^{\dagger\mathrm{S}}\hat{\mathrm{c}}_m^{\dagger\mathrm{S}}\hat{\mathrm{d}}_l^{\mathrm{S}}\hat{\mathrm{d}}_m^{\dagger\mathrm{S}}\right) + \left(-1 \cdot \hat{\mathrm{c}}_l^{\mathrm{S}}\hat{\mathrm{c}}_m^{\dagger\mathrm{S}}\hat{\mathrm{d}}_l^{\mathrm{S}}\hat{\mathrm{d}}_m^{\mathrm{S}}\hat{\mathrm{d}}_l^{\dagger\mathrm{S}}\hat{\mathrm{d}}_m^{\dagger\mathrm{S}}\right) + \\
& + \left(1 \cdot \hat{\mathrm{c}}_l^{\mathrm{S}}\hat{\mathrm{c}}_l^{\dagger\mathrm{S}}\hat{\mathrm{d}}_l^{\mathrm{S}}\hat{\mathrm{d}}_m^{\dagger\mathrm{S}}\right) + \left(2 \cdot \hat{\mathrm{c}}_m^{\mathrm{S}}\hat{\mathrm{c}}_m^{\dagger\mathrm{S}}\hat{\mathrm{d}}_l^{\mathrm{S}}\hat{\mathrm{d}}_m^{\dagger\mathrm{S}}\right) + \left(1 \cdot \hat{\mathrm{c}}_l^{\mathrm{S}}\hat{\mathrm{c}}_m^{\dagger\mathrm{S}}\hat{\mathrm{d}}_l^{\mathrm{S}}\hat{\mathrm{d}}_l^{\dagger\mathrm{S}}\right) + \left(2 \cdot \hat{\mathrm{c}}_l^{\mathrm{S}}\hat{\mathrm{c}}_m^{\dagger\mathrm{S}}\hat{\mathrm{d}}_m^{\mathrm{S}}\hat{\mathrm{d}}_m^{\dagger\mathrm{S}}\right) \\
\hat{\mathrm{V}}_{\text{Part C}}(l,m) \overset{\mathrm{MM}}{=}\ & \left(-2 \cdot \hat{\mathrm{c}}_l^{\mathrm{S}}\hat{\mathrm{c}}_m^{\dagger\mathrm{S}}\right) + \left(-2 \cdot \hat{\mathrm{d}}_l^{\mathrm{S}}\hat{\mathrm{d}}_m^{\dagger\mathrm{S}}\right) + \left(-1 \cdot \hat{\mathrm{c}}_l^{\mathrm{S}}\hat{\mathrm{c}}_m^{\mathrm{S}}\hat{\mathrm{c}}_l^{\dagger\mathrm{S}}\hat{\mathrm{c}}_m^{\dagger\mathrm{S}}\hat{\mathrm{d}}_l^{\mathrm{S}}\hat{\mathrm{d}}_m^{\dagger\mathrm{S}}\right) + \left(-1 \cdot \hat{\mathrm{c}}_l^{\mathrm{S}}\hat{\mathrm{c}}_m^{\dagger\mathrm{S}}\hat{\mathrm{d}}_l^{\mathrm{S}}\hat{\mathrm{d}}_m^{\mathrm{S}}\hat{\mathrm{d}}_l^{\dagger\mathrm{S}}\hat{\mathrm{d}}_m^{\dagger\mathrm{S}}\right) + \\
& + \left(2 \cdot \hat{\mathrm{c}}_l^{\mathrm{S}}\hat{\mathrm{c}}_l^{\dagger\mathrm{S}}\hat{\mathrm{d}}_l^{\mathrm{S}}\hat{\mathrm{d}}_m^{\dagger\mathrm{S}}\right) + \left(1 \cdot \hat{\mathrm{c}}_m^{\mathrm{S}}\hat{\mathrm{c}}_m^{\dagger\mathrm{S}}\hat{\mathrm{d}}_l^{\mathrm{S}}\hat{\mathrm{d}}_m^{\dagger\mathrm{S}}\right) + \left(2 \cdot \hat{\mathrm{c}}_l^{\mathrm{S}}\hat{\mathrm{c}}_m^{\dagger\mathrm{S}}\hat{\mathrm{d}}_l^{\mathrm{S}}\hat{\mathrm{d}}_l^{\dagger\mathrm{S}}\right) + \left(1 \cdot \hat{\mathrm{c}}_l^{\mathrm{S}}\hat{\mathrm{c}}_m^{\dagger\mathrm{S}}\hat{\mathrm{d}}_m^{\mathrm{S}}\hat{\mathrm{d}}_m^{\dagger\mathrm{S}}\right)
\end{aligned}$$

Optimization: Difference of V(t) for Hopping

Custom Python Scripts (SymPy)

- Monte-Carlo sampling requires transition probabilities between "adjacent" states

$$
\begin{aligned}
\alpha &= \frac{\mathrm{P}(\tilde{N},t)}{\mathrm{P}(N,t)} = \frac{f(\tilde{N},t)}{f(N,t)} \overset{2.39}{=} \frac{\left|e^{\mathcal{H}_{\text{eff}}(\tilde{N},t)}\right|^2 \left|\Psi_{\tilde{N}}\right|^2}{\left|e^{\mathcal{H}_{\text{eff}}(N,t)}\right|^2 \left|\Psi_{N}\right|^2} \\
&= \frac{\left|\Psi_{\tilde{N}}\right|^2}{\left|\Psi_{N}\right|^2} \frac{e^{\Re\left(\mathcal{H}_{\text{eff}}(\tilde{N},t)\right)+i\Im\left(\mathcal{H}_{\text{eff}}(\tilde{N},t)\right)+\Re\left(\mathcal{H}_{\text{eff}}(\tilde{N},t)\right)-i\Im\left(\mathcal{H}_{\text{eff}}(\tilde{N},t)\right)}}{e^{\Re(\mathcal{H}_{\text{eff}}(N,t))+i\Im(\mathcal{H}_{\text{eff}}(N,t))+\Re(\mathcal{H}_{\text{eff}}(N,t))-i\Im(\mathcal{H}_{\text{eff}}(N,t))}} \\
&= \frac{\left|\Psi_{\tilde{N}}\right|^2}{\left|\Psi_{N}\right|^2} e^{2\cdot\Re\left(\mathcal{H}_{\text{eff}}(\tilde{N},t)\right)-2\cdot\Re(\mathcal{H}_{\text{eff}}(N,t))} \\
&= \frac{\left|\Psi_{\tilde{N}}\right|^2}{\left|\Psi_{N}\right|^2} e^{2\cdot\Re\left(\mathcal{H}_{\text{eff}}(\tilde{N},t)-\mathcal{H}_{\text{eff}}(N,t)\right)}
\end{aligned}
$$

Optimization: Difference of V(t) for Hopping

Custom Python Scripts (SymPy)

- Monte-Carlo sampling requires transition probabilities between "adjacent" states
- These require differences of $\hat{V}^{\mathrm{I}}(t)$ and E_0

$$\alpha = \frac{\mathrm{P}(\tilde{N},t)}{\mathrm{P}(N,t)} = \frac{f(\tilde{N},t)}{f(N,t)} \overset{2.39}{=} \frac{\left|e^{\mathcal{H}_{\mathrm{eff}}(\tilde{N},t)}\right|^2 \left|\Psi_{\tilde{N}}\right|^2}{\left|e^{\mathcal{H}_{\mathrm{eff}}(N,t)}\right|^2 \left|\Psi_N\right|^2}$$

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

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

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

Optimization: Difference of V(t) for Hopping

Custom Python Scripts (SymPy)

- Monte-Carlo sampling requires transition probabilities between "adjacent" states
- These require differences of $\hat{V}^{\mathrm{I}}(t)$ and E_0
- Too many terms for simple evaluation by hand
- Intelligent pre-computation required to speed up processing

$$\begin{aligned}
\alpha &= \frac{\mathrm{P}(\tilde{N},t)}{\mathrm{P}(N,t)} = \frac{f(\tilde{N},t)}{f(N,t)} \overset{2.39}{=} \frac{\left|e^{\mathcal{H}_{\mathrm{eff}}(\tilde{N},t)}\right|^2 \left|\Psi_{\tilde{N}}\right|^2}{\left|e^{\mathcal{H}_{\mathrm{eff}}(N,t)}\right|^2 \left|\Psi_{N}\right|^2} \\
&= \frac{\left|\Psi_{\tilde{N}}\right|^2}{\left|\Psi_{N}\right|^2} \frac{e^{\Re\left(\mathcal{H}_{\mathrm{eff}}(\tilde{N},t)\right)+i\Im\left(\mathcal{H}_{\mathrm{eff}}(\tilde{N},t)\right)+\Re\left(\mathcal{H}_{\mathrm{eff}}(\tilde{N},t)\right)-i\Im\left(\mathcal{H}_{\mathrm{eff}}(\tilde{N},t)\right)}}{e^{\Re(\mathcal{H}_{\mathrm{eff}}(N,t))+i\Im(\mathcal{H}_{\mathrm{eff}}(N,t))+\Re(\mathcal{H}_{\mathrm{eff}}(N,t))-i\Im(\mathcal{H}_{\mathrm{eff}}(N,t))}} \\
&= \frac{\left|\Psi_{\tilde{N}}\right|^2}{\left|\Psi_{N}\right|^2} e^{2\cdot\Re\left(\mathcal{H}_{\mathrm{eff}}(\tilde{N},t)\right)-2\cdot\Re(\mathcal{H}_{\mathrm{eff}}(N,t))} \\
&= \frac{\left|\Psi_{\tilde{N}}\right|^2}{\left|\Psi_{N}\right|^2} e^{2\cdot\Re\left(\mathcal{H}_{\mathrm{eff}}(\tilde{N},t)-\mathcal{H}_{\mathrm{eff}}(N,t)\right)}
\end{aligned}$$

The process: Difference of V(t) for Hopping

Custom Python Scripts (SymPy)

$$
\begin{aligned}
E_0(N) - E_0(\tilde{N}) &= U \sum_{l} n_{l,\downarrow} n_{l,\uparrow} - U \sum_{l} \tilde{n}_{l,\downarrow} \tilde{n}_{l,\uparrow} + \sum_{l,\sigma} \varepsilon_l n_{l,\sigma} - \sum_{l,\sigma} \varepsilon_l \tilde{n}_{l,\sigma} \\
&\overset{2.45}{=} \left(\varepsilon_i - \varepsilon_j\right) \left(n_{i,\sigma_i} - n_{j,\sigma_j}\right) + U \cdot \begin{cases} \left(n_{i,\uparrow} - n_{j,\uparrow}\right) \left(n_{i,\downarrow} - n_{j,\downarrow}\right) & : \sigma_i = \sigma_j \\ \left(n_{i,\uparrow} - n_{j,\downarrow}\right) \left(n_{i,\downarrow} - n_{j,\uparrow}\right) & : \sigma_i \neq \sigma_j \end{cases} \\
&= \left(\varepsilon_i - \varepsilon_j\right) \left(n_{i,\sigma_i} - n_{j,\sigma_j}\right) + U \left(n_{i,\sigma_i} - n_{j,\sigma_j}\right) \left(n_{i,\overline{\sigma_i}} - n_{j,\overline{\sigma_j}}\right)
\end{aligned}
$$

- Setup difference

The process: Difference of V(t) for Hopping

Custom Python Scripts (SymPy)

$$
\begin{aligned}
E_0(N) - E_0(\tilde{N}) &= U \sum_l n_{l,\downarrow} n_{l,\uparrow} - U \sum_l \tilde{n}_{l,\downarrow} \tilde{n}_{l,\uparrow} + \sum_{l,\sigma} \varepsilon_l n_{l,\sigma} - \sum_{l,\sigma} \varepsilon_l \tilde{n}_{l,\sigma} \\
&\overset{2.45}{=} \left(\varepsilon_i - \varepsilon_j\right)\left(n_{i,\sigma_i} - n_{j,\sigma_j}\right) + U \cdot \begin{cases} \left(n_{i,\uparrow} - n_{j,\uparrow}\right)\left(n_{i,\downarrow} - n_{j,\downarrow}\right) & : \sigma_i = \sigma_j \\ \left(n_{i,\uparrow} - n_{j,\downarrow}\right)\left(n_{i,\downarrow} - n_{j,\uparrow}\right) & : \sigma_i \neq \sigma_j \end{cases} \\
&= \left(\varepsilon_i - \varepsilon_j\right)\left(n_{i,\sigma_i} - n_{j,\sigma_j}\right) + U\left(n_{i,\sigma_i} - n_{j,\sigma_j}\right)\left(n_{i,\overline{\sigma_i}} - n_{j,\overline{\sigma_j}}\right)
\end{aligned}
$$

$$
\tilde{n}_{l,\sigma} = \begin{cases} n_{i,\sigma_i} & : l = j \wedge \sigma = \sigma_j \\ n_{j,\sigma_j} & : l = i \wedge \sigma = \sigma_i \\ n_{l,\sigma} & : \text{else} \end{cases}
$$

- Setup difference
- Replace one by appropriate new occupation

The process: Difference of V(t) for Hopping

Custom Python Scripts (SymPy)

$$
\begin{aligned}
E_0(N) - E_0(\tilde{N}) &= U \sum_l n_{l,\downarrow} n_{l,\uparrow} - U \sum_l \tilde{n}_{l,\downarrow} \tilde{n}_{l,\uparrow} + \sum_{l,\sigma} \varepsilon_l n_{l,\sigma} - \sum_{l,\sigma} \varepsilon_l \tilde{n}_{l,\sigma} \\
&\overset{2.45}{=} \left(\varepsilon_i - \varepsilon_j\right) \left(n_{i,\sigma_i} - n_{j,\sigma_j}\right) + U \cdot \begin{cases} \left(n_{i,\uparrow} - n_{j,\uparrow}\right) \left(n_{i,\downarrow} - n_{j,\downarrow}\right) & : \sigma_i = \sigma_j \\ \left(n_{i,\uparrow} - n_{j,\downarrow}\right) \left(n_{i,\downarrow} - n_{j,\uparrow}\right) & : \sigma_i \neq \sigma_j \end{cases} \\
&= \left(\varepsilon_i - \varepsilon_j\right) \left(n_{i,\sigma_i} - n_{j,\sigma_j}\right) + U \left(n_{i,\sigma_i} - n_{j,\sigma_j}\right) \left(n_{i,\overline{\sigma_i}} - n_{j,\overline{\sigma_j}}\right)
\end{aligned}
$$

$$
\tilde{n}_{l,\sigma} = \begin{cases} n_{i,\sigma_i} & : l = j \wedge \sigma = \sigma_j \\ n_{j,\sigma_j} & : l = i \wedge \sigma = \sigma_i \\ n_{l,\sigma} & : \text{else} \end{cases}
$$

- Setup difference
- Replace one by appropriate new occupation
- Simplify as much as possible
- Sum over all possible neighbor combinations

The process: Difference of V(t) for Hopping

Custom Python Scripts (SymPy)

$$E_0(N) - E_0(\tilde{N}) = U \sum_{l} n_{l,\downarrow} n_{l,\uparrow} - U \sum_{l} \tilde{n}_{l,\downarrow} \tilde{n}_{l,\uparrow} + \sum_{l,\sigma} \varepsilon_l n_{l,\sigma} - \sum_{l,\sigma} \varepsilon_l \tilde{n}_{l,\sigma}$$

$$\overset{2.45}{=} \left(\varepsilon_i - \varepsilon_j\right)\left(n_{i,\sigma_i} - n_{j,\sigma_j}\right) + U \cdot \begin{cases} \left(n_{i,\uparrow} - n_{j,\uparrow}\right)\left(n_{i,\downarrow} - n_{j,\downarrow}\right) & : \sigma_i = \sigma_j \\ \left(n_{i,\uparrow} - n_{j,\downarrow}\right)\left(n_{i,\downarrow} - n_{j,\uparrow}\right) & : \sigma_i \neq \sigma_j \end{cases}$$

$$= \left(\varepsilon_i - \varepsilon_j\right)\left(n_{i,\sigma_i} - n_{j,\sigma_j}\right) + U\left(n_{i,\sigma_i} - n_{j,\sigma_j}\right)\left(n_{i,\overline{\sigma_i}} - n_{j,\overline{\sigma_j}}\right)$$

$$\tilde{n}_{l,\sigma} = \begin{cases} n_{i,\sigma_i} & : l = j \wedge \sigma = \sigma_j \\ n_{j,\sigma_j} & : l = i \wedge \sigma = \sigma_i \\ n_{l,\sigma} & : \text{else} \end{cases}$$

- Setup difference
- Replace one by appropriate new occupation
- Simplify as much as possible
- Sum over all possible neighbor combinations

Problem: number of terms/combinations: $3 \cdot 8 \cdot 4 \cdot 2 = 192$

Script-Generation: Difference of V(t) for Hopping

Custom Python Scripts (SymPy)

Generating Script

simplificationtermhelper.py

Generated Script

analyticalcalcfunctions.py

Beamer: LaTeX way of writing Presentations

Presentations? - Custom Beamer Template

- Write presentations like your papers/thesis in LaTeX

Beamer [2] Template [3]

Beamer: LaTeX way of writing Presentations

Presentations? - Custom Beamer Template

- Write presentations like your papers/thesis in LaTeX
- Reuse formulas/images/code/sources

Beamer [2] Template [3]

Beamer: LaTeX way of writing Presentations

Presentations? - Custom Beamer Template

- Write presentations like your papers/thesis in LaTeX
- Reuse formulas/images/code/sources
- Consistent style & references

Beamer [2] Template [3]

Beamer: LaTeX way of writing Presentations

Presentations? - Custom Beamer Template

- Write presentations like your papers/thesis in LaTeX
- Reuse formulas/images/code/sources
- Consistent style & references
- Version control

Beamer [2] Template [3]

Beamer: LaTeX way of writing Presentations

Presentations? - Custom Beamer Template

- Write presentations like your papers/thesis in LaTeX
- Reuse formulas/images/code/sources
- Consistent style & references
- Version control
- Easier collaboration

Beamer [2] Template [3]

Minimal example for beamer presentation

Presentations? - Custom Beamer Template

```latex
\documentclass[aspectratio=169]{beamer}

\usetheme[neutralbackground]{uniamntf}

\title[]{Title}
\subtitle{subtitle}
\author{Jonas Kell}
\institute[TP III]{Chair for theoretical Physics III}
\date[01.05.2024]{$1^{\text{st}}$ of Mai 2024}

\acknowledgement{
    Jonas Kell\\    Augsburg University\\
    jonas.kell@student.uni-augsburg.de\\    www.uni-augsburg.de
}

\begin{document}

    \begin{frame}[t,plain]
        \maketitle
    \end{frame}

    \section*{Summary \& Conclusion}
    {
        \setbeamertemplate{frametitle}[uniamntfack]
        \begin{frame}[plain]{Acknowledgment}
            Thank you for your kind attention
        \end{frame}
    }
\end{document}
```

Universität Augsburg
Mathematisch-Naturwissenschaftlich-Technische Fakultät

Thank you for your kind attention

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References I

Summary & Conclusion

[1] J. Kell, *Math-manipulator tool - info and repository*, (2024) https://github.com/jonas-kell/math-manipulator.

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

[4] J. Kell, *Latex sources for this presentation, the thesis and report*, (2024) https://github.com/jonas-kell/master-thesis-documents.

[5] J. Kell, *Thesis code implementation and reference*, (2024) https://github.com/jonas-kell/master-thesis-code.

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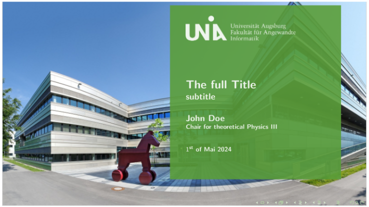
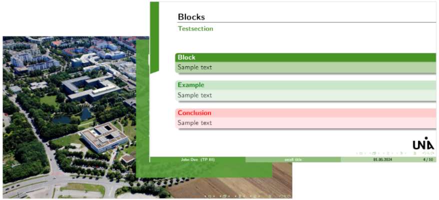
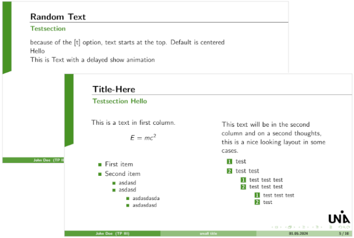
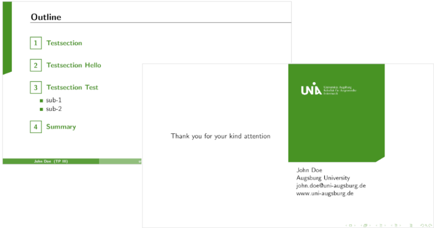
Theme alternative: Faculty of App. Computer Science

Extra slides









Backup-Solution Problem 1

Extra slides

```
eps comm((c# 1 c 2);(c# 1 c 1))- eps comm((c# 2 c 1);(c# 1 c 1)) + del comm((c# 1 c 2);(c# 2 c 1))-del comm((c# 2 c 1);( c# 1 c 2))
```

$$((eps\cdot[c_1^\dagger c_2, c_1^\dagger c_1]) + (-eps\cdot[c_2^\dagger c_1, c_1^\dagger c_1]) + (del\cdot[c_1^\dagger c_2, c_2^\dagger c_1]) + (-del\cdot[c_2^\dagger c_1, c_1^\dagger c_2]))$$

$$((eps\cdot[c_1^\dagger c_2, c_1^\dagger c_1]) - (eps\cdot[c_2^\dagger c_1, c_1^\dagger c_1]) + (del\cdot[c_1^\dagger c_2, c_2^\dagger c_1]) + (-del\cdot[c_2^\dagger c_1, c_1^\dagger c_2]))$$

$$((eps\cdot[c_1^\dagger c_2, c_1^\dagger c_1]) - (eps\cdot[c_2^\dagger c_1, c_1^\dagger c_1]) + (del\cdot[c_1^\dagger c_2, c_2^\dagger c_1]) - (del\cdot[c_2^\dagger c_1, c_1^\dagger c_2]))$$

$$((eps\cdot(c_1^\dagger c_2 c_1^\dagger c_1 - c_1^\dagger c_1 c_1^\dagger c_2)) - (eps\cdot[c_2^\dagger c_1, c_1^\dagger c_1]) + (del\cdot[c_1^\dagger c_2, c_2^\dagger c_1]) - (del\cdot[c_2^\dagger c_1, c_1^\dagger c_2]))$$

$$((eps\cdot(c_1^\dagger c_2 c_1^\dagger c_1 - c_1^\dagger c_1 c_1^\dagger c_2)) - (eps\cdot(c_2^\dagger c_1 c_1^\dagger c_1 - c_1^\dagger c_1 c_2^\dagger c_1)) + (del\cdot[c_1^\dagger c_2, c_2^\dagger c_1]) - (del\cdot[c_2^\dagger c_1, c_1^\dagger c_2]))$$

$$((eps\cdot(c_1^\dagger c_2 c_1^\dagger c_1 - c_1^\dagger c_1 c_1^\dagger c_2)) - (eps\cdot(c_2^\dagger c_1 c_1^\dagger c_1 - c_1^\dagger c_1 c_2^\dagger c_1)) + (del\cdot(c_1^\dagger c_2 c_2^\dagger c_1 - c_2^\dagger c_1 c_1^\dagger c_2)) - (del\cdot[c_2^\dagger c_1, c_1^\dagger c_2]))$$

$$((eps\cdot(c_1^\dagger c_2 c_1^\dagger c_1 - c_1^\dagger c_1 c_1^\dagger c_2)) - (eps\cdot(c_2^\dagger c_1 c_1^\dagger c_1 - c_1^\dagger c_1 c_2^\dagger c_1)) + (del\cdot(c_1^\dagger c_2 c_2^\dagger c_1 - c_2^\dagger c_1 c_1^\dagger c_2)) - (del\cdot(c_2^\dagger c_1 c_1^\dagger c_2 - c_1^\dagger c_2 c_2^\dagger c_1)))$$

$$((eps\cdot c_1^\dagger c_2 c_1^\dagger c_1) + (eps\cdot -c_1^\dagger c_1 c_1^\dagger c_2) - (eps\cdot(c_2^\dagger c_1 c_1^\dagger c_1 - c_1^\dagger c_1 c_2^\dagger c_1)) + (del\cdot(c_1^\dagger c_2 c_2^\dagger c_1 - c_2^\dagger c_1 c_1^\dagger c_2)) - (del\cdot(c_2^\dagger c_1 c_1^\dagger c_2 - c_1^\dagger c_2 c_2^\dagger c_1)))$$

$$((eps\cdot c_1^\dagger c_2 c_1^\dagger c_1) + (eps\cdot -c_1^\dagger c_1 c_1^\dagger c_2) - (eps\cdot c_2^\dagger c_1 c_1^\dagger c_1) - (eps\cdot -c_1^\dagger c_1 c_2^\dagger c_1) + (del\cdot(c_1^\dagger c_2 c_2^\dagger c_1 - c_2^\dagger c_1 c_1^\dagger c_2)) - (del\cdot(c_2^\dagger c_1 c_1^\dagger c_2 - c_1^\dagger c_2 c_2^\dagger c_1)))$$

$$((eps\cdot c_1^\dagger c_2 c_1^\dagger c_1) + (eps\cdot -c_1^\dagger c_1 c_1^\dagger c_2) - (eps\cdot c_2^\dagger c_1 c_1^\dagger c_1) - (eps\cdot -c_1^\dagger c_1 c_2^\dagger c_1) + (del\cdot c_1^\dagger c_2 c_2^\dagger c_1) + (del\cdot -c_2^\dagger c_1 c_1^\dagger c_2) - (del\cdot(c_2^\dagger c_1 c_1^\dagger c_2 - c_1^\dagger c_2 c_2^\dagger c_1)))$$

$$((eps\cdot c_1^\dagger c_2 c_1^\dagger c_1) + (eps\cdot -c_1^\dagger c_1 c_1^\dagger c_2) - (eps\cdot c_2^\dagger c_1 c_1^\dagger c_1) - (eps\cdot -c_1^\dagger c_1 c_2^\dagger c_1) + (del\cdot c_1^\dagger c_2 c_2^\dagger c_1) + (del\cdot -c_2^\dagger c_1 c_1^\dagger c_2) - (del\cdot c_2^\dagger c_1 c_1^\dagger c_2) - (del\cdot -c_1^\dagger c_2 c_2^\dagger c_1))$$

$$((eps\cdot c_1 c_2 c_1^\dagger c_1^\dagger) - (eps\cdot c_1^\dagger c_1 c_1^\dagger c_2) + (eps\cdot c_1 c_2^\dagger) - (eps\cdot c_1 c_1 c_1^\dagger c_2^\dagger) + (eps\cdot c_1^\dagger c_1 c_2^\dagger c_1) + (del\cdot c_2 c_2^\dagger) - (del\cdot c_2^\dagger c_1 c_1^\dagger c_2) - (del\cdot c_1 c_1^\dagger) + (del\cdot c_1^\dagger c_2 c_2^\dagger c_1))$$

$$((eps\cdot c_1 c_2 c_1^\dagger c_1^\dagger) + (eps\cdot c_2 c_1^\dagger) + (eps\cdot c_1 c_2 c_1^\dagger c_1^\dagger) - (eps\cdot c_1 c_1 c_1^\dagger c_2^\dagger) + (eps\cdot c_1 c_2^\dagger) - (eps\cdot c_1 c_1 c_1^\dagger c_2^\dagger) + (del\cdot c_2 c_2^\dagger) - (del\cdot c_1 c_1^\dagger) - (del\cdot c_1 c_1^\dagger) + (del\cdot c_2 c_2^\dagger))$$

$$((2\cdot eps\cdot c_1 c_2 c_1^\dagger c_1^\dagger) + (eps\cdot c_2 c_1^\dagger) - (2\cdot eps\cdot c_1 c_1 c_1^\dagger c_2^\dagger) + (eps\cdot c_1 c_2^\dagger) + (2\cdot del\cdot c_2 c_2^\dagger) - (2\cdot del\cdot c_1 c_1^\dagger))$$

$$(0 + (eps\cdot c_2 c_1^\dagger) - (2\cdot eps\cdot c_1 c_1 c_1^\dagger c_2^\dagger) + (eps\cdot c_1 c_2^\dagger) + (2\cdot del\cdot c_2 c_2^\dagger) - (2\cdot del\cdot c_1 c_1^\dagger))$$

$$(0 + (eps\cdot c_2 c_1^\dagger) - 0 + (eps\cdot c_1 c_2^\dagger) + (2\cdot del\cdot c_2 c_2^\dagger) - (2\cdot del\cdot c_1 c_1^\dagger))$$

$$((eps\cdot c_2 c_1^\dagger) + (eps\cdot c_1 c_2^\dagger) + (2\cdot del\cdot c_2 c_2^\dagger) - (2\cdot del\cdot c_1 c_1^\dagger))$$

$$(-(eps\cdot c_1^\dagger c_2) + (eps\cdot c_1 c_2^\dagger) + (2\cdot del\cdot c_2 c_2^\dagger) - (2\cdot del\cdot c_1 c_1^\dagger))$$

$$(-(eps\cdot c_1^\dagger c_2) - (eps\cdot c_2^\dagger c_1) + (2\cdot del\cdot c_2 c_2^\dagger) - (2\cdot del\cdot c_1 c_1^\dagger))$$

$$((eps\cdot(-c_1^\dagger c_2 - c_2^\dagger c_1)) + (2\cdot del\cdot c_2 c_2^\dagger) - (2\cdot del\cdot c_1 c_1^\dagger))$$

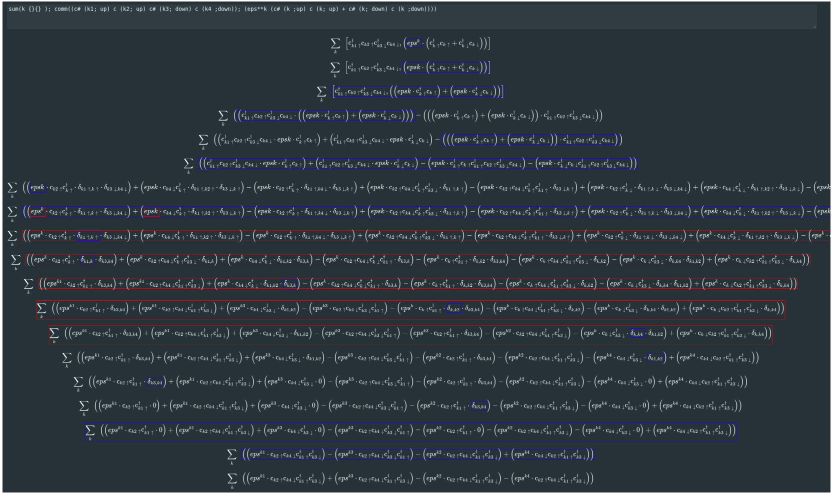
$$((2\cdot((del\cdot c_2 c_2^\dagger) - (del\cdot c_1 c_1^\dagger))) + (eps\cdot(-c_1^\dagger c_2 - c_2^\dagger c_1)))$$

$$((2\cdot del\cdot(c_2 c_2^\dagger - c_1 c_1^\dagger)) + (eps\cdot(-c_1^\dagger c_2 - c_2^\dagger c_1)))$$

$$((2\cdot del\cdot(c_2 c_2^\dagger - c_1 c_1^\dagger)) - (eps\cdot(c_1^\dagger c_2 + c_2^\dagger c_1)))$$

Backup-Solution Problem 2

Extra slides



Backup: Simplification V-Parts

Extra slides

```
-2 c l c# m -1 c l c# m d l d m d# l d# m + 2 c l c# m d l d# l +1 c l c# m d m d# m
```

$$\left(\left(-2\cdot \mathrm{c}_l\mathrm{c}_m^\dagger\right)+\left(-1\cdot \mathrm{c}_l\mathrm{c}_m^\dagger\mathrm{d}_l\mathrm{d}_m\mathrm{d}_l^\dagger\mathrm{d}_m^\dagger\right)+\left(2\cdot \mathrm{c}_l\mathrm{c}_m^\dagger\boxed{\mathrm{d}_l}\mathrm{d}_l^\dagger\right)+\left(1\cdot \mathrm{c}_l\mathrm{c}_m^\dagger\mathrm{d}_m\mathrm{d}_m^\dagger\right)\right)$$

$$\left(\left(-2\cdot \mathrm{c}_l\mathrm{c}_m^\dagger\right)+\left(-1\cdot \mathrm{c}_l\mathrm{c}_m^\dagger\mathrm{d}_l\mathrm{d}_m\mathrm{d}_l^\dagger\mathrm{d}_m^\dagger\right)+\left(2\cdot \mathrm{c}_l\mathrm{c}_m^\dagger\cdot\left(1+\mathrm{d}_l^\dagger\mathrm{d}_l\right)\right)+\left(1\cdot \mathrm{c}_l\mathrm{c}_m^\dagger\boxed{\mathrm{d}_m}\mathrm{d}_m^\dagger\right)\right)$$

$$\left(\left(-2\cdot \mathrm{c}_l\mathrm{c}_m^\dagger\right)+\left(-1\cdot \mathrm{c}_l\mathrm{c}_m^\dagger\mathrm{d}_l\boxed{\mathrm{d}_m}\mathrm{d}_l^\dagger\mathrm{d}_m^\dagger\right)+\left(2\cdot \mathrm{c}_l\mathrm{c}_m^\dagger\cdot\left(1+\mathrm{d}_l^\dagger\mathrm{d}_l\right)\right)+\left(\mathrm{c}_l\mathrm{c}_m^\dagger\cdot\left(1+\mathrm{d}_m^\dagger\mathrm{d}_m\right)\right)\right)$$

$$\left(\left(-2\cdot \mathrm{c}_l\mathrm{c}_m^\dagger\right)-\left(1\cdot \mathrm{c}_l\mathrm{c}_m^\dagger\boxed{\mathrm{d}_l}\mathrm{d}_l^\dagger\mathrm{d}_m\mathrm{d}_m^\dagger\right)+\left(2\cdot \mathrm{c}_l\mathrm{c}_m^\dagger\cdot\left(1+\mathrm{d}_l^\dagger\mathrm{d}_l\right)\right)+\left(\mathrm{c}_l\mathrm{c}_m^\dagger\cdot\left(1+\mathrm{d}_m^\dagger\mathrm{d}_m\right)\right)\right)$$

$$\left(\left(-2\cdot \mathrm{c}_l\mathrm{c}_m^\dagger\right)-\left(\mathrm{c}_l\mathrm{c}_m^\dagger\cdot\left(1+\mathrm{d}_l^\dagger\mathrm{d}_l\right)\cdot\boxed{\mathrm{d}_m}\mathrm{d}_m^\dagger\right)+\left(2\cdot \mathrm{c}_l\mathrm{c}_m^\dagger\cdot\left(1+\mathrm{d}_l^\dagger\mathrm{d}_l\right)\right)+\left(\mathrm{c}_l\mathrm{c}_m^\dagger\cdot\left(1+\mathrm{d}_m^\dagger\mathrm{d}_m\right)\right)\right)$$

$$\left(\left(-2\cdot \mathrm{c}_l\mathrm{c}_m^\dagger\right)-\boxed{\left(\mathrm{c}_l\mathrm{c}_m^\dagger\cdot\left(1+\mathrm{d}_l^\dagger\mathrm{d}_l\right)\cdot\left(1+\mathrm{d}_m^\dagger\mathrm{d}_m\right)\right)}+\left(2\cdot \mathrm{c}_l\mathrm{c}_m^\dagger\cdot\left(1+\mathrm{d}_l^\dagger\mathrm{d}_l\right)\right)+\left(\mathrm{c}_l\mathrm{c}_m^\dagger\cdot\left(1+\mathrm{d}_m^\dagger\mathrm{d}_m\right)\right)\right)$$

$$\left(\left(-2\cdot \mathrm{c}_l\mathrm{c}_m^\dagger\right)-\left(\mathrm{c}_l\mathrm{c}_m^\dagger\cdot 1\cdot 1\right)-\left(\mathrm{c}_l\mathrm{c}_m^\dagger\cdot 1\cdot \mathrm{d}_m^\dagger\mathrm{d}_m\right)-\left(\mathrm{c}_l\mathrm{c}_m^\dagger\mathrm{d}_l^\dagger\mathrm{d}_l\cdot 1\right)-\mathrm{c}_l\mathrm{c}_m^\dagger\mathrm{d}_l^\dagger\mathrm{d}_l\mathrm{d}_m^\dagger\mathrm{d}_m+\boxed{\left(2\cdot \mathrm{c}_l\mathrm{c}_m^\dagger\cdot\left(1+\mathrm{d}_l^\dagger\mathrm{d}_l\right)\right)}+\left(\mathrm{c}_l\mathrm{c}_m^\dagger\cdot\left(1+\mathrm{d}_m^\dagger\mathrm{d}_m\right)\right)\right)$$

$$\left(\left(-2\cdot \mathrm{c}_l\mathrm{c}_m^\dagger\right)-\left(\mathrm{c}_l\mathrm{c}_m^\dagger\cdot 1\cdot 1\right)-\left(\mathrm{c}_l\mathrm{c}_m^\dagger\cdot 1\cdot \mathrm{d}_m^\dagger\mathrm{d}_m\right)-\left(\mathrm{c}_l\mathrm{c}_m^\dagger\mathrm{d}_l^\dagger\mathrm{d}_l\cdot 1\right)-\mathrm{c}_l\mathrm{c}_m^\dagger\mathrm{d}_l^\dagger\mathrm{d}_l\mathrm{d}_m^\dagger\mathrm{d}_m+\left(2\cdot \mathrm{c}_l\mathrm{c}_m^\dagger\cdot 1\right)+\left(2\cdot \mathrm{c}_l\mathrm{c}_m^\dagger\mathrm{d}_l^\dagger\mathrm{d}_l\right)+\boxed{\left(\mathrm{c}_l\mathrm{c}_m^\dagger\cdot\left(1+\mathrm{d}_m^\dagger\mathrm{d}_m\right)\right)}\right)$$

$$\boxed{\left(\left(-2\cdot \mathrm{c}_l\mathrm{c}_m^\dagger\right)-\left(\mathrm{c}_l\mathrm{c}_m^\dagger\cdot 1\cdot 1\right)-\left(\mathrm{c}_l\mathrm{c}_m^\dagger\cdot 1\cdot \mathrm{d}_m^\dagger\mathrm{d}_m\right)-\left(\mathrm{c}_l\mathrm{c}_m^\dagger\mathrm{d}_l^\dagger\mathrm{d}_l\cdot 1\right)-\mathrm{c}_l\mathrm{c}_m^\dagger\mathrm{d}_l^\dagger\mathrm{d}_l\mathrm{d}_m^\dagger\mathrm{d}_m+\left(2\cdot \mathrm{c}_l\mathrm{c}_m^\dagger\cdot 1\right)+\left(2\cdot \mathrm{c}_l\mathrm{c}_m^\dagger\mathrm{d}_l^\dagger\mathrm{d}_l\right)+\left(\mathrm{c}_l\mathrm{c}_m^\dagger\cdot 1\right)+\mathrm{c}_l\mathrm{c}_m^\dagger\mathrm{d}_m^\dagger\mathrm{d}_m\right)}$$

$$\boxed{\left(-\mathrm{c}_l\mathrm{c}_m^\dagger\mathrm{d}_l^\dagger\mathrm{d}_l-\mathrm{c}_l\mathrm{c}_m^\dagger\mathrm{d}_l^\dagger\mathrm{d}_l\mathrm{d}_m^\dagger\mathrm{d}_m+\left(2\cdot \mathrm{c}_l\mathrm{c}_m^\dagger\mathrm{d}_l^\dagger\mathrm{d}_l\right)\right)}$$

$$\left(\mathrm{c}_l\mathrm{c}_m^\dagger\mathrm{d}_l^\dagger\mathrm{d}_l-\mathrm{c}_l\mathrm{c}_m^\dagger\mathrm{d}_l^\dagger\mathrm{d}_l\mathrm{d}_m^\dagger\mathrm{d}_m\right)$$

Variables:

Macros:

+

c#	bc("c"; #0)
c	ba("c"; #0)
d#	bc("d"; #0)
d	ba("d"; #0)
displayl	l\mathrm{}
displaym	m\mathrm{}
l	dist(displayl)
m	dist(displaym)

$$\hat{\mathrm{V}}_{\text{Part A}}(l,m) \overset{\mathrm{MM}}{=} \sum_{\sigma\in\{\uparrow,\downarrow\}} \hat{\mathrm{c}}^{\mathrm{S}}_{l,\sigma}\hat{\mathrm{c}}^{\dagger\mathrm{S}}_{m,\sigma}\left(1+2\cdot\hat{\mathrm{n}}^{\mathrm{S}}_{l,\overline{\sigma}}\hat{\mathrm{n}}^{\mathrm{S}}_{m,\overline{\sigma}}-\hat{\mathrm{n}}^{\mathrm{S}}_{l,\overline{\sigma}}-\hat{\mathrm{n}}^{\mathrm{S}}_{m,\overline{\sigma}}\right)$$

$$\hat{\mathrm{V}}_{\text{Part B}}(l,m) \overset{\mathrm{MM}}{=} \sum_{\sigma\in\{\uparrow,\downarrow\}} \hat{\mathrm{c}}^{\mathrm{S}}_{l,\sigma}\hat{\mathrm{c}}^{\dagger\mathrm{S}}_{m,\sigma}\left(\hat{\mathrm{n}}^{\mathrm{S}}_{m,\overline{\sigma}}-\hat{\mathrm{n}}^{\mathrm{S}}_{l,\overline{\sigma}}\hat{\mathrm{n}}^{\mathrm{S}}_{m,\overline{\sigma}}\right)$$

$$\hat{\mathrm{V}}_{\text{Part C}}(l,m) \overset{\mathrm{MM}}{=} \sum_{\sigma\in\{\uparrow,\downarrow\}} \hat{\mathrm{c}}^{\mathrm{S}}_{l,\sigma}\hat{\mathrm{c}}^{\dagger\mathrm{S}}_{m,\sigma}\left(\hat{\mathrm{n}}^{\mathrm{S}}_{l,\overline{\sigma}}-\hat{\mathrm{n}}^{\mathrm{S}}_{l,\overline{\sigma}}\hat{\mathrm{n}}^{\mathrm{S}}_{m,\overline{\sigma}}\right)$$