Exercise Session 1

IESM Fall 2025-2026

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September 9, 2025

Welcome to the IESM course!

- Lecturer: Prof. Ursula Röthlisberger
- TAs:
  - Salomé Guilbert
  - Qihao Zhang
  - Thibault Kläy
  - Evan Vasey
  - Different PostDocs from LCBC lab

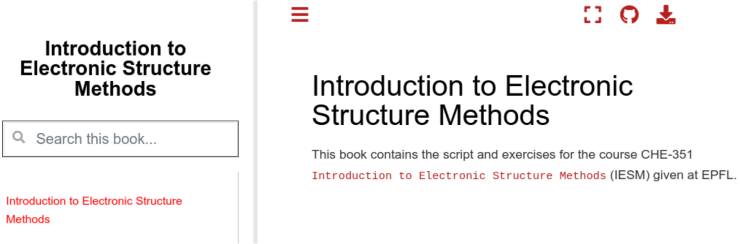
- Mondays from 8:15 to 10:00 and Tuesdays from 10:15 to 12:00
- Course schedule for the semester available on Moodle and the exercise webpage

- Moodle page


EPFL
MOODLE
FR EN
Introduction to electronic structure methods
Dashboard › Courses › Chimie, Génie Chimique (CGC) › CGC - Bachelor › CH-353

Exercise sessions

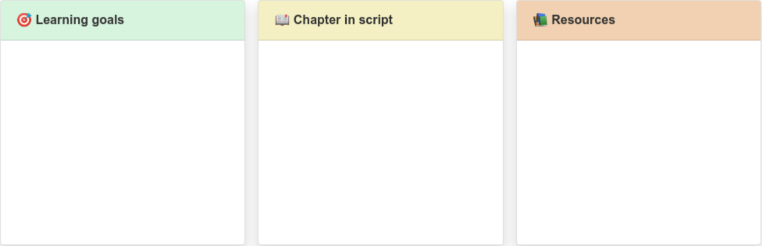
- Exercise website: **https://lcbc-epfl.github.io/iesm-public/**



Exercise structure

Introduction

- Learning goals
- Chapter in script
- Resources



Exercise structure

Theory section

- Relevant theory for the exercise
- Theoretical exercises

Practical exercises

- “Coding” exercises
- Interpretation of results

Exercise evaluation

- Examples:

Exercise 9

Give the commutator of the position and linear momentum operators in the position representation (consider one dimension only).

Bonus Exercise 10

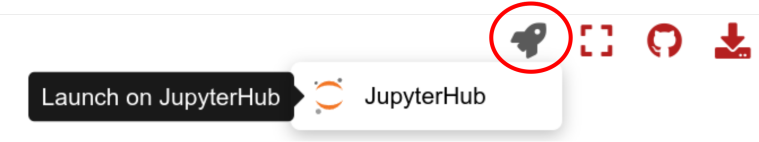
Show that the potential energy operator $\hat{V}(\mathbf{r})$ is multiplicative when applied to the real-space wavefunction.

```python
# Check Orthogonality
ϕ1ϕ2 = 0 # Replace with vector operation
print(f'<ϕ1|ϕ2> = {ϕ1ϕ2}')
```

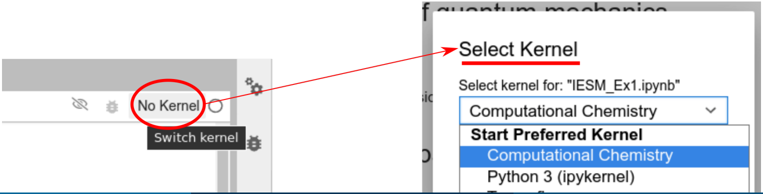
- Exercises account for 1/3 of the final grade (2/3 from exams, 1 written 1 oral)
- Submit report
  - `pdf` document answering the questions completely with relevant results
    - Handwritten portions ok (please verify legibility)
    - We provide report templates on Overleaf and Google Docs
  - Due date is usually the next exercise session (check Moodle!)
  - Interviews during next exercise session
    - Test your understanding and discuss your doubts/questions
  - Detailed feedback via Moodle after the interview

Computer environment

- We will use a virtual environment that you can directly launch from the exercise website
- Click the rocket button on the top right of the code files and choose JupyterHub to launch noto.epfl.ch

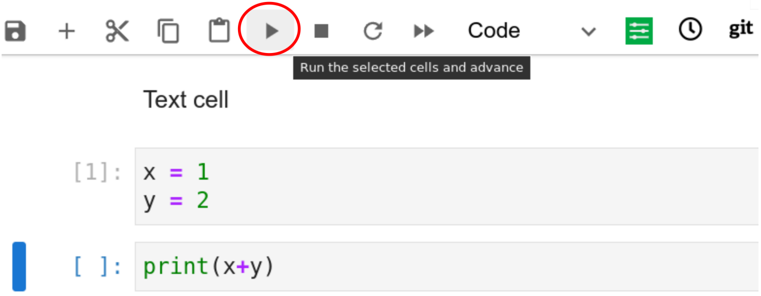


- On noto.epfl.ch your work will be saved on your EPFL storage
- Make sure to always activate (top right) the `Computational Chemistry` kernel



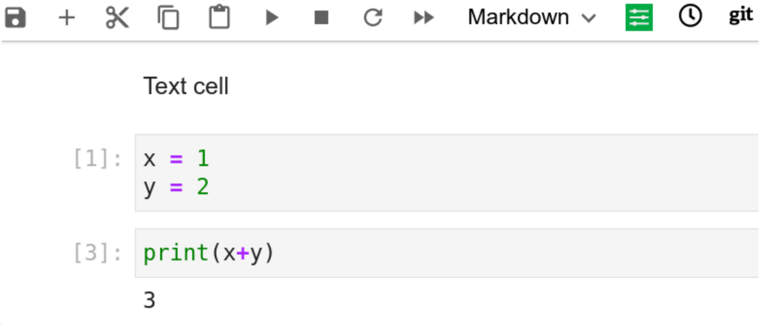
Jupyter notebooks

- `.iynb` files organized in cells
  - Markdown (text)
  - Code
- Run a code cell by pressing `Play` button (or `Ctrl+Enter`)



Jupyter notebooks

- `.iynb` files organized in cells
  - Markdown (text)
  - Code
- Run a code cell by pressing :arrow_forward: (or `Ctrl+Enter`)



Exercise 1 - Overview

Linear Algebra in Quantum Mechanics - Exercise page

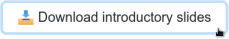
- Linear Algebra in Quantum Mechanics
- Basic Concepts in Quantum Mechanics
- Working with vectors using Numpy

🎯 Learning goals	📖 Chapter in script	📚 Resources
Review basic concept of linear algebra Review basic notation of quantum mechanics	Chapter 2 - Basic principles of Quantum Mechanics Appendix A.1 - Vector space and scalar product	Cohen-Tannoudji, C., Diu, B., & Laloe, F. (1986). Quantum Mechanics, Volume 1. • Chapter II B - State space, Dirac notation • Chapter II C - Representations in the state space • Chapter II D - Eigenvalue equations, observables • Chapter II E - Two important examples of represantations and observables • Chapter II Complement $\mathrm{D_{II}}$ - A more detailed study of the $\{\|r\rangle\}$ and $\{\|p\rangle\}$ representations • Chapter II Complement $\mathrm{E_{II}}$ - Some general properties of two observables, Q and P, whose commutator is equal to $i\hbar$

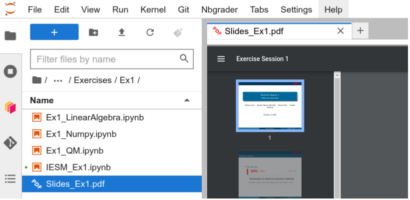
Exercise 1 - Tips

Tips!

- Start from Section 1.3 - Working with vectos using Numpy to get familiar with Noto environment and Jupyter Notebooks
- How to get the slides:
  - Download from the exercise page



  - Once you open Noto, in the exercise folder



  - Will be uploaded on the Moodle page

Exercise 1 - Tips

- We provide templates for the exercise reports, you can access them from the exercise page

  Report Template Google Docs

  Report Template Overleaf

- The answers can be short, for a full mark we don't expect more than what is explicitly asked
- You can ask for help anytime on the exercises and also the theory!
  - During the exercise session
  - During the week, on the Moodle Forum (public, so everyone can benefit from the answers and in principle you can help each other!)
  - At least one of us will be always present at the lectures, you can ask us questions before/after or during the break

Exercise Sessions - Important Information

- The final grade from the exercises will be given by the best 8 out of 9 exercises. Hence in principle, you have a "free" exercise that you can decide to skip
- We will send a schedule for the interviews before each exercise session
- Please let us know in advance if you will not be able to be there for the interview
- In case of overlaps with other courses, we can schedule interviews also outside the exercise hours
- In case you don't show up at the interview and you don't contact us via email to reschedule the interview, the grade for that report will be 0