Universität Konstanz

Mixed quantum states, relaxation and decoherence

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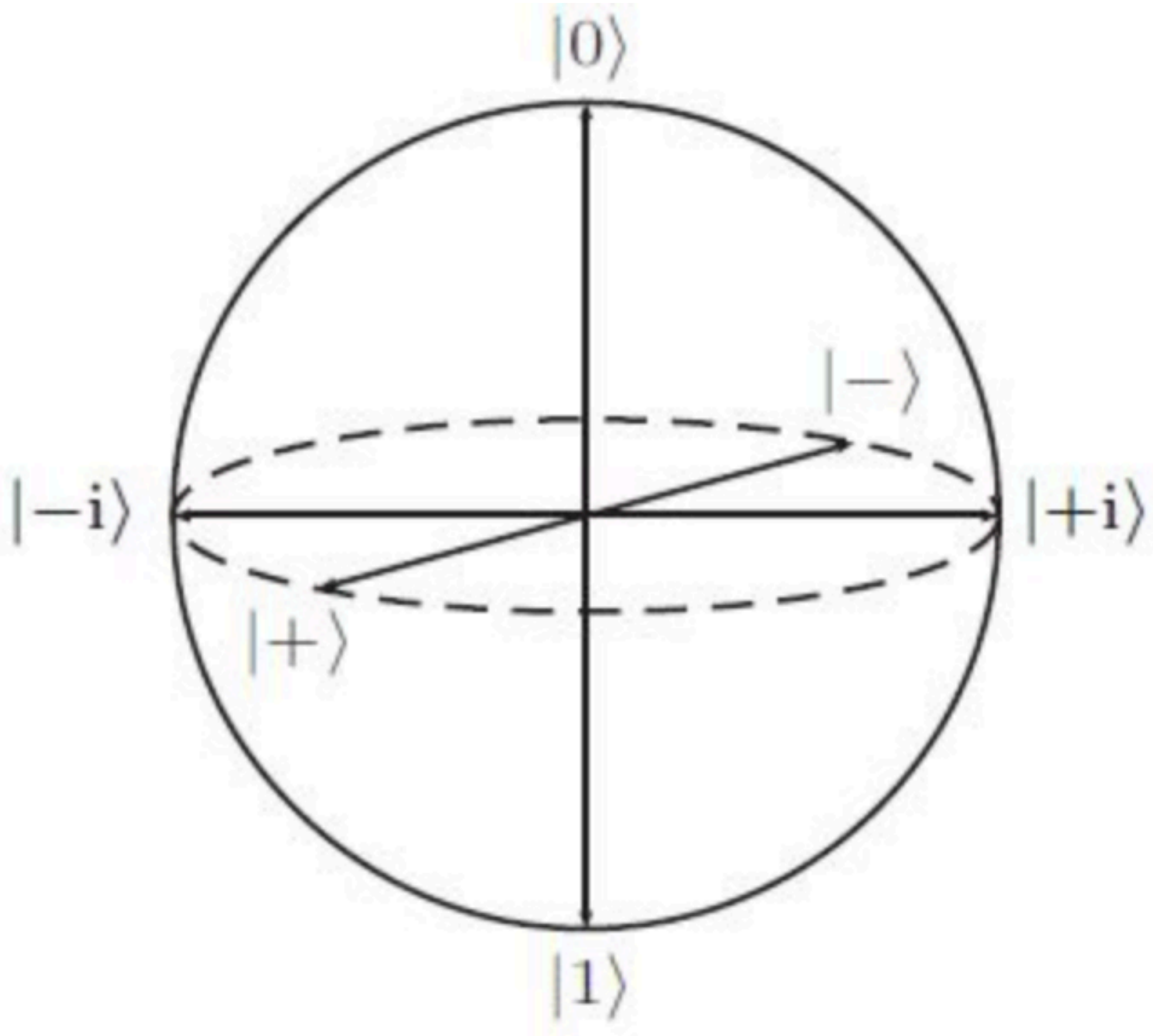
Pure vs. mixed states

- Well known: quantum state as a vector $|\psi\rangle = \sum_i c_i |i\rangle$ with $\sum_i |c_i|^2 = 1$

  Pure state

- Imagine qubit in state $|\psi\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$
- Measurement in $\{|0\rangle, |1\rangle\}$-basis with outcome probabilities $p_0 = p_1 = 1/2$
- Measurement result is discarded
  ⇒state after measurement is $|0(1)\rangle$ with probability $p_{0(1)}$
- Second measurement has same outcome probabilities
- Qubit state is **not** $|\psi\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$
- Need method to
  - incoherently superimpose (mix) pure states
  - respect observer's knowledge



Kevin Garapo, Mhlambululi Mafu, Francesco Petruccione. (2016). Intercept-resend attack on six-state quantum key distribution over collective-rotation noise channels. 中国物理b：英文版, (7), 131-137, CC BY-SA 4.0, https://commons.wikimedia.org/w/index.php?curid=52147296

The density operator

$$\langle A \rangle = \langle \psi | A | \psi \rangle$$

- **Density operator** $\rho = \sum_{ij} c_i c_j^* |i\rangle\langle j| = |\psi\rangle\langle\psi|$ describes same physics as $|\psi\rangle$
- Properties of density operator: 1. $\rho^\dagger = \rho$
  2. $\forall |x\rangle \in \mathcal{H} : \ \langle x|\rho|x\rangle \geq 0$
  3. $\mathrm{tr}\, \rho = 1$
- General form $\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$ with $\sum_i p_i = 1$

  Probability to find state i

The density operator of mixed states

- Measured qubit from earlier (p.2)
- Before measurement: pure state $|\psi\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right)$

„populations“

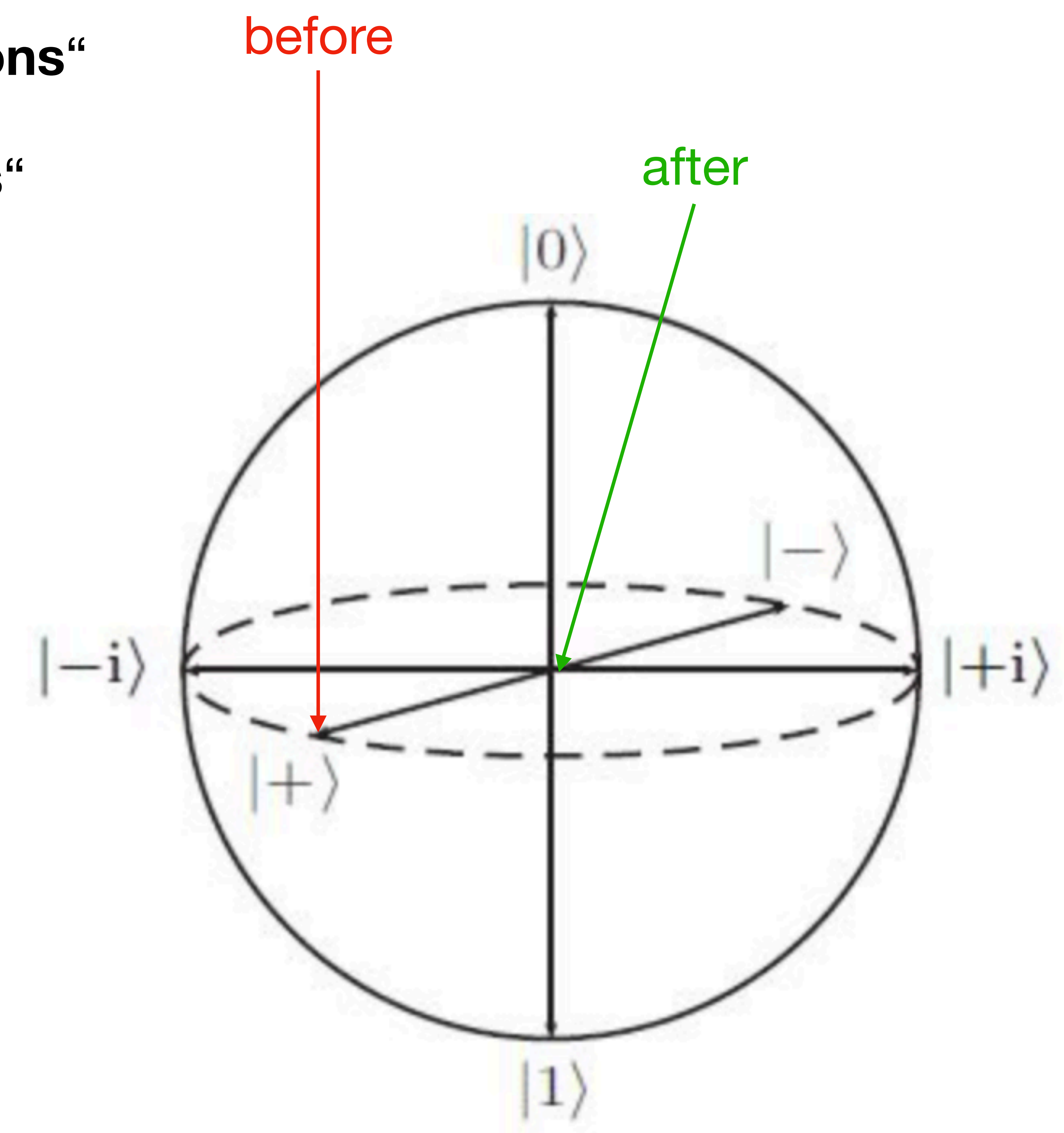
„coherences“

$$\rho = \frac{1}{\sqrt{2}^2}\left(|0\rangle + |1\rangle\right)\left(\langle 0| + \langle 1|\right) = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$$

- After measurement: mixed state of $|0(1)\rangle$ with probabilities $p_{0(1)}$

$$\rho = p_0|0\rangle\langle 0| + p_1|1\rangle\langle 1| = \frac{1}{2}\mathbb{1}$$

- Bloch vector $\vec{p} = (\langle\sigma_x\rangle, \langle\sigma_y\rangle, \langle\sigma_z\rangle)$
- Bloch representation $\rho = \frac{1}{2}(\mathbb{1} + \vec{p}\cdot\vec{\sigma}) = \frac{1}{2}\begin{pmatrix} 1+p_z & p_x - ip_y \\ p_x + ip_y & 1 - p_z \end{pmatrix}$
- General property of **mixed state:** $\mathrm{tr}\rho^2 < 1 \Leftrightarrow \rho = \sum_i p_i|\psi_i\rangle\langle\psi_i| \neq |\phi\rangle\langle\phi|$



Multipartite systems

- Consider bipartite Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$ with density operator

$$\rho = \sum_{ijkl} \rho_{ij,kl} |i\rangle_A |j\rangle_B \, {}_A\langle k|_B\langle l|$$

- Calculate expectation value $\langle O_A \otimes \mathbb{1} \rangle = \mathrm{tr}[\rho(O_A \otimes 1)] = \sum_{ij,kl} \rho_{ij,kl} \, {}_A\langle k|O_A|i\rangle_A \, {}_B\langle l|j\rangle_B$

- Density operator of reduced system A given by **partial trace** $\rho_A = \mathrm{tr}_B \rho = \sum_i \, {}_B\langle i|\rho|i\rangle_B$

- **State purification**: every mixed state in $\mathcal{H}$ can be written as pure state in $\mathcal{H} \otimes \mathcal{H}_C$

$$\rho = \sum_{i=1}^{r} p_i |\psi_i\rangle\langle\psi_i| = \mathrm{tr}_c |\psi\rangle\langle\psi| \text{ where } |\psi\rangle = \sum_{i=1}^{r} \sqrt{p_i} |\psi_i\rangle|\phi_i\rangle$$

Generalized measurements

- For each possible measurement outcome m there is one **measurement operator** M_m

  Completeness relation $\sum_m M_m^\dagger M_m = \mathbb{1}$

  Probability for outcome m: $p_m = \mathrm{tr}\left(M_m \rho M_m^\dagger\right)$

  State after measurement: $\rho_f = \frac{M_m \rho M_m^\dagger}{p_m}$

- Simplest example: orthogonal **projective measurements** $M_m M_n = \delta_{mn} M_m$

  system state is projected to eigenstate of observable

  Born's rule $p_m = \mathrm{tr}\left(M_m^\dagger M_m \rho\right) = \mathrm{tr}\left(M_m M_m \rho\right) = \mathrm{tr}\left(M_m \rho\right) = \langle M_m \rangle$

- In general: **weak measurements**

- Remember measurement with discarded outcomes? $\rho_i = \frac{1}{2}\left(|0\rangle + |1\rangle\right)\left(\langle 0| + \langle 1|\right) \rightarrow \rho_f = \frac{1}{2}\left(|0\rangle\langle 0| + |1\rangle\langle 1|\right)$
- **Non-selective measurement**: $\rho_f = \sum_m M_m \rho_i M_m^\dagger$

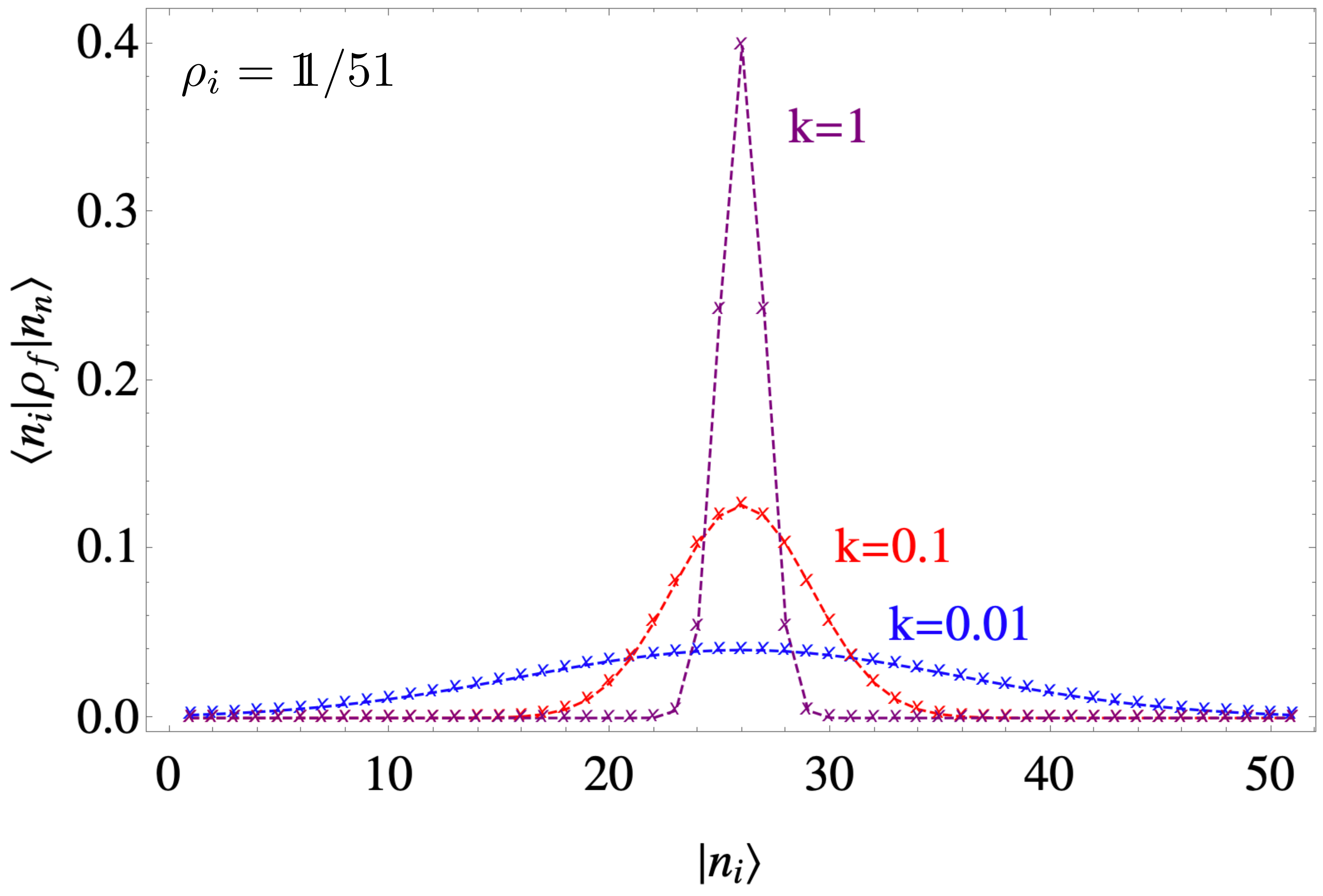
- $\{F_m, \forall m\} := \{M_m^\dagger M_m, \forall m\}$ often referred as **POVM** (positive operator valued measure)

Examples for general measurements

- Measurement operator weighted sum of projectors $M_m = \frac{1}{N}\sum_n e^{-k(n-m)^2/4}|n\rangle\langle n|$
- Choose initial state $\rho_i = \mathbb{1}/N$
- Final state mixture of basis states with Gaussian distribution

$$\rho_f = \frac{M_m \rho_i M_m^\dagger}{\mathrm{tr}\left(M_m \rho_i M_m^\dagger\right)} = \frac{1}{N}\sum_n e^{-k(n-m)^2/2}|n\rangle\langle n|$$

- $k \to 0$: no information gain
  $k \to \infty$: projective measurement
- k is **measurement strength**



Time evolution beyond unitaries

- Time evolution in closed quantum systems is unitary $|\psi'\rangle = U|\psi\rangle$

$$\rho' = |\psi'\rangle\langle\psi'| = U|\psi\rangle\langle\psi|U^\dagger$$

- Time evolution in closed systems does not create or annihilate information

What if subsystems are added or removed? $\rho \mapsto \rho \otimes \rho_B$

$$\rho \mapsto \rho_A = \mathrm{tr}_B\ \rho$$

- Consider state $\rho = \rho_A \otimes |0\rangle\langle 0|$ in bipartite Hilbert space $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$

- Time evolution in subsystem A: $\rho'_A = \mathrm{tr}_B \left[U_{AB}(\rho_{AB} \otimes |0\rangle\langle 0|) U^\dagger_{AB} \right]$

- **Kraus representation** of linear **superoperator** Λ with **Kraus operators** M_μ

Time evolution beyond unitaries

$$\rho'_A = \sum_\mu M_\mu \rho_A M_\mu^\dagger$$

$$M_\mu = {}_B\langle \mu | U_{AB} | 0 \rangle_B$$

- Maps density operators to density operators, $\sum_\mu M_\mu^\dagger M_\mu = \mathbb{1}_A$

$$1.\ (\rho'_A)^\dagger = \rho'_A$$
$$2.\ \forall |x\rangle \in \mathcal{H}_A :\ \langle x|\rho'_A|x\rangle \geq 0$$
$$3.\ \mathrm{tr}\ \rho'_A = 1$$

- Not necessarily unitary: information can be transferred into or out of subsystem

- Non-selective measurement as superoperator $\rho_f = \sum_\mu M_\mu \rho M_\mu^\dagger = \Lambda \rho$

  Interaction with inaccessible environment = re-preparation of system state, transfer of information to environment

Amplitude damping

- Qubit excitation is transferred to environment with probability p, $U_A : \begin{cases} |0\rangle_Q|0\rangle_E \mapsto |0\rangle_Q|0\rangle_E \\ |1\rangle_Q|0\rangle_E \mapsto \sqrt{1-p}|1\rangle_Q|0\rangle_E + \sqrt{p}|0\rangle_Q|1\rangle_E \end{cases}$

$$M^A_\mu = {}_E\langle\mu|U_A|0\rangle_E \quad \Rightarrow \quad M^A_0 = \begin{pmatrix} 1 & 0 \\ 0 & \sqrt{1-p} \end{pmatrix},\ M^A_1 = \begin{pmatrix} 0 & \sqrt{p} \\ 0 & 0 \end{pmatrix}$$

- Initial density operator ρ evolves to

$$\rho' = M^A_0 \rho \left(M^A_0\right)^\dagger + M^A_1 \rho \left(M^A_1\right)^\dagger = \begin{pmatrix} \rho_{00} + p\rho_{11} & \sqrt{1-p}\,\rho_{01} \\ \sqrt{1-p}\,\rho_{10} & (1-p)\rho_{11} \end{pmatrix}$$

- Continuous interaction with environment

$$\rho'^n = \begin{pmatrix} \rho_{00} + [1-(1-p)^n]\rho_{11} & (1-p)^{n/2}\rho_{01} \\ (1-p)^{n/2}\rho_{10} & (1-p)^n\rho_{11} \end{pmatrix} \xrightarrow{n\to\infty} \begin{pmatrix} \rho_{00} + [1-e^{-\Gamma_1 t}]\rho_{11} & e^{-\Gamma_2 t}\rho_{01} \\ e^{-\Gamma_2 t}\rho_{10} & e^{-\Gamma_1 t}\rho_{11} \end{pmatrix}$$

with infinitesimal probability $\dfrac{t}{np} = \dfrac{1}{\Gamma_1} = T_1$ **Relaxation time:** 1/(decay rate of populations)

$= \dfrac{1}{2\Gamma_2} = T_2/2$ **(Phase) coherence time:** 1/(decay rate of coherences)

Phase damping

- Interaction with environment with probability p', $U_P : \begin{cases} |0\rangle_Q|0\rangle_E \mapsto |0\rangle_Q|0\rangle_E \\ |1\rangle_Q|0\rangle_E \mapsto \sqrt{1-p'}|1\rangle_Q|0\rangle_E + \sqrt{p'}|1\rangle_Q|1\rangle_E \end{cases}$

$$M_\mu^P = {}_E\langle\mu|U_P|0\rangle_E \quad \Rightarrow \quad M_0^A = \begin{pmatrix} 1 & 0 \\ 0 & \sqrt{1-p} \end{pmatrix},\ M_1^A = \begin{pmatrix} 0 & 0 \\ 0 & \sqrt{p} \end{pmatrix}$$

- Consider qubit with amplitude & phase damping

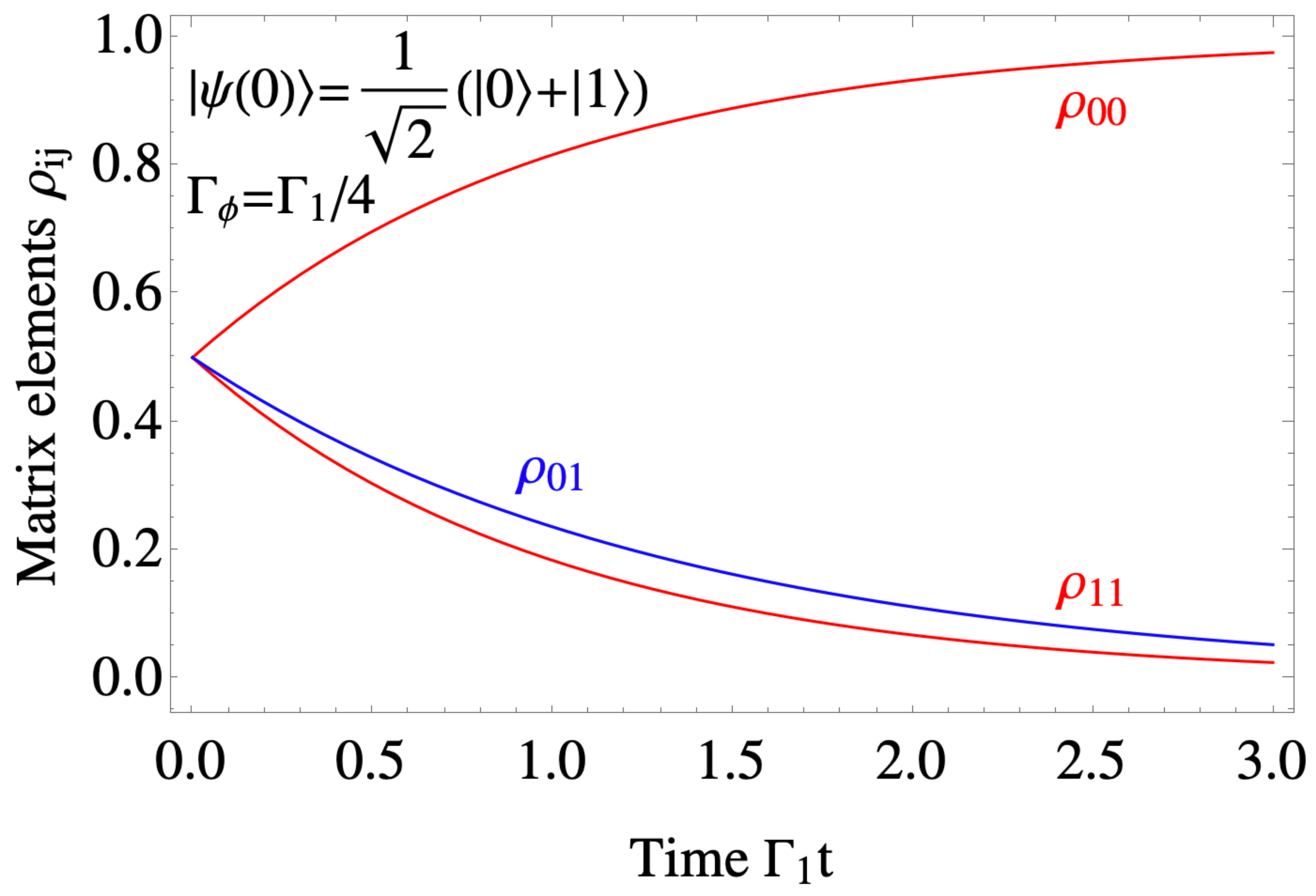
$$\rho''^n = \begin{pmatrix} \rho_{00} + [1-(1-p)^n]\rho_{11} & (1-p)^{n/2}(1-p')^{n/2}\rho_{01} \\ (1-p)^{n/2}(1-p')^{n/2}\rho_{10} & (1-p)^n\rho_{11} \end{pmatrix} \xrightarrow{n\to\infty} \begin{pmatrix} \rho_{00} + [1-e^{-\Gamma_1 t}]\rho_{11} & e^{-\frac{\Gamma_1+2\Gamma_\phi}{2}t}\rho_{01} \\ e^{-\frac{\Gamma_1+2\Gamma_\phi}{2}t}\rho_{10} & e^{-\Gamma_1 t}\rho_{11} \end{pmatrix}$$

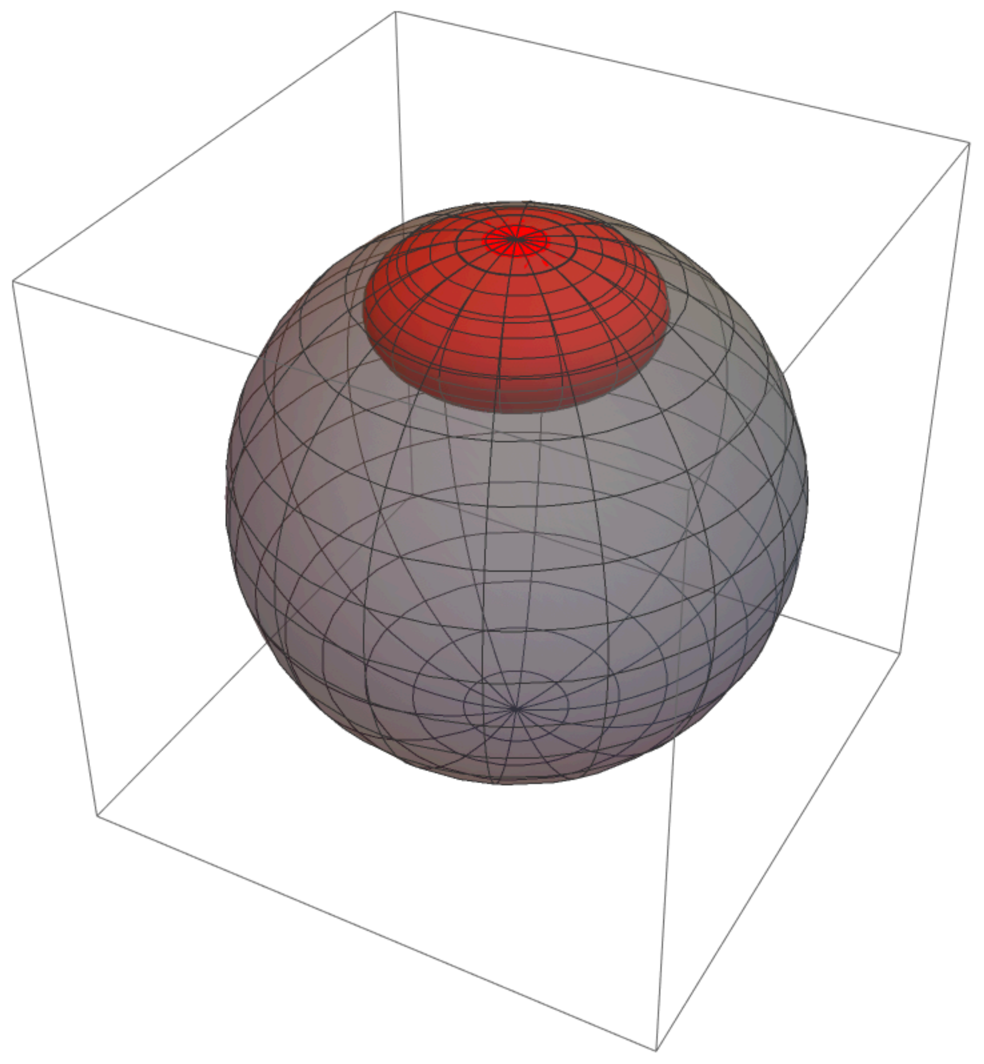
with infinitesimal probability $p' = 2\Gamma_\phi t/n$

- Decay rate of off-diagonal elements $\Gamma_2 = \Gamma_1/2 + \Gamma_\phi$ **Pure dephasing rate**

Relaxation and decoherence

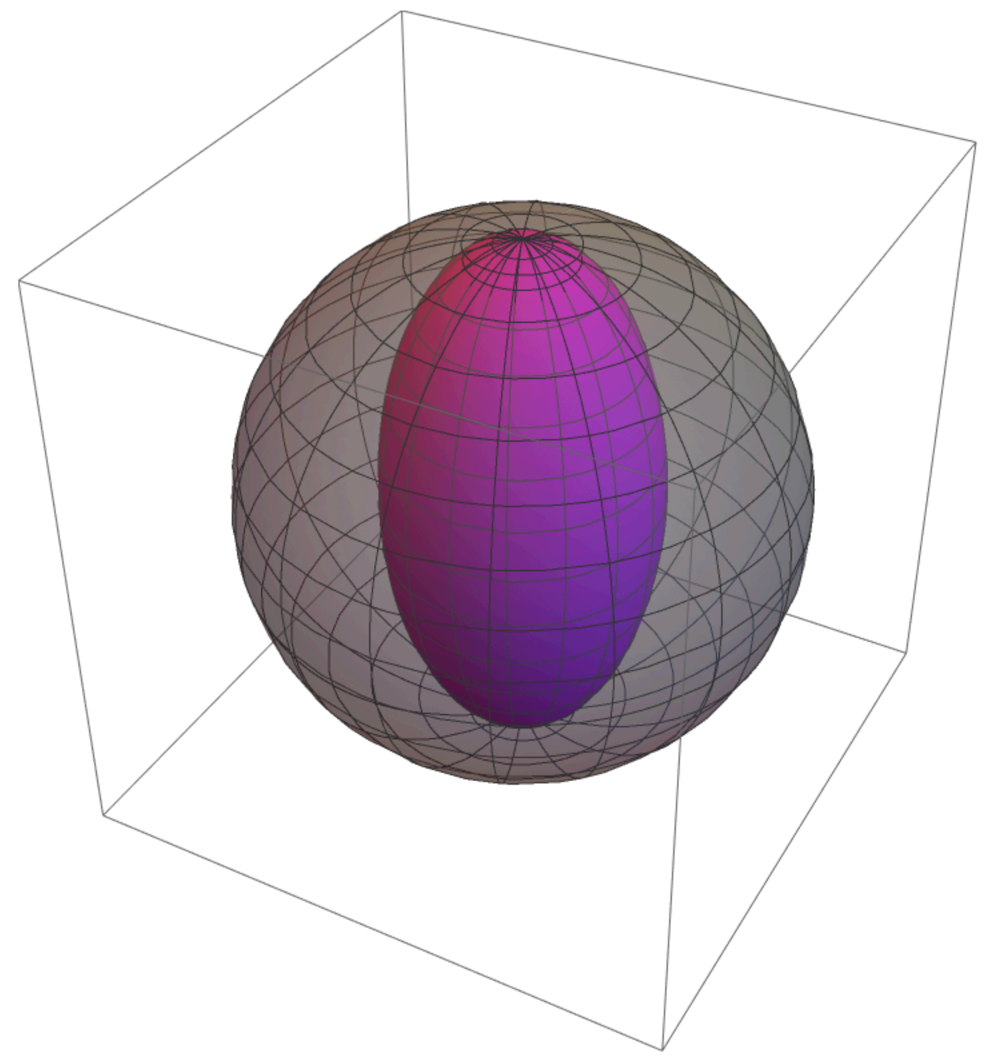
$$\frac{1}{T_2} = \frac{1}{2T_1} + \frac{1}{T_\phi}$$





Relaxation

$$\vec{p} \rightarrow \begin{pmatrix} \sqrt{1-p}\, p_x \\ \sqrt{1-p}\, p_y \\ p + (1-p) p_z \end{pmatrix}$$



Pure dephasing

$$\vec{p} \rightarrow \begin{pmatrix} \sqrt{1-p}\, p_x \\ \sqrt{1-p}\, p_y \\ p_z \end{pmatrix}$$

Infinitesimal time evolution

- Unitary time evolution generated by **Liouville equation** (**Liouville superoperator** $\mathcal{L}$)

$$\partial_t \rho = \frac{i}{\hbar}[\rho, H] = \mathcal{L}\rho$$

- Consider system S and environment E, projection superoperators $P\rho = \rho_S,\ Q\rho = (1-P)\rho = \rho_E$

Can write Liouville equation as $\partial_t \begin{pmatrix} \rho_S \\ \rho_E \end{pmatrix} = \begin{pmatrix} P \\ Q \end{pmatrix} \mathcal{L} \begin{pmatrix} P \\ Q \end{pmatrix} \rho + \begin{pmatrix} P \\ Q \end{pmatrix} \mathcal{L} \begin{pmatrix} Q \\ P \end{pmatrix} \rho$

Formally integrate second line $\rho_E = e^{Q\mathcal{L}t}\rho_E(t=0) + \int_0^t \mathrm{d}t'\, e^{Q\mathcal{L}t'} Q\mathcal{L}P\rho(t-t')$

Plug into first line ⇒ **Nakajima–Zwanzig equation**

$$\partial_t \rho_S = P\mathcal{L}\rho_S + \int_0^t \mathrm{d}t'\, \mathcal{K}(t')\rho_S(t-t')$$

$$\mathcal{K}(t) = P\mathcal{L}e^{Q\mathcal{L}t}Q\mathcal{L}P$$

Infinitesimal time evolution

- Solve Nakajima–Zwanzig eq.: hard $$\partial_t \rho_S = P\mathcal{L}\rho_S + \int_0^t \mathrm{d}t' \, \mathcal{K}(t')\rho_S(t-t')$$

- **Markov approximation**: timescale of environment dynamics much faster than system dynamics

$$\mathcal{K}(t) \approx \delta(t)\mathcal{K}$$

- Find **Lindblad equation** (**Lindblad superoperator** L)

$$\partial_t \rho_S = \frac{i}{\hbar}[\rho_S, H_S] + \mathcal{K}\rho_s = L\rho_S$$

- Most common form from Kraus representation, Lindbladian operators L_μ

$$\partial_t \rho_S = L\rho_S = \frac{i}{\hbar}[\rho_S, H_S] + \sum_\mu \left(L_\mu \rho_S L_\mu^\dagger - \frac{1}{2}\left(L_\mu^\dagger L_\mu \rho_s + \rho_S L_\mu^\dagger L_\mu\right)\right)$$

Relaxation and decoherence II

- Master equation $\partial_t \rho = \sum_\mu \left(L_\mu \rho L_\mu^\dagger - \frac{1}{2}\left(L_\mu^\dagger L_\mu \rho + \rho L_\mu^\dagger L_\mu \right) \right)$ describes amplitude and phase damping of qubit with

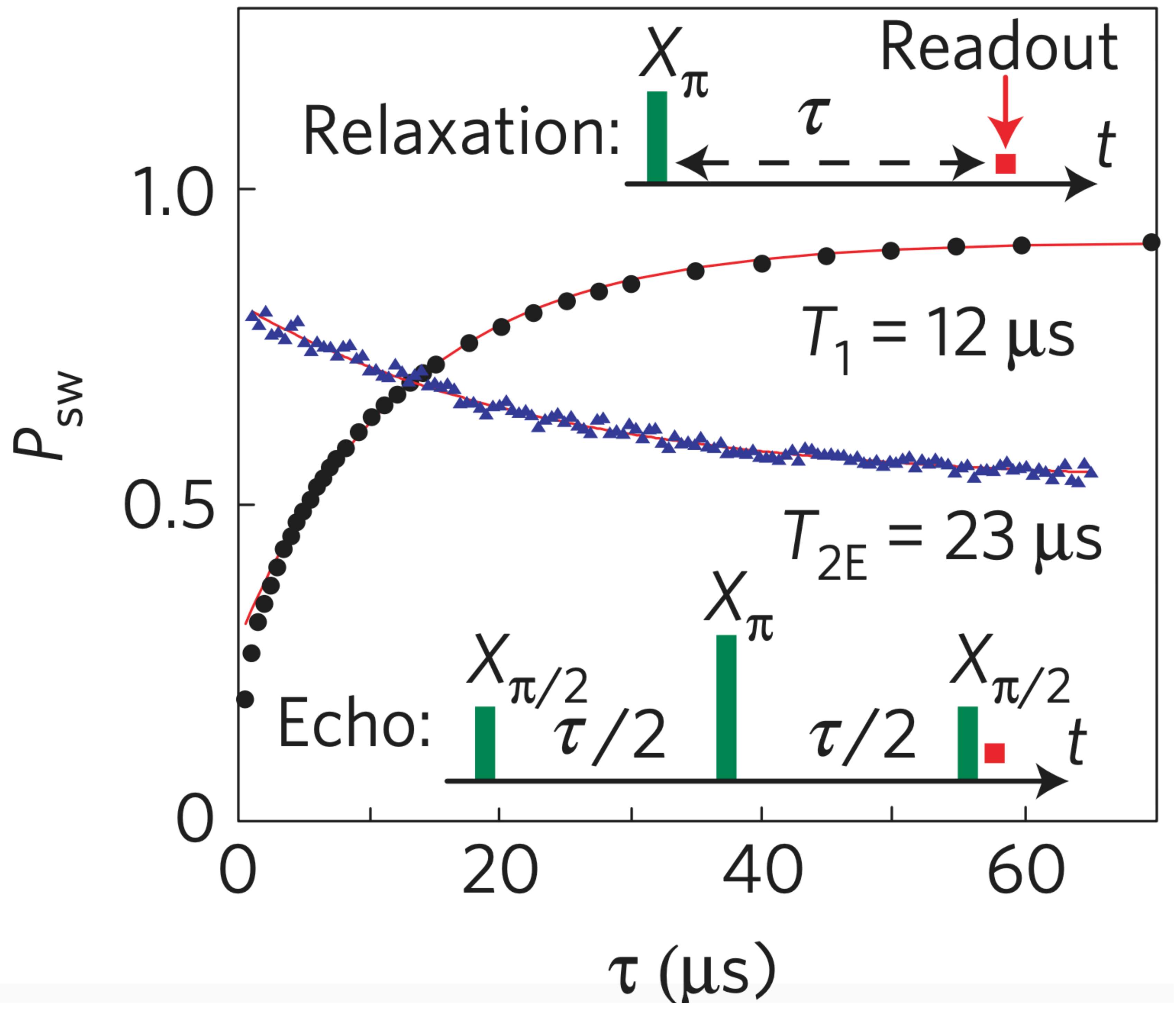
$$L_1 = \sqrt{\Gamma_\phi} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

$$L_2 = \sqrt{\frac{\Gamma_1}{2}} \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

$$L_3 = \sqrt{\frac{\Gamma_1}{2}} \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$

Measurement of T_1 & T_2

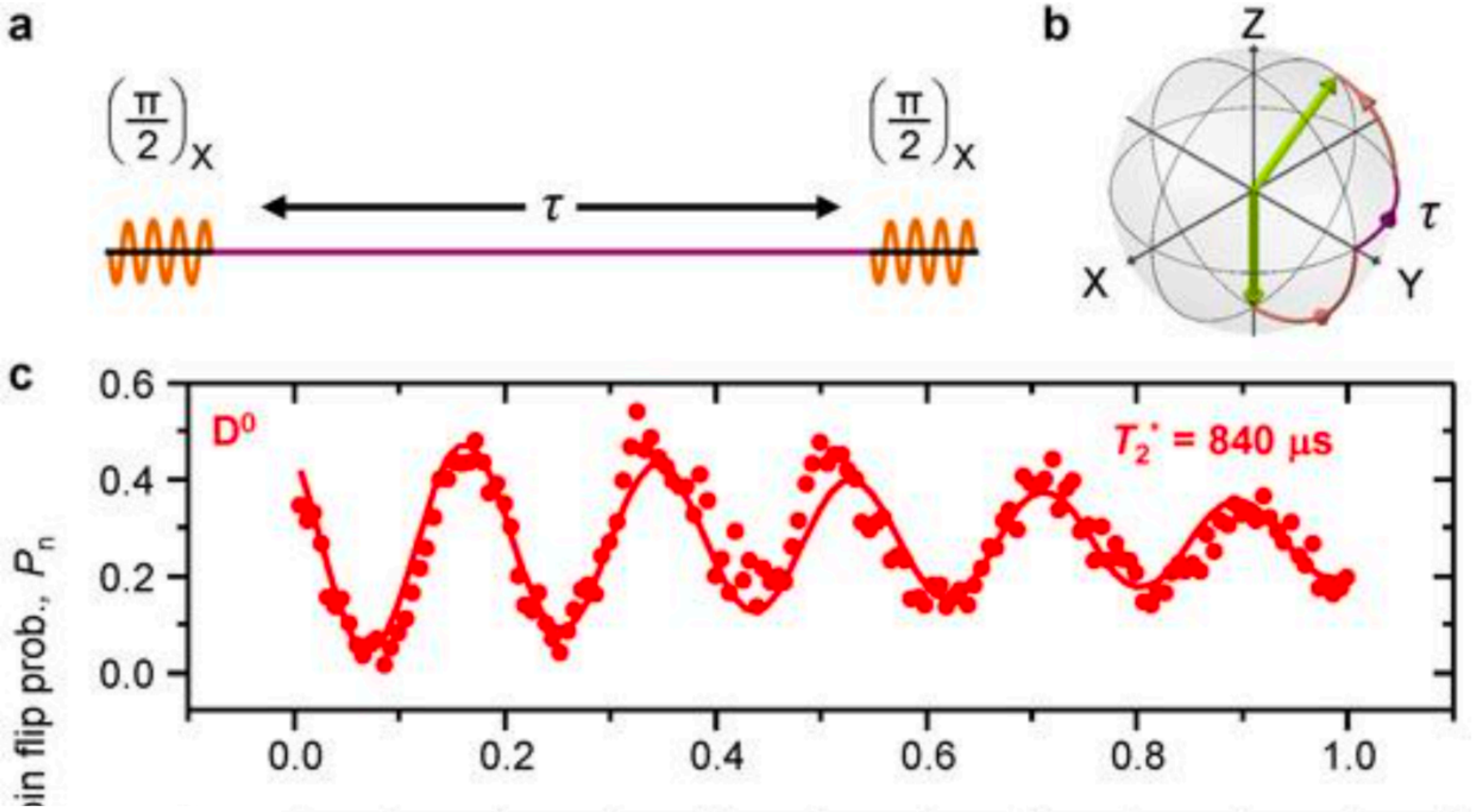
- T_1: Inversion recovery
  - Excite qubit (π-pulse)
  - Wait for time τ
  - Measure & repeat



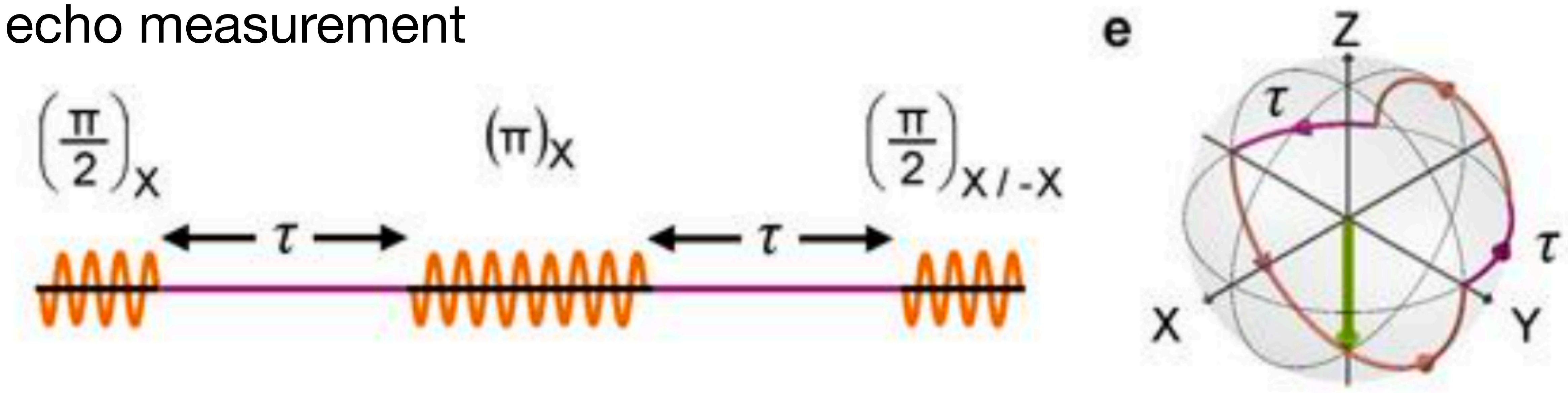
J. Bylander *et al.*, Nature Physics **7**, 565 (2011)

- $T_2^* = \left(T_2^{-1} + \Delta T_2^{-1}\right)^{-1}$: Free induction decay
  - Rotate around x-axis by $\pi/2$
  - Wait for time τ
  - Another $(\pi/2)_x$-pulse, measure, repeat

J. Pla *et al.*, Nature **496**, 334 (2013)



- T_2: Hahn echo measurement



Further reading

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