

UNA

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

2024-09-05

Computer aided calculations

1. Welcome
2. Presentation of "Project Work" (Projektarbeit)
3. Runs parallel to the "Practical Training" (Fachpraktikum)
4. Presentation in this Group-Slot

Outline

1 Introduction of the problem



└ Outline

1. Introduction of theme worked on in Project-Work, Practical Training and Master Thesis
 - The mathematical Problem of Many-Body Physics
2. Focus of the report is on the mathematical details. I have a history in Computer-Science, therefore would like here to present some techniques I learned in my work as well as studies as a Computer scientist, that I think might be quite useful to apply in the context of such a working group.
 - The computational/notational problem of "doing maths easily"
3. What was there to make it easier (Off the shelf solutions)
4. What I did:
 - Math Manipulator
 - Tricks to use to improve your Python
 - Latex for presentations
5. Gist: after I (somewhat of a computer scientist by trade) learned the process of being a theoretical physicist, I want to bring back some tools/workflows to maybe improve someones life here at TP III

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2 Solutions: Off the shelf

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3 Math-Manipulator

- What did I do?
- How can you use it
- Interactive Demonstration



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- 1** [Introduction of the problem](#)
- 2** [Solutions: Off the shelf](#)
- 3** [Math-Manipulator](#)
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- 4** [Custom Python Scripts \(SymPy\)](#)



Computer aided calculations

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4 Custom Python Scripts (SymPy)

5 Presentations? - Custom Beamer Template



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Physics of what we calculate

Introduction of the problem

- Content of my Practical Training (Fachpraktikum)

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

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

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



2024-09-05

Computer aided calculations
 └ Introduction of the problem
 └ Physics of what we calculate

1. Hubbard-Model Hamiltonian with externally applied electric field
2. Hard-Core Bosonic Operators (will be explained in later slide, do not need to elaborate on)
3. Spin-dependent lattice Model
4. External electric field acts symmetric on both spin directions
 - This will be important later, multiple times
 - All terms always need to be symmetric in terms of spin up/down

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Physics of what we calculate

Introduction of the problem

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- 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

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

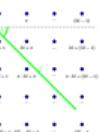
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Computer aided calculations
 └ Introduction of the problem
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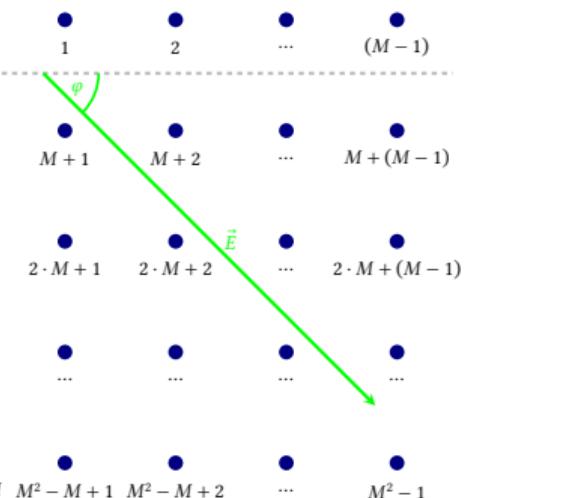
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Physics of what we calculate

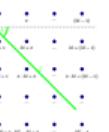
Introduction of the problem

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



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Computer aided calculations
└ Introduction of the problem
 └ Physics of what we calculate

1. 2-dimensional square geometry
2. Program supports already for general size inputs
3. Thanks to the Monte-Carlo Sampling we can even efficiently evaluate larger systems already

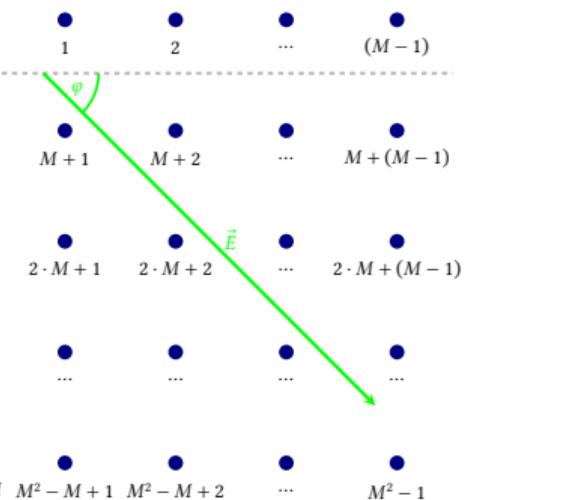


Physics of what we calculate

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



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Computer aided calculations
└ Introduction of the problem

└ Physics of what we calculate

1. 2-dimensional square geometry
2. Program supports already for general size inputs
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$$[\hat{c}_{l,\sigma}, \hat{c}_{l',\sigma'}] = [\hat{c}_{l,\sigma}^\dagger, \hat{c}_{l',\sigma'}^\dagger] = 0$$
$$[\hat{c}_{l,\sigma}, \hat{c}_{l',\sigma'}^\dagger] = \delta(l,l') \cdot \delta(\sigma,\sigma')$$

Physics of what we calculate

Introduction of the problem

■ Hard-Core Bosonic operators

$$[\hat{c}_{l,\sigma}, \hat{c}_{l',\sigma'}] = [\hat{c}_{l,\sigma}^\dagger, \hat{c}_{l',\sigma'}^\dagger] = 0$$

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- Computer aided calculations
 - └ Introduction of the problem
 - └ Physics of what we calculate

1. Operators are hard-core bosonic
 - standard commutation relations
 - occupations are only either zero or one
2. fermionic operators (anti-commutation) would work equivalent
3. other notation to rewrite the two spin degrees of freedom into two operators of different dof makes it more readable and comfortable to apply computationally in some cases



$$\begin{aligned} [\hat{c}_{l,\sigma}, \hat{c}_{l',\sigma'}] &= [\hat{c}_{l,\sigma}^\dagger, \hat{c}_{l',\sigma'}^\dagger] = 0 \\ [\hat{c}_{l,\sigma}, \hat{c}_{l',\sigma'}^\dagger] &= \delta(l,l') \cdot \delta(\sigma,\sigma') \end{aligned}$$

Physics of what we calculate

Introduction of the problem

■ Hard-Core Bosonic operators

- (Would work analogously with Fermionic operators)

$$\begin{aligned} [\hat{c}_{l,\sigma}, \hat{c}_{l',\sigma'}] &= [\hat{c}_{l,\sigma}^\dagger, \hat{c}_{l',\sigma'}^\dagger] = 0 \\ [\hat{c}_{l,\sigma}, \hat{c}_{l',\sigma'}^\dagger] &= \delta(l,l') \cdot \delta(\sigma,\sigma') \end{aligned}$$

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$\hat{c}_{l,\sigma}^{(1)} \leftrightarrow \hat{c}_l^{(1)}$ $\hat{c}_{l,\sigma}^{(1)} \leftrightarrow \hat{d}_l^{(1)}$

$\hat{c}_{l,\sigma}^{(2)} \leftrightarrow \hat{c}_l^{(2)}$ $\hat{c}_{l,\sigma}^{(2)} \leftrightarrow \hat{d}_l^{(2)}$

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

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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

$$[\hat{c}_{l,\sigma}, \hat{c}_{l',\sigma'}] = [\hat{c}_{l,\sigma}^\dagger, \hat{c}_{l',\sigma'}^\dagger] = 0$$

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Working on paper: A Computer-Scientists view

Introduction of the problem

Doing Theoretical Physics often requires lengthy analytical calculations

Computer aided calculations
└ Introduction of the problem
 └ Working on paper: A Computer-Scientists view

2024-09-05

1. Comparison of advantages/disatvantages of doing calculations "by hand"
2. Advantages
 - No skills required to learn, writing is natural, every new symbol can just be written
 - Operational Libery (cross out stuff as please, swap whatever without "proof")
 - For completely different approaches no new tool is needed (lern that integral cannot be solved with a specific strategy that you tool doesn't support: out of luck)
 - Hard to loose access to taken notes, produce them without internet/power
3. Disatvantages
 - Many tasks are repetitive, trivial and unfunny to do, paper cannot automate
 - Sign errores, copy errors happen too often
 - Sharing and archiving is non-standart. Many standarts exist for e.g. sharing latex
 - No version-control (git): hard for people that are used to it like me. Cannot just do stuff and later revert if it didn't work
 - Need to write the pretty version in the computer anyway



Working on paper: A Computer-Scientists view

Introduction of the problem

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Advantages of working on paper:

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- Fast iteration for high variation workload
- "Offline" available

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Problems of working on paper:

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- Error-prone and time-consuming to fix mistakes
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Computer aided calculations

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$$\begin{aligned} [S, H] &= [c_1^t c_2 - c_2^t c_1, \epsilon c_1^t c_1 + \Delta (c_1^t c_2 + c_2^t c_1)] \Rightarrow [c_1^t c_2, c_1^t c_1] = 0, \text{ obvious, usu.} \\ &= \epsilon [c_1^t c_2, c_1^t c_1] - \epsilon [c_2^t c_1, c_1^t c_1] + \Delta [c_1^t c_2, c_1^t c_1] - \Delta [c_2^t c_1, c_1^t c_1] \\ &\quad \left| \begin{array}{l} c_1^t c_2 c_1^t c_1 - c_2^t c_1 c_1^t c_2 = c_1^t c_2 \\ = -c_1^t c_2 \\ \hline \end{array} \right| \left| \begin{array}{l} c_1^t c_2 c_1^t c_1 - c_1^t c_1 c_1^t c_2 = \\ + c_1^t c_1 \\ \hline \end{array} \right| \left| \begin{array}{l} c_1^t c_2 c_1^t c_1 - c_2^t c_2 + c_2^t c_1 c_1^t c_2 = \\ -c_1^t c_2 \\ \hline \end{array} \right| \left| \begin{array}{l} c_1^t c_2 + c_2^t c_1 c_1^t c_2 - c_1^t c_2 - c_1^t c_1 c_1^t c_2 = c_1^t c_2 - c_1^t c_2 \\ \hline \end{array} \right| \end{aligned}$$

$$\begin{aligned} &\rightarrow \epsilon c_1^t c_2 - \epsilon c_2^t c_1 + 2\Delta (c_1^t c_1 - c_2^t c_2) \\ &= \epsilon (c_1^t c_2 - c_2^t c_1) + 2\Delta (c_1^t c_1 - c_2^t c_2) \\ &= \frac{\epsilon}{\Delta} V + 2\Delta (c_1^t c_1 - c_2^t c_2) \end{aligned}$$

Examples from "Theoretical Solid State Physics"

Introduction of the problem

$$\begin{aligned} [S, H] &= [c_1^t c_2 - c_2^t c_1, \epsilon c_1^t c_1 + \Delta (c_1^t c_2 + c_2^t c_1)] \Rightarrow [c_1^t c_2, c_1^t c_1] = 0, \text{ obvious, usu.} \\ &= \epsilon [c_1^t c_2, c_1^t c_1] - \epsilon [c_2^t c_1, c_1^t c_1] + \Delta [c_1^t c_2, c_1^t c_1] - \Delta [c_2^t c_1, c_1^t c_1] \\ &\quad \left| \begin{array}{l} c_1^t c_2 c_1^t c_1 - c_2^t c_1 c_1^t c_2 = c_1^t c_2 \\ = -c_1^t c_2 \\ \hline \end{array} \right| \left| \begin{array}{l} c_1^t c_2 c_1^t c_1 - c_1^t c_1 c_1^t c_2 = \\ + c_1^t c_1 \\ \hline \end{array} \right| \left| \begin{array}{l} c_1^t c_2 c_1^t c_1 - c_2^t c_2 + c_2^t c_1 c_1^t c_2 = \\ -c_1^t c_2 \\ \hline \end{array} \right| \left| \begin{array}{l} c_1^t c_2 + c_2^t c_1 c_1^t c_2 - c_1^t c_2 - c_1^t c_1 c_1^t c_2 = c_1^t c_2 - c_1^t c_2 \\ \hline \end{array} \right| \end{aligned}$$

$$\begin{aligned} \hat{c}_{k\sigma}^\dagger(t) &= e^{iHt} c_{k\sigma}^\dagger e^{-iHt} && \rightarrow \text{complicated} \\ \hat{c}_{k\sigma}^\dagger(t) &= e^{iHt} \hat{c}_{k\sigma}^\dagger e^{-iHt} && \rightarrow \text{easier} \end{aligned}$$

$$\hat{c}_{k\sigma}^\dagger = e^{\hat{c}_{k\sigma}^\dagger} e^{-\hat{S}} \approx c_{k\sigma}^\dagger + [\hat{S}, c_{k\sigma}^\dagger] + O(U^2)$$

$$[\hat{S}, c_{k\sigma}^\dagger] = \frac{U}{N} \sum'_{k_1, k_2, k_3, k_4} \delta(k_1 - k_2 + k_3 - k_4) [c_{k_1}^\dagger c_{k_2}^\dagger c_{k_3}^\dagger c_{k_4}, c_{k\sigma}^\dagger] =$$

$$c_{k_1}^\dagger c_{k_2}^\dagger c_{k_3}^\dagger c_{k_4} S_{k_1} S_{k_2} + c_{k_1}^\dagger c_{k_2}^\dagger c_{k_3}^\dagger c_{k_4} S_{k_1} S_{k_2}$$

$$c_{k\sigma}^\dagger = e^{\hat{S}} c_{k\sigma}^\dagger e^{-\hat{S}} = c_{k\sigma}^\dagger + \frac{U}{N} \sum'_{k_1, k_2, k_3} \frac{\delta(k_1 - k_2 + k_3 - k_\sigma)}{\epsilon_{k_1} - \epsilon_{k_2} + \epsilon_{k_3} - \epsilon_{k\sigma}}$$

$$= c_{k\sigma}^\dagger + \frac{U}{N} \sum'_{k_1, k_2, k_3} \frac{\delta(k_1 - k_2 + k_3 - k_\sigma)}{\epsilon_{k_1} - \epsilon_{k_2} + \epsilon_{k_3} - \epsilon_{k\sigma}} \delta_{kk_1} c_{k_1}^\dagger c_{k_2}^\dagger c_{k_3}^\dagger c_{k\sigma}$$

$$= c_{k\sigma}^\dagger + \frac{U}{N} \sum'_{k_1, k_2, k_3} \frac{1}{\epsilon_{k_1} - \epsilon_{k_2} + \epsilon_{k_3} - \epsilon_{k\sigma}} c_{k_1}^\dagger c_{k_2}^\dagger c_{k_3}^\dagger c_{k\sigma}$$

$$\text{ii) } \bar{H} = \alpha H_u + e^{\hat{S}} H c^{-\hat{S}} = H + [\hat{S}, H_0] + O(U^2) \quad [\hat{S}, V] \rightarrow \text{second order}$$

$$[\hat{S}, H_0] = \frac{U}{N} \sum'_{k_1, k_2, k_3, k_4} \frac{\delta(k_1 - k_2 + k_3 - k_4)}{\epsilon_{k_1} - \epsilon_{k_2} + \epsilon_{k_3} - \epsilon_{k_4}} [c_{k_1}^\dagger c_{k_2}^\dagger c_{k_3}^\dagger c_{k_4}, \sum_{k\sigma} \epsilon_{k\sigma} n_{k\sigma}]$$

$$\rightarrow \text{use } [c_{k\sigma}^\dagger, h_{k'\sigma'}^\dagger] = -(\epsilon_{k_1} - \epsilon_{k_2} + \epsilon_{k_3} - \epsilon_{k_4}) c_{k_1}^\dagger c_{k_2}^\dagger c_{k_3}^\dagger c_{k_4}$$

Examples from "Theoretical Solid State Physics"

Introduction of the problem

Final transform?

$$\begin{aligned} c_{k\sigma}^\dagger(t) &= e^{iHt} c_{k\sigma}^\dagger e^{-iHt} && \rightarrow \text{complicated} \\ \hat{c}_{k\sigma}^\dagger(t) &= e^{iHt} \hat{c}_{k\sigma}^\dagger e^{-iHt} && \rightarrow \text{easier} \end{aligned}$$

$$\hat{c}_{k\sigma}^\dagger = e^{\hat{c}_{k\sigma}^\dagger} e^{-\hat{S}} \approx c_{k\sigma}^\dagger + [\hat{S}, c_{k\sigma}^\dagger] + O(U^2)$$

$$[\hat{S}, c_{k\sigma}^\dagger] = \frac{U}{N} \sum'_{k_1, k_2, k_3, k_4} \delta(k_1 - k_2 + k_3 - k_4) [c_{k_1}^\dagger c_{k_2}^\dagger c_{k_3}^\dagger c_{k_4}, c_{k\sigma}^\dagger] =$$

$$c_{k_1}^\dagger c_{k_2}^\dagger c_{k_3}^\dagger c_{k_4} S_{k_1} S_{k_2} + c_{k_1}^\dagger c_{k_2}^\dagger c_{k_3}^\dagger c_{k_4} S_{k_1} S_{k_2}$$

$$c_{k\sigma}^\dagger = e^{\hat{S}} c_{k\sigma}^\dagger e^{-\hat{S}} = c_{k\sigma}^\dagger + \frac{U}{N} \sum'_{k_1, k_2, k_3} \frac{\delta(k_1 - k_2 + k_3 - k_\sigma)}{\epsilon_{k_1} - \epsilon_{k_2} + \epsilon_{k_3} - \epsilon_{k\sigma}}$$

$$= c_{k\sigma}^\dagger + \frac{U}{N} \sum'_{k_1, k_2, k_3} \frac{\delta(k_1 - k_2 + k_3 - k_\sigma)}{\epsilon_{k_1} - \epsilon_{k_2} + \epsilon_{k_3} - \epsilon_{k\sigma}} \delta_{kk_1} c_{k_1}^\dagger c_{k_2}^\dagger c_{k_3}^\dagger c_{k\sigma}$$

$$= c_{k\sigma}^\dagger + \frac{U}{N} \sum'_{k_1, k_2, k_3} \frac{1}{\epsilon_{k_1} - \epsilon_{k_2} + \epsilon_{k_3} - \epsilon_{k\sigma}} c_{k_1}^\dagger c_{k_2}^\dagger c_{k_3}^\dagger c_{k\sigma}$$

$$\text{ii) } \bar{H} = \alpha H_u + e^{\hat{S}} H c^{-\hat{S}} = H + [\hat{S}, H_0] + O(U^2) \quad [\hat{S}, V] \rightarrow \text{second order}$$

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■ Goal: produce time evolution
of operator

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

Examples from the Practical Training

Introduction of the problem

- Goal: produce time evolution
of operator

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

1. Want to calculate the Time-Evolution of the operator V in the interaction Picture
2. Basically comes down to inserting definitions (however already derived from MM)
3. Distributing and re-ordering is a painful, time-intensive process
4. How to time-evolve operator in the Interaction Picture $\{\cdot\}(t) = e^{iH_0 t} \{\cdot\} e^{-iH_0 t}$

Examples from the Practical Training

Introduction of the problem

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

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

$$\hat{c}_m^{\dagger I}(t) = e^{i\epsilon_m t} \left(1 + (e^{iUt} - 1) \hat{d}_m^{\dagger S} \hat{d}_m^S \right) \hat{c}_m^{\dagger S}$$

$$\hat{c}_m^I(t) = e^{-i\epsilon_m t} \left(1 + (e^{-iUt} - 1) \hat{d}_m^{\dagger S} \hat{d}_m^S \right) \hat{c}_m^S$$

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

$$\begin{aligned}\hat{V} &= -J \cdot \sum_{\langle l,m \rangle} \left(\hat{c}_l^\dagger \hat{c}_m + \hat{c}_m^\dagger \hat{c}_l + \hat{d}_l^\dagger \hat{d}_m + \hat{d}_m^\dagger \hat{d}_l \right) \\ \hat{d}_m^{\dagger I}(t) &= e^{i\omega_m t} \left(1 + (e^{iUt} - 1) \hat{d}_m^{\dagger S} \hat{d}_m^S \right) \hat{d}_m^S \\ \hat{d}_m^I(t) &= e^{-i\omega_m t} \left(1 + (e^{-iUt} - 1) \hat{d}_m^{\dagger S} \hat{d}_m^S \right) \hat{d}_m^S \\ \hat{d}_m^{\dagger I}(t) &= e^{i\omega_m t} \left(1 + (e^{iUt} - 1) \hat{c}_m^{\dagger S} \hat{c}_m^S \right) \hat{d}_m^S \\ \hat{d}_m^I(t) &= e^{-i\omega_m t} \left(1 + (e^{-iUt} - 1) \hat{c}_m^{\dagger S} \hat{c}_m^S \right) \hat{d}_m^S\end{aligned}$$

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

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

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

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

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2024-09-05

- Computer aided calculations
 └ Introduction of the problem
 └ Examples from the Practical Training

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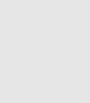
$\hat{V} = -J \cdot \sum_{\langle l, m \rangle} \left(\hat{c}_l^\dagger \hat{c}_m + \hat{c}_m^\dagger \hat{c}_l + \hat{d}_l^\dagger \hat{d}_m + \hat{d}_m^\dagger \hat{d}_l \right)$

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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

Computer aided calculations
└ Solutions: Off the shelf

└ Paper-like writing on digital devices

- 2024-09-05
- 1. Taking notes digitally can have many benefits
 - 2. OneNote, Xournalpp, Notion and many more examples
 - 3. Still lacks "true" automatization
 - 4. Great danger of Vendor-Locking, losing access
 - Cloud-Driven offers do not work without internet
 - Often times even tied to the device (Apple-Notes I-pad, personal experience with one-note)
 - Countless stories about providers ending support, users getting blocked and more
 - 5. Conclusion: very great choice to boost productivity. But TIP: archive everything as pdf if you ever plan to use it later. It may save you weeks of work/complete loss of data.



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2024-09-05

Computer aided calculations

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TIP:

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

2024-09-05

Computer aided calculations

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Computer-Algebra Systems

Solutions: Off the shelf

- Proprietary Software (Often payed):

- Computer aided calculations
 - Solutions: Off the shelf
 - Computer-Algebra Systems

- Standalone Online Calculators

1. There exist already countless possible attempts at solving the worlds problems
2. All of them are great at what they are designed for, I will not attempt competing with any of the m in terms of any metric except maybe usability (and probably still fail)
3. Chat-GPT is included in the list, because it can do many calculations by now, however is extremely unreliable
4. Central, reoccurring Problems (multiple ore some for everything)
 - Paid access
 - Non-reliable
 - Difficult to "cite" / use in paper/thesis
 - Limited in scope, because software is very spezialized to the task
 - Require training/ prior (export) knowlede to properly take advantage of



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- Standalone Online Calculators

- Integralrechner.de (Integral-Calculator)
 - Matrix-Calculators
 - ...

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 └ Computer-Algebra Systems

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What is Math-Manipulator?
Math-Manipulator - What did I do?

What is Math-Manipulator?

Math-Manipulator - What did I do?

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

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

[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

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



Computer aided calculations

└ Math-Manipulator

 └ What did I do?

 └ What is Math-Manipulator?

1. I wrote a custom tool that should help with the process of doing math paper-like, but with the help of computers

2. Features/Properties

- Relatively smart initial text-input
 - Omit implied multiplication
 - Omit implied zeros
 - Parameter autoboxing
 - Bracket culling
 - → Way less stringent as e.g. input to many Computer-Algebra-Systems requires

– Once initial input is set, operations with mouse

- Rename, Pack, Move elements with mouse interactions
- Execute operator-specific operations (distribute, delta/qm-op stuff)

– Many pre-defined Functions/Symbols

– Automatic Macro and Variable system

– In-Browser Help with interactive Playground

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

Computer aided calculations
└ Math-Manipulator
 └ How can you use it
 └ In the Browser

2024-09-05

1. Source code available
2. (Relatively) easily extensible, tutorial and issues available
3. Instantly usable, offline and online



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Available here
<https://jonas-kell.github.io/math-manipulator/>

In the Browser

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Computer aided calculations

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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

2024-09-05

Computer aided calculations
└ Math-Manipulator
 └ How can you use it
 └ Usage as VS-Code Extension

1. For more serious use, integrated in the code-editor VS-Code as an Extension
2. Allows for all features, but includes
 - Offline use out of the box
 - Storage of files (with that version control)
 - Multiple parallel projects
3. Has already taken entry into my personal workflow by now
 - Probably I will never make back my WHOLE time-investment
 - But I already saved hours upon hours when I noticed sign mistakes, symmetry issues or similar in calculations I did with it



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

Note

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

Computer aided calculations

- └ Math-Manipulator
 - └ How can you use it
 - └ Usage as VS-Code Extension

2024-09-05

Usage as VS-Code Extension
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$$= \epsilon [c_1^t c_2, c_1^t c_2] - \epsilon [c_2 + c_3 - c_4^t c_1] + D [c_1^t c_2, c_2^t c_3] - D [c_1^t c_3, c_3^t c_2]$$

$$[c_1^t c_2, c_1^t c_2, \sum \epsilon_k u_{kk}] \\ - (c_1^t c_2 + c_3^t c_1) + 2D (c_1^t c_3 - c_3^t c_2)$$

2024-09-05

1. Go to Demo in VS-Code folder math-manipulator-calculations in the presentation subfolder
2. Think of disabling spellchecker
3. Think to first split deltas before evaluating !!!!!
4. Macros and other optimizations are possible, but not really necessary
5. Input for simple demo: distribute, cleanup, order op string,
 $(x+y)(4*x -z+y)(-z + 1+ x)$
6. Input for simple operators:

```
fc("") 1fa("") 1) ;|; fc("") 1)fa("") m) ;|; fc("") 1)fa("") 2) ;|; fa("") 2)fc("") 2);|; fc("") 1)fa("") 1)fc("") 3)fa("") 3)fa("") 2)fc("") 1)
```

Demo Problems from before

Math-Manipulator - Interactive Demonstration

$$= \epsilon [c_1^t c_2, c_1^t c_2] - \epsilon [c_2 + c_3 - c_4^t c_1] + D [c_1^t c_2, c_2^t c_3] - D [c_1^t c_3, c_3^t c_2]$$

$$= \epsilon (c_1^t c_2 - c_2^t c_1) + 2D (c_1^t c_3 - c_3^t c_2)$$

$$[c_1^t c_2, c_1^t c_2, c_3^t c_3, c_4^t c_4, \sum \epsilon_k u_{kk}] \\ - (c_1^t c_2 + c_3^t c_1) + 2D (c_1^t c_3 - c_3^t c_2)$$

Usage for the Practical Training

Math-Manipulator - Interactive Demonstration

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

Computer aided calculations
 └ Math-Manipulator
 └ Interactive Demonstration
 └ Usage for the Practical Training

2024-09-05

1. Go to Demo in VS-Code submodule mm-calculations.
2. Think of disabling spellchecker
3. Show process of how V is calculated
4. Story: at the end at first result was no longer symmetrical in up and down, but it should have been. Mistake was in the very first input. But because of the upfront configuration (and in my case programming) effort, re-calculating the endresult took 20min instead of one week

$$\hat{V}(t) = \left\{ \hat{V}^S \right\}(t) \stackrel{2.11}{=} -J \cdot \sum_{[l,m]} \left\{ \left(\hat{c}_l^{\dagger S} \hat{c}_m^S + \hat{d}_l^{\dagger S} \hat{d}_m^S \right) \right\}(t)$$

$$\hat{V}_{\text{Part A}}(l, m) \stackrel{\text{MM}}{=} (1 \cdot \hat{c}_l^S \hat{c}_m^{\dagger S}) + (1 \cdot \hat{d}_l^S \hat{d}_m^{\dagger S}) + (2 \cdot \hat{c}_l^S \hat{c}_m^S \hat{c}_l^{\dagger S} \hat{c}_m^{\dagger S} \hat{d}_l^S \hat{d}_m^{\dagger S}) + \\ + (-3 \cdot \hat{c}_l^S \hat{c}_l^{\dagger S} \hat{d}_m^S \hat{d}_m^{\dagger S}) + (-3 \cdot \hat{c}_m^S \hat{c}_m^{\dagger S} \hat{d}_l^S \hat{d}_l^{\dagger S}) + (-3 \cdot \hat{c}_l^S \hat{c}_m^S \hat{d}_l^S \hat{d}_l^{\dagger S}) + (-3 \cdot \hat{c}_l^S \hat{c}_m^{\dagger S} \hat{d}_m^S \hat{d}_m^{\dagger S})$$

$$\hat{V}_{\text{Part B}}(l, m) \stackrel{\text{MM}}{=} (-2 \cdot \hat{c}_l^S \hat{c}_m^{\dagger S}) + (-2 \cdot \hat{d}_l^S \hat{d}_m^{\dagger S}) + (-1 \cdot \hat{c}_l^S \hat{c}_m^S \hat{c}_l^{\dagger S} \hat{c}_m^{\dagger S} \hat{d}_l^S \hat{d}_m^{\dagger S}) + \\ + (1 \cdot \hat{c}_l^S \hat{c}_l^{\dagger S} \hat{d}_m^S \hat{d}_m^{\dagger S}) + (2 \cdot \hat{c}_m^S \hat{c}_m^{\dagger S} \hat{d}_l^S \hat{d}_l^{\dagger S}) + (-1 \cdot \hat{c}_l^S \hat{c}_m^S \hat{d}_l^S \hat{d}_l^{\dagger S}) + (2 \cdot \hat{c}_l^S \hat{c}_m^{\dagger S} \hat{d}_m^S \hat{d}_m^{\dagger S})$$

$$\hat{V}_{\text{Part C}}(l, m) \stackrel{\text{MM}}{=} (-2 \cdot \hat{c}_l^S \hat{c}_m^{\dagger S}) + (-2 \cdot \hat{d}_l^S \hat{d}_m^{\dagger S}) + (-1 \cdot \hat{c}_l^S \hat{c}_m^S \hat{c}_l^{\dagger S} \hat{c}_m^{\dagger S} \hat{d}_l^S \hat{d}_m^{\dagger S}) + \\ + (2 \cdot \hat{c}_l^S \hat{c}_l^{\dagger S} \hat{d}_m^S \hat{d}_m^{\dagger S}) + (1 \cdot \hat{c}_m^S \hat{c}_m^{\dagger S} \hat{d}_l^S \hat{d}_l^{\dagger S}) + (2 \cdot \hat{c}_m^S \hat{c}_m^{\dagger S} \hat{d}_l^S \hat{d}_l^{\dagger S}) + (1 \cdot \hat{c}_l^S \hat{c}_m^{\dagger S} \hat{d}_m^S \hat{d}_m^{\dagger S})$$

Usage for the Practical Training

Math-Manipulator - Interactive Demonstration

$$\hat{V}^I(t) = \left\{ \hat{V}^S \right\}(t) \stackrel{2.11}{=} -J \cdot \sum_{[l,m]} \left\{ \left(\hat{c}_l^{\dagger S} \hat{c}_m^S + \hat{d}_l^{\dagger S} \hat{d}_m^S \right) \right\}(t)$$

$$= -J \cdot \sum_{[l,m]} \left(\hat{c}_l^{\dagger I}(t) \hat{c}_m^I(t) + \hat{d}_l^{\dagger I}(t) \hat{d}_m^I(t) \right)$$

$$\stackrel{\text{MM}}{=} -J \cdot \sum_{[l,m]} \left[e^{i(\varepsilon_m - \varepsilon_l) \cdot t} \cdot \hat{V}_{\text{Part A}}(l, m) + e^{i(\varepsilon_m - \varepsilon_l + U) \cdot t} \cdot \hat{V}_{\text{Part B}}(l, m) + e^{i(\varepsilon_m - \varepsilon_l - U) \cdot t} \cdot \hat{V}_{\text{Part C}}(l, m) \right]$$

$$\hat{V}_{\text{Part A}}(l, m) \stackrel{\text{MM}}{=} (5 \cdot \hat{c}_l^S \hat{c}_m^{\dagger S}) + (5 \cdot \hat{d}_l^S \hat{d}_m^{\dagger S}) + (2 \cdot \hat{c}_l^S \hat{c}_m^S \hat{c}_l^{\dagger S} \hat{c}_m^{\dagger S} \hat{d}_l^S \hat{d}_m^{\dagger S}) + (2 \cdot \hat{c}_l^S \hat{c}_m^{\dagger S} \hat{d}_l^S \hat{d}_m^S \hat{d}_l^{\dagger S} \hat{d}_m^{\dagger S}) + \\ + (-3 \cdot \hat{c}_l^S \hat{c}_l^{\dagger S} \hat{d}_m^S \hat{d}_m^{\dagger S}) + (-3 \cdot \hat{c}_m^S \hat{c}_m^{\dagger S} \hat{d}_l^S \hat{d}_l^{\dagger S}) + (-3 \cdot \hat{c}_l^S \hat{c}_m^S \hat{d}_l^S \hat{d}_l^{\dagger S}) + (-3 \cdot \hat{c}_l^S \hat{c}_m^{\dagger S} \hat{d}_m^S \hat{d}_m^{\dagger S})$$

$$\hat{V}_{\text{Part B}}(l, m) \stackrel{\text{MM}}{=} (-2 \cdot \hat{c}_l^S \hat{c}_m^{\dagger S}) + (-2 \cdot \hat{d}_l^S \hat{d}_m^{\dagger S}) + (-1 \cdot \hat{c}_l^S \hat{c}_m^S \hat{c}_l^{\dagger S} \hat{c}_m^{\dagger S} \hat{d}_l^S \hat{d}_m^{\dagger S}) + (-1 \cdot \hat{c}_l^S \hat{c}_m^{\dagger S} \hat{d}_l^S \hat{d}_m^S \hat{d}_l^{\dagger S} \hat{d}_m^{\dagger S}) + \\ + (1 \cdot \hat{c}_l^S \hat{c}_l^{\dagger S} \hat{d}_m^S \hat{d}_m^{\dagger S}) + (2 \cdot \hat{c}_m^S \hat{c}_m^{\dagger S} \hat{d}_l^S \hat{d}_l^{\dagger S}) + (1 \cdot \hat{c}_l^S \hat{c}_m^{\dagger S} \hat{d}_l^S \hat{d}_l^{\dagger S}) + (2 \cdot \hat{c}_l^S \hat{c}_m^{\dagger S} \hat{d}_m^S \hat{d}_m^{\dagger S})$$

$$\hat{V}_{\text{Part C}}(l, m) \stackrel{\text{MM}}{=} (-2 \cdot \hat{c}_l^S \hat{c}_m^{\dagger S}) + (-2 \cdot \hat{d}_l^S \hat{d}_m^{\dagger S}) + (-1 \cdot \hat{c}_l^S \hat{c}_m^S \hat{c}_l^{\dagger S} \hat{c}_m^{\dagger S} \hat{d}_l^S \hat{d}_m^{\dagger S}) + (-1 \cdot \hat{c}_l^S \hat{c}_m^{\dagger S} \hat{d}_l^S \hat{d}_m^S \hat{d}_l^{\dagger S} \hat{d}_m^{\dagger S}) + \\ + (2 \cdot \hat{c}_l^S \hat{c}_l^{\dagger S} \hat{d}_m^S \hat{d}_m^{\dagger S}) + (1 \cdot \hat{c}_m^S \hat{c}_m^{\dagger S} \hat{d}_l^S \hat{d}_l^{\dagger S}) + (2 \cdot \hat{c}_m^S \hat{c}_m^{\dagger S} \hat{d}_l^S \hat{d}_l^{\dagger S}) + (1 \cdot \hat{c}_l^S \hat{c}_m^{\dagger S} \hat{d}_m^S \hat{d}_m^{\dagger S})$$

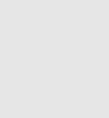
Computer aided calculations

Math-Manipulator

Interactive Demonstration

- Usage for the Practical Training

2024-09-05



Optimization: Difference of $V(t)$ for Hopping

Custom Python Scripts (SymPy)

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

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

Computer aided calculations

└ Custom Python Scripts (SymPy)

└ Optimization: Difference of $V(t)$ for Hopping

2024-09-05

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

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

- "Adjacent" states because from one Monte-Carlo step to the next we require a small change of one or two particle-sites. Could come from hopping or flipping.
- The E_0 differences are quickly calculated by hand in the report



Optimization: Difference of $V(t)$ for Hopping

Custom Python Scripts (SymPy)

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

- These require differences of $\hat{V}^I(t)$ and E_0

$$\begin{aligned}\alpha &= \frac{P(\tilde{N}, t)}{P(N, t)} = \frac{f(\tilde{N}, t)}{f(N, t)} \stackrel{2.39}{=} \frac{\left| e^{H_{\text{eff}}(\tilde{N}, t)} \right|^2 |\Psi_{\tilde{N}}|^2}{\left| e^{H_{\text{eff}}(N, t)} \right|^2 |\Psi_N|^2} \\ &= \frac{|\Psi_{\tilde{N}}|^2 e^{\Re(H_{\text{eff}}(\tilde{N}, t)) + i\Im(H_{\text{eff}}(\tilde{N}, t)) + \Re(H_{\text{eff}}(\tilde{N}, t)) - i\Im(H_{\text{eff}}(\tilde{N}, t))}}{|\Psi_N|^2 e^{\Re(H_{\text{eff}}(N, t)) + i\Im(H_{\text{eff}}(N, t)) + \Re(H_{\text{eff}}(N, t)) - i\Im(H_{\text{eff}}(N, t))}} \\ &= \frac{|\Psi_{\tilde{N}}|^2}{|\Psi_N|^2} e^{2\Re(H_{\text{eff}}(\tilde{N}, t)) - 2\Re(H_{\text{eff}}(N, t))} \\ &= \frac{|\Psi_{\tilde{N}}|^2}{|\Psi_N|^2} e^{2\Re(H_{\text{eff}}(\tilde{N}, t) - H_{\text{eff}}(N, t))}\end{aligned}$$

Computer aided calculations

Custom Python Scripts (SymPy)

Optimization: Difference of $V(t)$ for Hopping

2024-09-05

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

These require differences of $\hat{V}^I(t)$ and E_0

$$\begin{aligned}\alpha &= \frac{P(\tilde{N}, t)}{P(N, t)} = \frac{f(\tilde{N}, t)}{f(N, t)} = \frac{\left| e^{H_{\text{eff}}(\tilde{N}, t)} \right|^2 |\Psi_{\tilde{N}}|^2}{\left| e^{H_{\text{eff}}(N, t)} \right|^2 |\Psi_N|^2} \\ &= \frac{|\Psi_{\tilde{N}}|^2 e^{\Re(H_{\text{eff}}(\tilde{N}, t)) + i\Im(H_{\text{eff}}(\tilde{N}, t)) + \Re(H_{\text{eff}}(\tilde{N}, t)) - i\Im(H_{\text{eff}}(\tilde{N}, t))}}{|\Psi_N|^2 e^{\Re(H_{\text{eff}}(N, t)) + i\Im(H_{\text{eff}}(N, t)) + \Re(H_{\text{eff}}(N, t)) - i\Im(H_{\text{eff}}(N, t))}} \\ &= \frac{|\Psi_{\tilde{N}}|^2}{|\Psi_N|^2} e^{2\Re(H_{\text{eff}}(\tilde{N}, t)) - 2\Re(H_{\text{eff}}(N, t))} \\ &= \frac{|\Psi_{\tilde{N}}|^2}{|\Psi_N|^2} e^{2\Re(H_{\text{eff}}(\tilde{N}, t) - H_{\text{eff}}(N, t))}\end{aligned}$$

1. "Adjacent" states because from one Monte-Carlo step to the next we require a small change of one or two particle-sites. Could come from hopping or flipping.
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Optimization: Difference of $V(t)$ for Hopping

Custom Python Scripts (SymPy)

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

$$\begin{aligned}\alpha &= \frac{P(\tilde{N}, t)}{P(N, t)} = \frac{f(\tilde{N}, t)}{f(N, t)} \stackrel{2.39}{=} \frac{\left| e^{H_{\text{eff}}(\tilde{N}, t)} \right|^2 |\Psi_{\tilde{N}}|^2}{\left| e^{H_{\text{eff}}(N, t)} \right|^2 |\Psi_N|^2} \\ &= \frac{|\Psi_{\tilde{N}}|^2 e^{\Re(H_{\text{eff}}(\tilde{N}, t)) + i\Im(H_{\text{eff}}(\tilde{N}, t)) + \Re(H_{\text{eff}}(\tilde{N}, t)) - i\Im(H_{\text{eff}}(\tilde{N}, t))}}{|\Psi_N|^2 e^{\Re(H_{\text{eff}}(N, t)) + i\Im(H_{\text{eff}}(N, t)) + \Re(H_{\text{eff}}(N, t)) - i\Im(H_{\text{eff}}(N, t))}} \\ &= \frac{|\Psi_{\tilde{N}}|^2}{|\Psi_N|^2} e^{2\Re(H_{\text{eff}}(\tilde{N}, t)) - 2\Re(H_{\text{eff}}(N, t))} \\ &= \frac{|\Psi_{\tilde{N}}|^2}{|\Psi_N|^2} e^{2\Re(H_{\text{eff}}(\tilde{N}, t) - H_{\text{eff}}(N, t))}\end{aligned}$$

Computer aided calculations

Custom Python Scripts (SymPy)

Optimization: Difference of $V(t)$ for Hopping

2024-09-05

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

These require differences of $\hat{V}^I(t)$ and E_0

Too many terms for simple evaluation by hand

Intelligent pre-computation required to speed up processing

$$\begin{aligned}\alpha &= \frac{P(\tilde{N}, t)}{P(N, t)} = \frac{f(\tilde{N}, t)}{f(N, t)} \stackrel{2.39}{=} \frac{\left| e^{H_{\text{eff}}(\tilde{N}, t)} \right|^2 |\Psi_{\tilde{N}}|^2}{\left| e^{H_{\text{eff}}(N, t)} \right|^2 |\Psi_N|^2} \\ &= \frac{|\Psi_{\tilde{N}}|^2 e^{\Re(H_{\text{eff}}(\tilde{N}, t)) + i\Im(H_{\text{eff}}(\tilde{N}, t)) + \Re(H_{\text{eff}}(\tilde{N}, t)) - i\Im(H_{\text{eff}}(\tilde{N}, t))}}{|\Psi_N|^2 e^{\Re(H_{\text{eff}}(N, t)) + i\Im(H_{\text{eff}}(N, t)) + \Re(H_{\text{eff}}(N, t)) - i\Im(H_{\text{eff}}(N, t))}} \\ &= \frac{|\Psi_{\tilde{N}}|^2}{|\Psi_N|^2} e^{2\Re(H_{\text{eff}}(\tilde{N}, t)) - 2\Re(H_{\text{eff}}(N, t))} \\ &= \frac{|\Psi_{\tilde{N}}|^2}{|\Psi_N|^2} e^{2\Re(H_{\text{eff}}(\tilde{N}, t) - H_{\text{eff}}(N, t))}\end{aligned}$$

1. "Adjacent" states because from one Monte-Carlo step to the next we require a small change of one or two particle-sites. Could come from hopping or flipping.
2. The E_0 differences are quickly calculated by hand in the report



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

Setup difference

The process: Difference of $V(t)$ for Hopping

Custom Python Scripts (SymPy)

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

■ Setup difference

Computer aided calculations

└ Custom Python Scripts (SymPy)

└ The process: Difference of $V(t)$ for Hopping

2024-09-05

1. The V differences are $3 \cdot 8 = 32 \cdot 4 = 96 \cdot 2 = 192$ terms
2. The process is relatively straight forward:
 - write down the terms
 - replace
 - simplify difference
3. Still quite complicated and a lot of work, but:
 - way faster to write because non-repetitive logic
 - verifiably correct calculations
 - multiple times re-done on changes to underlying code, each time only took seconds
 - sometimes brute-force NEEDS to work, before optimization can be found



$$\begin{aligned} E_0(N) - E_0(\tilde{N}) &= U \sum_l n_{l,\downarrow} n_{l,\uparrow} - U \sum_l \tilde{n}_{l,\downarrow} \tilde{n}_{l,\uparrow} + \sum_{l,\sigma} \varepsilon_l n_{l,\sigma} - \sum_{l,\sigma} \varepsilon_l \tilde{n}_{l,\sigma} \\ &\stackrel{2.45}{=} (\varepsilon_i - \varepsilon_j) (n_{i,\sigma_i} - n_{j,\sigma_j}) + U \cdot \begin{cases} (n_{i,\uparrow} - n_{j,\uparrow})(n_{i,\downarrow} - n_{j,\downarrow}) & : \sigma_i = \sigma_j \\ (n_{i,\uparrow} - n_{j,\downarrow})(n_{i,\downarrow} - n_{j,\uparrow}) & : \sigma_i \neq \sigma_j \end{cases} \quad \tilde{n}_{l,\sigma} = \begin{cases} n_{i,\sigma_i} & : l = j \wedge \sigma = \sigma_j \\ n_{j,\sigma_j} & : l = i \wedge \sigma = \sigma_i \\ n_{l,\sigma} & : \text{else} \end{cases} \\ &= (\varepsilon_i - \varepsilon_j) (n_{i,\sigma_i} - n_{j,\sigma_j}) + U (n_{i,\sigma_i} - n_{j,\sigma_j}) (n_{i,\bar{\sigma}_i} - n_{j,\bar{\sigma}_j}) \end{aligned}$$

Setup difference
Replace one by appropriate new occupation

The process: Difference of V(t) for Hopping

Custom Python Scripts (SymPy)

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

$$\stackrel{2.45}{=} (\varepsilon_i - \varepsilon_j) (n_{i,\sigma_i} - n_{j,\sigma_j}) + U \cdot \begin{cases} (n_{i,\uparrow} - n_{j,\uparrow})(n_{i,\downarrow} - n_{j,\downarrow}) & : \sigma_i = \sigma_j \\ (n_{i,\uparrow} - n_{j,\downarrow})(n_{i,\downarrow} - n_{j,\uparrow}) & : \sigma_i \neq \sigma_j \end{cases} \quad \tilde{n}_{l,\sigma} = \begin{cases} n_{i,\sigma_i} & : l = j \wedge \sigma = \sigma_j \\ n_{j,\sigma_j} & : l = i \wedge \sigma = \sigma_i \\ n_{l,\sigma} & : \text{else} \end{cases}$$

- Setup difference
- Replace one by appropriate new occupation

Computer aided calculations

Custom Python Scripts (SymPy)

The process: Difference of V(t) for Hopping

1. The V differences are $3 \cdot 8 = 32 \cdot 4 = 96 \cdot 2 = 192$ terms
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The process: Difference of $V(t)$ for Hopping

Custom Python Scripts (SymPy)

$$\begin{aligned} E_0(N) - E_0(\tilde{N}) &= U \sum_l n_{l,\downarrow} n_{l,\uparrow} - U \sum_l \tilde{n}_{l,\downarrow} \tilde{n}_{l,\uparrow} + \sum_{l,\sigma} \varepsilon_l n_{l,\sigma} - \sum_{l,\sigma} \varepsilon_l \tilde{n}_{l,\sigma} \\ &\stackrel{2.45}{=} (\varepsilon_i - \varepsilon_j) (n_{i,\sigma_i} - n_{j,\sigma_j}) + U \cdot \begin{cases} (n_{i,\uparrow} - n_{j,\uparrow})(n_{i,\downarrow} - n_{j,\downarrow}) & : \sigma_i = \sigma_j \\ (n_{i,\uparrow} - n_{j,\downarrow})(n_{i,\downarrow} - n_{j,\uparrow}) & : \sigma_i \neq \sigma_j \end{cases} \quad \tilde{n}_{l,\sigma} = \begin{cases} n_{i,\sigma_i} & : l = j \wedge \sigma = \sigma_j \\ n_{j,\sigma_j} & : l = i \wedge \sigma = \sigma_i \\ n_{l,\sigma} & : \text{else} \end{cases} \\ &= (\varepsilon_i - \varepsilon_j) (n_{i,\sigma_i} - n_{j,\sigma_j}) + U (n_{i,\sigma_i} - n_{j,\sigma_j}) (n_{i,\bar{\sigma}_i} - n_{j,\bar{\sigma}_j}) \end{aligned}$$

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



Computer aided calculations

- └ Custom Python Scripts (SymPy)

- └ The process: Difference of $V(t)$ for Hopping

2024-09-05

The process: Difference of $V(t)$ for Hopping
Custom Python Scripts (SymPy)

$E(N) - E(\tilde{N}) = U \sum_l n_{l,\sigma} \cdot \tilde{n}_{l,\sigma} + \sum_l \tilde{n}_{l,\sigma} \cdot n_{l,\sigma}$
 $\stackrel{!}{=} (\varepsilon_i - \varepsilon_j) (n_{i,\sigma_i} - n_{j,\sigma_j}) + U \cdot \begin{cases} (n_{i,\uparrow} - n_{j,\uparrow})(n_{i,\downarrow} - n_{j,\downarrow}) & : \sigma_i = \sigma_j \\ (n_{i,\uparrow} - n_{j,\downarrow})(n_{i,\downarrow} - n_{j,\uparrow}) & : \sigma_i \neq \sigma_j \end{cases}$
 $\tilde{n}_{l,\sigma} = \begin{cases} n_{i,\sigma_i} & : l = j \wedge \sigma = \sigma_j \\ n_{j,\sigma_j} & : l = i \wedge \sigma = \sigma_i \\ n_{l,\sigma} & : \text{else} \end{cases}$

- 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)

$$\begin{aligned} E_0(N) - E_0(\tilde{N}) &= U \sum_l n_{l,\downarrow} n_{l,\uparrow} - U \sum_l \tilde{n}_{l,\downarrow} \tilde{n}_{l,\uparrow} + \sum_{l,\sigma} \varepsilon_l n_{l,\sigma} - \sum_{l,\sigma} \varepsilon_l \tilde{n}_{l,\sigma} \\ &\stackrel{2.45}{=} (\varepsilon_i - \varepsilon_j) (n_{i,\sigma_i} - n_{j,\sigma_j}) + U \cdot \begin{cases} (n_{i,\uparrow} - n_{j,\uparrow})(n_{i,\downarrow} - n_{j,\downarrow}) & : \sigma_i = \sigma_j \\ (n_{i,\uparrow} - n_{j,\downarrow})(n_{i,\downarrow} - n_{j,\uparrow}) & : \sigma_i \neq \sigma_j \end{cases} \quad \tilde{n}_{l,\sigma} = \begin{cases} n_{i,\sigma_i} & : l = j \wedge \sigma = \sigma_j \\ n_{j,\sigma_j} & : l = i \wedge \sigma = \sigma_i \\ n_{l,\sigma} & : \text{else} \end{cases} \\ &= (\varepsilon_i - \varepsilon_j) (n_{i,\sigma_i} - n_{j,\sigma_j}) + U (n_{i,\sigma_i} - n_{j,\sigma_j}) (n_{i,\bar{\sigma}_i} - n_{j,\bar{\sigma}_j}) \end{aligned}$$

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

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



Computer aided calculations

Custom Python Scripts (SymPy)

The process: Difference of $V(t)$ for Hopping

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The process: Difference of $V(t)$ for Hopping
Custom Python Scripts (SymPy)

$$E(N) - E(\tilde{N}) = U \sum_l n_{l,\sigma} \cdot \tilde{n}_{l,\sigma} + \sum_l \varepsilon_l \cdot n_{l,\sigma}$$
$$\stackrel{!}{=} (\varepsilon_i - \varepsilon_j) (n_{i,\sigma_i} - n_{j,\sigma_j}) + U \cdot \begin{cases} (n_{i,\uparrow} - n_{j,\uparrow})(n_{i,\downarrow} - n_{j,\downarrow}) & : \sigma_i = \sigma_j \\ (n_{i,\uparrow} - n_{j,\downarrow})(n_{i,\downarrow} - n_{j,\uparrow}) & : \sigma_i \neq \sigma_j \end{cases}$$
$$\tilde{n}_{l,\sigma} = \begin{cases} n_{i,\sigma_i} & : l = j \wedge \sigma = \sigma_j \\ n_{j,\sigma_j} & : l = i \wedge \sigma = \sigma_i \\ n_{l,\sigma} & : \text{else} \end{cases}$$

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

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

1. The V differences are $3 \cdot 8 = 32 \cdot 4 = 96 \cdot 2 = 192$ terms
2. The process is relatively straight forward:
 - write down the terms
 - replace
 - simplify difference
3. Still quite complicated and a lot of work, but:
 - way faster to write because non-repetitive logic
 - verifiably correct calculations
 - multiple times re-done on changes to underlying code, each time only took seconds
 - sometimes brute-force NEEDS to work, before optimization can be found

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

Custom Python Scripts (SymPy)

Generating Script

simplificationtermhelper.py

Generated Script

analyticalcalcfuctions.py

Computer aided calculations

└ Custom Python Scripts (SymPy)

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

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1. simplificationtermhelper.py script to generate the script
2. analyticalcalcfuctions.py script is generated and used in the code
3. Generated file: 1556 lines, script that generates: 534 lines
4. Show the script that generates/is generated → simplification with Sympy
5. Parallel to computer-science practice "Vendored" code



Beamer: LaTeX way of writing Presentations

Presentations? - Custom Beamer Template

- Write presentations like your papers/thesis in \LaTeX



1. Re-use tooling, editor, setup (even this on overleaf alone much better than shared powerpoint presentation)
2. This presentation, report and thesis all live in one git-repository and share resources
3. Everything I ever work on is hosted in Git.
 - Without Version Control it is no longer possible for me to work effectively
 - Every workflow is massively ensured by it
 - Also for single-person work, but built in collaboration, synchronization and backup

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└ Presentations? - Custom Beamer Template

└ Beamer: LaTeX way of writing Presentations

Beamer: LaTeX way of writing Presentations

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Beamer: LaTeX way of writing Presentations

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- Easier collaboration



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└ Presentations? - Custom Beamer Template

└ Beamer: LaTeX way of writing Presentations

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

Minimal example for beamer presentation

Presentations? - Custom Beamer Template

```
1 \documentclass[aspectratio=169]{beamer}
2
3 \usetheme[neutralbackground]{uniamntf}
4
5 \title[]{Title}
6 \subtitle{subtitle}
7 \author{Jonas Kell}
8 \institute[TP III]{Chair for theoretical Physics III}
9 \date[01.05.2024]{\$1^{\text{st}}\$ of Mai 2024}
10
11 \acknowledgement{
12   Jonas Kell\\ Augsburg University\\
13   jonas.kell@student.uni-augsburg.de\\ www.uni-augsburg.de
14 }
15
16 \begin{document}
17
18 \begin{frame}[t,plain]
19   \maketitle
20 \end{frame}
21
22 \section*{Summary \& Conclusion}
23 {
24   \setbeamertemplate{frametitle}{uniamntfack}
25   \begin{frame}[plain]{Acknowledgment}
26     Thank you for your kind attention
27   \end{frame}
28 }
29 \end{document}
```



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Computer aided calculations

└ Presentations? - Custom Beamer Template

└ Minimal example for beamer presentation

1. 29 lines gets you a basic presentation
2. First time very much slower as putting together by hand in PowerPoint
3. If you want to do crazy stuff, possible but really hard
4. Actually quite a timesaver when you have an example/template to work of and do not require crazy levels of features
5. When it works, perfectly portable (just a pdf), high performant and versatile (output rendering of presentation, notes, animations from one source)
6. If proper presentation tools, has all the bells and whistles (presentation timer, pointer, multi-view presentation and more)

Minimal example for beamer presentation
Presentations? - Custom Beamer Template

Thank you for your kind attention



Jonas Kell
University of Augsburg
jonas.kell@student.uni-augsburg.de
www.uni-augsburg.de



Universität Augsburg
Mathematisch-Naturwissenschaftlich-
Technische Fakultät



References I

Summary & Conclusion

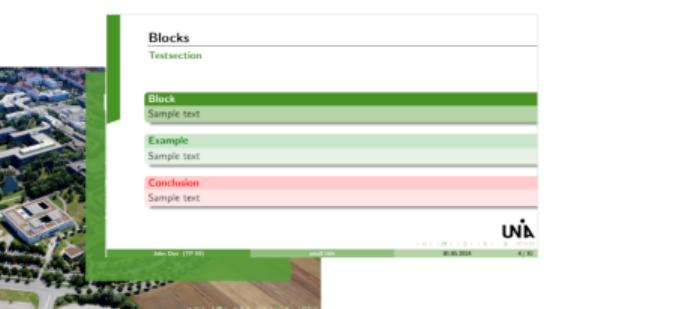
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Theme alternative: Faculty of App. Computer Science

Extra slides



Random Text
Testsection
because of the [t] option, text starts at the top. Default is centered.
Hello
This is Text with a delayed show animation.

Title-Here
Testsection Hello

This is a text in first column.
 $E = mc^2$

This text will be in the second column and on a second thoughts, this is a nice looking layout in some cases.

First item
Second item
and
and
and
and
and

Outline

- 1 Testsection
- 2 Testsection Hello
- 3 Testsection Test
 - sub-1
 - sub-2
- 4 Summary

John Doe (TP III) small icon 15.05.2024 A / 10

Thank you for your kind attention

John Doe
Augsburg University
john.doe@uni-augsburg.de
www.uni-augsburg.de

John Doe (TP III) small icon 15.05.2024 A / 10

Backup-Solution Problem 1

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└ Backup-Solution Problem 1



$$\hat{v}_{\text{part},i}(l,m) = \sum_{\sigma \in \{\uparrow, \downarrow\}} \hat{c}_{l,\sigma}^S \hat{c}_{m,\sigma}^{\dagger S} (1 + 2 \cdot \hat{n}_{l,\sigma}^S \hat{n}_{m,\sigma}^S - \hat{n}_{l,\sigma}^S - \hat{n}_{m,\sigma}^S)$$

$$\hat{v}_{\text{part},i}(l,m) = \sum_{\sigma \in \{\uparrow, \downarrow\}} \hat{c}_{l,\sigma}^S \hat{c}_{m,\sigma}^{\dagger S} (\hat{n}_{l,\sigma}^S - \hat{n}_{m,\sigma}^S)$$

$$\hat{v}_{\text{part},i}(l,m) = \sum_{\sigma \in \{\uparrow, \downarrow\}} \hat{c}_{l,\sigma}^S \hat{c}_{m,\sigma}^{\dagger S} (\hat{n}_{l,\sigma}^S - \hat{n}_{m,\sigma}^S)$$

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 n d# n

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

$$((-2 \cdot c_l c_m^l) + (-1 \cdot c_l c_m^l d_l d_m d_n^l) + (2 \cdot c_l c_m^l d_l d_n^l) + (1 \cdot c_l c_m^l d_m d_n^l))$$

$$((-2 \cdot c_l c_m^l) + (-1 \cdot c_l c_m^l d_l d_m d_n^l) + (2 \cdot c_l c_m^l \cdot (1 + d_l^l d_l)) + (1 \cdot c_l c_m^l \cdot d_m d_n^l))$$

$$((-2 \cdot c_l c_m^l) + (-1 \cdot c_l c_m^l d_l d_m d_n^l) + (2 \cdot c_l c_m^l \cdot (1 + d_l^l d_l)) + (c_l c_m^l \cdot (1 + d_m^l d_n)))$$

$$((-2 \cdot c_l c_m^l) - (1 \cdot c_l c_m^l d_l d_m d_n^l) + (2 \cdot c_l c_m^l \cdot (1 + d_l^l d_l)) + (c_l c_m^l \cdot (1 + d_m^l d_n)))$$

$$((-2 \cdot c_l c_m^l) - (c_l c_m^l \cdot (1 + d_l^l d_l)) + (2 \cdot c_l c_m^l \cdot (1 + d_l^l d_l)) + (c_l c_m^l \cdot (1 + d_m^l d_n)))$$

$$((-2 \cdot c_l c_m^l) - (c_l c_m^l \cdot 1 \cdot 1) - (c_l c_m^l \cdot 1 \cdot d_m^l d_n) - (c_l c_m^l \cdot d_l^l \cdot 1) - c_l c_m^l d_l^l d_m^l d_n + (2 \cdot c_l c_m^l \cdot (1 + d_m^l d_n)))$$

$$((-2 \cdot c_l c_m^l) - (c_l c_m^l \cdot 1 \cdot 1) - (c_l c_m^l \cdot 1 \cdot d_m^l d_n) - (c_l c_m^l d_l^l d_l \cdot 1) - c_l c_m^l d_l^l d_m^l d_n + (2 \cdot c_l c_m^l \cdot 1) + (c_l c_m^l \cdot (1 + d_m^l d_n)))$$

$$((-2 \cdot c_l c_m^l) - (c_l c_m^l \cdot 1 \cdot 1) - (c_l c_m^l \cdot 1 \cdot d_m^l d_n) - (c_l c_m^l d_l^l d_l \cdot 1) - c_l c_m^l d_l^l d_m^l d_n + (2 \cdot c_l c_m^l \cdot 1) + (c_l c_m^l \cdot (1 + d_m^l d_n)) + (c_l c_m^l \cdot 1) + c_l c_m^l d_m^l d_n)$$

$$((-2 \cdot c_l c_m^l) - (c_l c_m^l \cdot 1 \cdot 1) - (c_l c_m^l \cdot 1 \cdot d_m^l d_n) - (c_l c_m^l d_l^l d_l \cdot 1) - c_l c_m^l d_l^l d_m^l d_n + (2 \cdot c_l c_m^l \cdot 1) + (c_l c_m^l \cdot (1 + d_m^l d_n)) + (c_l c_m^l \cdot 1) + c_l c_m^l d_m^l d_n)$$

$$(-c_l c_m^l d_l^l d_l - c_l c_m^l d_l^l d_m^l d_n + (2 \cdot c_l c_m^l d_l^l d_l))$$

$$(c_l c_m^l d_l^l d_l - c_l c_m^l d_l^l d_m^l d_n)$$

Variables:

Macros:

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

Computer aided calculations
└ Extra slides

└ Backup: Simplification V-Parts

2024-09-05

1. Better optimization was found, rewriting in number operators DOES save on terms (however only for B and C, A still same number of terms and computational requirement, even if it looks nicer)
2. Doesn't help at all with computing more efficiently, so python script still exceptionally useful
3. Wouldn't have come so far, if simple "brute-force" solution wasn't done in the first place

