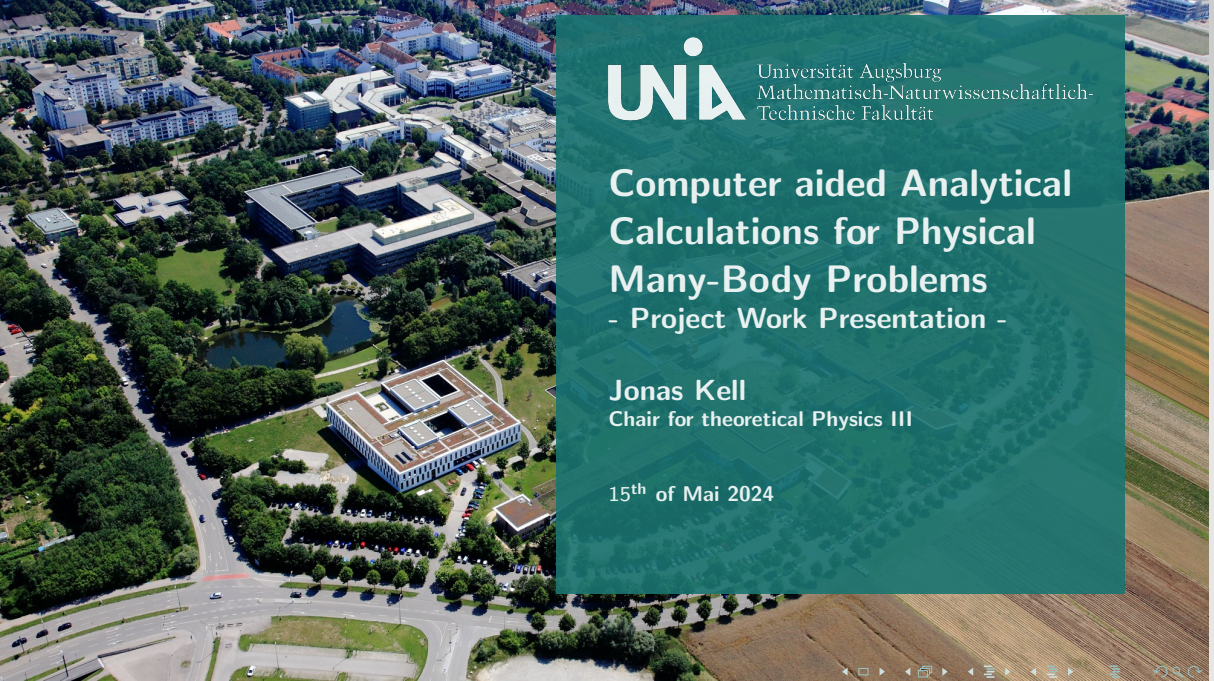

Universität Augsburg
Mathematisch-Naturwissenschaftlich-Technische Fakultät

Computer aided Analytical Calculations for Physical Many-Body Problems

- Project Work Presentation -

Jonas Kell
Chair for theoretical Physics III

15^{th} of Mai 2024

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

Outline

Outline
1 Introduction of the problem

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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- How can you use it
- Interactive Demonstration

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5 Presentations? - Custom Beamer Template

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Physics of what we calculate

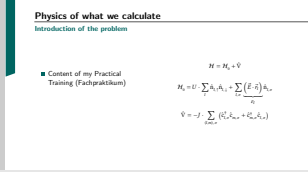
Introduction of the problem

- Content of my Practical Training (Fachpraktikum)

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

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

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



1. Hubbard-Model Hamiltonian with exterally applied electric field
2. Hard-Core Bosinic 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

Physics of what we calculate

Introduction of the problem

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

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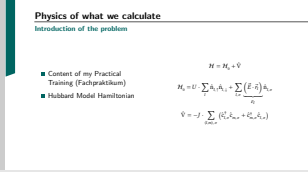

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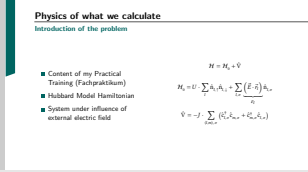

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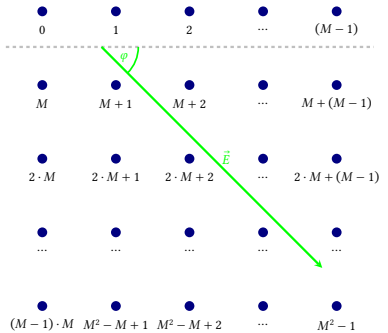
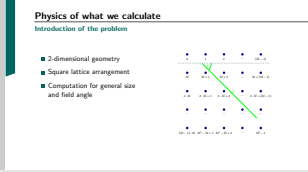
Physics of what we calculate

Introduction of the problem

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





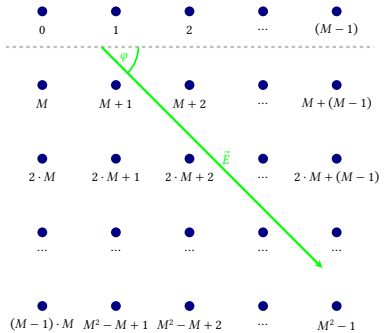
1. 2-dimensional square geometry
2. Program supports already for general size inputs
3. Thanks to the Monte-Carlo Sampling we can even efficiently evaluate larger systems already

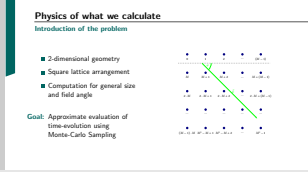
Physics of what we calculate

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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Physics of what we calculate

Introduction of the problem

- Hard-Core Bosonic operators

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

1. Operators are hard-core bosonic
   - standard commutation relations
   - occupations are only either zero ore 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

Physics of what we calculate

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Physics of what we calculate

Introduction of the problem

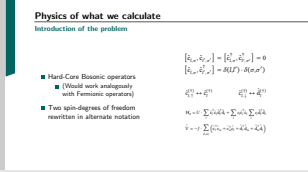
- Hard-Core Bosonic operators
  - (Would work analogously with Fermionic operators)
- Two spin-degrees of freedom rewritten in alternate notation

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

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

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

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



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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
Introduction of the problem
Doing Theoretical Physics often requires lengthy analytical calculations

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 repetetive, trivial and unfunny to do, paper cannot automize
   - 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

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
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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
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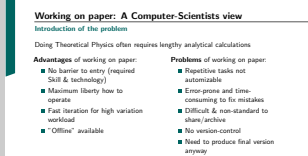

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Examples from "Theoretical Solid State Physics"

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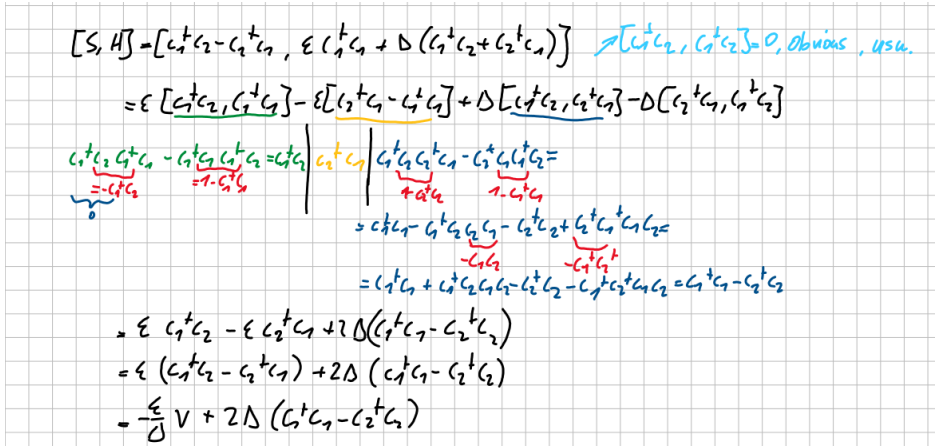
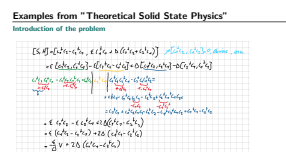
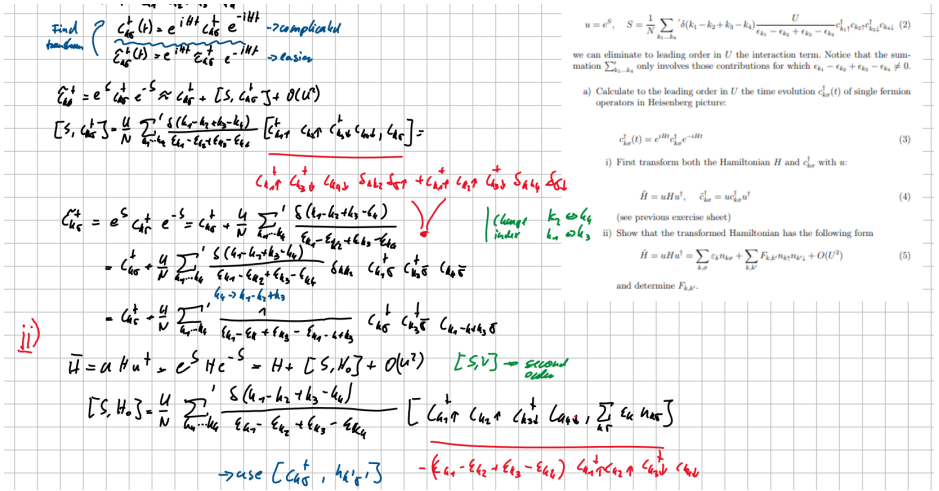




1. From the lecture "Theoretical Solid State Physics" (Theoretische Festkörperphysik), helt by Markus Heyl in WS 22/23
2. Sheet 3, Problem 2: Schrieffer-Wolf transformation
3. Rather simple calculation, still contains sing mistakes (that here luckily averaged out)

Examples from "Theoretical Solid State Physics"

Introduction of the problem



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

we can eliminate to leading order in U the interaction term. Notice that the summation $\sum'_{k_1\ldots k_4}$ 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:

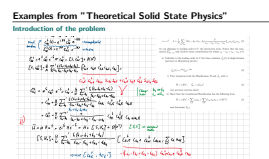
$$\tilde{H} = uHu^\dagger, \quad \tilde{c}^\dagger_{k\sigma} = uc^\dagger_{k\sigma}u^\dagger \quad (4)$$

(see previous exercise sheet)

ii) Show that the transformed Hamiltonian has the following form

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

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



1. From the lecture "Theoretical Solid State Physics" (Theoretische Festkörperphysik), helt by Markus Heyl in WS 22/23
2. Sheet 8, Problem 1: Schrieffer-Wolf transformation of the Hubbard Model
3. Just written down steps done by someone else (Tutor/other pupil, often shared the terms to calculate them all, still time)

Examples from the Practical Training

Introduction of the problem

- Goal: produce time evolution of operator

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

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

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

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

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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

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

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

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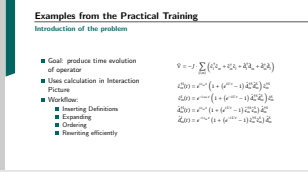

1. Want to calculate the Time-Evolution of the operator V in the interaction Picture
2. Basically comes down to inserting definitions (however already derived from MM)
3. Distributing and re-ordering is a painful, time-intensive process
4. How to time-evolve operator in the Interaction Picture $\{\cdot\}(t)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

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

Paper-like writing on digital devices
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Can give benefits that paper lacks
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1. Taking notes digially 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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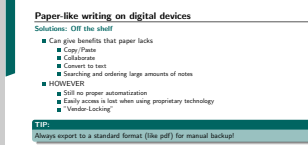
TIP:

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



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Computer-Algebra Systems

Solutions: Off the shelf

- Proprietary Software (Often payed):
- Standalone Online Calculators

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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, reoccuring 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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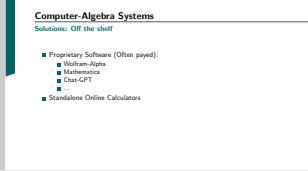

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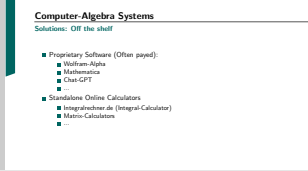
  - Integralrechner.de (Integral-Calculator)
  - Matrix-Calculators
  - ...



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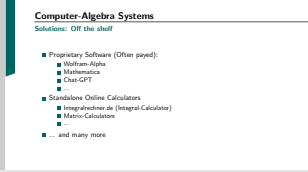
  - Matrix-Calculators
  - ...
- ... and many more



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What is Math-Manipulator?

Math-Manipulator - What did I do?

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

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

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

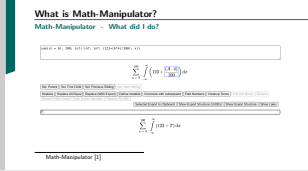
Rename With Swap | Pack Same Variables | Replace All With

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]



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

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

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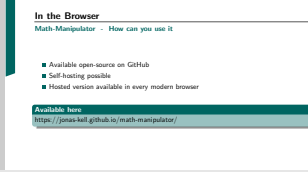
Available here

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



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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

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

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

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Math-Manipulator - How can you use it

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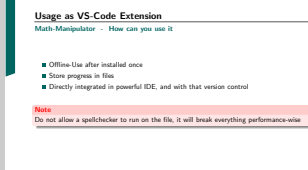
Note

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



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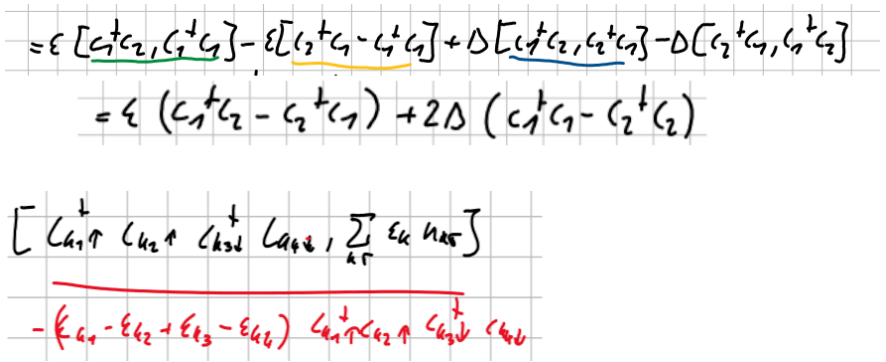
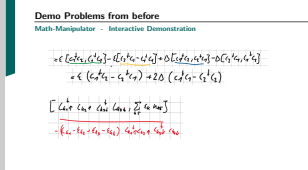
Demo Problems from before

Math-Manipulator - Interactive Demonstration



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("" 1)fa("" 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)`



Usage for the Practical Training

Math-Manipulator - Interactive Demonstration

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

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 upfornt configuration (and in my case programming) effort, re-calculating the endresult took 20min instead of one week

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

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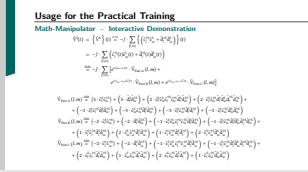

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Optimization: Difference of V(t) for Hopping

Custom Python Scripts (SymPy)

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

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

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

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

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

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

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

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\begin{aligned}
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&= \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))}} \\
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The process: Difference of V(t) for Hopping

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\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} \\
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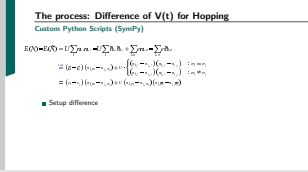
\end{aligned}
$$

- Setup difference



1. The V differences are $3 \cdot 8 \cdot = 32 \cdot 4 = 96 \cdot 2 = 192$ 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 bacuse non-repetetive logic
   - verifiably correct calculations
   - multiple times re-done on changes to underlying code, each time only took seconds
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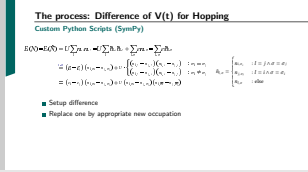
\end{aligned}
$$

- Setup difference
- Replace one by appropriate new occupation



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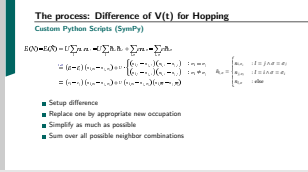
\end{aligned}
$$

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



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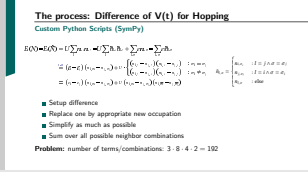
- Sum over all possible neighbor combinations

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



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

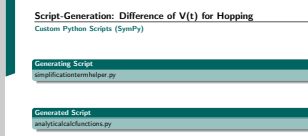
Custom Python Scripts (SymPy)

Generating Script

simplificationtermhelper.py

Generated Script

analyticalcalcfunctions.py



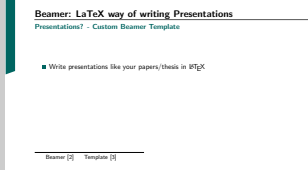
1. `simplificationtermhelper.py` script to generate the script
2. `analyticalcalcfunctions.py` script is generated and used in the code
3. Generated file: 1556 lines, script that generates: 534 lines
4. Show the script that generates/is generated → simplification with Sympy
5. Parallel to computer-science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

Beamer: LaTeX way of writing Presentations

Presentations? - Custom Beamer Template

- Write presentations like your papers/thesis in LaTeX

Beamer [2] Template [3]



1. Re-use tooling, editor, setup (even this on overleaf alone much better that 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

Beamer: LaTeX way of writing Presentations

Presentations? - Custom Beamer Template

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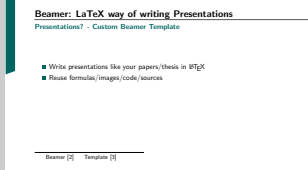
Beamer [2] Template [3]



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Presentations? - Custom Beamer Template

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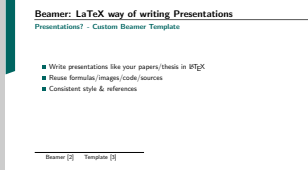
- Consistent style & references

Beamer [2] Template [3]



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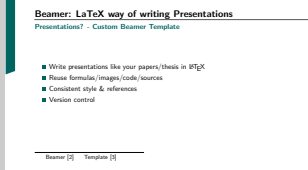

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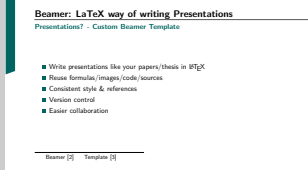
Presentations? - Custom Beamer Template

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

Beamer [2] Template [3]



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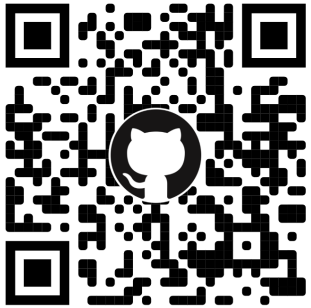
Minimal example for beamer presentation

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}
```

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)

Thank you for your kind attention



Universität Augsburg
Mathematisch-Naturwissenschaftlich-Technische Fakultät

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

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

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.

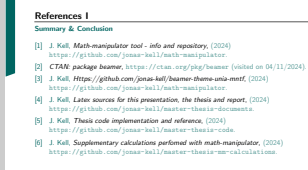
[2] *CTAN: package beamer*, https://ctan.org/pkg/beamer (visited on 04/11/2024).

[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.

[6] J. Kell, *Supplementary calculations perfomed with math-manipulator*, (2024) https://github.com/jonas-kell/master-thesis-mm-calculations.


References I
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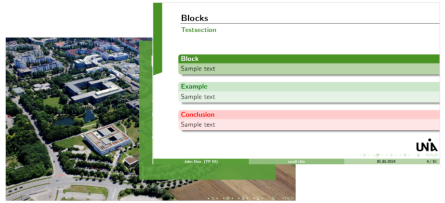
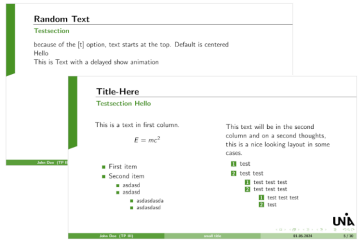
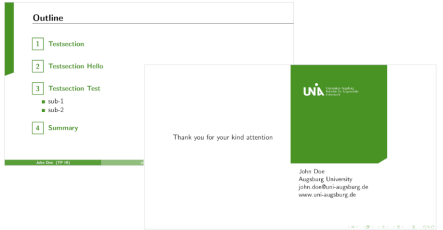
[5] J. Kell, Thesis code implementation and reference, (2024) https://github.com/jonas-kell/master-thesis-code.
[6] J. Kell, Supplementary calculations perfomed with math-manipulator, (2024) https://github.com/jonas-kell/master-thesis-mm-calculations.

Theme alternative: Faculty of App. Computer Science

Extra slides



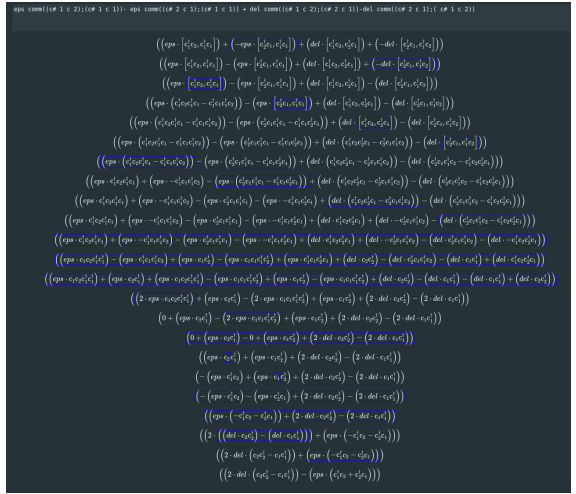




1. Template does also do "Faculty of Applied Computer Science" presentations out of the box
2. Alternate styles (e.g. title slide) available

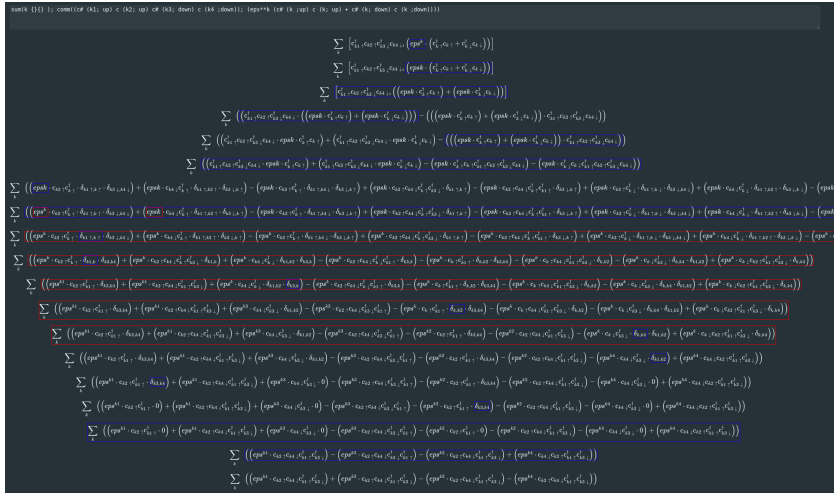
Backup-Solution Problem 1

Extra slides

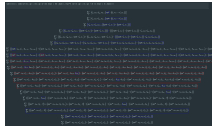


Backup-Solution Problem 2

Extra slides

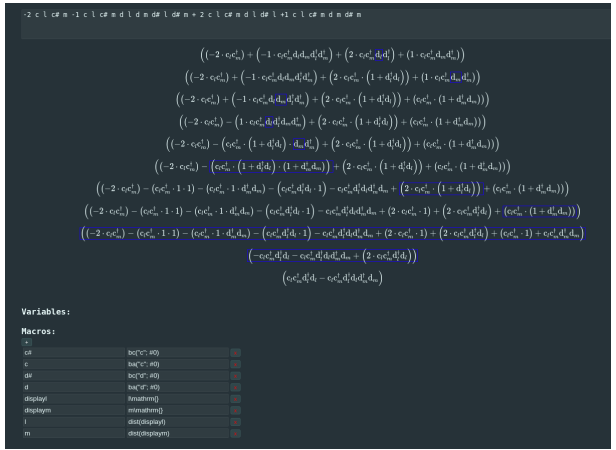


Backup-Solution Problem 2
Extra slides



Backup: Simplification V-Parts

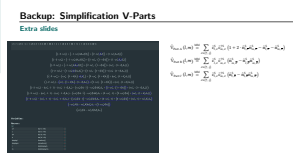
Extra slides



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

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

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



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 exceptinally usefull
3. Wouldn't have come so far, if simple "brute-force" solution wasn't done in the first place