

Exercise Session 1

IESM Fall 2023-2024

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- Moodle page



The screenshot shows the top navigation bar of the EPFL Moodle system. On the left is a red vertical bar with a white right-pointing chevron. Next to it is the EPFL logo in red, followed by the word MOODLE in red. On the right side of the bar are the language links FR and EN (highlighted in red), and two small icons: a bell for notifications and a speech bubble for messages. Below the navigation bar is a white box containing the course title 'Introduction to electronic structure methods' and a breadcrumb trail: '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 sessions

- 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
```

```
 $\phi_1\phi_2 = 0$  # Replace with vector operation
```

```
print(f'< $\phi_1|\phi_2$ > = { $\phi_1\phi_2$ }')
```

- 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)
 - You can type responses in the noto notebook and save as a pdf
 - 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)



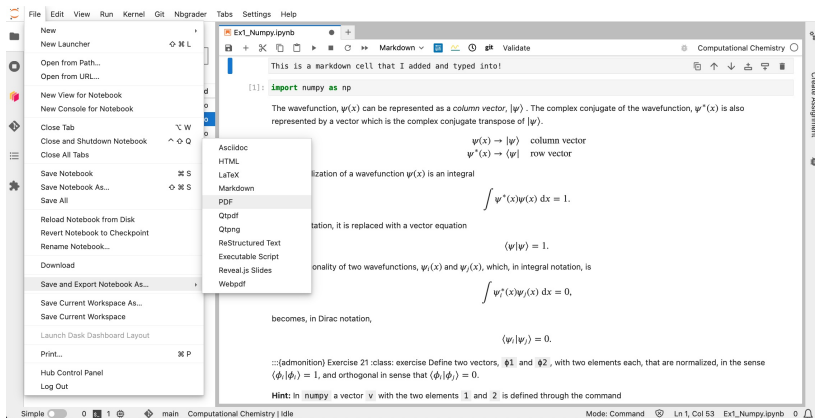
Text cell

```
[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](#)