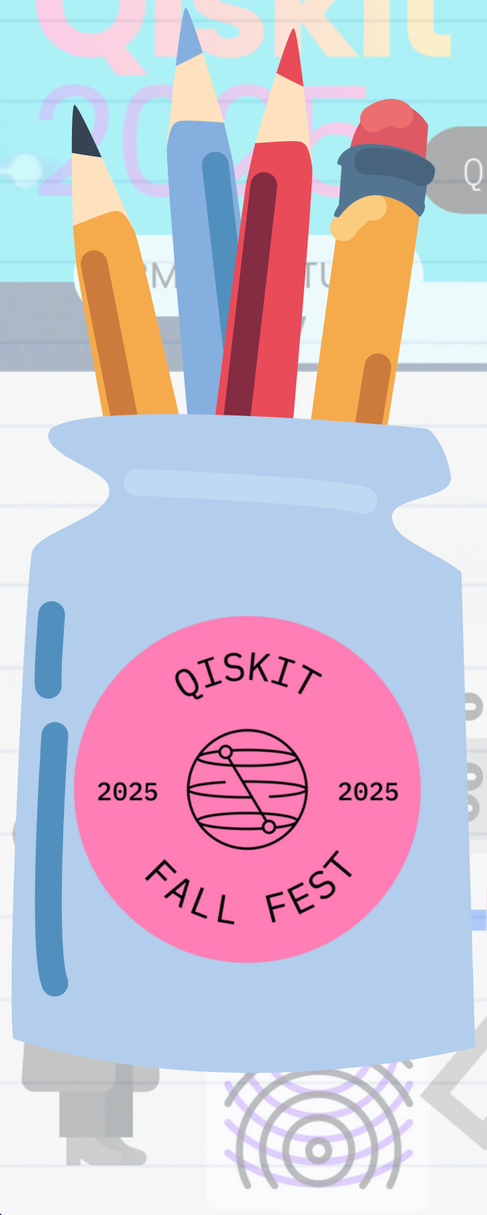


QFF2025 VARIATIONAL ALGORITHM

Notebook Exercises

Variational Quantum Algorithms

Le Duc-Truyen

PhD student

iTHEMS, RIKEN

Background: Theoretical Physics, High Energy Physics

Research Topics: Quantum Field Theory, Particle Physics Phenomenology, Quantum Computing For Quantum Field Theory, Intedisplinary Mathematical Applications

Email: leductruyenhep@gmail.com

QFF2025

Useful resources

Quantum chemistry with VQE and SQD:

- https://quantum.cloud.ibm.com/learning/en/courses/utility-scale-quantum-computing/variational-quantum-algorithms
- https://quantum.cloud.ibm.com/learning/en/courses/quantum-chem-with-vqehttps://quantum.cloud.ibm.com/learning/en/courses/quantum-diagonalization-algorithms/vqe,
- https://quantum.cloud.ibm.com/learning/en/courses/quantum-diagonalization-algorithms/sqd-overview.

Max-cut problems with QAOA and Utility-scale QAOA (100-Qubit) :

- https://quantum.cloud.ibm.com/docs/en/tutorials/quantum-approximate-optimization-algorithm
- https://quantum.cloud.ibm.com/learning/en/courses/utility-scale-quantum-computing/variational-quantum-algorithms, https://quantum.cloud.ibm.com/learning/en/courses/quantum-computing-in-practice/utility-scale-qaoa,
- https://billtcheng2013.medium.com/from-hello-world-to-maxcut-solving-graph-problems-with-qiskit-3837191aa04c

Access the GitHub link below to run the notebook:

https://github.com/vbinvu68/Qiskit-fall-fest-25-at-Univ-Paris-Saclay/tree/main/Day1

ENJOY YOUR QUANTUM DAYS!

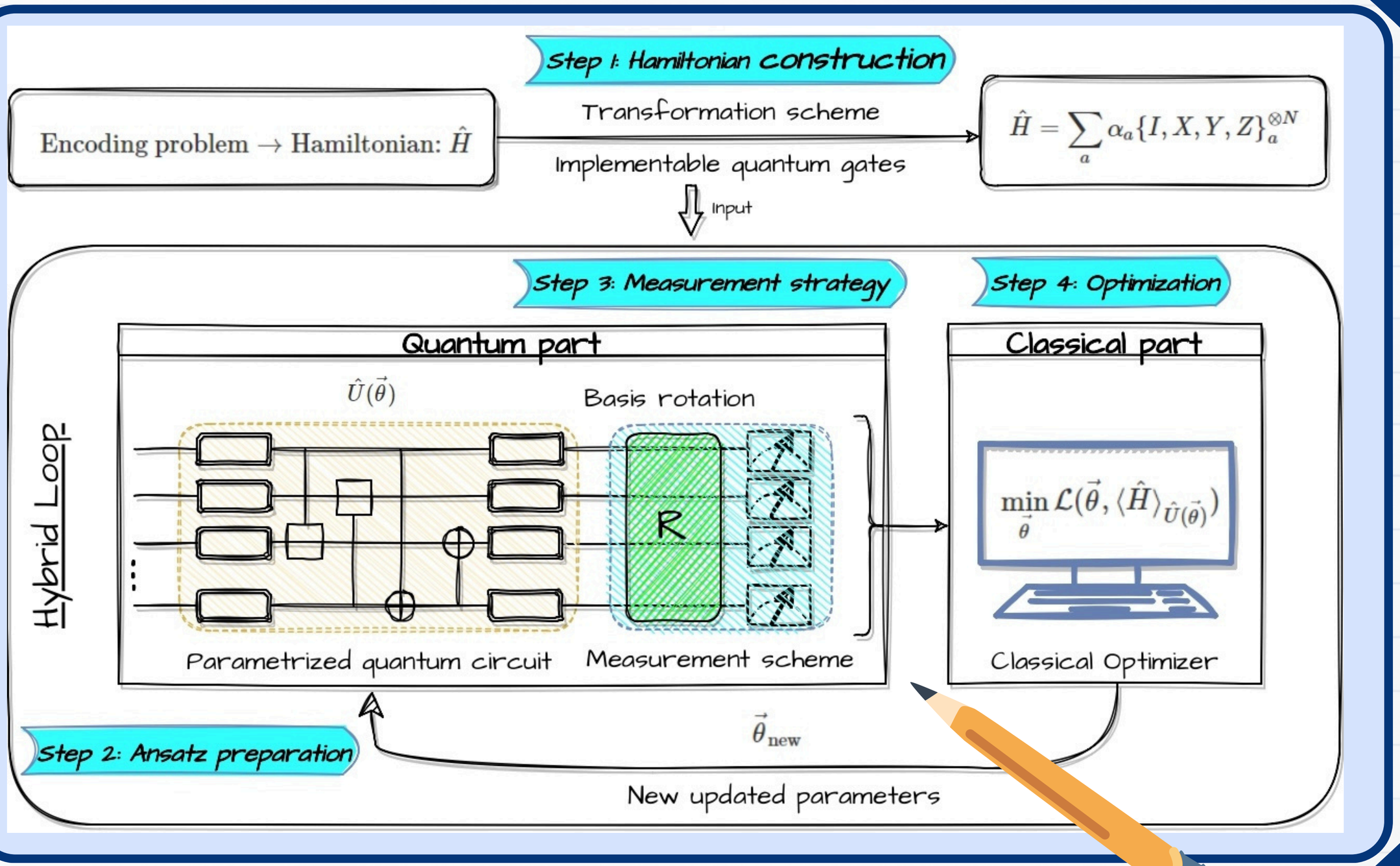
LEARNING OBJECTIVES PART-1

Learn how to use Qiskit packages to implement VQAs

Understand the VQA workflow

Get your hands on an optimization problem using QAOA technique

VQA/VQE



Cre: arXiv:2412.19176

EXCERCISE VQAS

COMPUTING SIMPLE HAMILTONIAN USING VQE

Exercise 1: Build cost function for hybrid VQE loop

Exercise 2: Apply to other simple Hamiltonian

MAXCUT PROBLEM

Exercise 3: Construct the Maxcut problem

Exercise 4: Maxcut as QUBO optimization problem

FROM QUBO TO HAMILTONIAN

Exercise 5: Construct a variational form to QAOA ansatz

Exercise 6: Construct Hamiltonian based on QUBO optimization

RUN QAOA ON QISKIT

Exercise 7: Construct Cost function for QAOA optimization

EXTRA EXCERCISE

Exercise*: Try different ansatz with different hyperparameters

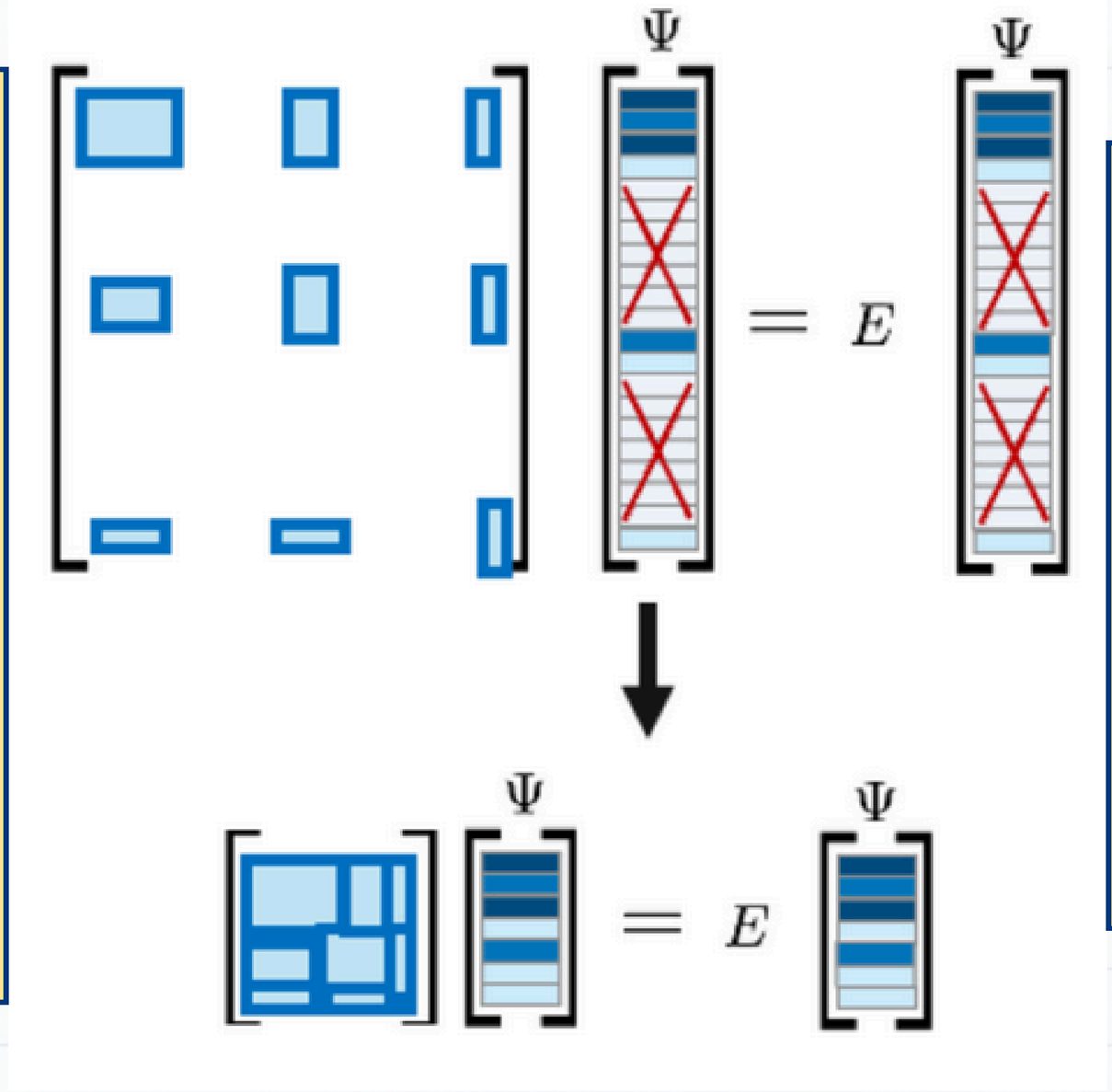
LEARNING OBJECTIVES PART-2

Learn how to use Qiskit packages to solve molecular problem

Understand the Sample-based Quantum Diagonalization (SQD) methods.

Analyze and compare how the choice of ansatz and initial parameters affects on SQD result.

SAMPLE



BASED

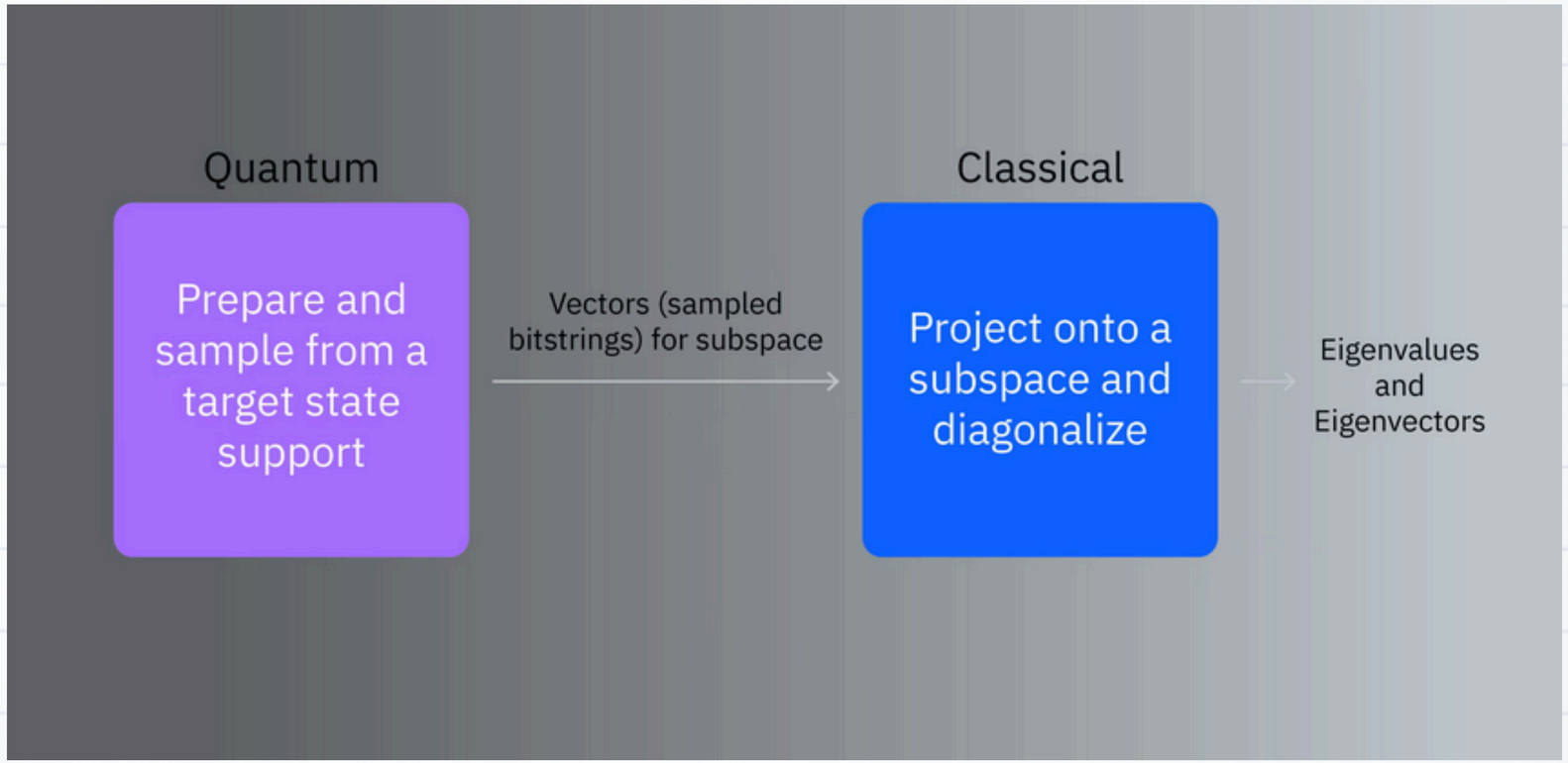
Cre: QGSS2025-lab3

SQD STEPS

Step 1: Initialize circuits and operators

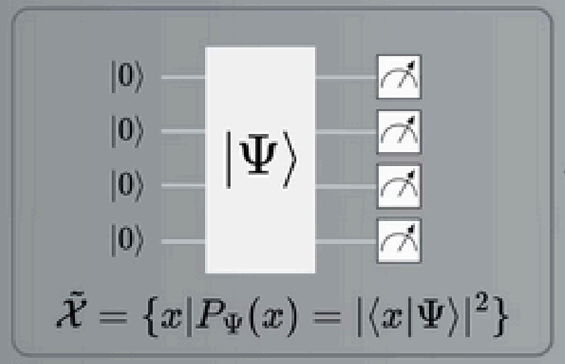
Step 2: Sample configurations of subspace from the circuit

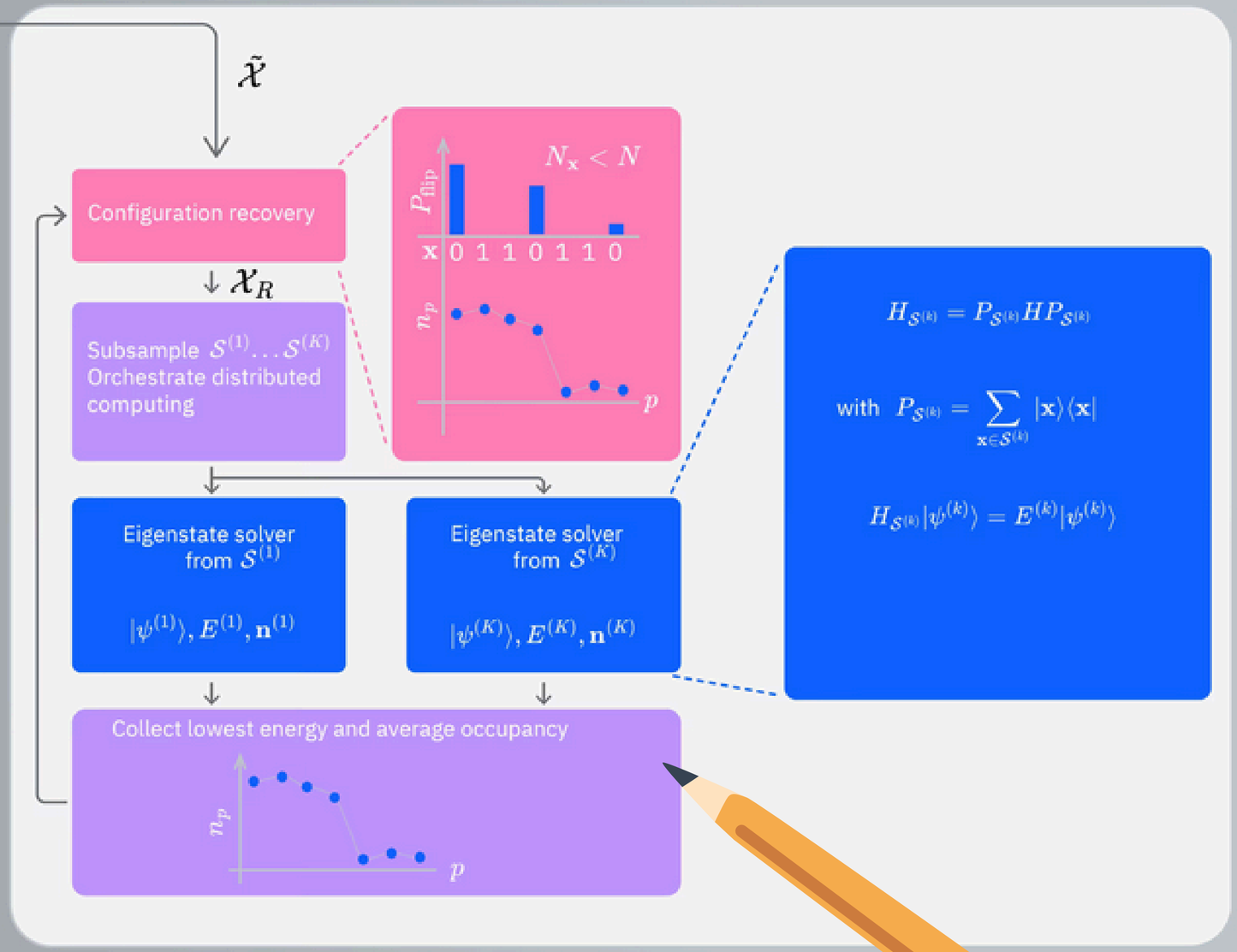
Step 3: Iterative post-process



Cre: Qiskit notebook

PROCESS





Cre: Qiskit notebook

EXCERCISE
QUANTUM CHEMISTRY WITH SQD

Exercise 1: Identify the molecule configuration information using *PySCF*

Exercise 2: Convert molecule into qubit operator using *ffsim*

Exercise 3: Create a Hardware-Efficient Ansatz (RealAmplitudes) for SQD

Exercise 4: Initialize an Informed UCJ Ansatz

EXTRA EXCERCISE

Exercise*: Try to build the hybrid loop of SQD

Packages: PySCF, *ffsim*, *qiskit_addon_sqd*

QFF2025

THANK YOU FOR YOUR ATTENDANCE AND STAY IN THE LOOP

Access the GitHub link below to run the notebook:

https://github.com/vbinvu68/Qiskit-fall-fest-25-at-Univ-Paris-Saclay/tree/main/Day1

ENJOY YOUR QUANTUM DAYS!