

# QUANTUM COMPLEXITY

\* Complexity classes - classical and quantum

\* Hamiltonian simulation

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What is a complexity class?

Set of decision problems with similar hardness

↑  
given instance  $x$ , "decide" (Y/N) whether instance has a specific property / is in some set " $L$ "

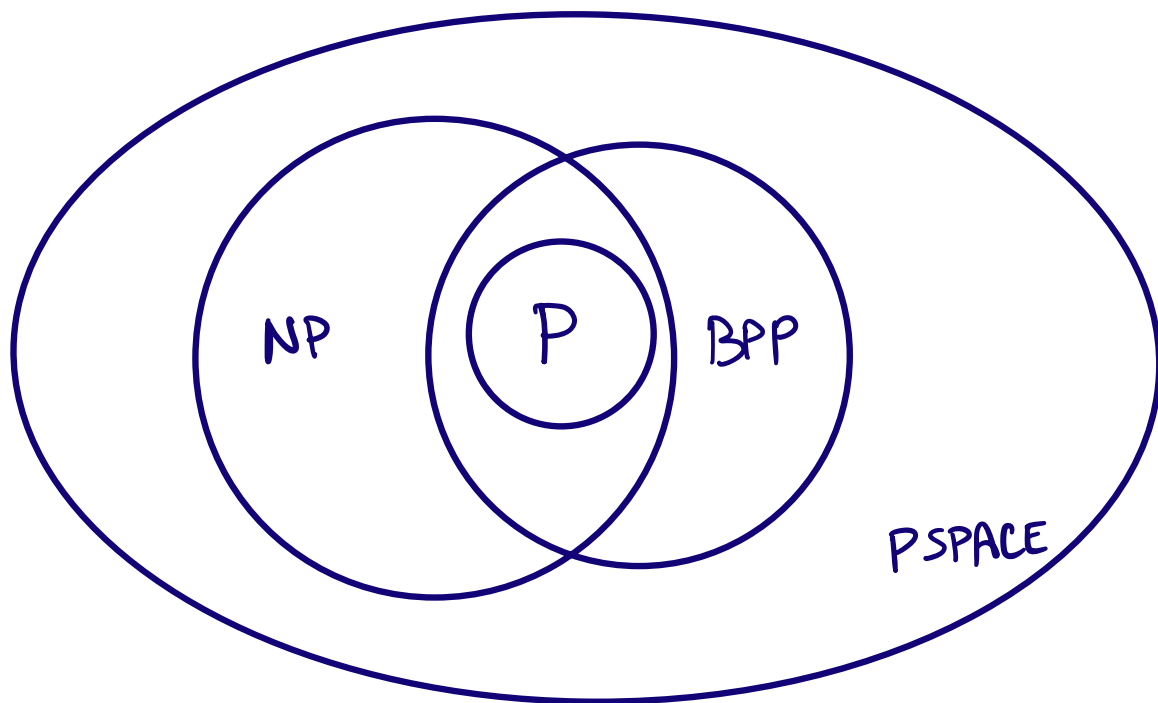
## EXAMPLES

P : Solved by classical computers in (deterministic, i.e. not randomized) polynomial time

BPP : solved by randomized computers in polynomial time (with error probability  $< 1/3$  on every input)

NP : for instances  $x$  in  $L$ , there is a polynomial-length "witness" that convinces a polynomial-time computer that  $x \in L$ .

PSPACE : solved by deterministic computer in polynomial space



Quantum analogues :

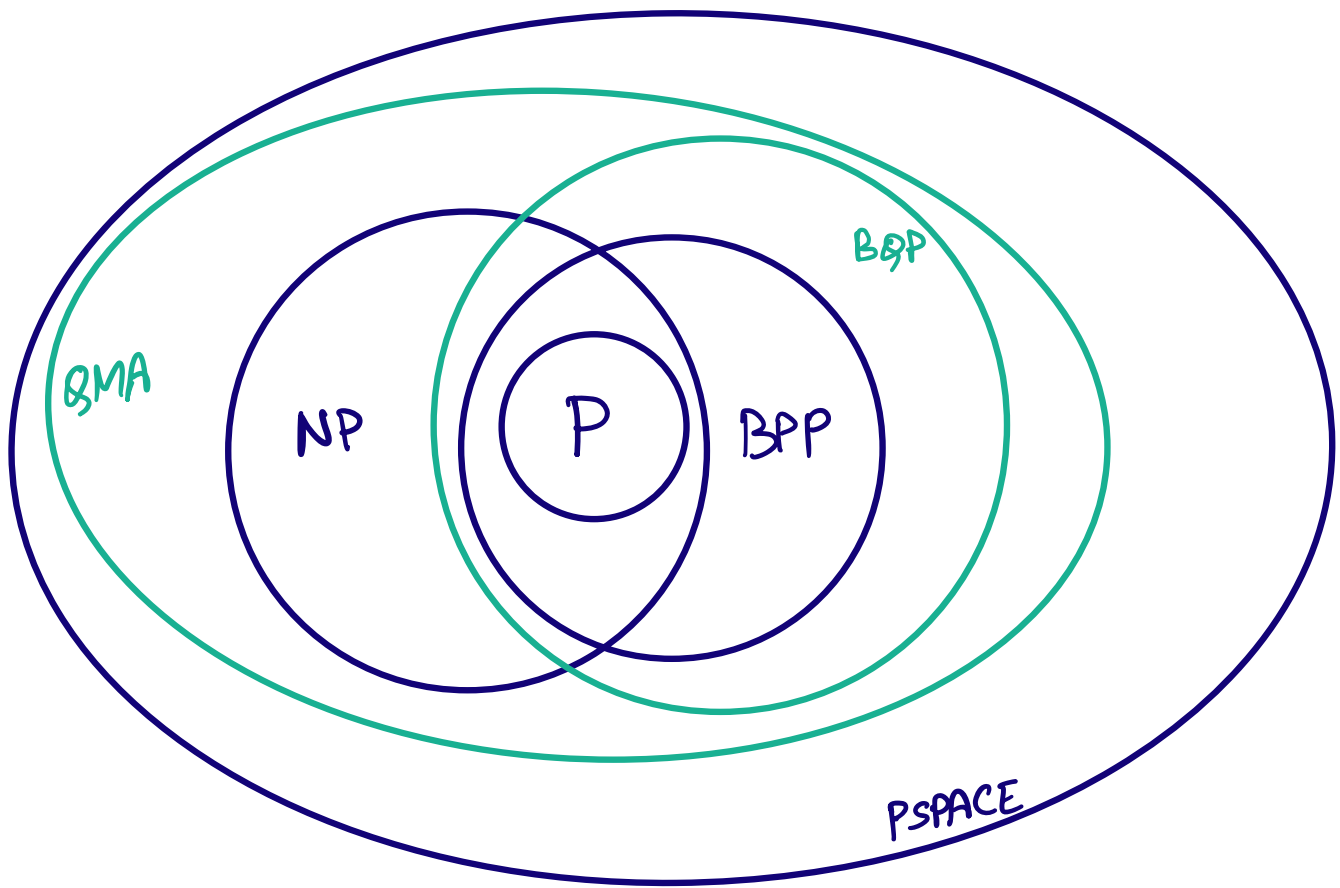
BQP : BPP, except, quantum computers

Example : factoring

"Quantum" NP ?

QMA : For every  $x \in L$ , there is "quantum witness" that convinces polytime verifier with error  $\leq \frac{1}{3}$ .

Eg : Decide if lowest eigenvalue of  $k$ -local Hamiltonian is  $\leq a$  or  $\geq a + \frac{1}{\text{poly}}$ .



We will now take a detour into Hamiltonian complexity.

A killer app of quantum computing:

Hamiltonian simulation

evolve a quantum state over time according to a Hamiltonian

↑  
encodes information about how a collection of particles interact with each other over time

The Hamiltonian  $H$  determines which unitary will actually occur in a given physical system.

System starts at state  $|\psi_0\rangle$

State at time  $t$  is  $|\psi_t\rangle$ , governed by

$$|\psi_t\rangle = U|\psi_0\rangle$$

where  $U = e^{-iHt}$  ↗ unitary when  $H$  is Hermitian

So basically  $|\psi_1\rangle = e^{-iH}|\psi_0\rangle$

$$|\psi_2\rangle = e^{-iH}|\psi_1\rangle = e^{-iH \cdot 2}|\psi_0\rangle$$

and so on...

[ $t$  need not be discrete]

# Application : Quantum chemistry

figure out how a quantum system will evolve over time  
many important applications

\* Material sciences

\* Drug discovery

\* Energy industry

\* Fertilizer production

1-3% of world's energy

(eg. Nitrogen fixation, turn nitrogen into ammonia through catalyst)

## HAMILTONIAN SIMULATION

Input : Hamiltonian  $H$ , state  $|\psi_0\rangle$  on  $n$  qubits,  
time  $t$

Output :  $e^{iHt} |\psi_0\rangle$

unfortunately, since  $H$  is  $2^n \times 2^n$  matrix for large  $n$ , classical computers cannot efficiently compute the output. (Require time exponential in  $n$ ).

What about quantum computers?

The unitary  $e^{iHt}$  is not efficiently implementable in general, for arbitrary  $H$ .

However,  $H$  that occur in nature have structure

They are typically "local": particles interact with nearby particles only

$$H = H_1 + H_2 \dots + H_m \quad m = \text{poly}(n)$$

each  $H_i$  captures "constraint" on a few qubits only

"k"-local  $\Rightarrow$  Acts nontrivially on  $k$  qubits only

i.e., each  $H_i = h_i \otimes I$

$\downarrow$   
k-qubit matrix

for constant  $k$ , there is now a quantum

algorithm with runtime  $\text{poly}(n, m, t, \log(\frac{1}{\epsilon}))$   
 $\uparrow$   
error