

Exercise Session 1

IESM Fall 2025-2026

Salomé, Qihao, Thibault, Evan

September 9, 2025

Introduction to Electronic Structure Methods

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

Exercise sessions

- Moodle page



Exercise sessions

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



Introduction to Electronic Structure Methods

 Search this book...

Introduction to Electronic Structure
Methods

Introduction to Electronic Structure Methods

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.

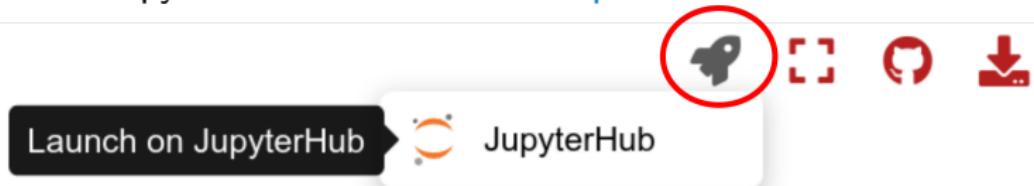
Check Orthogonality

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

- 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)

The screenshot shows a Jupyter Notebook interface. At the top is a toolbar with various icons: file, new, open, save, play (highlighted with a red circle), stop, refresh, cell, cell type, dropdown, git, and help. Below the toolbar, a text cell contains the text "Text cell". Underneath, two code cells are shown. The first code cell has the output: [1]:
x = 1
y = 2. The second code cell has the input: []: print(x+y).

Jupyter notebooks

- .ipynb files organized in cells
 - Markdown (text)
 - Code
- Run a code cell by pressing :arrow_forward: (or Ctrl+Enter)
A horizontal toolbar with various icons: a square, a plus sign, a minus sign, a double minus sign, a double square, a double arrow, a double right arrow, a double left arrow, a double right double left arrow, a double left double right arrow, a double right double left double right arrow, a double left double right double left double right arrow, a green square with three horizontal lines, a blue circle with a dot, and a red square with the word "git".

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

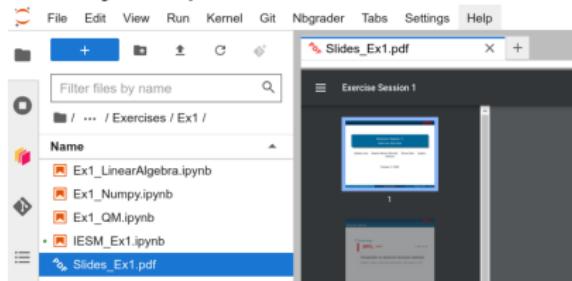
Learning goals	Chapter in script	Resources
<p>Review basic concept of linear algebra</p> <p>Review basic notation of quantum mechanics</p>	<p>Chapter 2 - Basic principles of Quantum Mechanics</p> <p>Appendix A.1 - Vector space and scalar product</p>	<p>Cohen-Tannoudji, C., Diu, B., & Laloe, F. (1986). Quantum Mechanics, Volume 1.</p> <ul style="list-style-type: none">• 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 vectors 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