

# Exercise Session 1

## IESM Fall 2023-2024

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- Moodle page



The screenshot shows the top section of an EPFL Moodle course page. On the left, there 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. On the far right of this header area, the text "FR | EN" is displayed in grey, followed by a bell icon and a speech bubble icon. Below this header, a horizontal line separates it from the main content area. The main content area has a light grey background and contains the title "Introduction to electronic structure methods" in a large, bold, black font. Below the title, a breadcrumb trail is shown in a smaller, grey font: "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
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)
    - 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](https://noto.epfl.ch)



- On [noto.epfl.ch](https://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
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- 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<sub>II</sub> - A more detailed study of the  $\{|r\rangle\}$  and  $\{|p\rangle\}$  representations
- Chapter II Complement E<sub>II</sub> - 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](#)