

Exercise Session 1

IESM Fall 2025-2026

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Welcome to the IESM course!

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

Introduction to Electronic Structure Methods

- 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



The screenshot shows the top navigation bar of the EPFL Moodle 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 the navigation bar, there are links for 'FR' and 'EN' in red, and two icons: a bell for notifications and a speech bubble for messages. Below the navigation bar, the main content area is enclosed in a light gray border. It features the course title 'Introduction to electronic structure methods' in a large, bold, black font. Underneath the title is a breadcrumb trail: 'Dashboard > Courses > Chimie, Génie Chimique (CGC) > CGC - Bachelor > CH-353'.

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

The screenshot shows the website interface for "Introduction to Electronic Structure Methods". On the left, there is a search bar with the placeholder text "Search this book...". Below the search bar, the title "Introduction to Electronic Structure Methods" is displayed in red. On the right, there is a navigation menu icon (three horizontal lines) and three icons: a square with a plus sign, a circular arrow, and a download arrow. The main title "Introduction to Electronic Structure Methods" is prominently displayed. Below the title, a paragraph states: "This book contains the script and exercises for the course CHE-351 Introduction to Electronic Structure Methods (IESM) given at EPFL."

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:

1 Exercise 9

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

1 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'⟨ $\phi_1$  |  $\phi_2$ ⟩ = { $\phi_1\phi_2$ }')
```

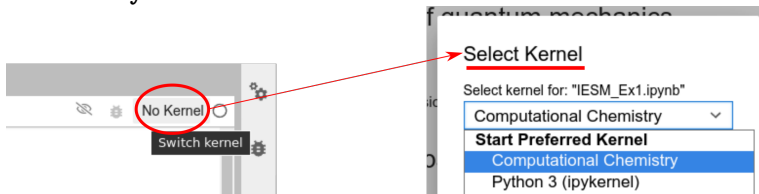
- Exercises account for 1/3 of the final grade (2/3 from exams, 1 written 1 oral)
- Submit report
 - pdf document answering the questions completely with relevant results
 - Handwritten portions ok (please verify legibility)
 - We provide report templates on Overleaf and Google Docs
 - Due date is usually 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

- .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

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 $i\hbar$

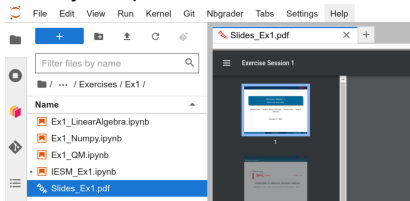
Exercise 1 - Tips

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