

Exercise Session 1

IESM Fall 2024-2025

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Introduction to Electronic Structure Methods

Welcome to the IESM course!

- Lecturer: Prof. Ursula Röthlisberger
- TAs:
 - Yuri Cho
 - Salomé Guilbert
 - Sophia Johnson
 - Andrea Levy
 - Víctor Sabanza Gil
 - Qihao Zhang
 - Different PostDocs from LCBC lab

Introduction to Electronic Structure Methods

- Mondays and Tuesdays from 10h15 to 12h00
- Course schedule for the semester available on Moodle and the exercise webpage
- Tomorrow we'll have the first lecture (in BCH3303) with more practical details on the course

- Moodle page



The screenshot shows the EPFL Moodle interface. On the left is a red vertical bar with a white right-pointing chevron. To its right is the EPFL logo in red, followed by a vertical line and the word 'MOODLE' in red. Further right are the language links 'FR' and 'EN' in red, followed by a bell icon and a speech bubble icon. Below this header is a large white box with a thin grey border. Inside the box, the title 'Introduction to electronic structure methods' is displayed in a large, bold, black font. Below the title, a breadcrumb trail is shown: 'Dashboard > Courses > Chimie, Génie Chimique (CGC) > CGC - Bachelor > CH-353'.

> EPFL | MOODLE FR EN  

Introduction to electronic structure methods

Dashboard > Courses > Chimie, Génie Chimique (CGC) > CGC - Bachelor > CH-353

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



Exercise structure

Introduction

- Learning goals
- Chapter in script
- Resources

 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.

```
# Check orthogonality
phi1phi2 = 0 # Replace with vector operation
print(f'<phi1|phi2> = {phi1phi2}')
```

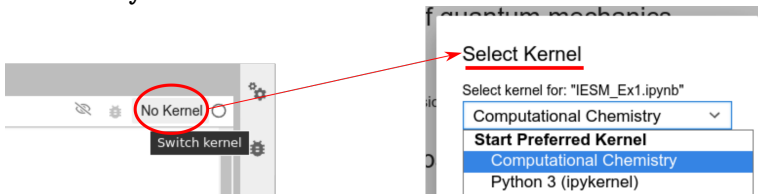
- Exercises contribute to 1/3 of final grade
- Submit report
 - pdf document answering the questions completely with relevant results
 - Handwritten portions ok (please verify legibility)
 - We provide report templates on Overleaf and Google Docs
 - Due date is usually the next exercise session (check Moodle!)
 - Interviews during next exercise session
 - Test your understanding and discuss your doubts/questions
 - Detailed feedback via Moodle after the interview
 - No grade, but comments and detailed corrections

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

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



Text cell

```
[1]: x = 1  
     y = 2
```

```
[ ]: print(x+y)
```

Jupyter notebooks

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



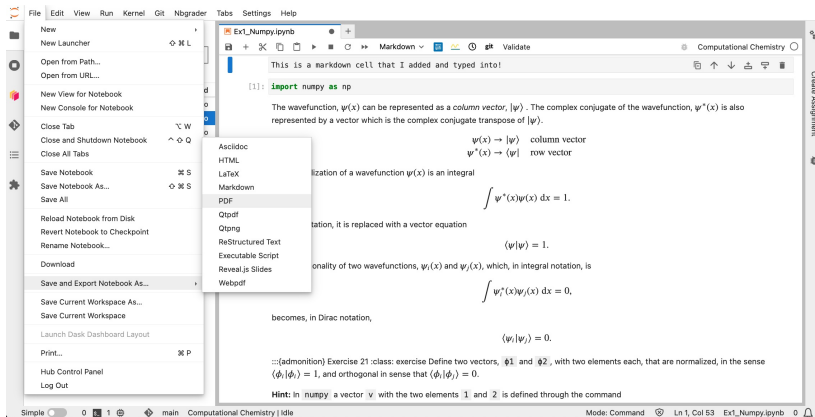
Text cell

```
[1]: x = 1  
     y = 2
```

```
[3]: print(x+y)
```

3

Saving Jupyter notebooks as PDFs



- Run a code cell by pressing :arrow_forward: (or Ctrl+Enter)



Text cell

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

Review basic concept of linear algebra

Review basic notation of quantum mechanics

Chapter in script

Chapter 2 - Basic principles of Quantum Mechanics

Appendix A.1 - Vector space and scalar product

Resources

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 representations and observables
- Chapter II Complement D_{II} - A more detailed study of the $\{|r\rangle\}$ and $\{|p\rangle\}$ representations
- Chapter II Complement E_{II} - Some general properties of two observables, Q and P , whose commutator is equal to $i\hbar$

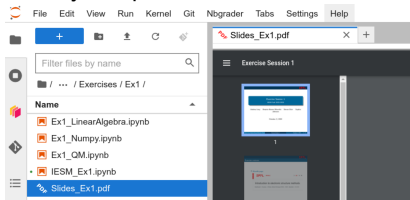
Exercise 1 - Tips

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