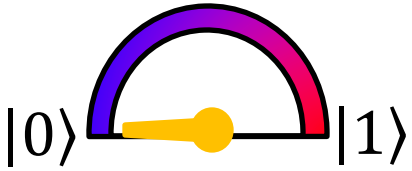
Electron paramagnetic resonance spectroscopy for molecular qubits

Valentin Novikov

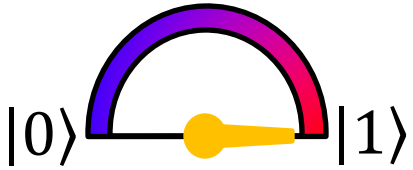
Common myths about quantum computers:

- Quantum computers are faster at *everything*
- “Quantum parallelism” provides *exponential speedup*
- A qubit is “both $|0\rangle$ and $|1\rangle$” *at the same time*
- *Schrödinger’s cat* is a good analogy for a qubit

Possible states of qubits: flipping a coin



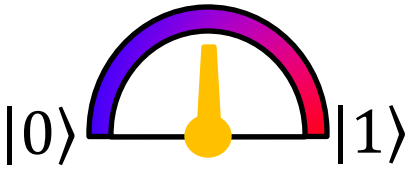
100% of being in $|0\rangle$ state



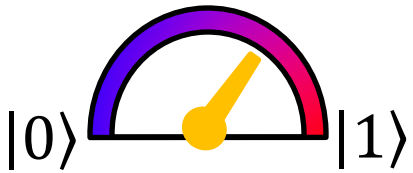
100% of being in $|1\rangle$ state

Only when we measure (catch the coin), the result is determined

Before we caught it:



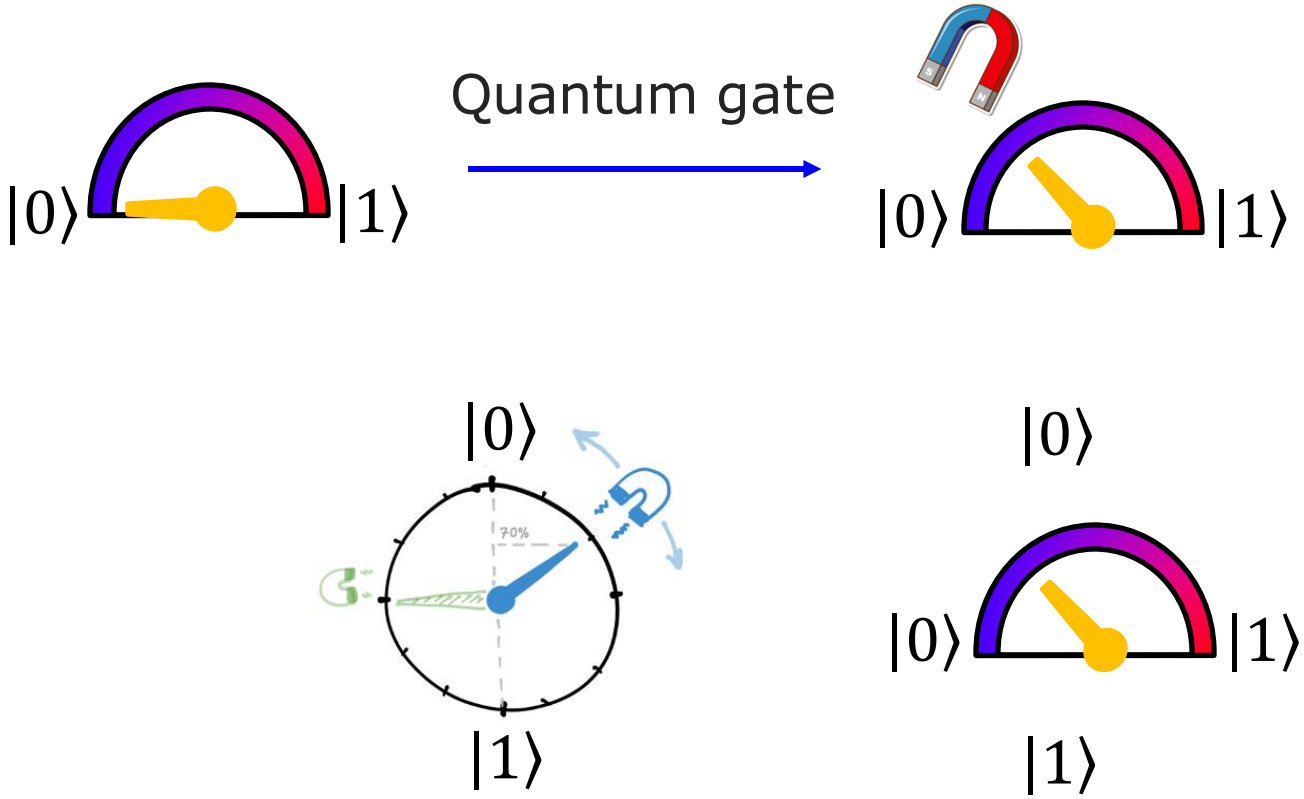
Fair coin:
50 / 50

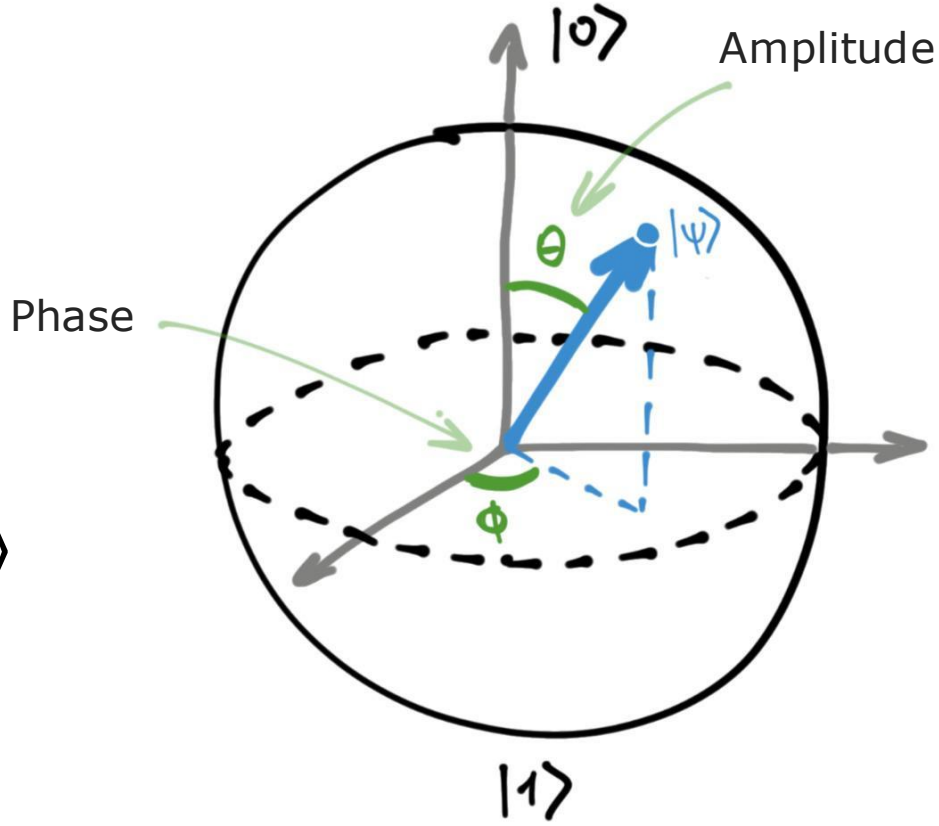


Unfair coin:
30 / 70

Schrödinger's ~~cat~~ Harvey Dent

Qubit manipulation and a Bloch sphere





$$|\psi\rangle = \cos\left(\frac{\theta}{2}\right)|0\rangle + e^{i\phi}\sin\left(\frac{\theta}{2}\right)|1\rangle$$

What can we do with a spin?

Doing nothing:

$a|0\rangle+b|1\rangle$ $\quad$ $a|0\rangle+b|1\rangle$

Even this “operation” is quite hard for quantum system

Measuring:

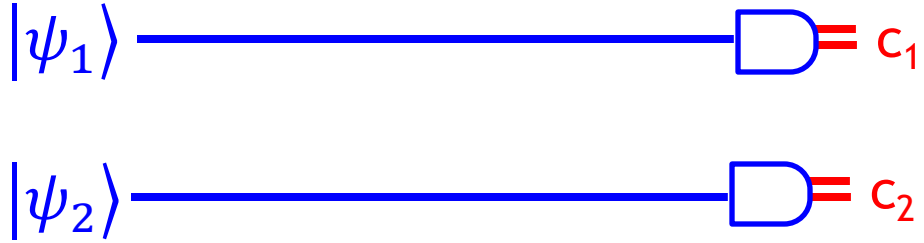
$a|0\rangle+b|1\rangle$

Result is classical bit

$|0\rangle$ in a^2 cases

$|1\rangle$ in b^2 cases

Several qubits:



$|0\rangle \; or \; |1\rangle$

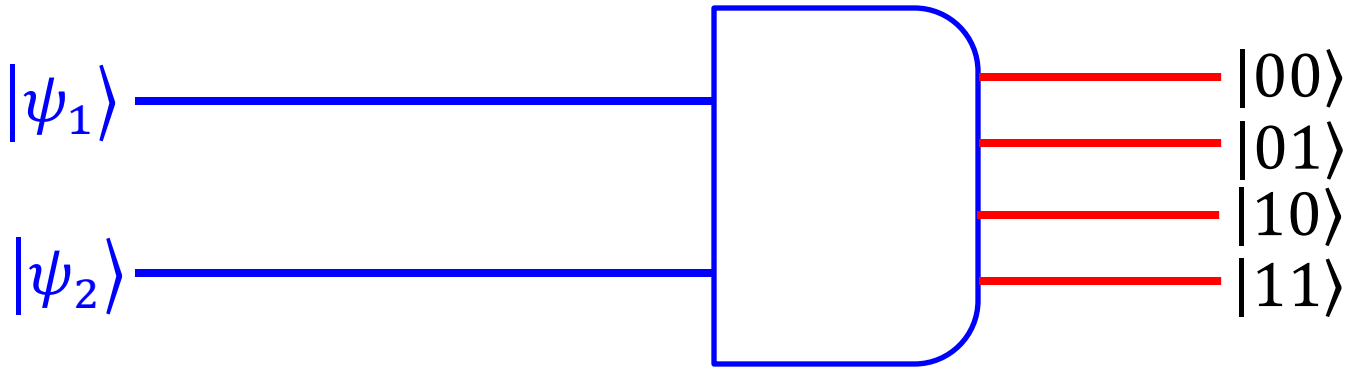
$|0\rangle \; or \; |1\rangle$

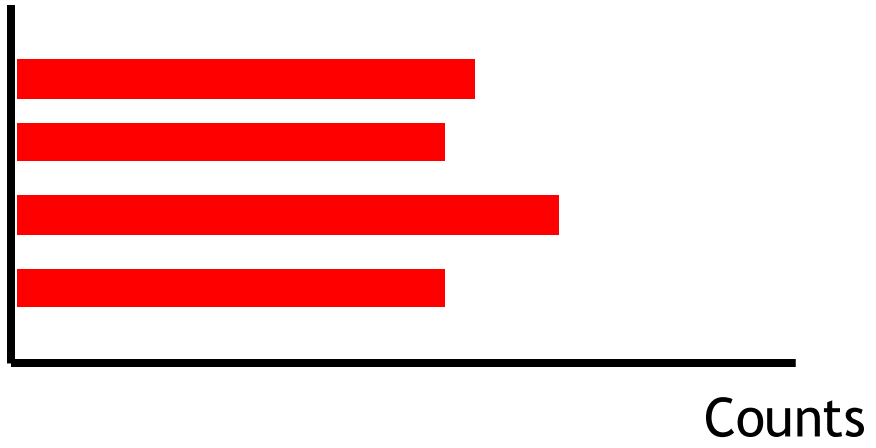
Possible outputs:

$|00\rangle, |10\rangle, |01\rangle, |11\rangle$

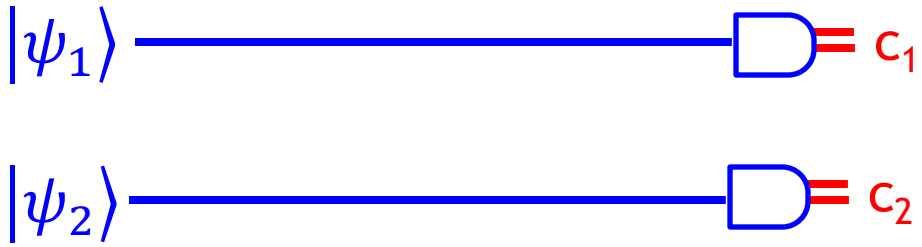
What can we do with two spins?

We may repeat the measurements many times and each time get one of the possible outputs.





Several qubits:



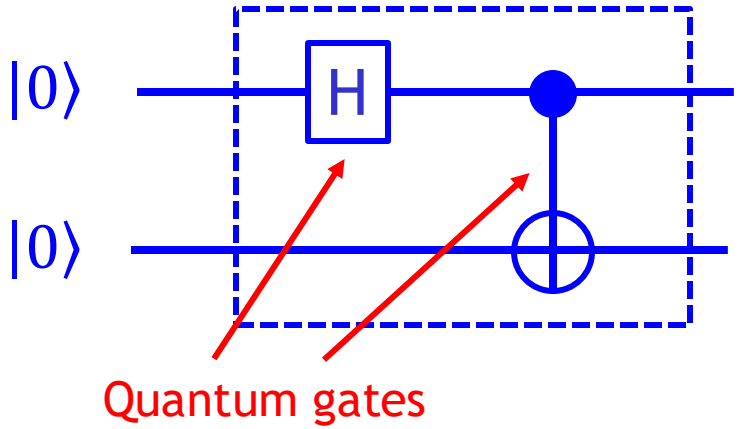
$|0\rangle \; or \; |1\rangle$

$|0\rangle \; or \; |1\rangle$

Possible outputs:

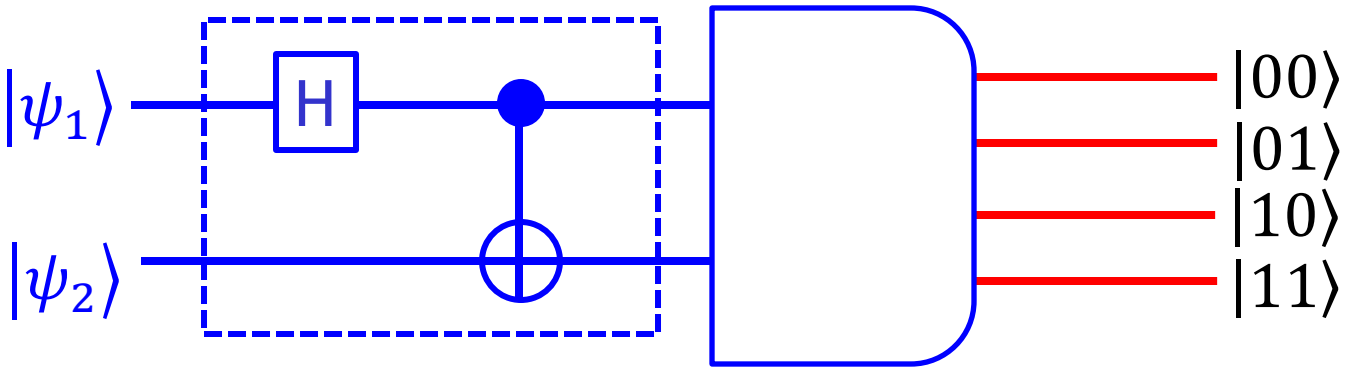
$|00\rangle, |10\rangle, |01\rangle, |11\rangle$

Entanglement



$$|\psi\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$$

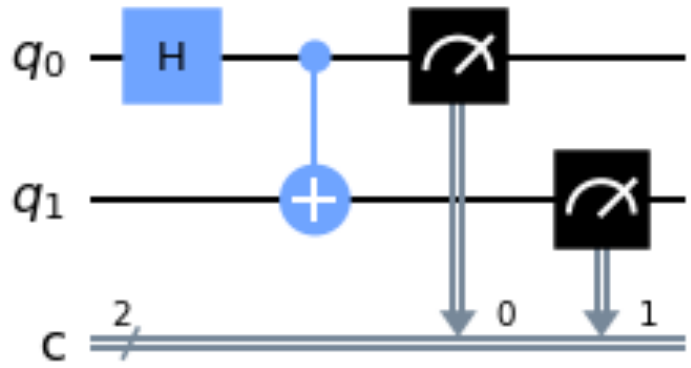
Both qubits after measurement will be in the same state, but we don't know which one.

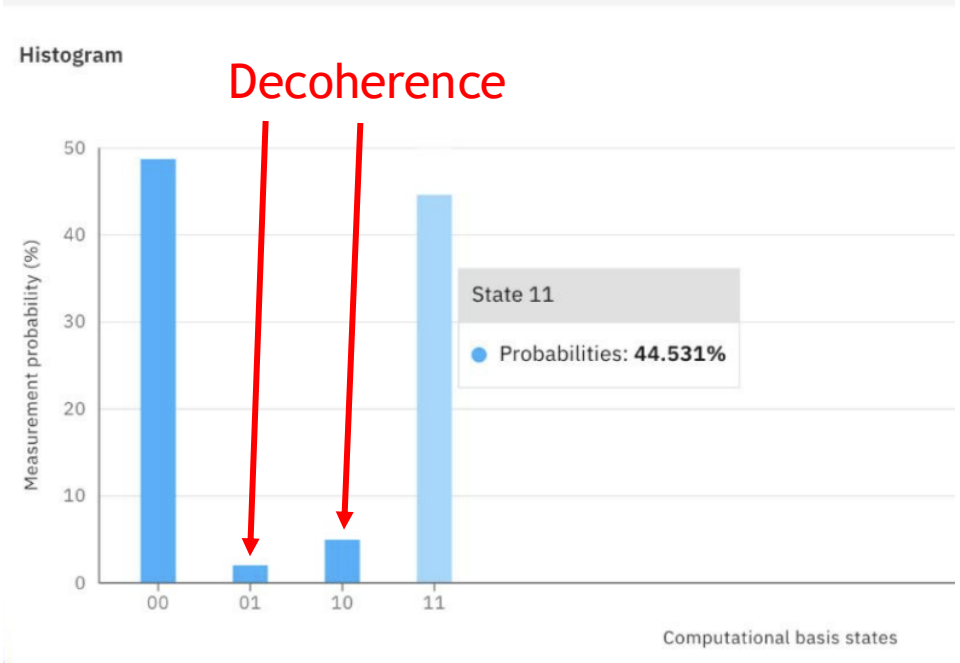


Now only $|00\rangle$ or $|11\rangle$ are possible

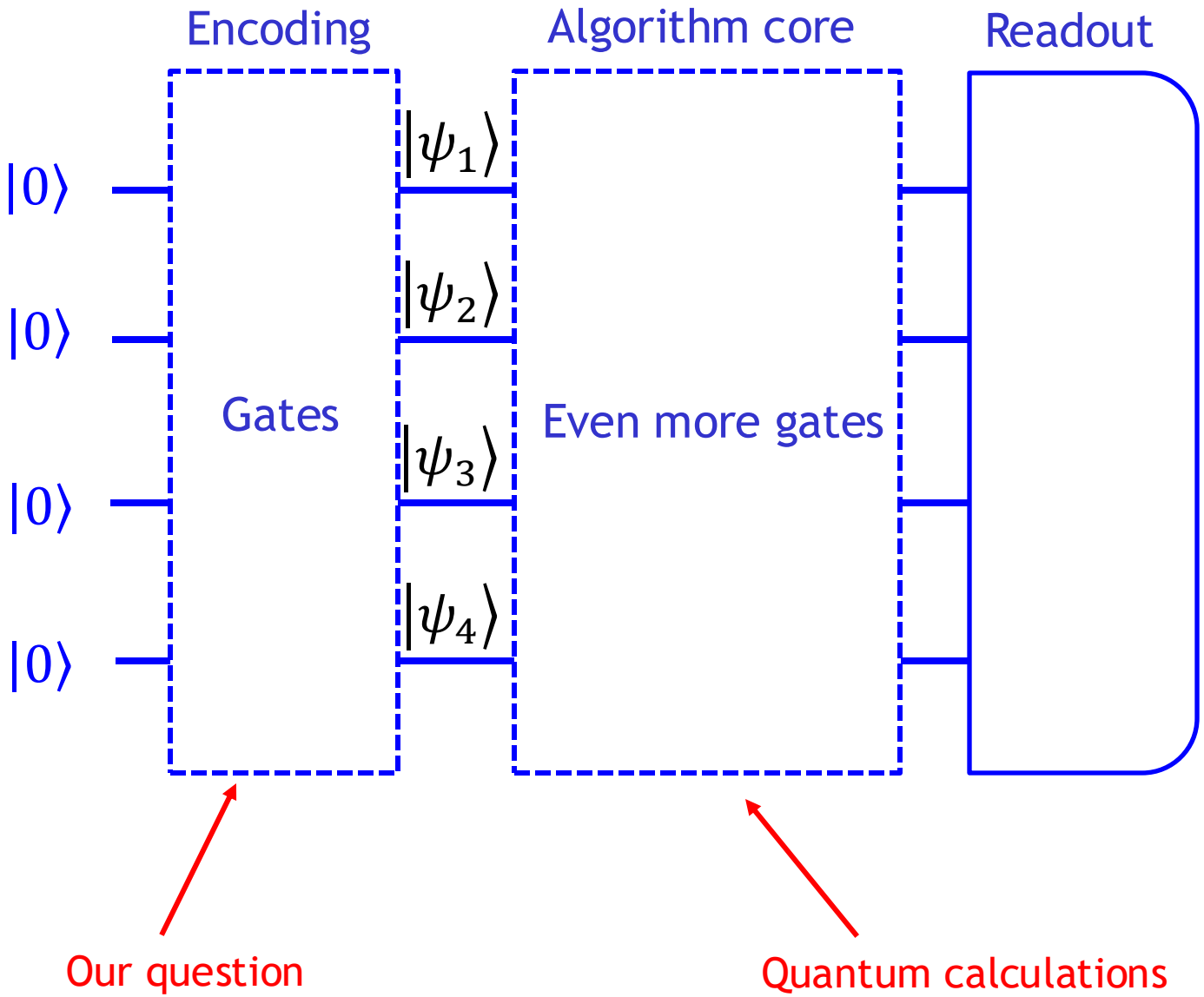
Calculation using real quantum computer from IBM with Qiskit

```python
from qiskit import QuantumCircuit
from qiskit.quantum_info import SparsePauliOp
from qiskit.transpiler import generate_preset_pass_manager
from qiskit_ibm_runtime import EstimatorV2 as Estimator
from qiskit_ibm_runtime import QiskitRuntimeService
from qiskit.visualization import matplotlib as qiskit_matplotlib
from qiskit_ibm_runtime import QiskitRuntimeService

qc = QuantumCircuit(2)
qc.h(0)
qc.cx(0, 1)
qc.draw("mpl")

QiskitRuntimeService.save_account(
    token=token,
    instance="Test1",
    name="novikov84@gmail.com",
    set_as_default=True,
    overwrite=True,
)

service = QiskitRuntimeService()
backend = service.least_busy(simulator=False, operational=True)
pm = generate_preset_pass_manager(backend=backend, optimization_level=1)
isa_circuit = pm.run(qc)
isa_circuit.draw("mpl", idle_wires=False)

estimator = Estimator(mode=backend)
estimator.options.resilience_level = 1
estimator.options.default_shots = 5000

mapped_observables = [
    observable.apply_layout(isa_circuit.layout) for observable in observables
]

job = estimator.run([(isa_circuit, mapped_observables)])
```

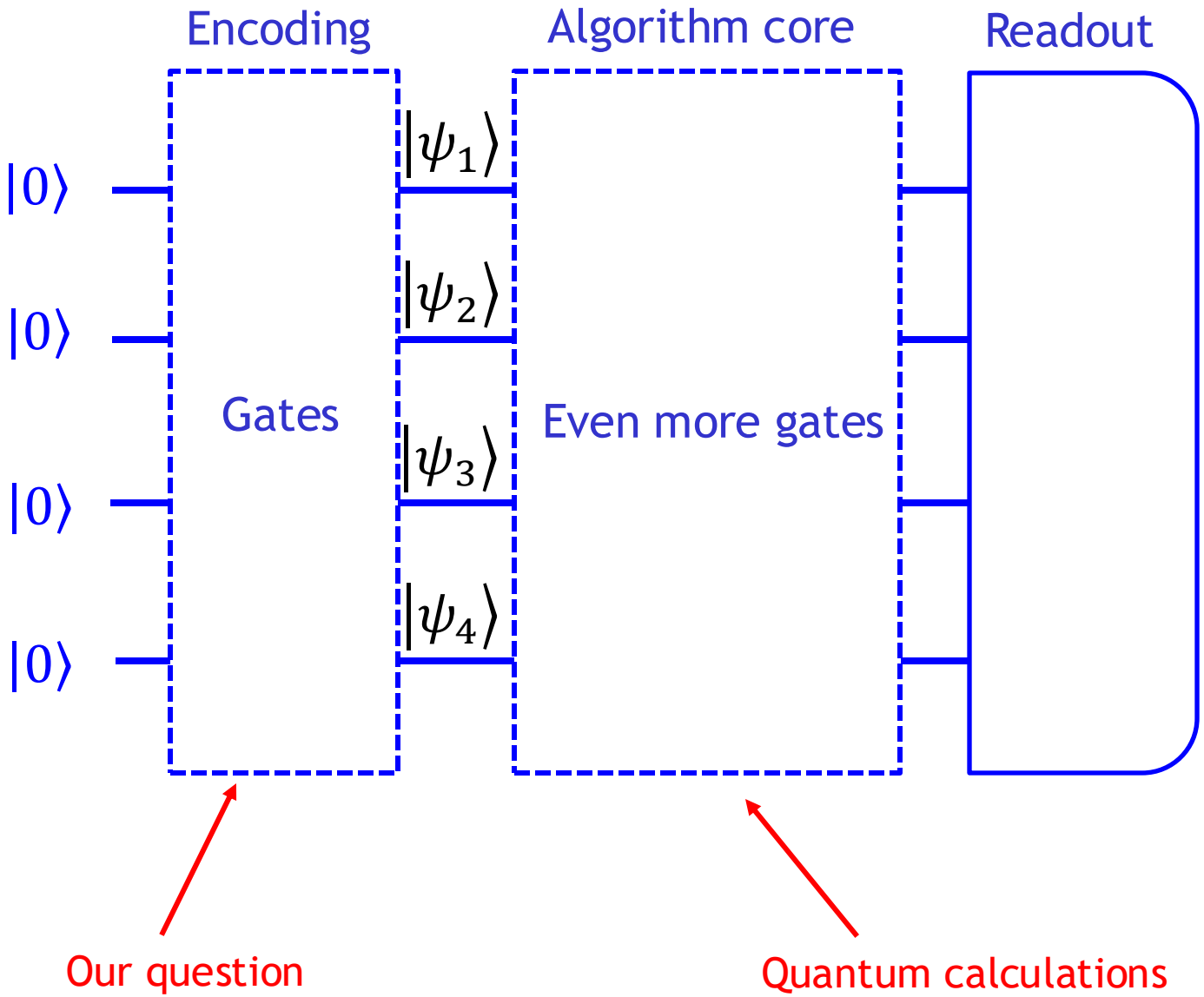


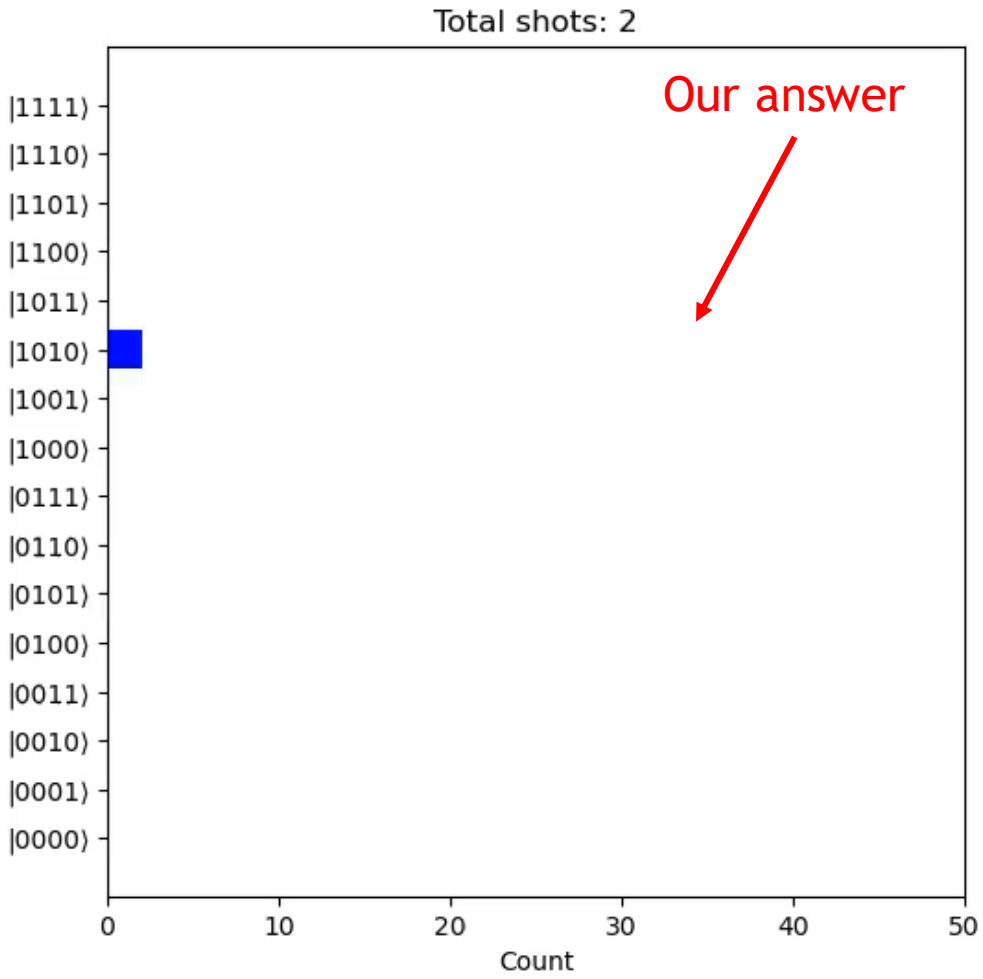


Four qubit algorithm

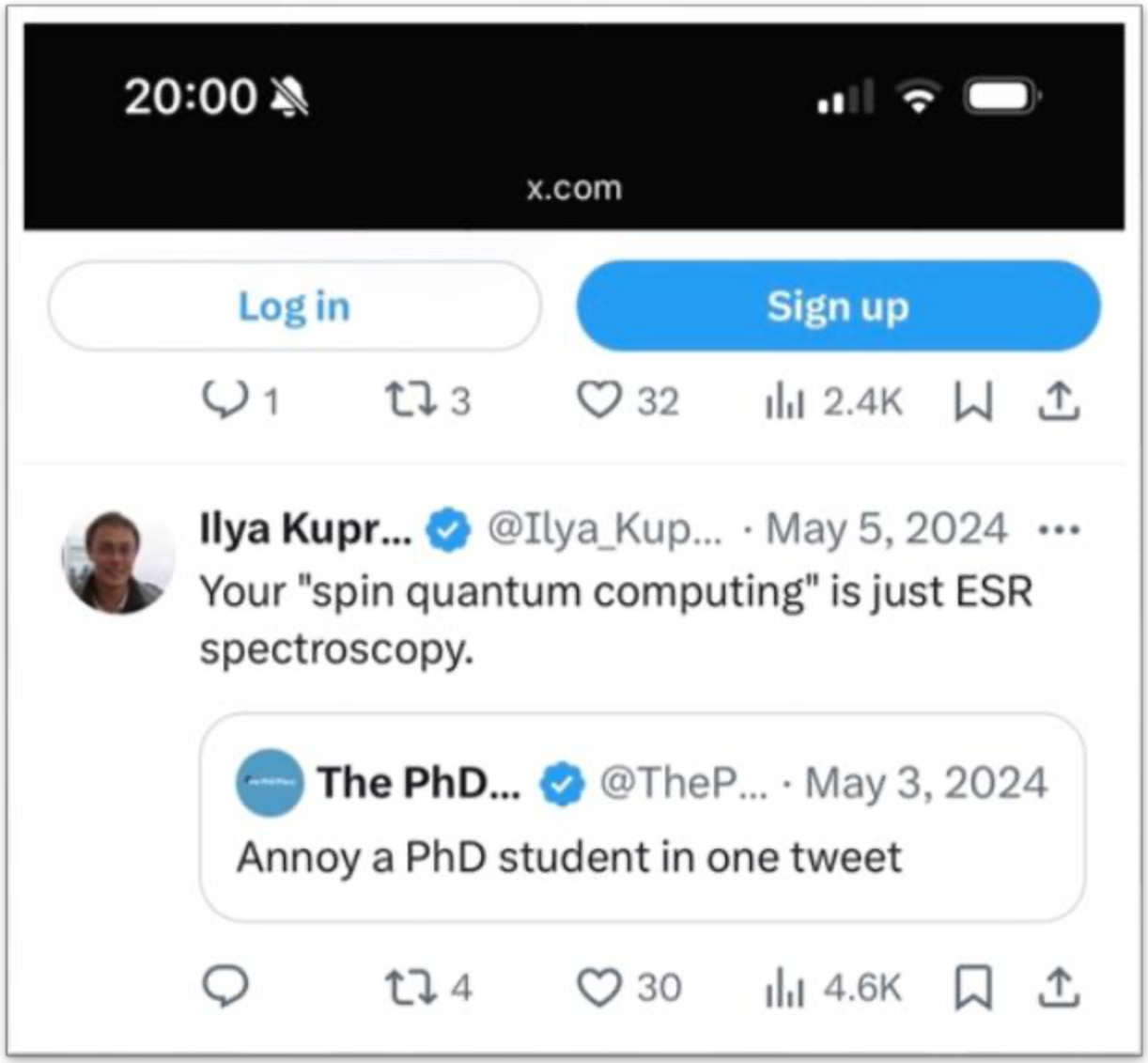


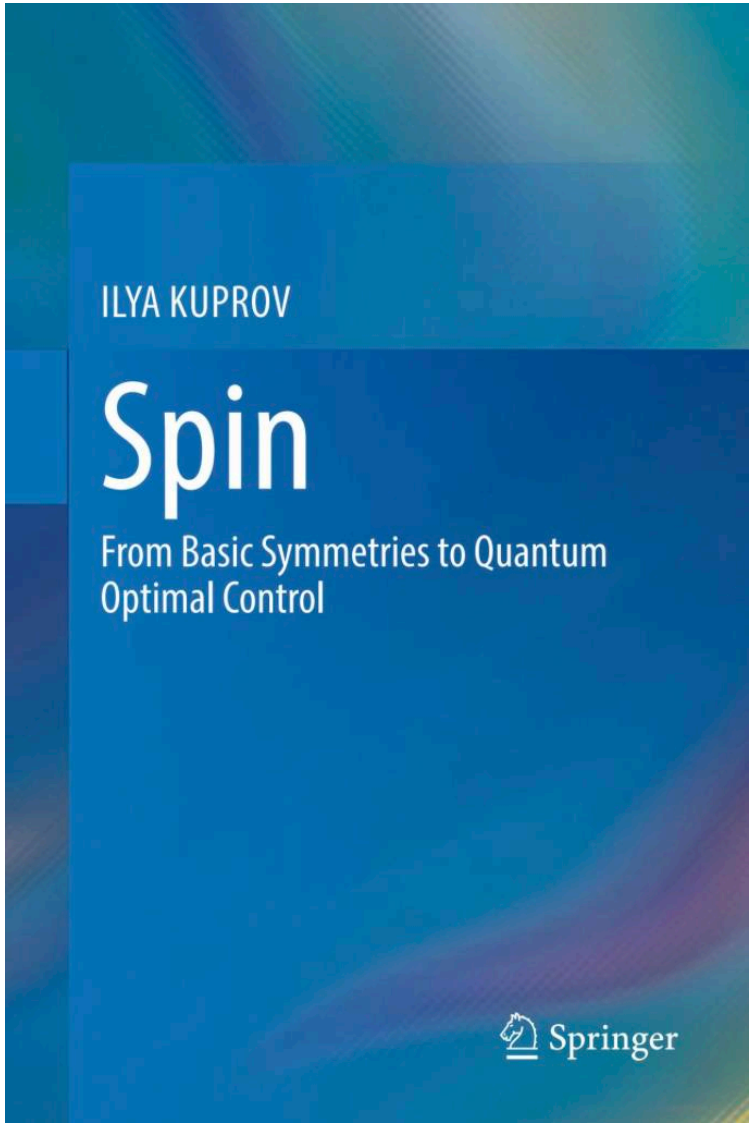
Four qubit algorithm



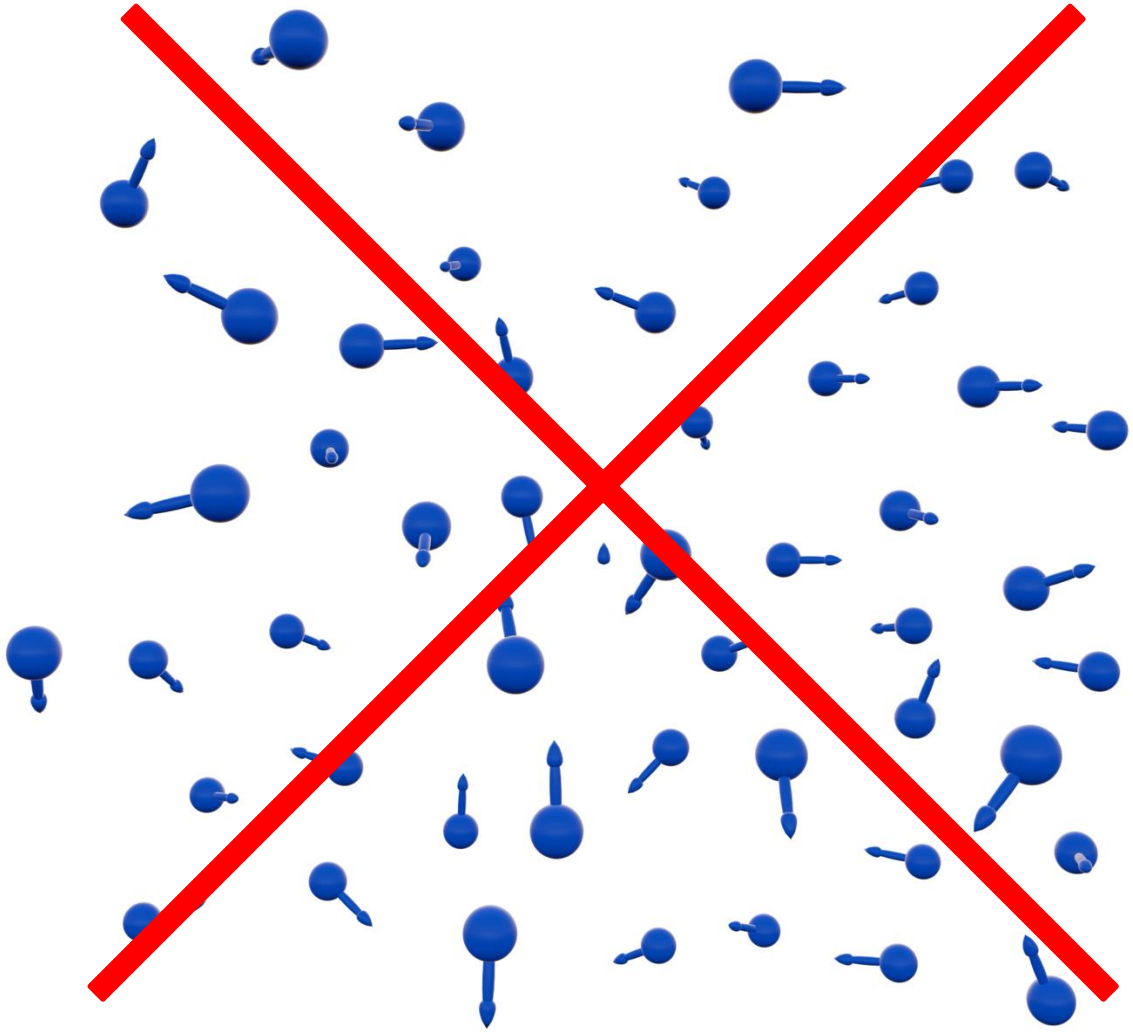


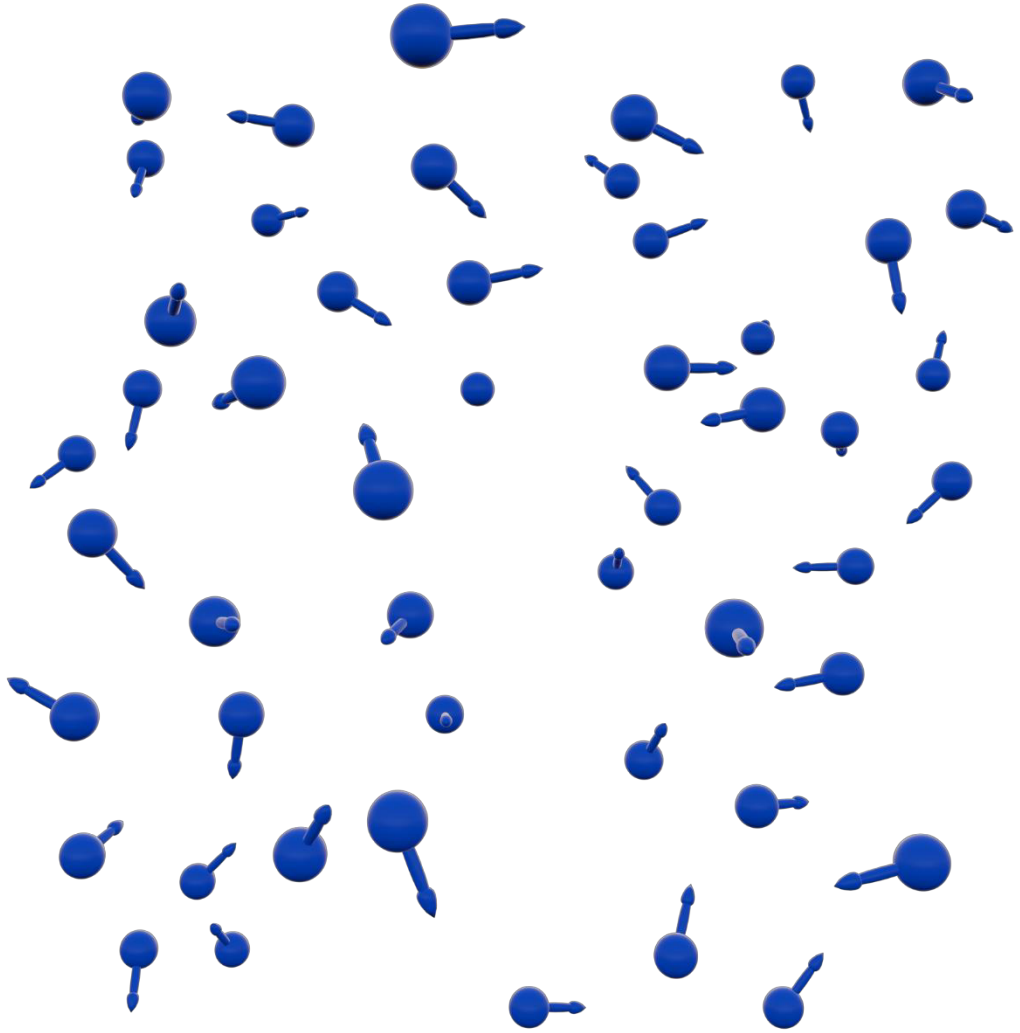
But what it has to do with EPR?



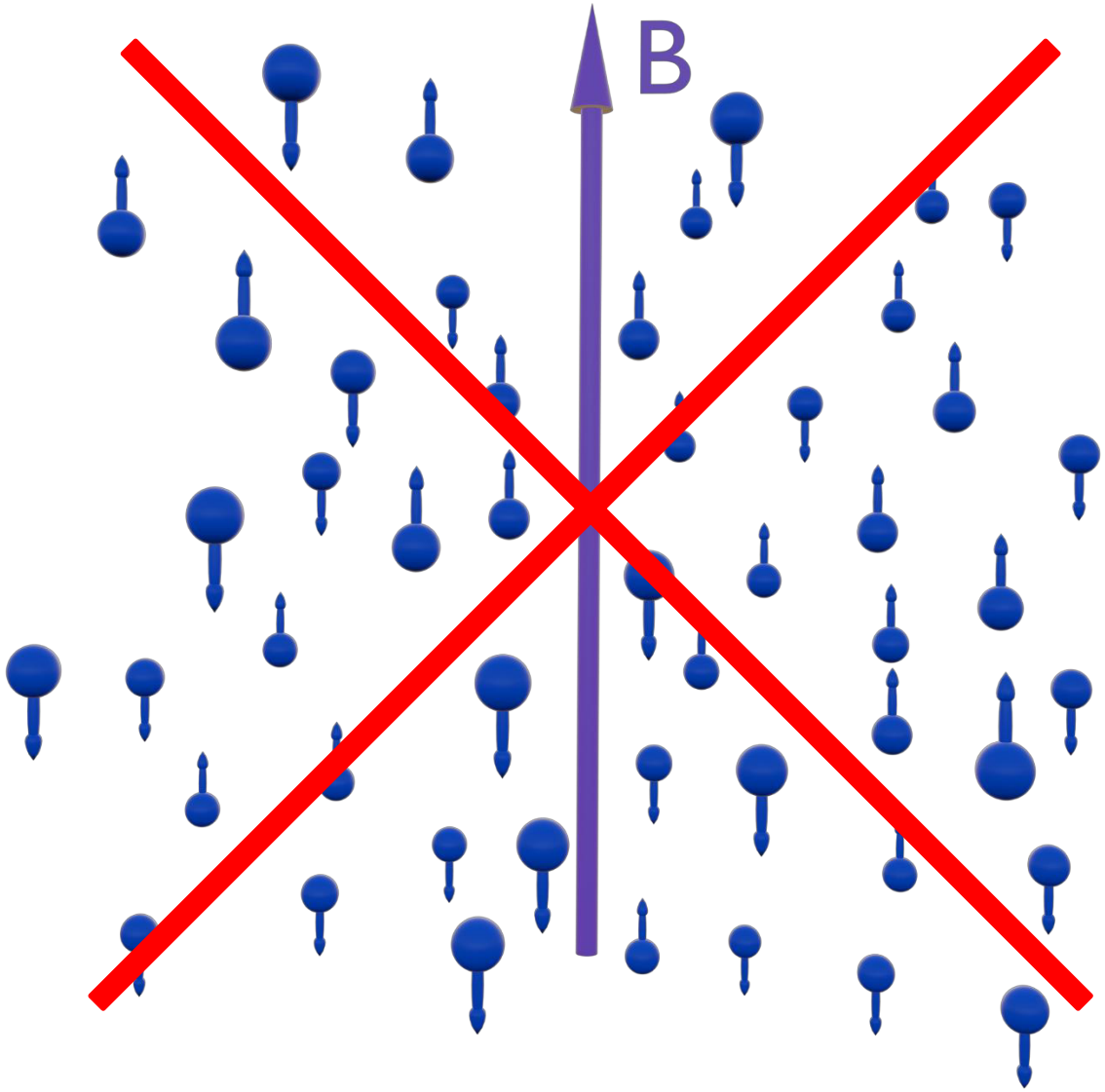


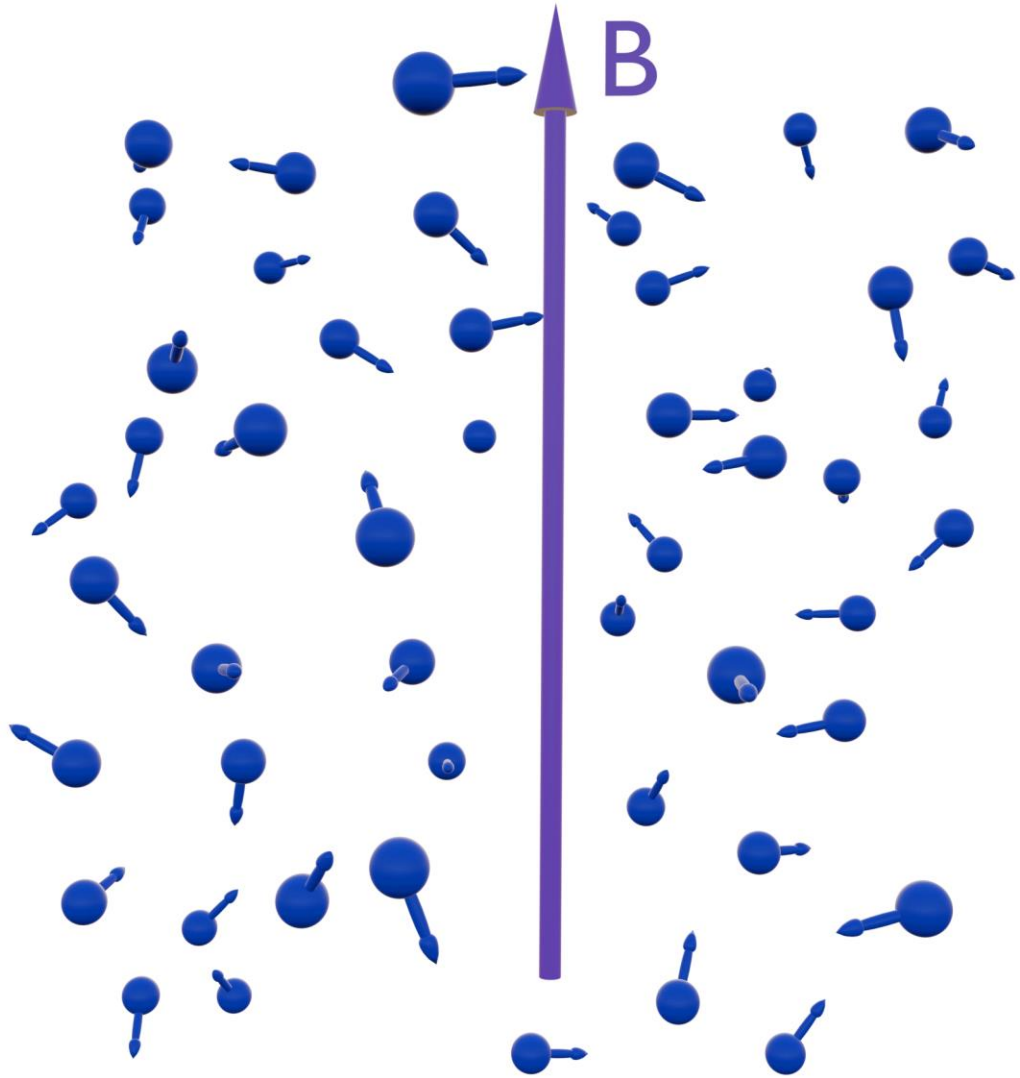
Spins in magnetic field



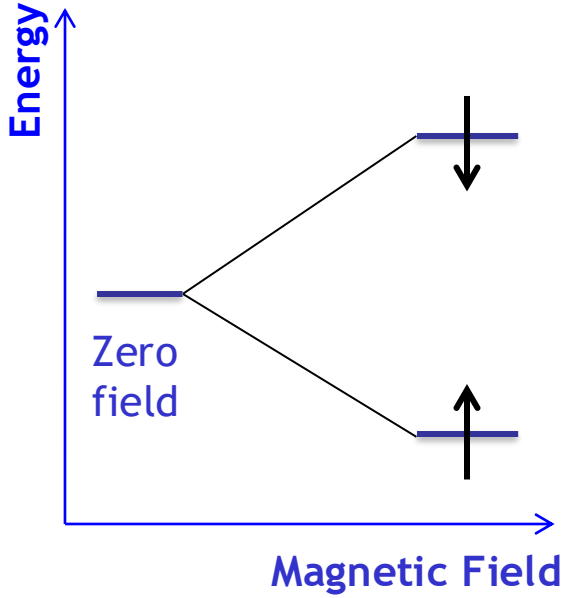


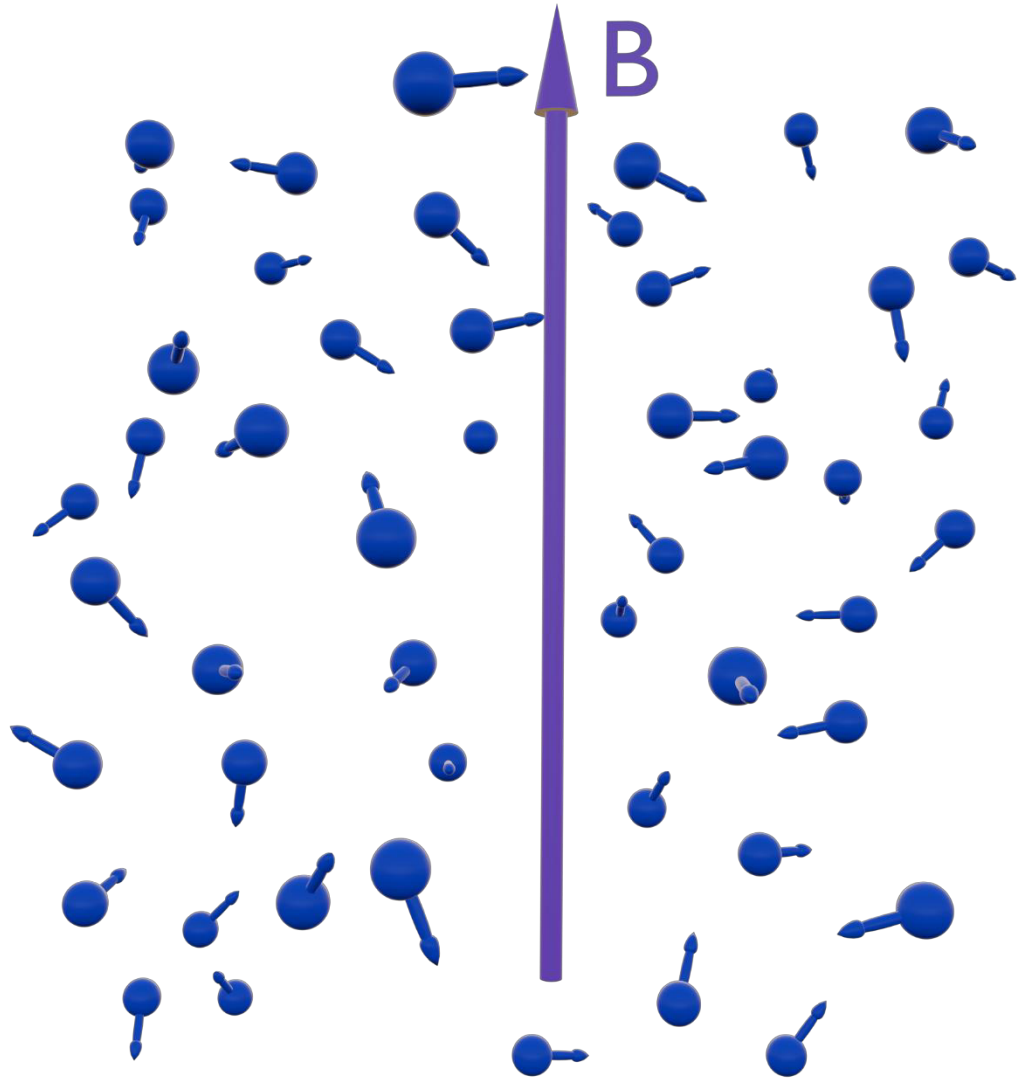
Spins in magnetic field





Spins in magnetic field

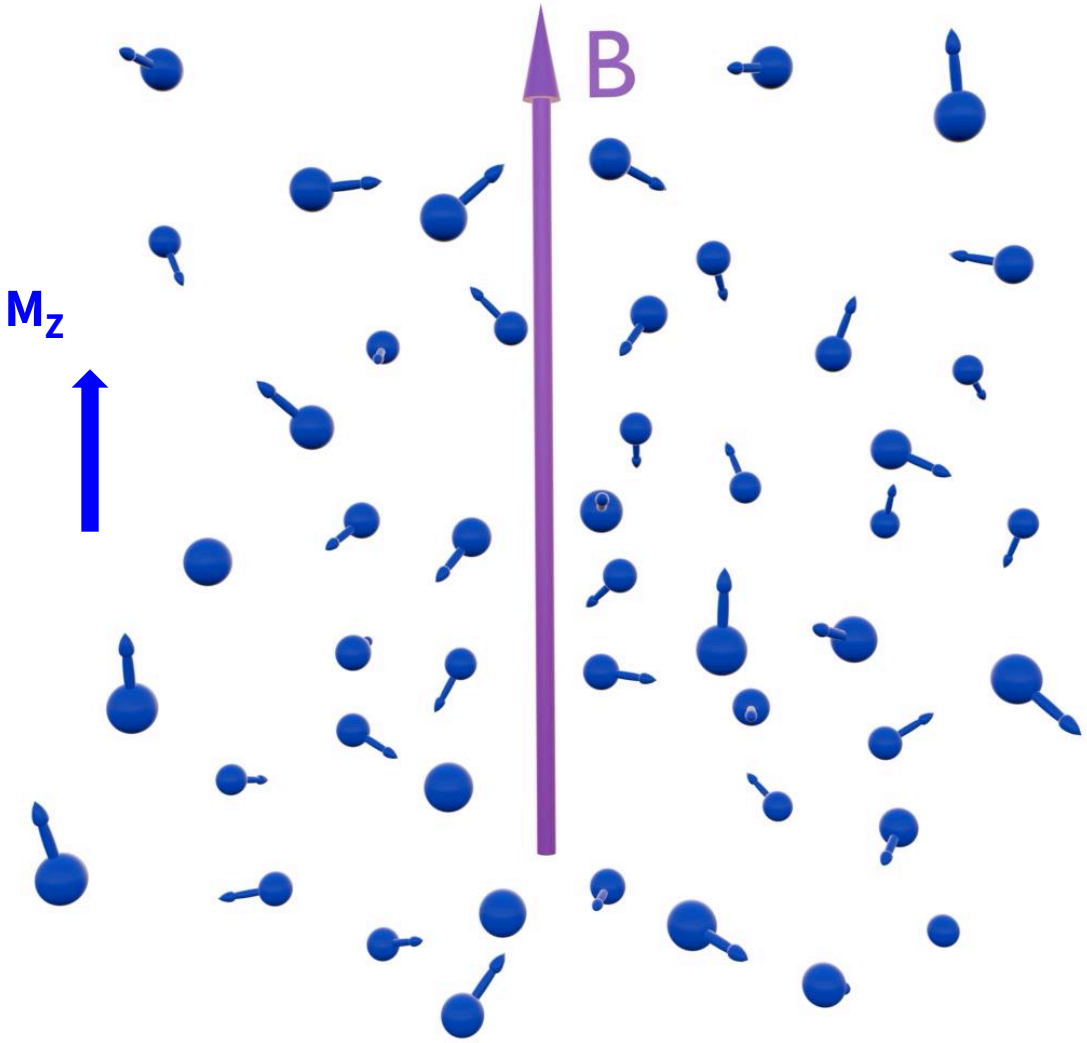




Small fluctuation fields:

Random change of cone angle

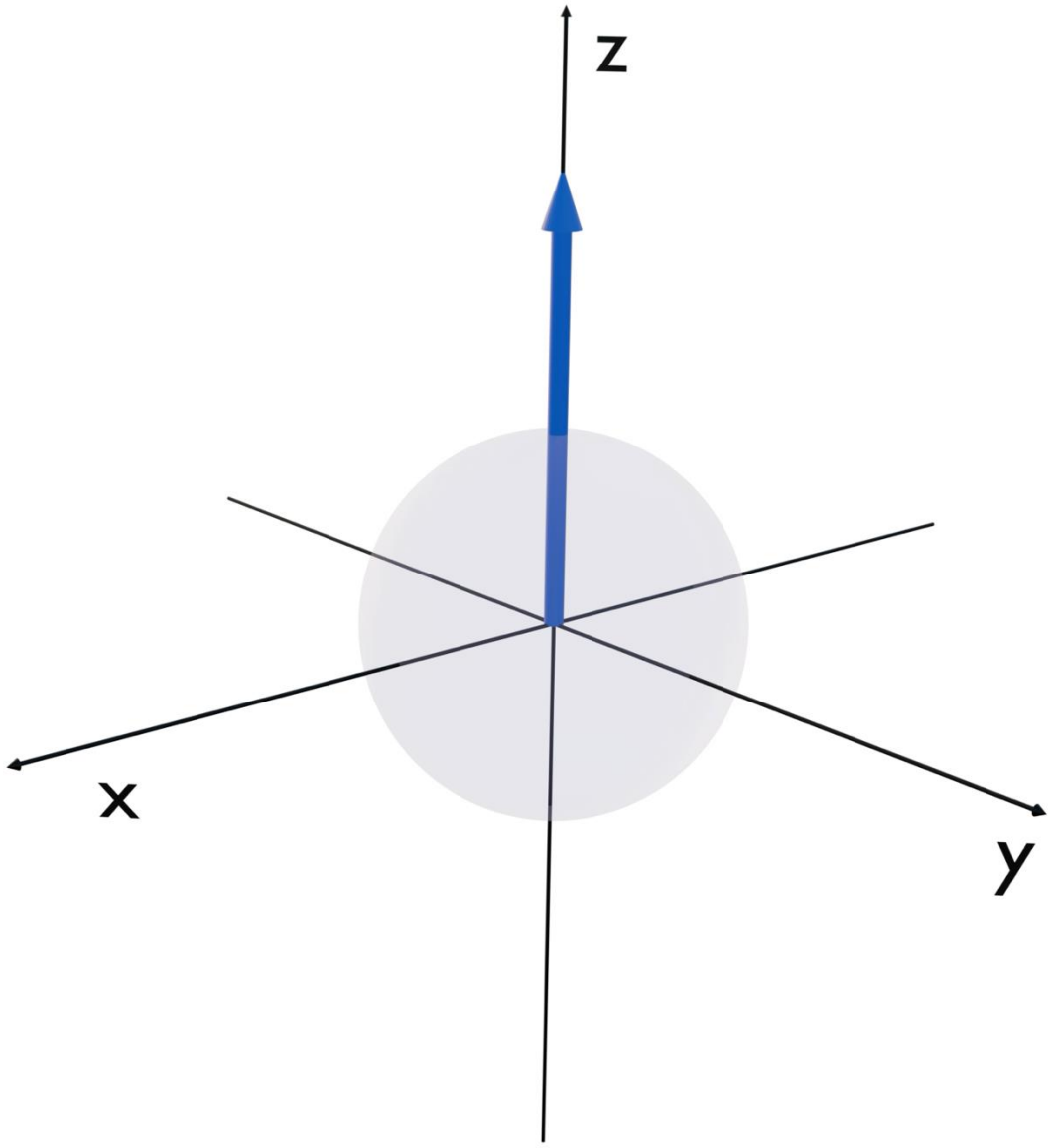
Spins in magnetic field



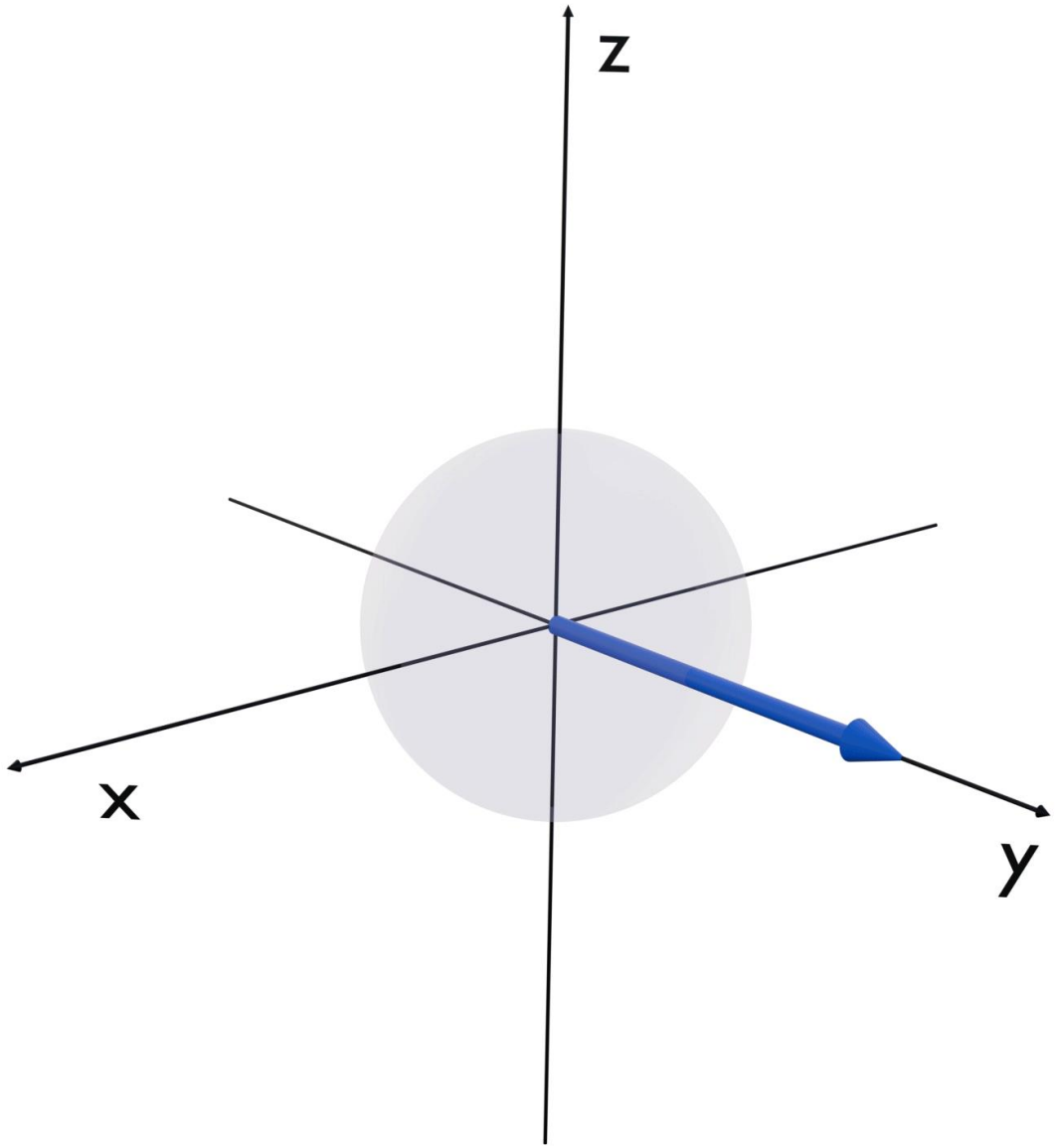
Small fluctuation fields:
Random change of cone angle

Slow build-up of macroscopic magnetization

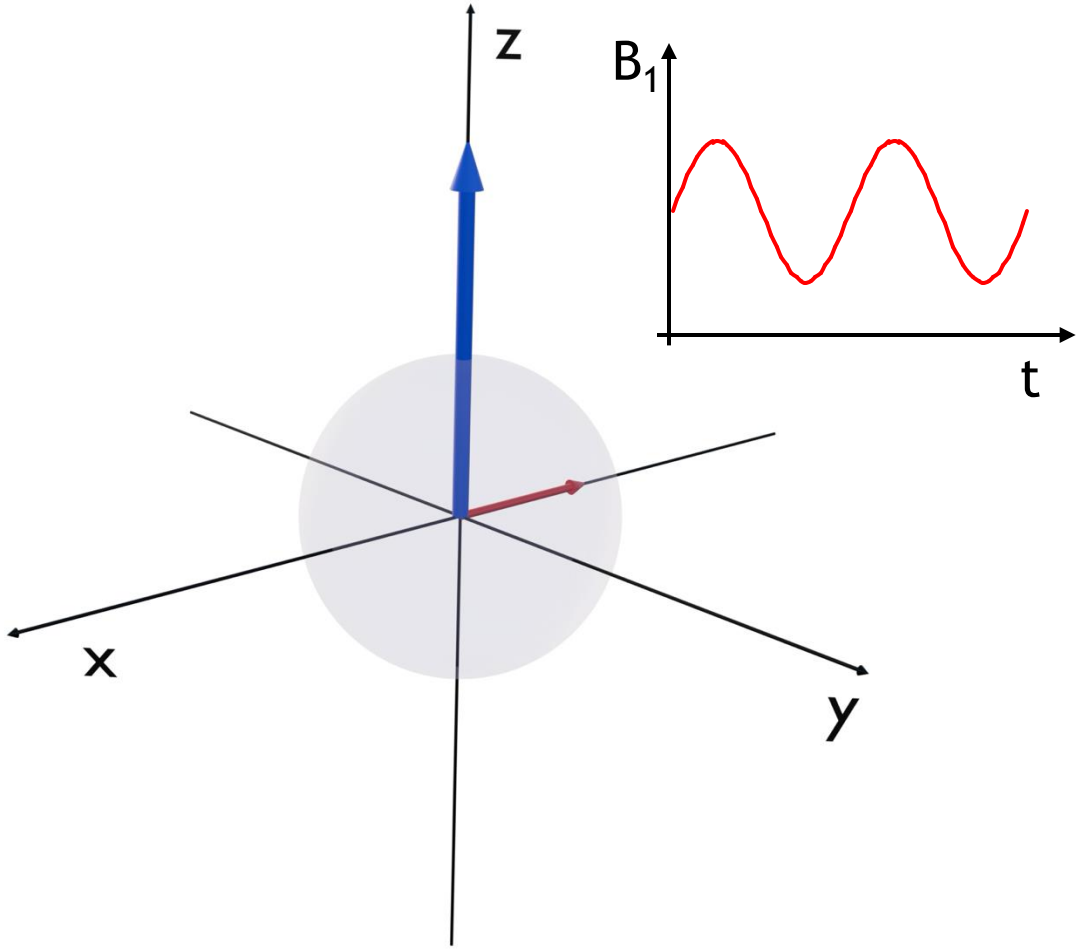
Macroscopic magnetisation rotation



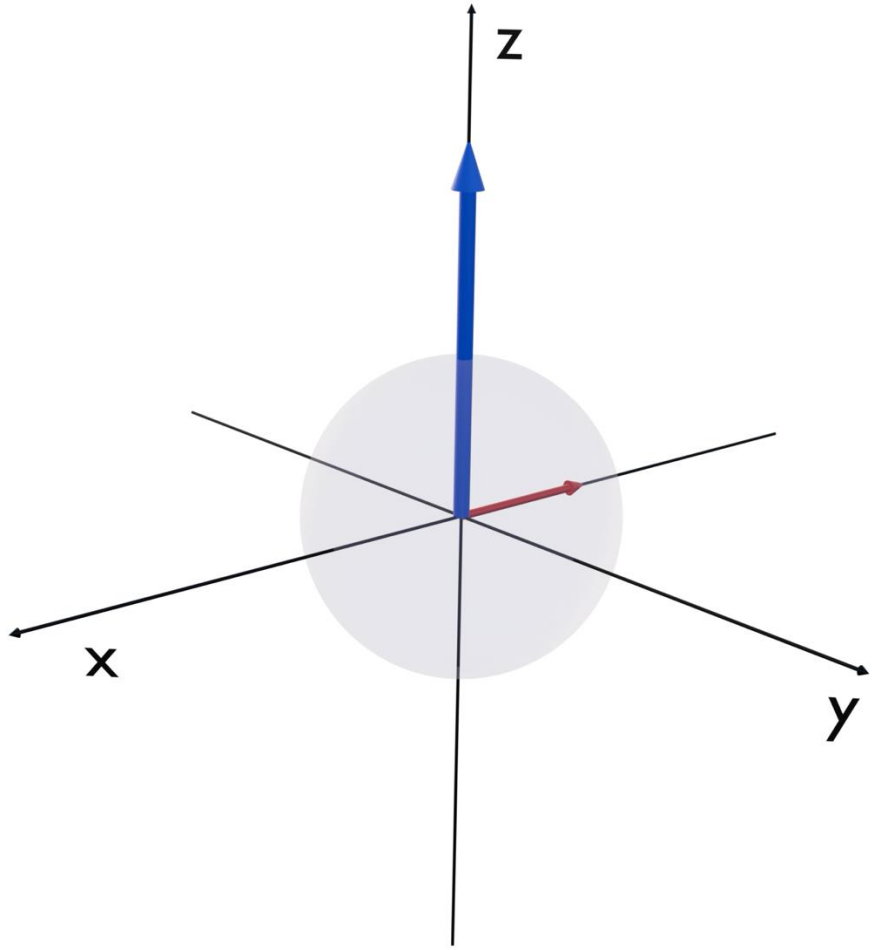
Macroscopic magnetisation rotation



Laboratory frame:



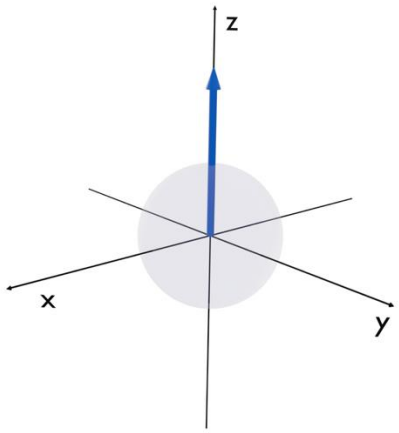
Rotating frame:

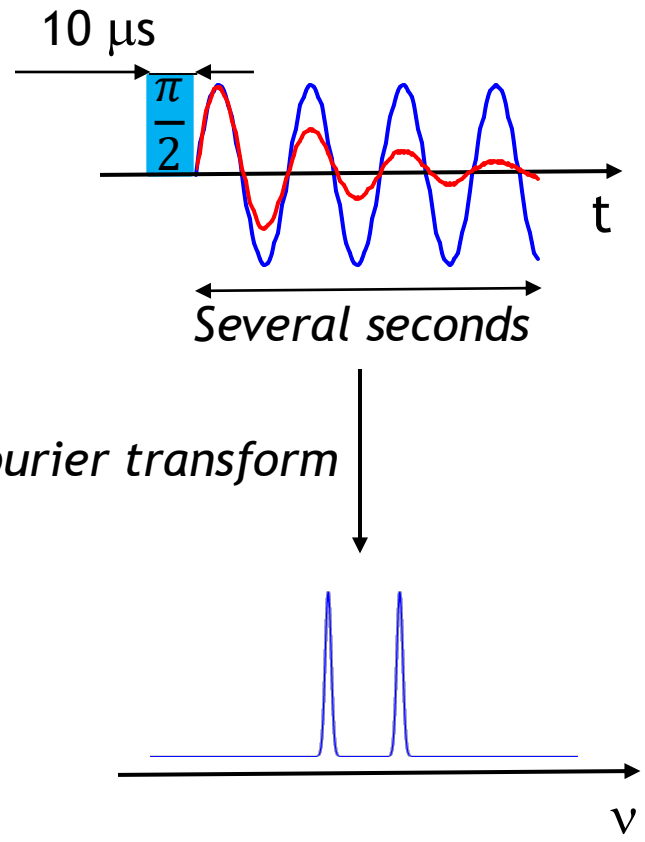


Axis of rotation (additional field B_1) rotates with time ⟶ A microwave pulse

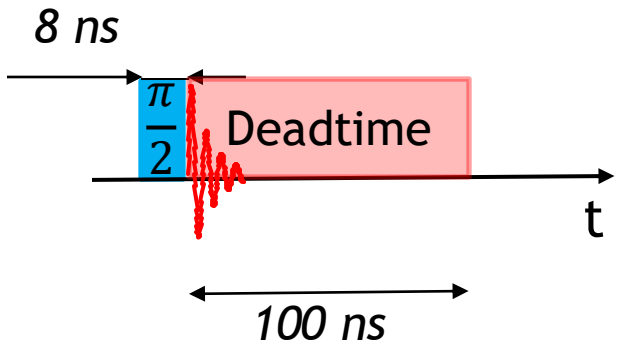
Pulsed Fourier spectroscopy

NMR

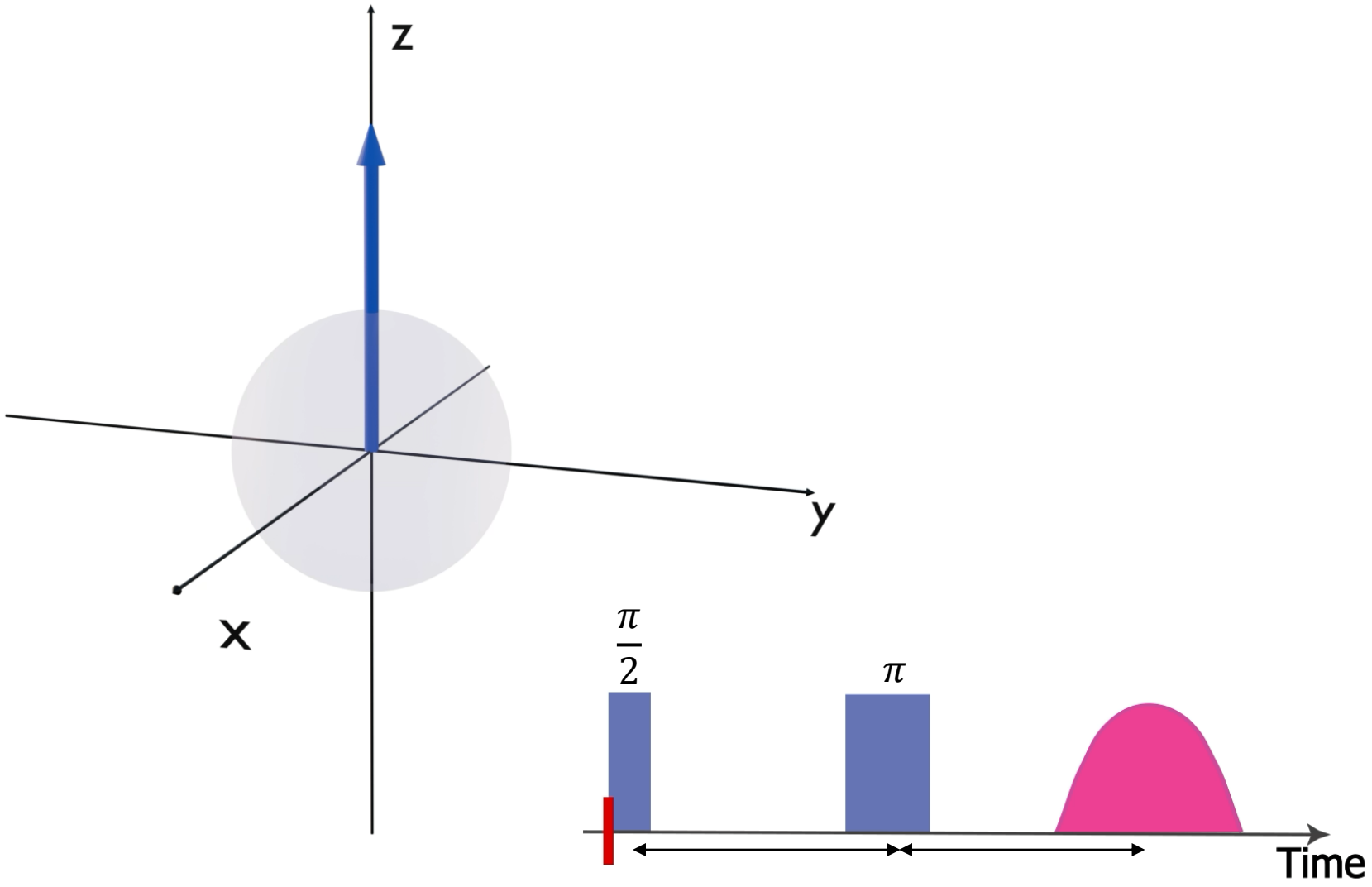




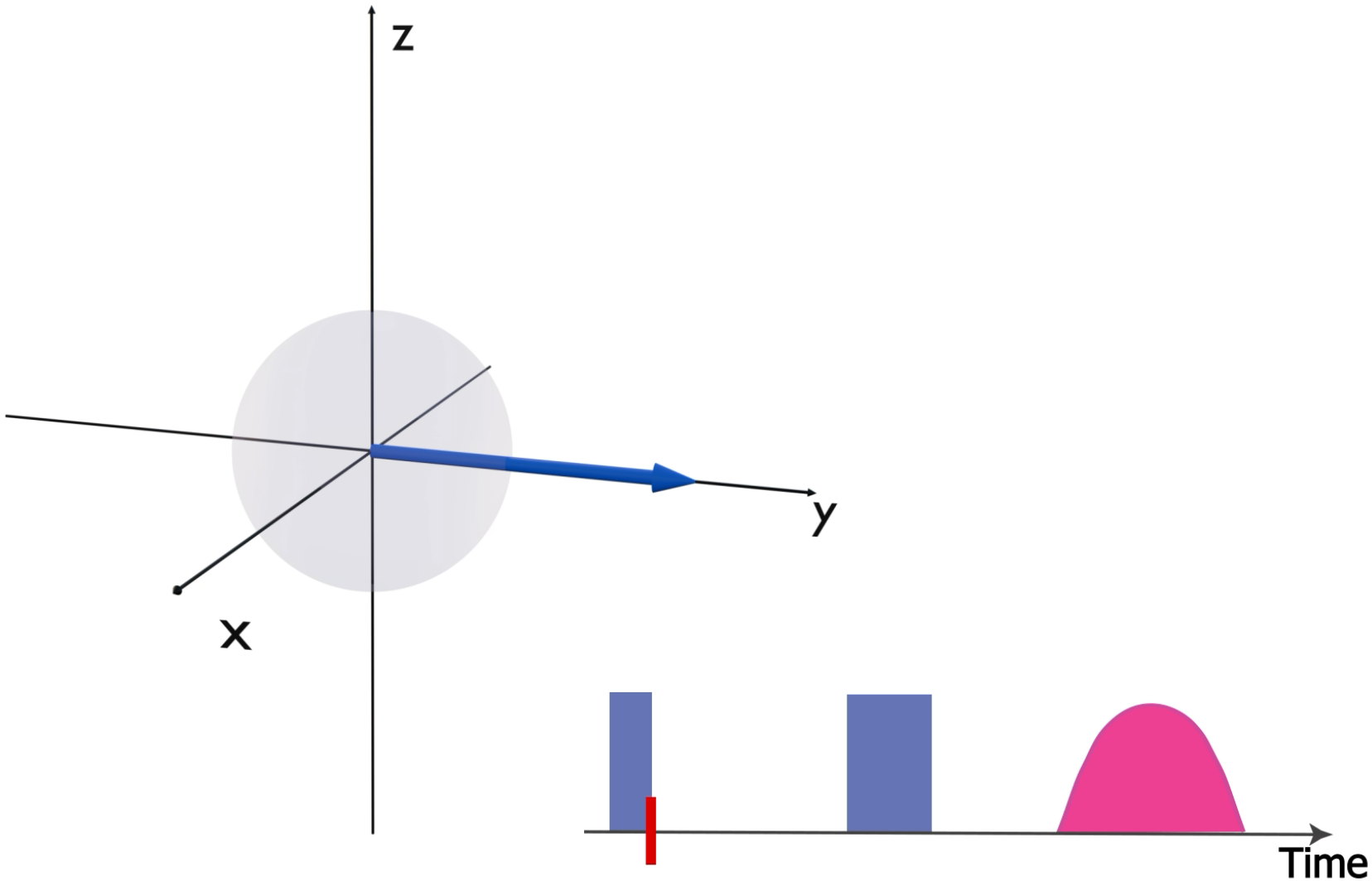
EPR



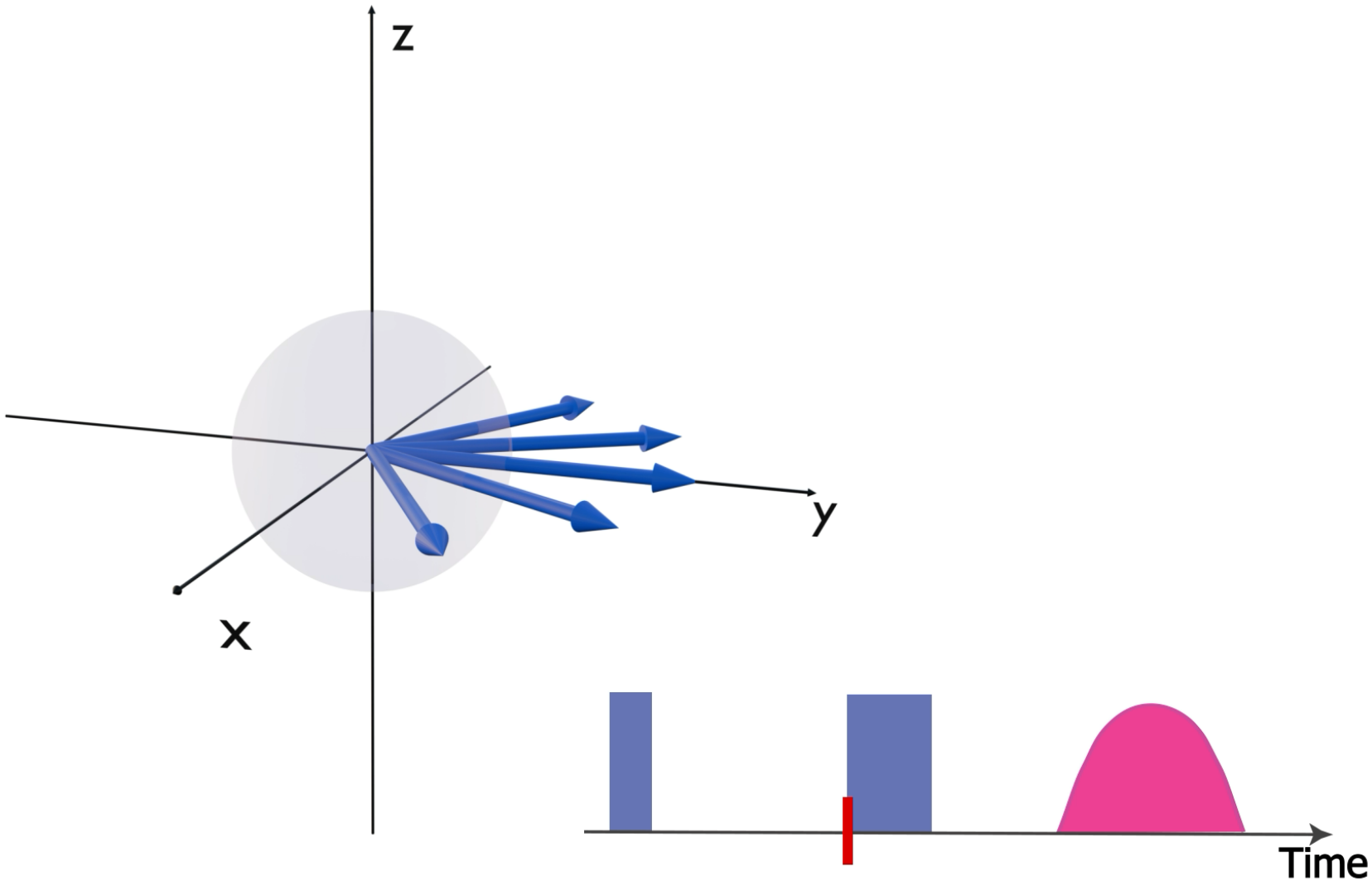
Hahn spin echo in a rotating frame



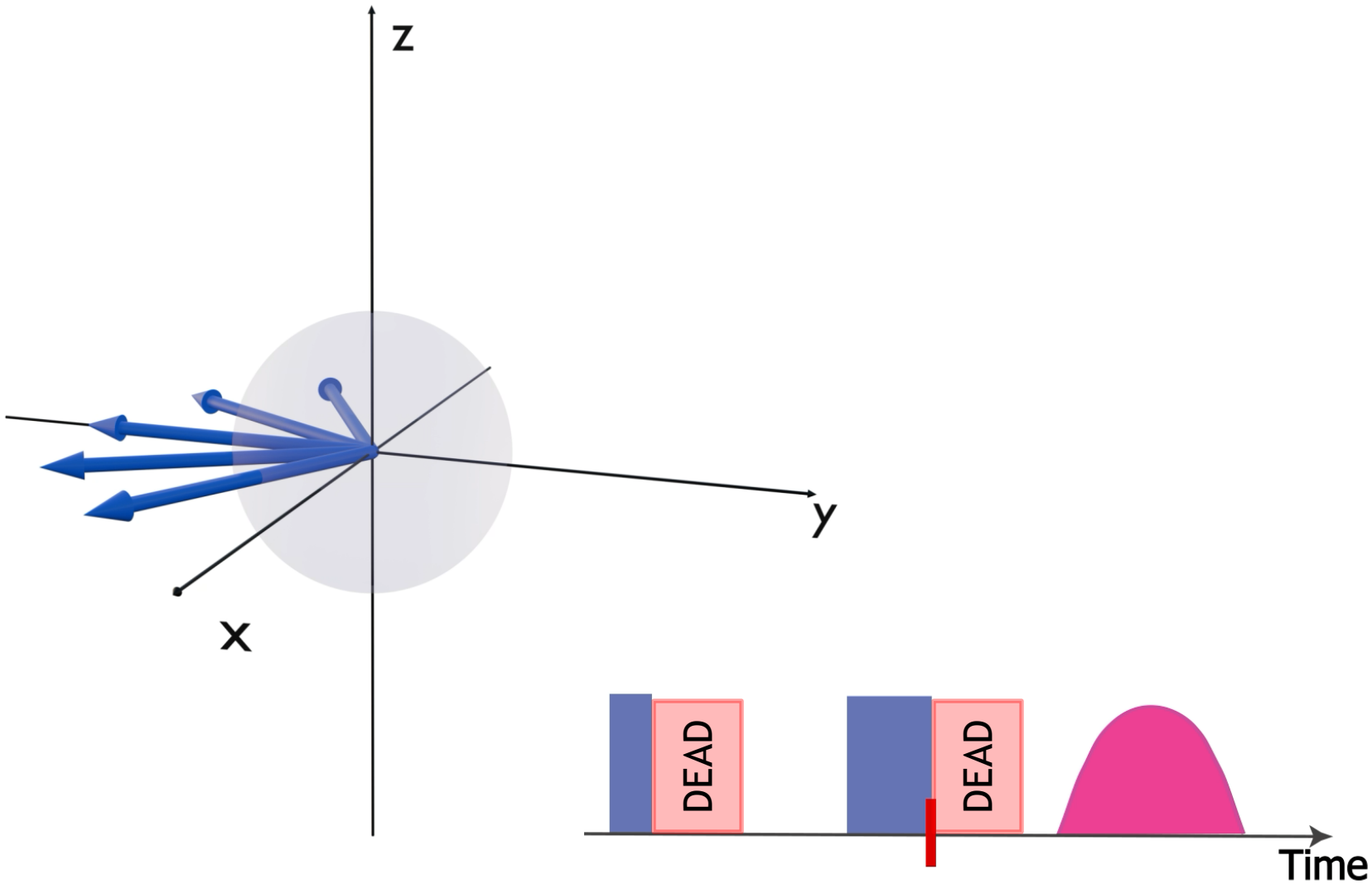
Hahn spin echo



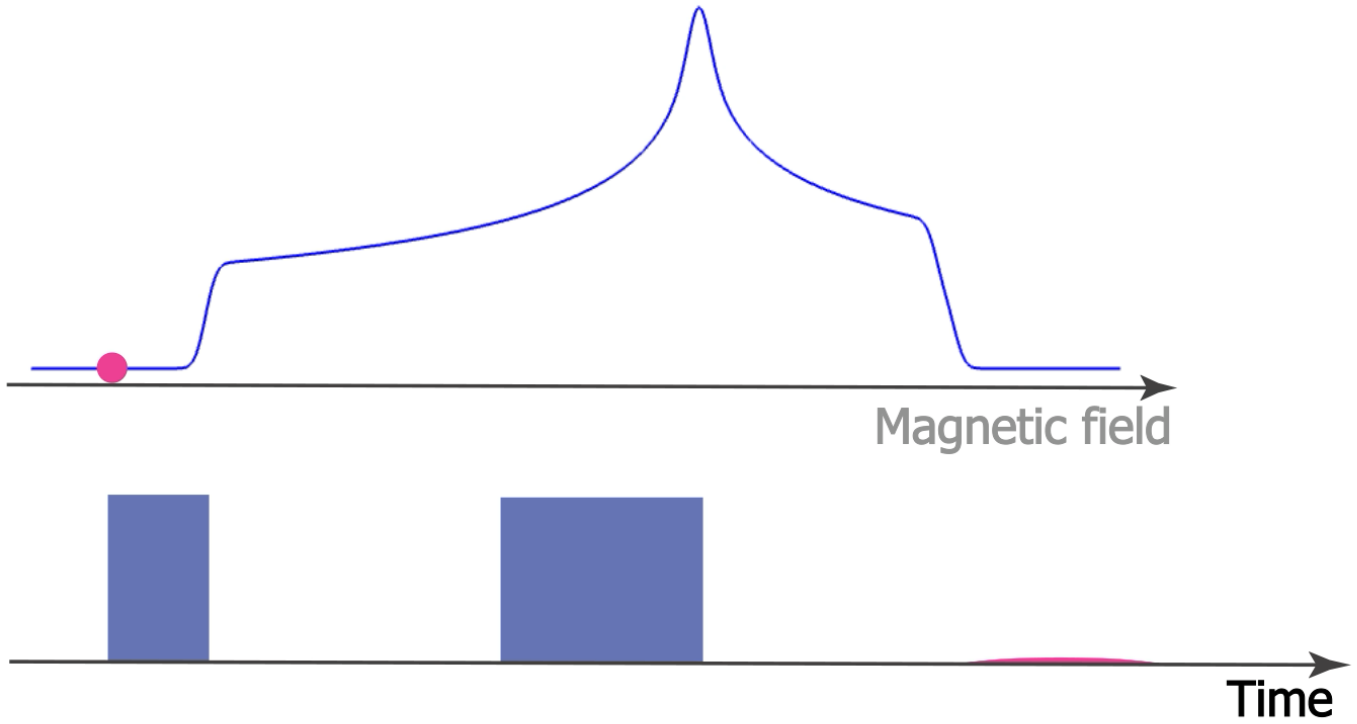
Hahn spin echo



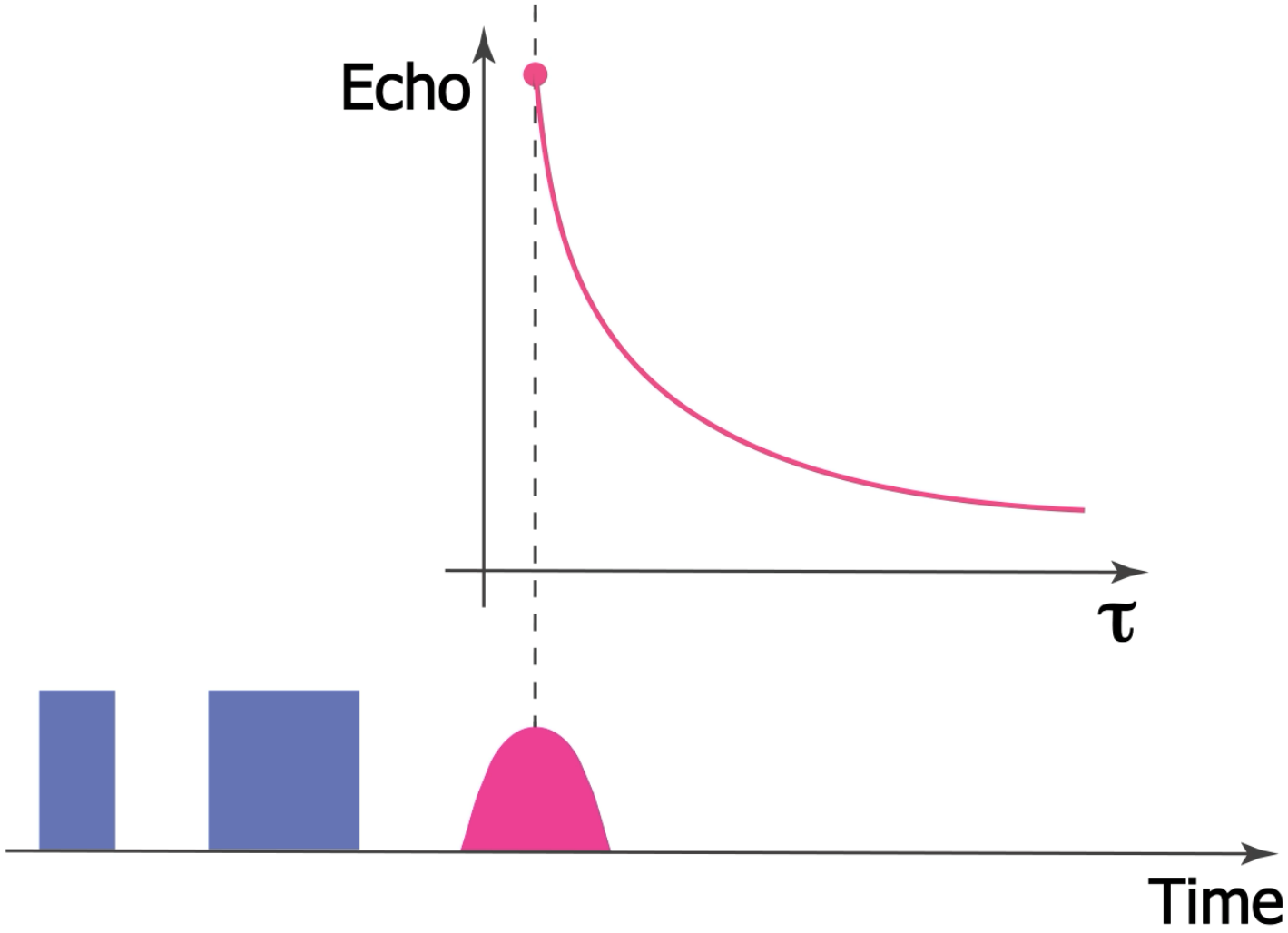
Hahn spin echo

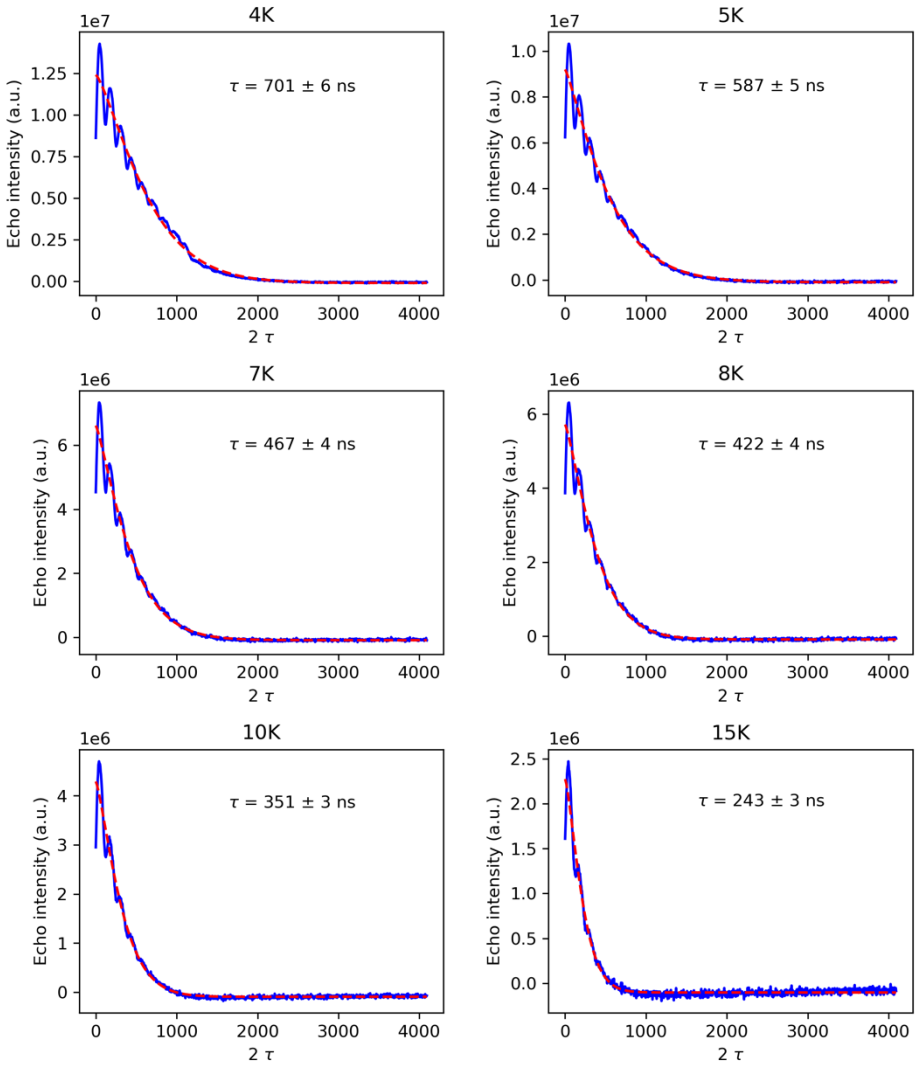


Echo-detected field-sweep spectra



T_m relaxation measurement





How to increase spin phase memory time

Problem	Possible solution

• Electron–electron dipolar interactions	• Dilute the paramagnetic centers
	  • In a solution
	  • In a diamagnetic solid matrix

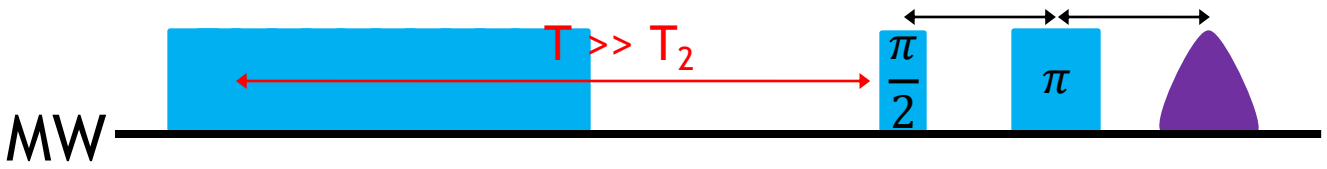
• Interactions with nuclear spins	• Use nuclear-spin-free isotopes
	  • Isotopically purified samples
	  • Or at least deuterated solvent

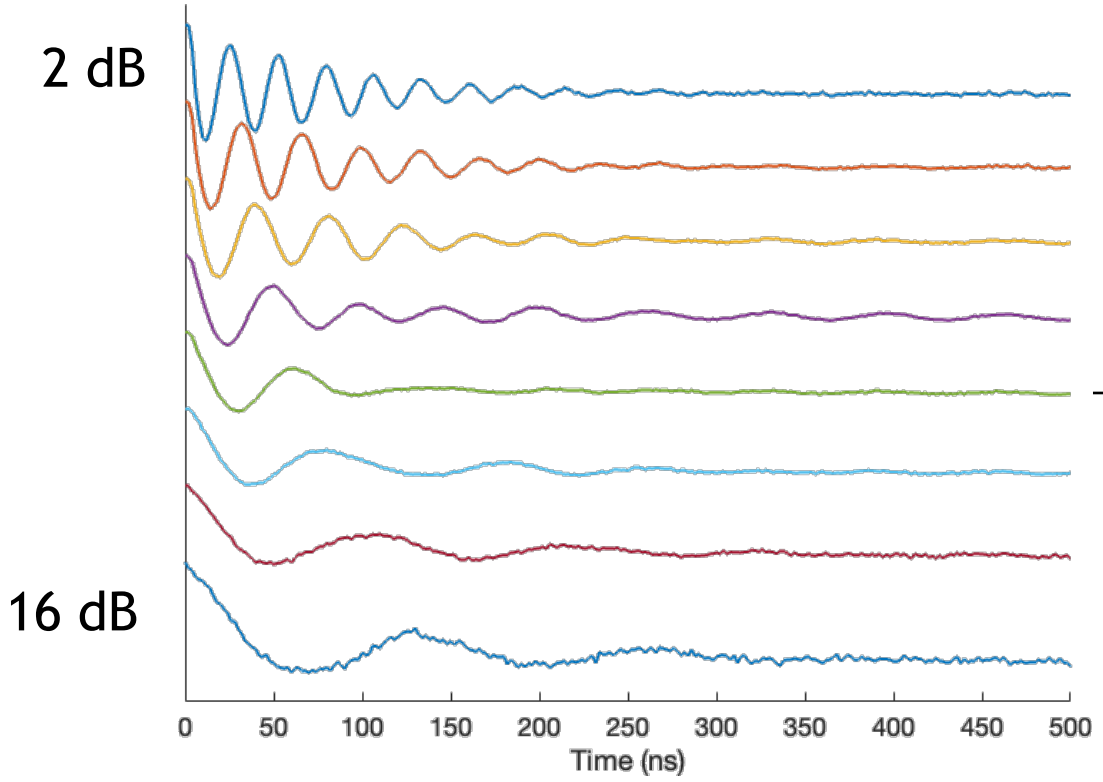
• Phonon-induced decoherence (vibrations)	• Low temperature

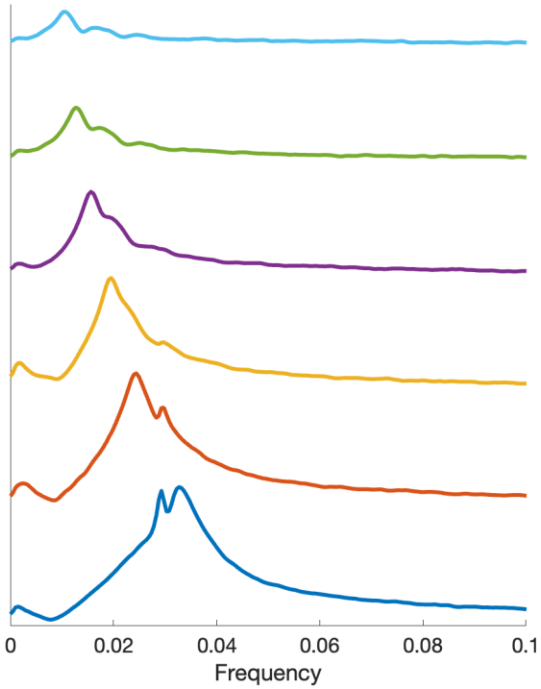
A long T_m is necessary but not sufficient for quantum computing

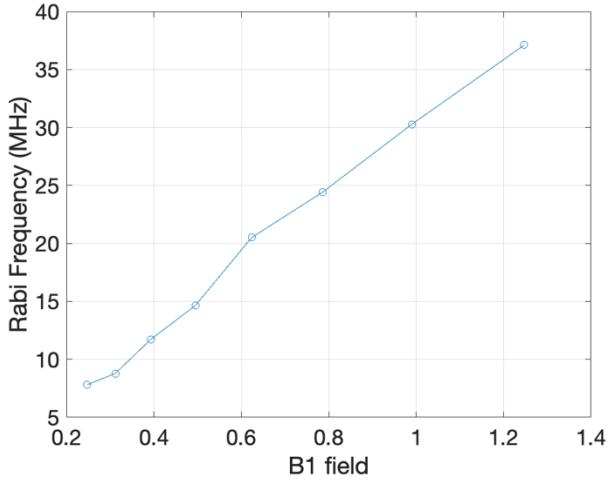
Quantum decoherence ≠ EPR relaxation

Rabi oscillations

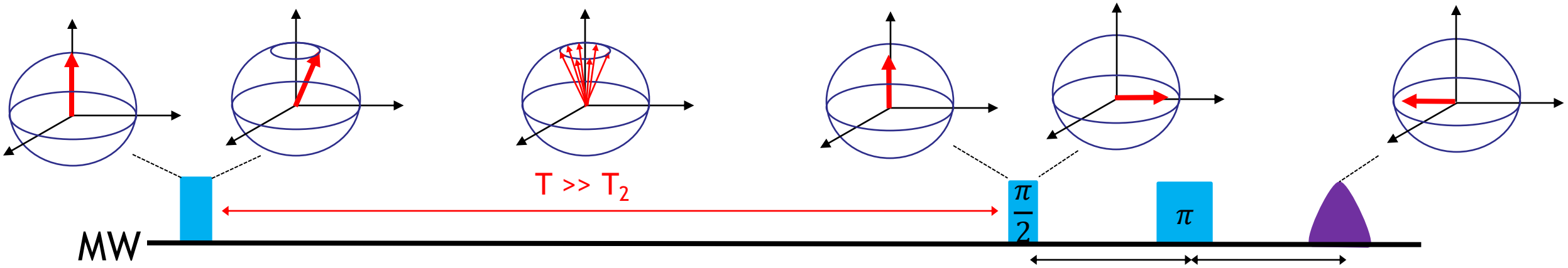




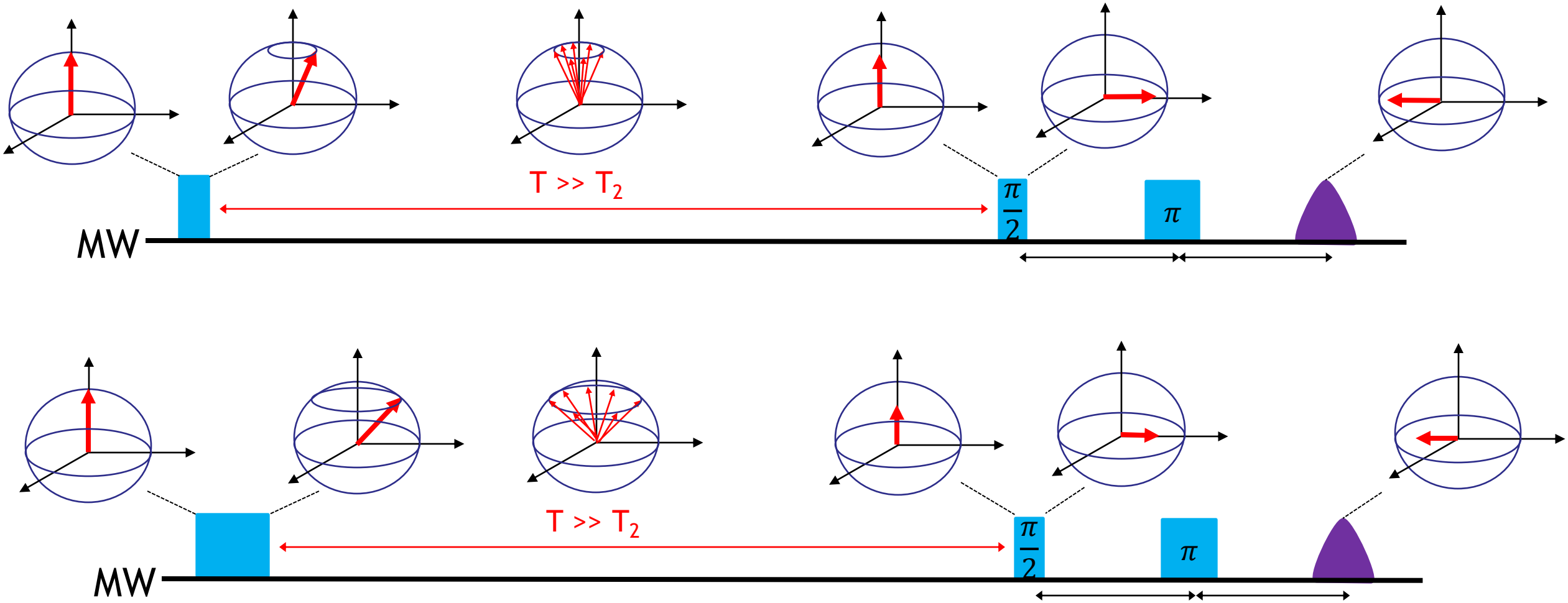




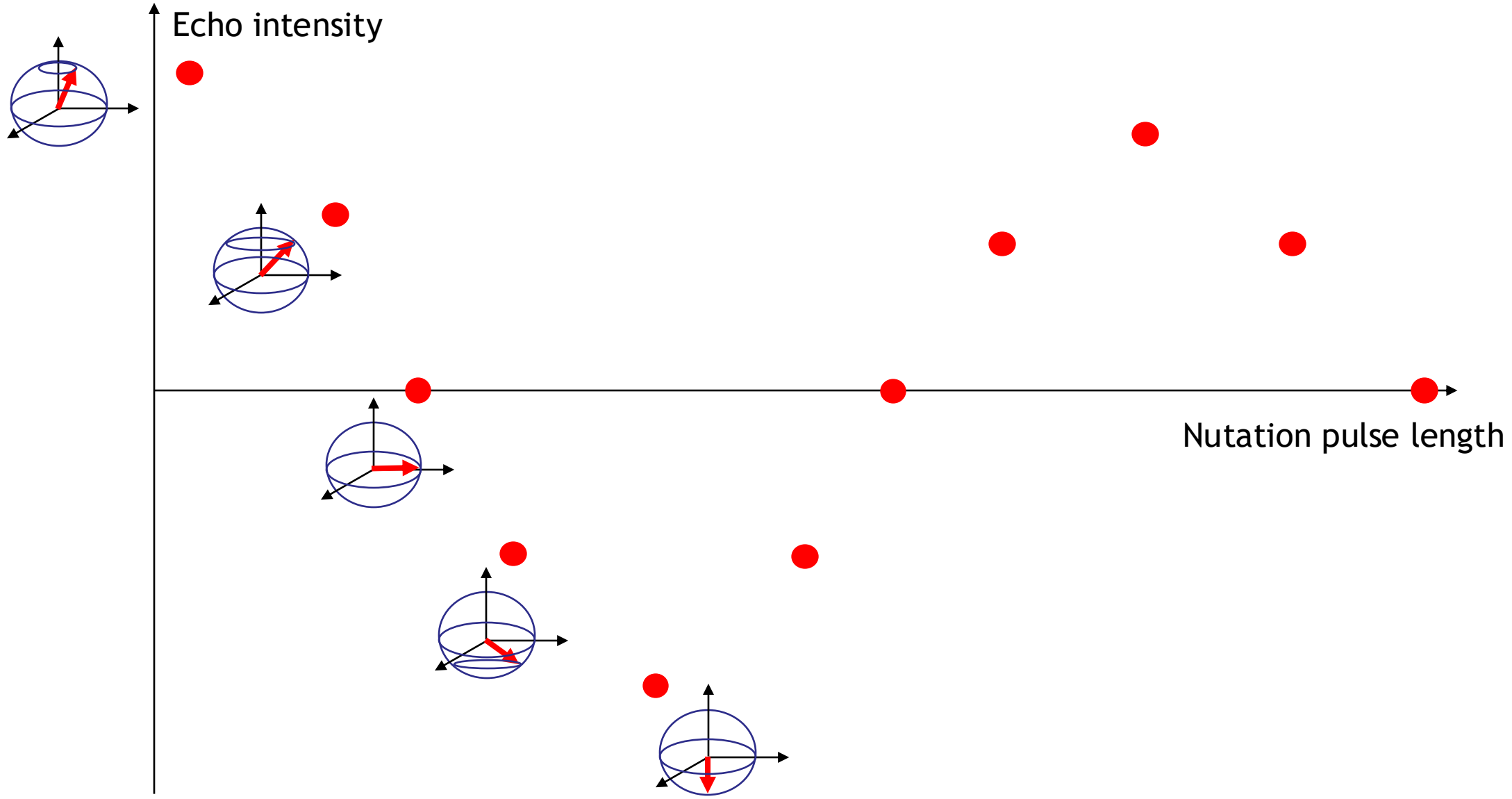
Rabi oscillations



Rabi oscillations



Rabi oscillations



Conclusions

Measuring EPR is not doing quantum computing

EPR spectroscopy and quantum computing share concepts like spin manipulation, coherence, and decoherence, but they serve very different purposes

EPR is macroscopic

Pulsed EPR manipulates large ensembles of spins and detects classical magnetization, not individual quantum states

Relaxation is not quantum decoherence

Hahn echo and phase memory time describe ensemble-averaged dephasing, not true quantum decoherence or entanglement loss

No arbitrary spin state by Rabi oscillations

Rabi oscillations in EPR represent classical population transfer in a spin ensemble, not single-qubit rotations or superposition control

Additional reading (watching) on quantum computing

But what is quantum computing? (Grover's Algorithm)

1.1M views • 12 days ago

3Blue1Brown

Timestamps: 0:00 - Misconceptions 6:03 - The state vector 12:00 - Qubits 15:52 ·

4K Subtitles

10 chapters Misconceptions | The state vector | Qubits | The vibe ·