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Nonadiabatic Molecular Dynamics: Concepts, Methods, and Emerging Tools

IV– From quantum to classical

What does happen to a quantum state when it is measured?

A quantum state may follow two types of time evolution:

1. On itself, it evolves with the **Schrödinger equation** (unitary and deterministic)

2. During a measurement, it evolves with the **Born rule** (non-unitary and stochastic)


Can Particles be Quantum Entangled Across Time?
Brian Greene
World
Science
Festival
9:22 / 35:18 • History of the Beginnings of Quantum Mechanics ›
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• Relational interpretation
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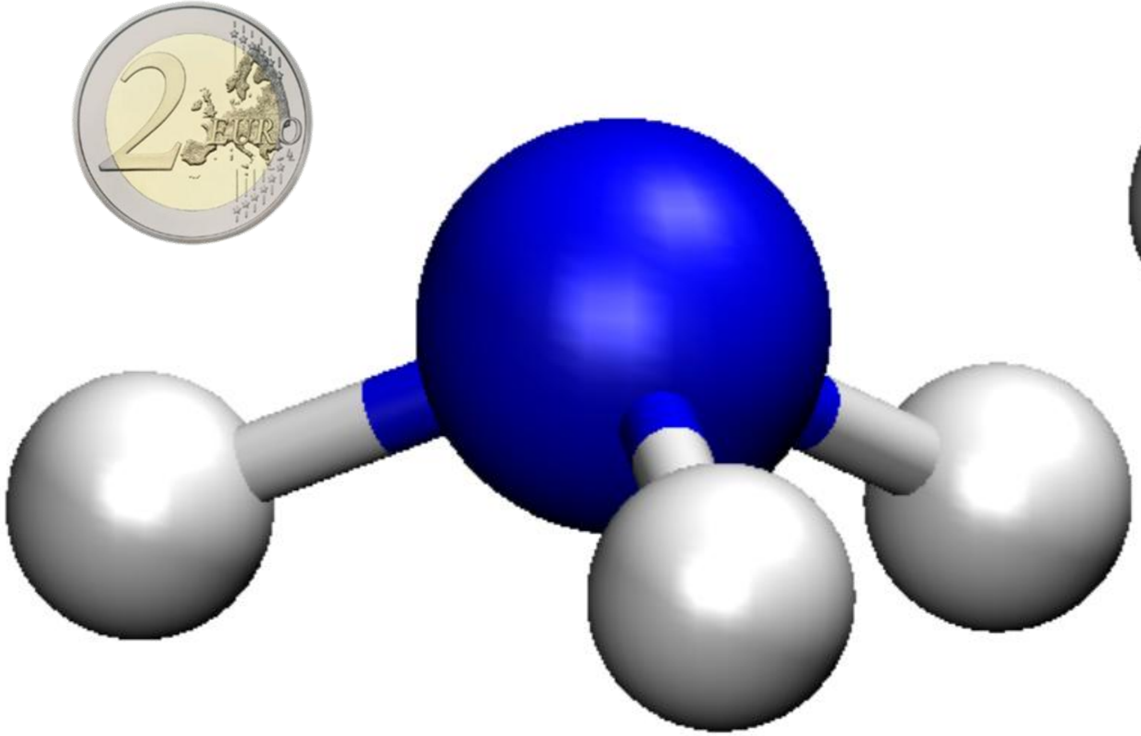
Decoherence
Many worlds
Objective collapse
Relational interpretation
. . .

Proposed Solutions to the Measurement Problem

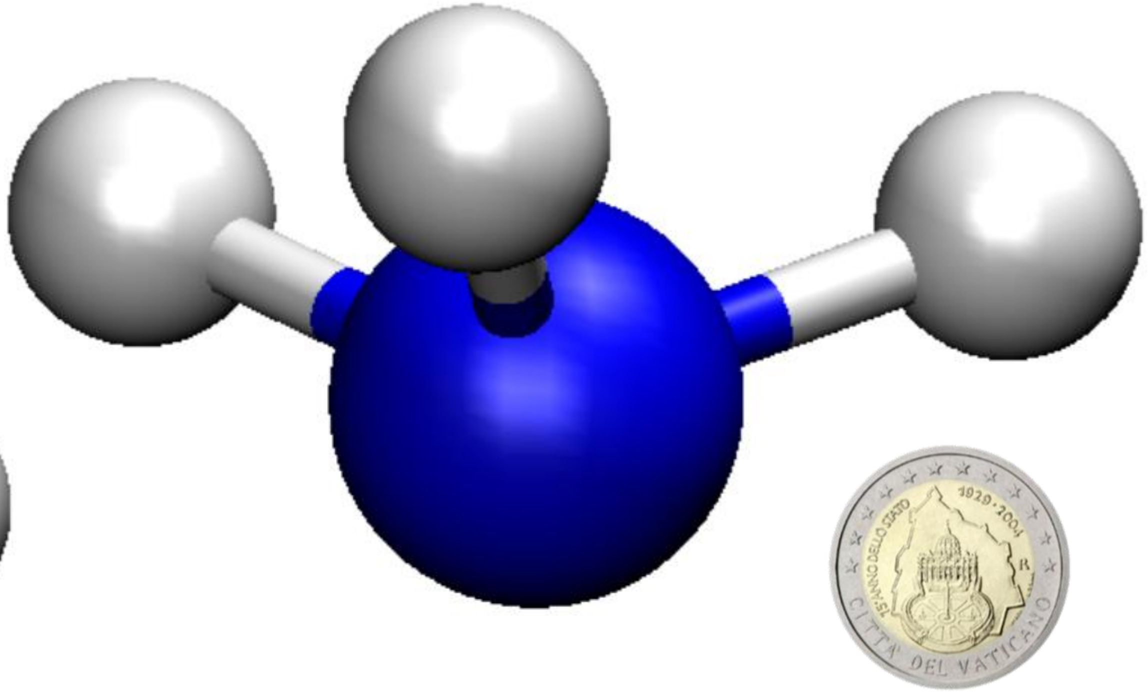
Interpretation	Year published	Author(s)	Deterministic?	Ontic wave-function?	Unique history?	Hidden variables?	Collapsing wave-functions?	Observer role?	Local dynamics?	Counter-factually definite?	Extant universal wave-function?
Consciousness causes collapse	1961–1993	John von Neumann, Eugene Wigner, Henry Stapp	No	Yes	Yes	No	Yes	Causal	No	No	Yes
Consistent histories	1984	Robert B. Griffiths	No	No	No	No	No	No	Yes	No	Yes
Copenhagen interpretation	1927–	Niels Bohr, Werner Heisenberg	No	Some	Yes	No	Some	No	Yes	No	No
de Broglie–Bohm theory	1927–1952	Louis de Broglie, David Bohm	Yes	Yes	Yes	Yes	Phenomen-ological	No	No	Yes	Yes
Ensemble interpretation	1926	Max Born	Agnostic	No	Yes	Agnostic	No	No	No	No	No
Many-minds interpretation	1970	H. Dieter Zeh	Yes	Yes	No	No	No	Interpre-tational	Yes	Ill-posed	Yes
Many-worlds interpretation	1957	Hugh Everett	Yes	Yes	No	No	No	No	Yes	Ill-posed	Yes
Objective-collapse theories	1986–1989	Ghirardi–Rimini–Weber, Penrose interpretation	No	Yes	Yes	No	Yes	No	No	No	No
QBism	2010	Christopher Fuchs, Rüdiger Schack	No	No	Agnostic	No	Yes	Intrinsic	Yes	No	No
Quantum logic	1936	Garrett Birkhoff	Agnostic	Agnostic	Yes	No	No	Interpre-tational	Agnostic	No	No
Relational interpretation	1994	Carlo Rovelli	No	No	Agnostic	No	Yes	Intrinsic	Possibly	No	No
Time-symmetric theories	1955	Satosi Watanabe	Yes	No	Yes	Yes	No	No	No	No	Yes
Transactional interpretation	1986	John G. Cramer	No	Yes	Yes	No	Yes	No	No	Yes	No

en.wikipedia.org/wiki/Interpretations_of_quantum_mechanics

Stating the Measurement Problem



$|\text{up}\rangle$



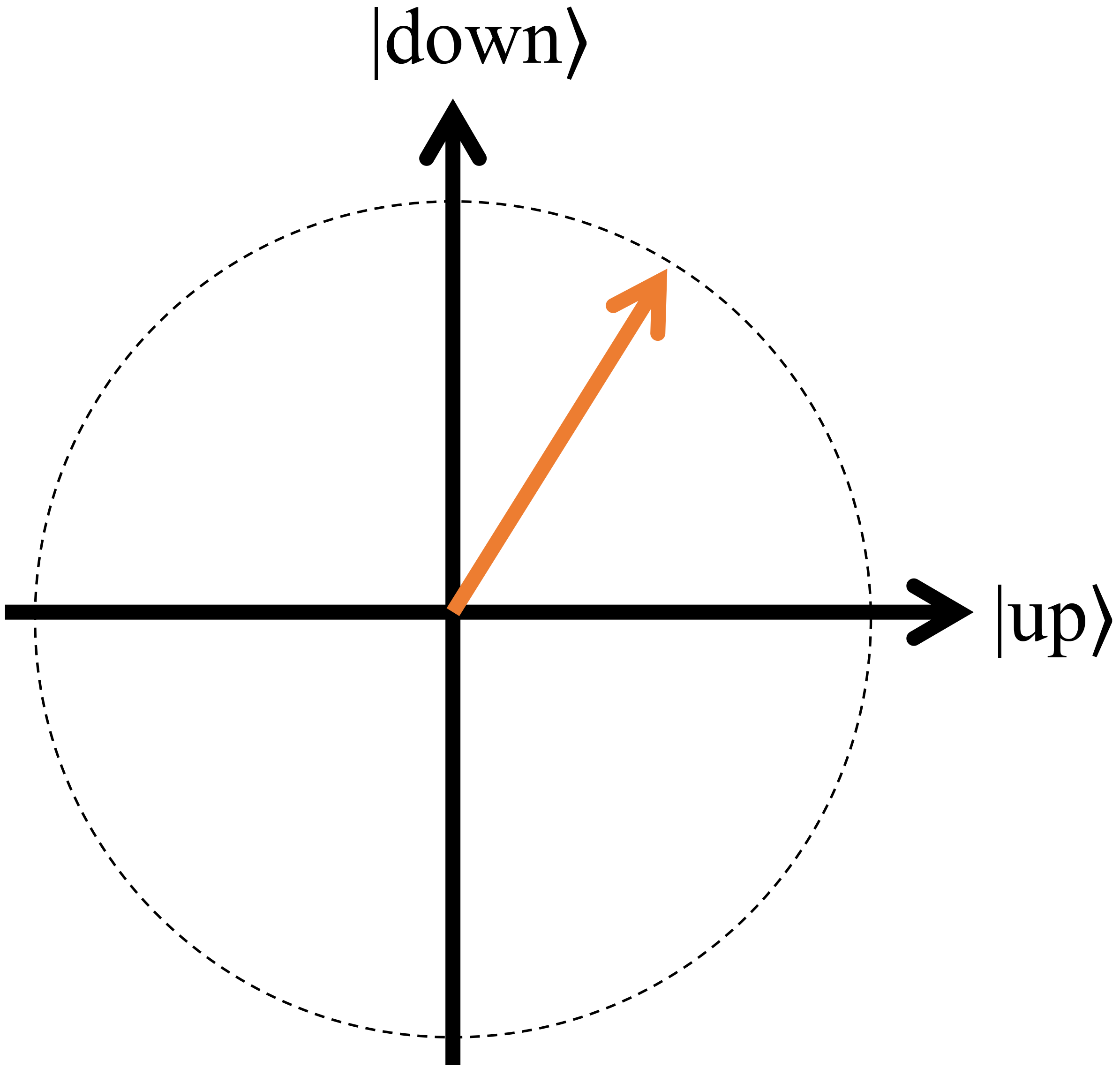
$|\text{down}\rangle$

The Feynman Lectures on Physics III, Ch. 8 & 9

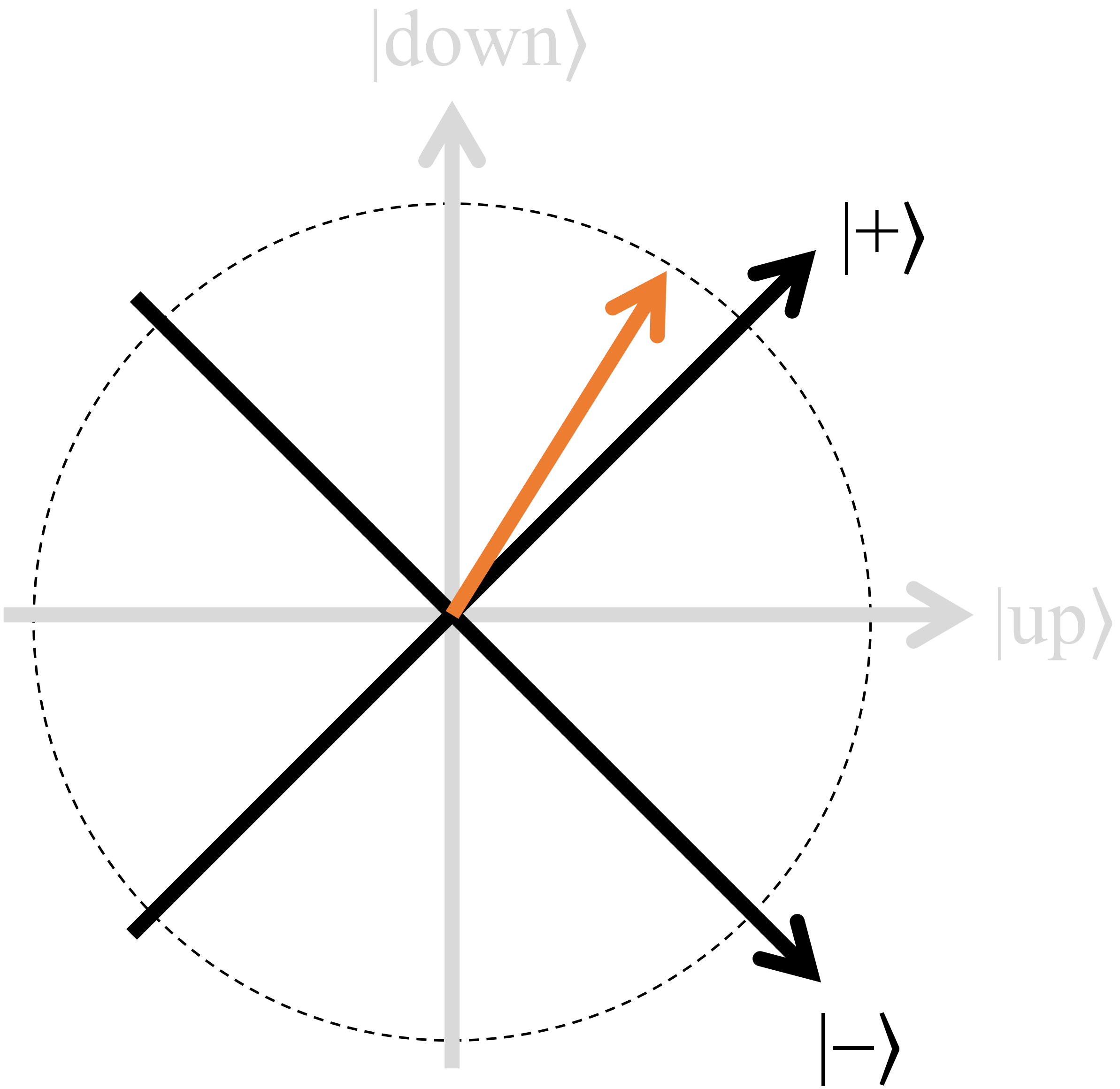
The measurement problem

- The problem of **outcomes**:
  How and why a single outcome is chosen?

Schlosshauer. *Decoherence,* **2007**



|down⟩
|up⟩



The quantum state can be written in any basis in the Hilbert space

$$|+\rangle = |up\rangle + |down\rangle$$

$$|-\rangle = |up\rangle - |down\rangle$$

The measurement problem

- The problem of **outcomes**:
  How and why a single outcome is chosen?

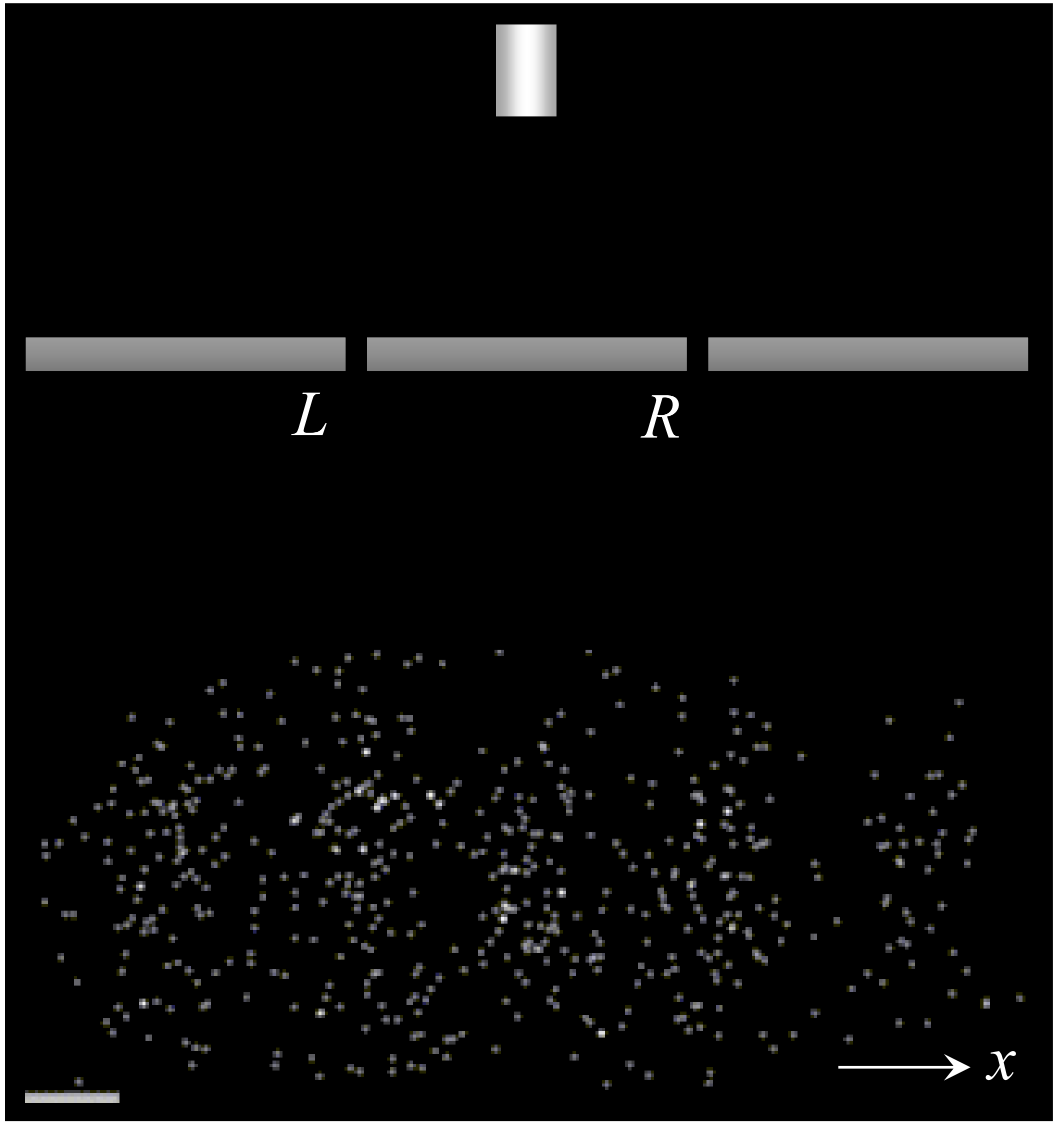
- The problem of **preferred basis**:
  What singles out preferred outcomes in nature?

Schlosshauer. *Decoherence,* **2007**

Double-slit experiment

$$|\Psi\rangle = \frac{1}{\sqrt{2}}\left(|\psi_L\rangle + |\psi_R\rangle\right)$$

$$\begin{aligned} P(x) &= \left|\langle x|\Psi\rangle\right|^2 \\ &= \frac{1}{2}\left|\psi_L(x) + \psi_R(x)\right|^2 \\ &= \frac{1}{2}\left|\psi_L(x)\right|^2 + \frac{1}{2}\left|\psi_R(x)\right|^2 \\ &\quad + \mathrm{Re}\left[\psi_L(x)\psi_R^*(x)\right] \end{aligned}$$



The measurement problem

- The problem of **outcomes**:
  How and why a single outcome is chosen?

- The problem of **preferred basis**:
  What singles out preferred outcomes in nature?

- The problem of **nonobservability of interference**:
  Why don’t we see superposition effects everywhere?

Schlosshauer. *Decoherence*, **2007**

Decoherence:
A quantum world in disguise

Decoherence transfers quantum information to the environment and suppresses the interference terms

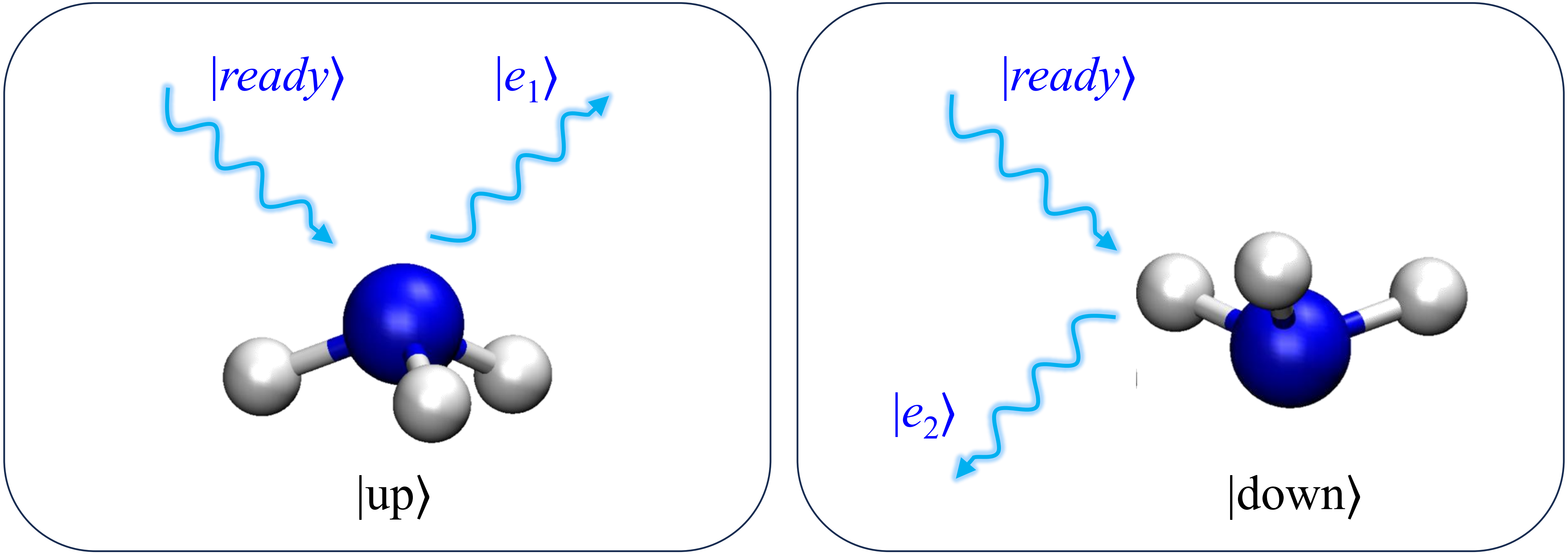
$$\overbrace{\left|\Psi\right\rangle = \left(a\left|up\right\rangle + b\left|down\right\rangle\right)}^{\text{System}} \otimes \overbrace{\left|ready\right\rangle}^{\text{Environment}}$$

$$= a\left|up\right\rangle\left|e_1\right\rangle + b\left|down\right\rangle\left|e_2\right\rangle$$

System's reduced density matrix

$$\rho_S = \mathrm{Tr}_E\left[\left|\Psi\right\rangle\left\langle\Psi\right|\right]$$

$$= \begin{bmatrix} |a|^2 & ab^*\left\langle e_2 | e_1\right\rangle \\ ba^*\left\langle e_1 | e_2\right\rangle & |b|^2 \end{bmatrix}$$



$$\langle e_1 | e_2 \rangle \to 0$$

System Environment

$$|\Psi\rangle = \underbrace{\left(a|up\rangle + b|down\rangle\right)}_{\text{System}} \otimes \underbrace{|ready\rangle}_{\text{Environment}}$$

$$= a|up\rangle|e_1\rangle + b|down\rangle|e_2\rangle$$

System's reduced density matrix

$$\rho_S = \mathrm{Tr}_E\left[|\Psi\rangle\langle\Psi|\right]$$

$$= \begin{bmatrix} |a|^2 & ab^* \langle e_2|e_1\rangle \\ ba^* \langle e_1|e_2\rangle & |b|^2 \end{bmatrix} \xrightarrow{\text{Decoherence}} \begin{bmatrix} |a|^2 & 0 \\ 0 & |b|^2 \end{bmatrix}$$

Lindblad evolution

$$\rho_S = \mathrm{Tr}_E\left[\rho\right]$$

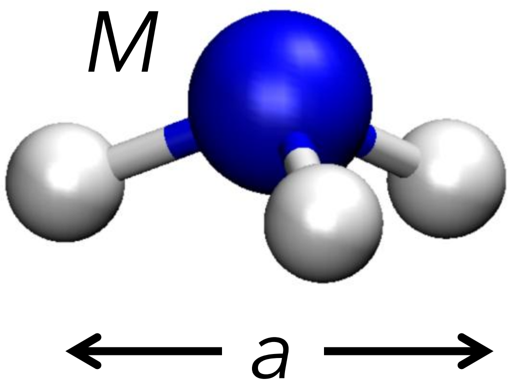
$$\frac{d\rho_S}{dt} = -\frac{i}{\hbar}\left[\hat{H},\rho_S\right] + \sum_k \Gamma_k \left(\hat{L}_k \rho_S \hat{L}_k^\dagger - \frac{1}{2}\left\{ \hat{L}_k^\dagger \hat{L}_k, \rho_S \right\} \right)$$

This term is responsible for decoherence

Decoherence is fast!

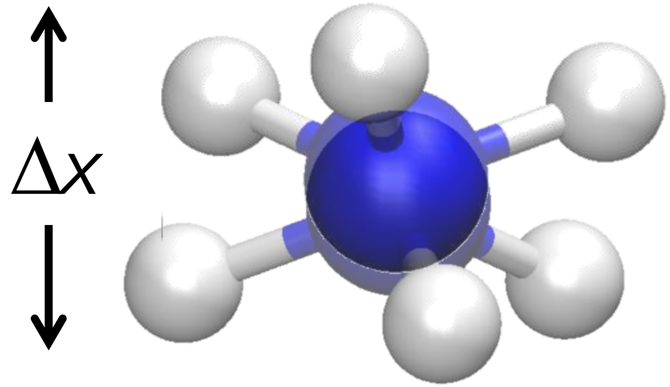
Off-diagonal terms

$$\rho_S(up,down,t)=\rho_S(up,down,0)e^{-t/\tau_D}$$



$$\tau_D=\frac{1}{\frac{8}{3\hbar^2}\frac{N}{V}(2\pi M)^{1/2}a^2\Delta x^2(k_BT)^{3/2}}$$

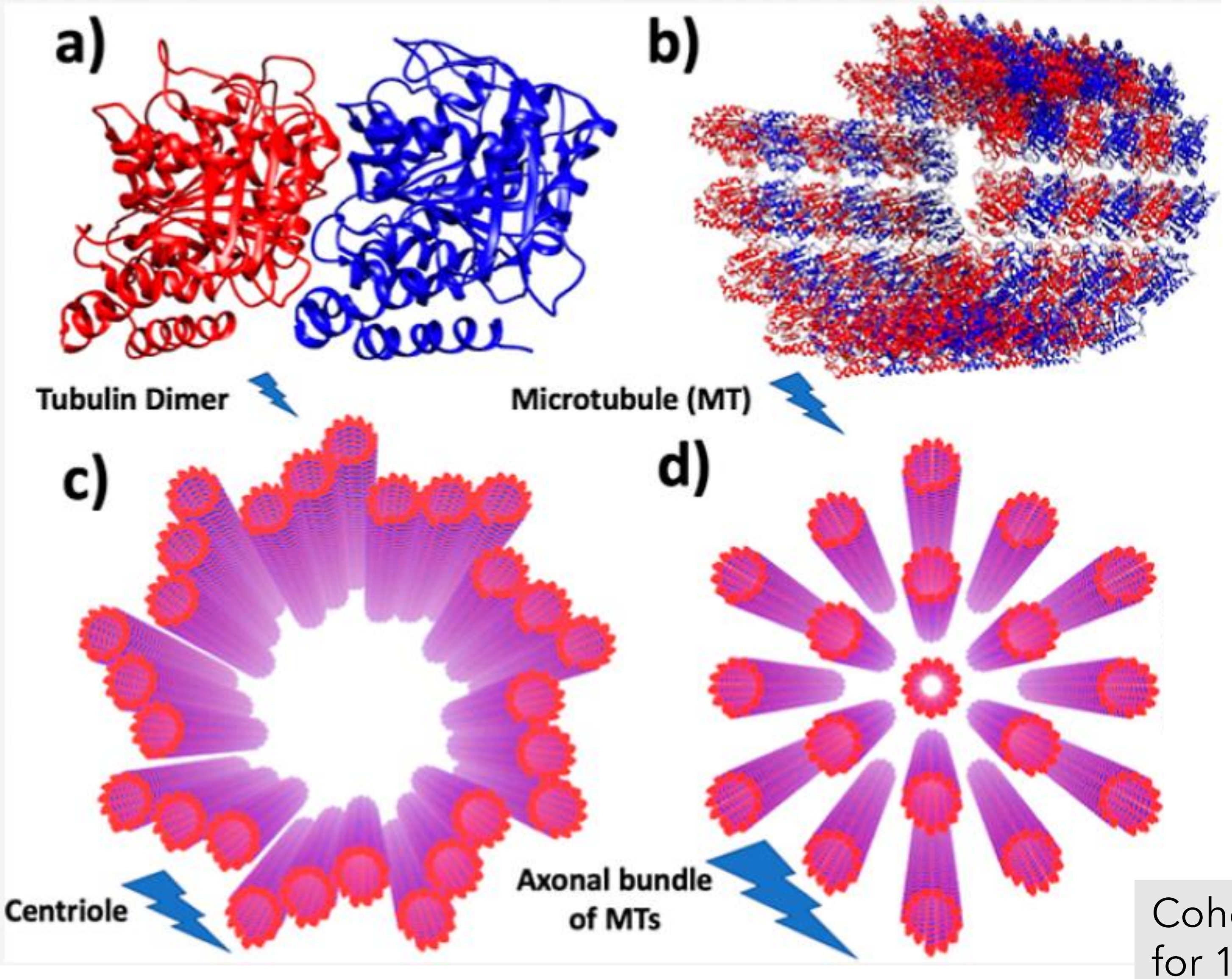
$$=10^{-19}\ \mathrm{s}$$



Joos; Zeh. *Z Phys B* **1985**, *59*, 223

But sometimes,
decoherence may take longer

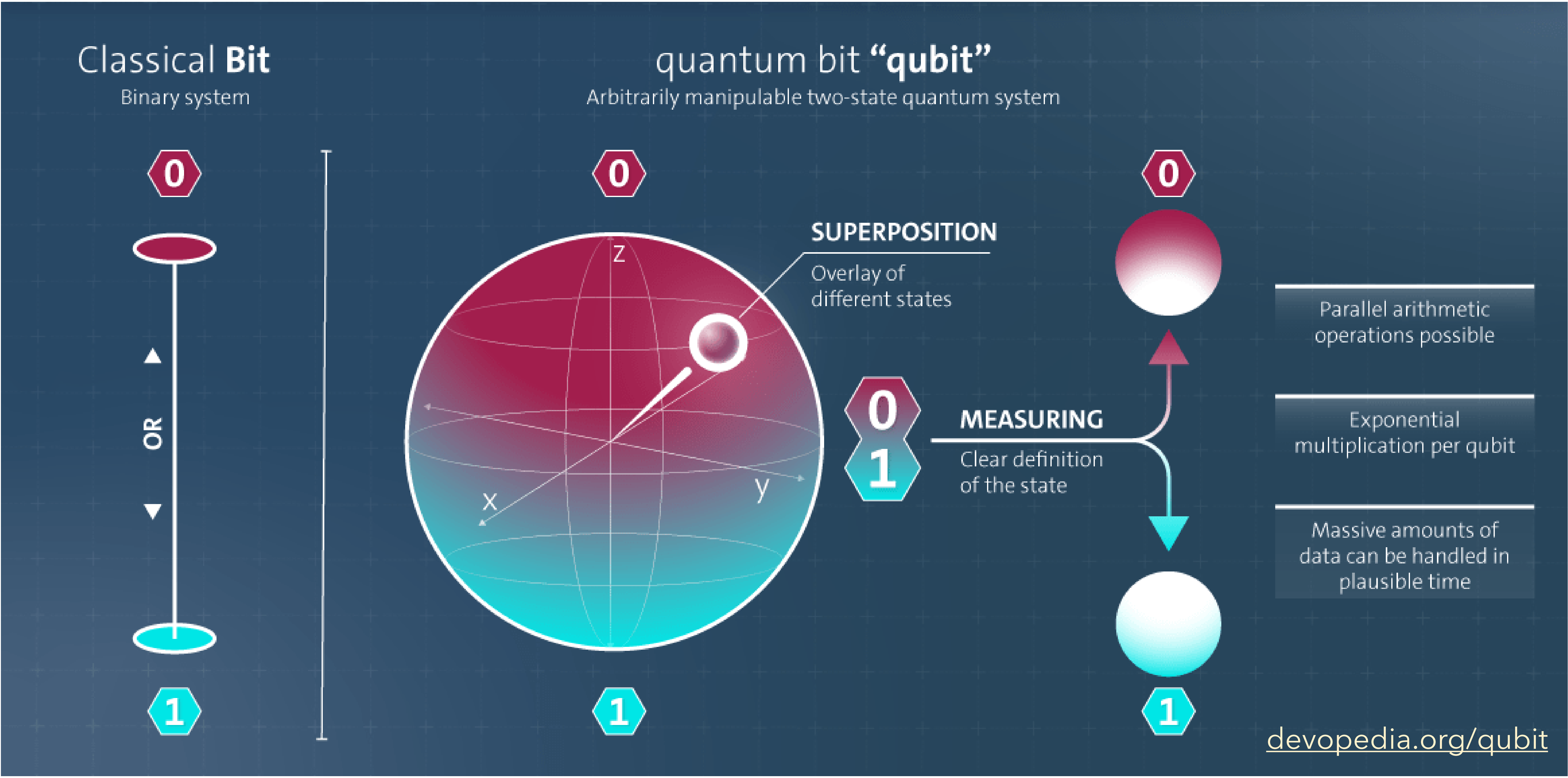
Superradiance in Trp protein architectures



Coherences should live for 100 fs to explain the results

Babcock *et al.* *J Phys Chem B* **2024**, *128*, 4035

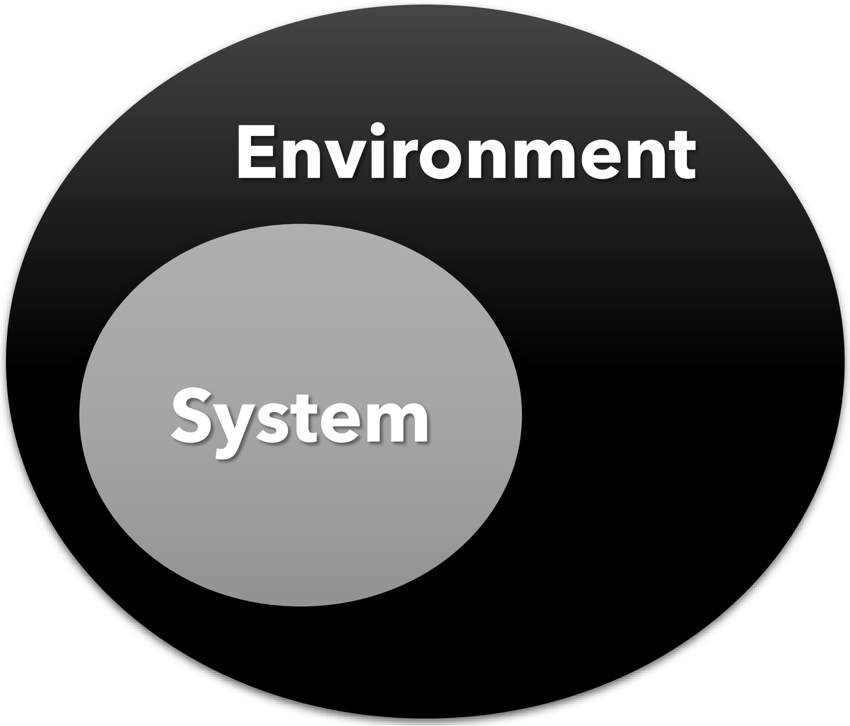
Long-lived coherences are the heart of quantum computing



On which basis does decoherence occur?

Einselection:
Decoherence drives the quantum state to the basis **least entangled** with the environment

Zurek. *Phys Rev D* **1981**, *24*, 1516



Basis on which decoherence occurs

1. $\hat{H}_{system} \gg \hat{H}_{int}$	$\hat{H}_{system}$ (energy) eigenstates
2. $\hat{H}_{system} \ll \hat{H}_{int}$	$\hat{H}_{int}$ eigenstates (position)
3. $\hat{H}_{system} \approx \hat{H}_{int}$	Coherent states

Coherent states are quantum states of the harmonic oscillator that most closely resemble classical oscillations, thereby minimizing the uncertainty relation and achieving equal variances in position and momentum.

Paz; Zurek. *Phys Rev Lett* **1999**, *82*, 5181

In a molecule, electrons lose coherence to nuclear vibrations because $\hat{H}_{elec} \gg \hat{H}_{vib}$

The *least entangled basis* is $\hat{H}_{elec}$ eigenstates (**electronic energy**)

In a gas, a molecule loses coherence to the environment because $\hat{H}_{int} \gg \hat{H}_{mol}$

The *least entangled basis* is $\hat{H}_{int}$ eigenstates (**molecular position**)

Decoherence solves:

- The problem of **preferred basis**:
  What singles out preferred outcomes in nature?

- The problem of **nonobservability of interference**:
  Why don’t we see superposition effects everywhere?

Decoherence does NOT solve:

- The problem of **outcomes**:
  How and why a single outcome is chosen?

The problem of outcomes

$$\rho_S = \mathrm{Tr}_E\left[\hat{\rho}\right]$$

$$= \begin{bmatrix} |a|^2 & ab^*\langle e_2|e_1\rangle \\ ba^*\langle e_1|e_2\rangle & |b|^2 \end{bmatrix} \xrightarrow{\text{Decoherence}} \begin{bmatrix} |a|^2 & 0 \\ 0 & |b|^2 \end{bmatrix}$$

Collapse

$$\begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \qquad \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$$

Collapse is not a consensus

QBism

$$\rho_S = \mathrm{Tr}_S\left[\hat{\rho}\right]$$

$$= \begin{bmatrix} |a|^2 & ab^*\langle e_2|e_1\rangle \\ ba^*\langle e_1|e_2\rangle & |b|^2 \end{bmatrix} \xrightarrow{\text{Decoherence}} \begin{bmatrix} |a|^2 & 0 \\ 0 & |b|^2 \end{bmatrix}_S$$

Knowledge update

$$\begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \qquad \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$$

Many-worlds interpretation

$$\rho_S = \mathrm{Tr}_S\left[\hat{\rho}\right]$$

$$= \begin{bmatrix} |a|^2 & ab^*\langle e_2|e_1\rangle \\ ba^*\langle e_1|e_2\rangle & |b|^2 \end{bmatrix} \xrightarrow{\text{Decoherence}} \begin{bmatrix} |a|^2 & 0 \\ 0 & |b|^2 \end{bmatrix}_S$$

Universe branching

$$\begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}_{S+O} \qquad \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}_{S+O}$$

Objective collapse

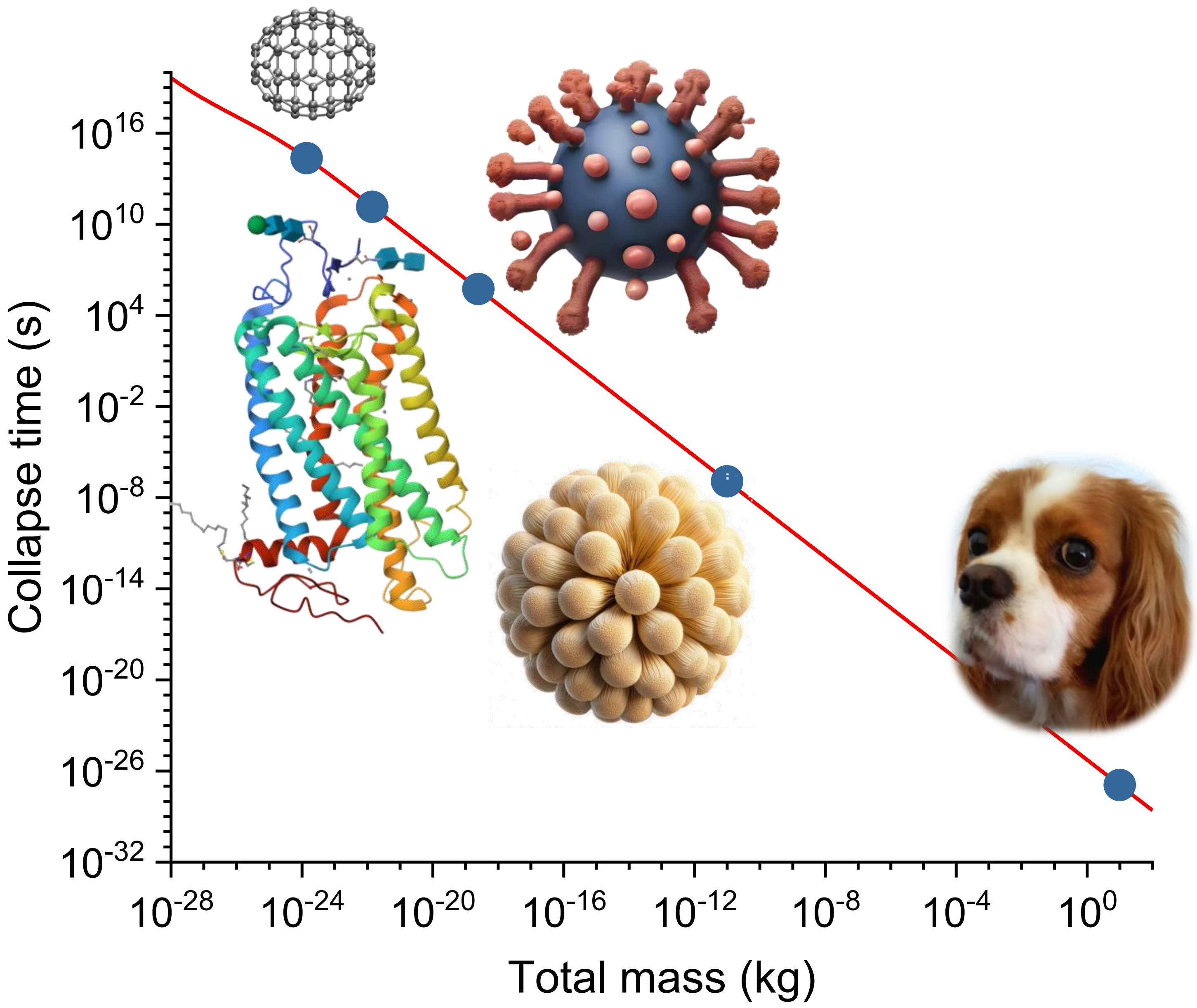
$$\rho_S = \mathrm{Tr}_S\left[\hat{\rho}\right]$$

$$= \begin{bmatrix} |a|^2 & ab^*\langle e_2|e_1\rangle \\ ba^*\langle e_1|e_2\rangle & |b|^2 \end{bmatrix} \xrightarrow{\text{Decoherence}} \begin{bmatrix} |a|^2 & 0 \\ 0 & |b|^2 \end{bmatrix}_S$$

Field perturbation

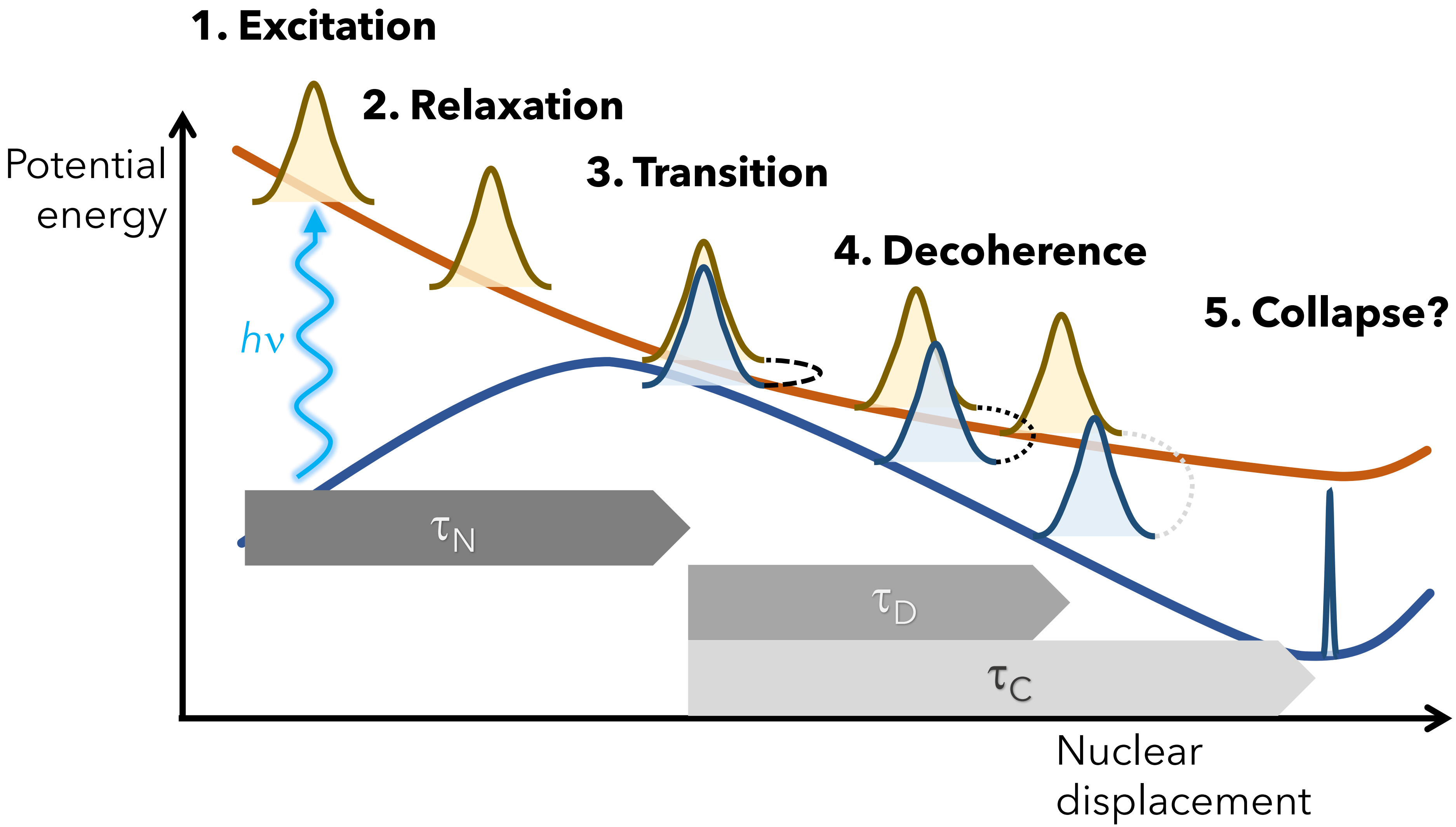
$$\begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \qquad \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$$

Diósi-Penrose gravity-induced collapse

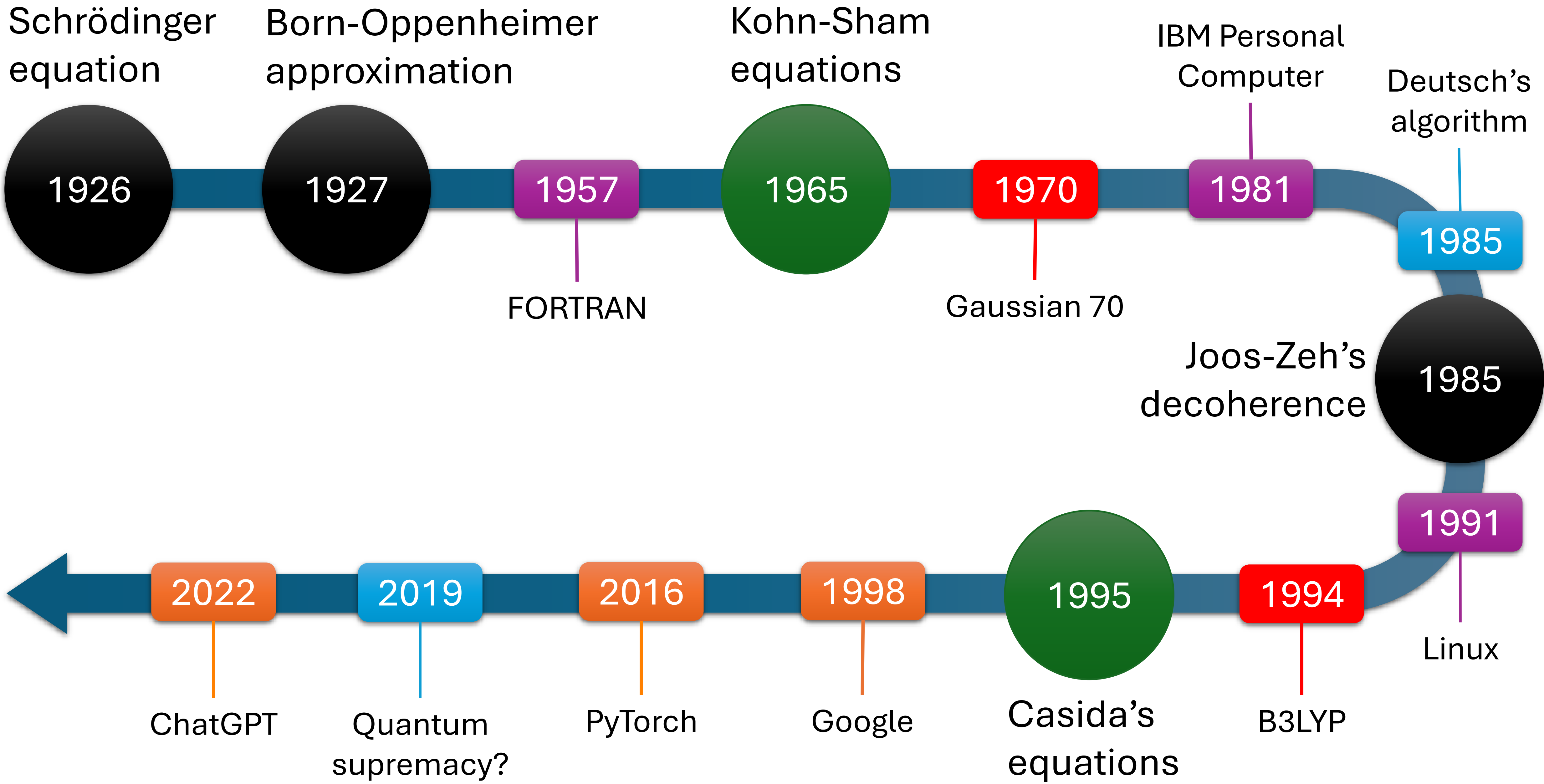


Tomaz; Mattos; Barbatti. *PCCP* **2024**, *26*, 20785

A quasi-classical world



Quantum chemistry in context



Barbatti. *Pure Appl Chem* **2025**

To know more:

The measurement problem

- Tomaz; Mattos; Barbatti. *arXiv [quant-ph]* **2025**

Decoherence in molecular context

- Shu; Truhlar. *JCTC* **2023**, *19*, 380

Insights into quantum chemistry

- Barbatti. *Pure Appl Chem* **2025**

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