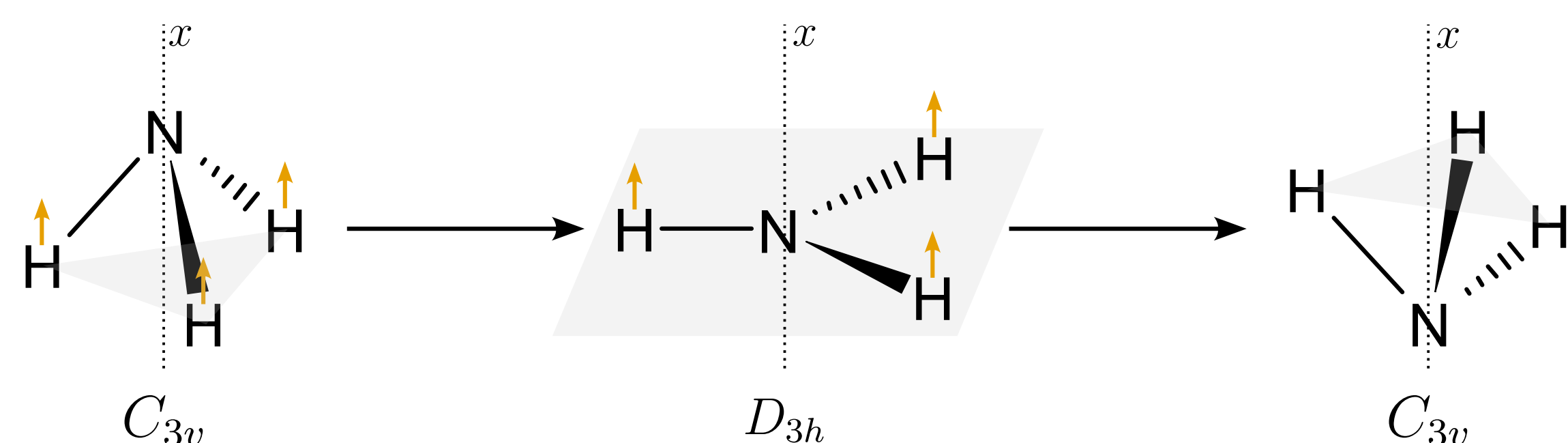


Tunnelling is present since the evolution of the primitive Universe, allowing the origin and evolution of life [1].

Introduction and main objective

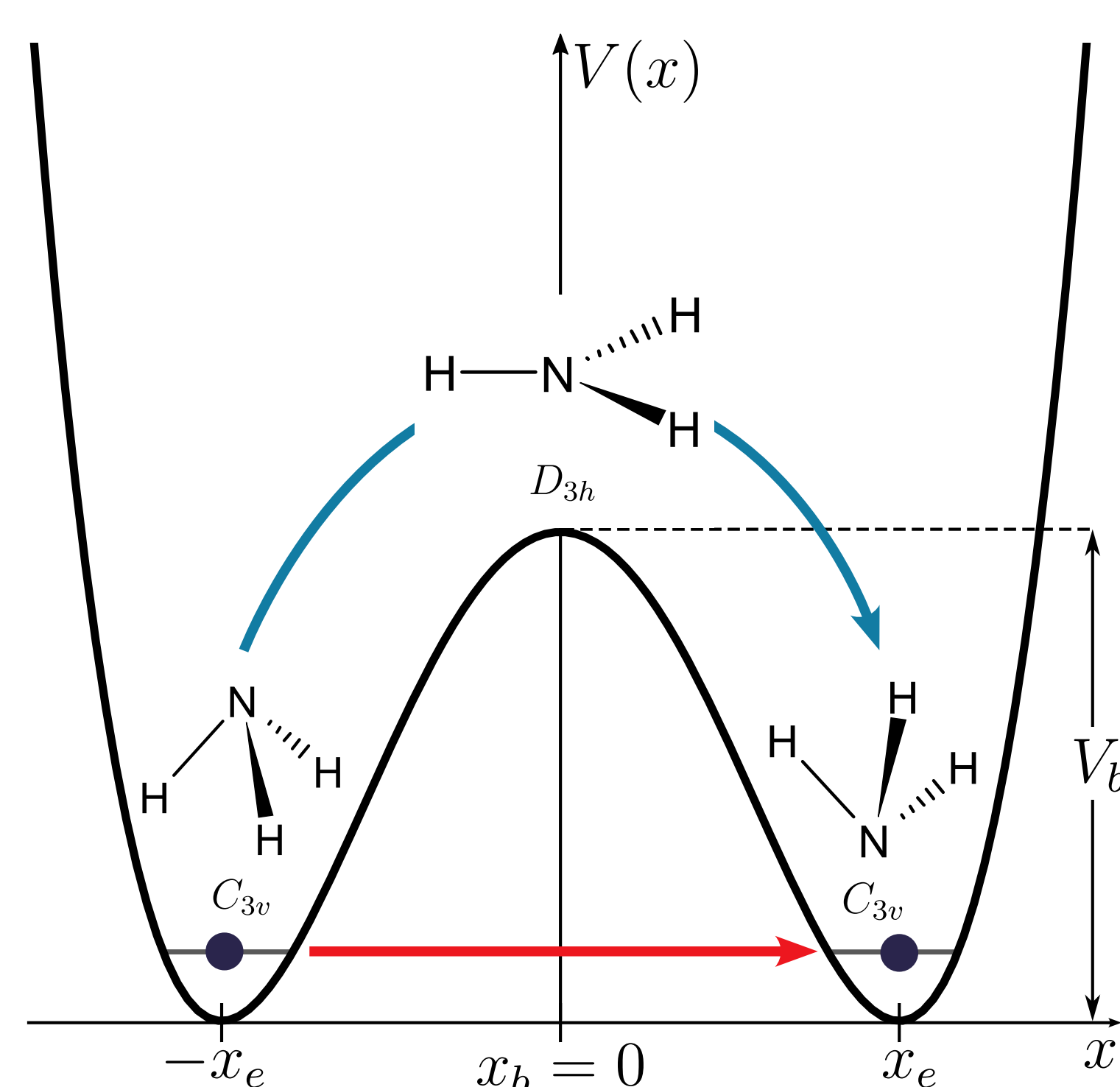
- Study tunnelling in a realistic example, the inversion motion of NH₃, which gave birth to the first MASER [2]



- Double symmetric potential well:** lower energy equilibrium C_{3v} (wells) and higher energy D_{3h} (barrier)

Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2\mu} \frac{d^2}{dx^2} + \frac{V_b}{x_e^4} x^4 - \frac{2V_b}{x_e^2} x^2 + V_b$$



Classic
VS
Quantum

- Visualize tunnelling, in real time, with your own eyes

Method & Results

Stationary states and Non-stationary states

SS $|\psi_v\rangle$: expansion in HO basis $\{\varphi_k\}_N$

$$|\psi_v\rangle = \sum_{k=0}^N c_k^{(v)} |\varphi_k\rangle$$

NS $|\Psi\rangle$: superposition of SS

$$|\Psi\rangle = \sum_n a_n |\psi_n\rangle$$

NS's are constructed from the first 4 SS as

$$|\Psi\rangle = \frac{1}{\sqrt{2}} \{ \cos \alpha (|\psi_0\rangle + |\psi_1\rangle) + \sin \alpha (|\psi_2\rangle + |\psi_3\rangle) \}$$

with energy

$$\langle E \rangle = \sum_n |a_n|^2 E_n$$

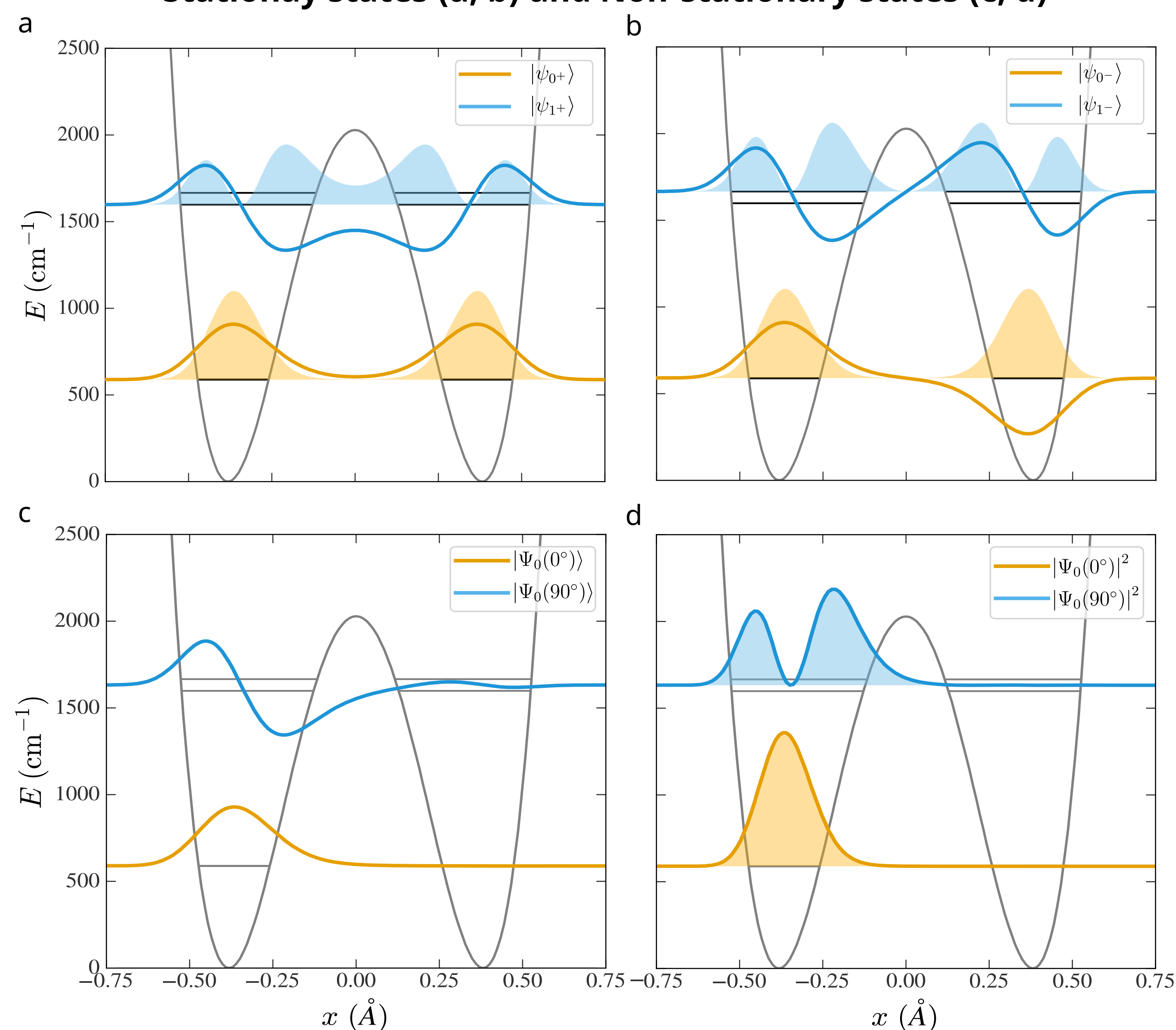
Time dynamics of non-stationary states

- TD NS: superposition of TD SS

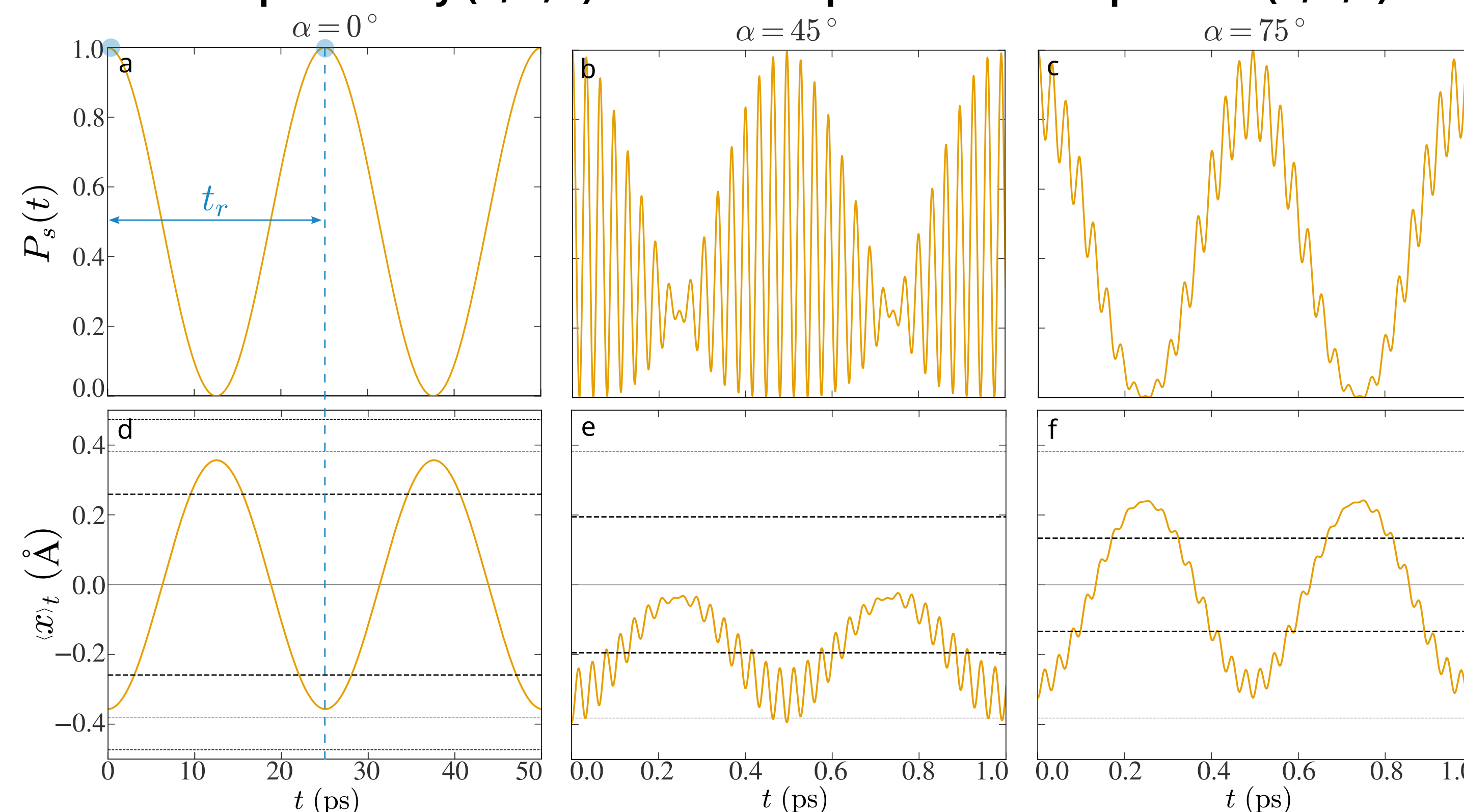
$$|\Psi(t; \alpha)\rangle = \sum_i a_i |\psi_i(t)\rangle = \sum_i a_i |\varphi_i\rangle e^{-iE_i t/\hbar}$$

- Derived analytical expressions for time evolution of expectation values, $\langle x \rangle_t$, survival probability, $P_s(t)$, and recurrence time, t_r .

Stationary states (a, b) and Non-stationary states (c, d)



Survival probability (a, b, c) and Time-expected value of position (d, e, f)



Conclusions

- Localized NS evolve over t crossing the barrier by **tunnelling**
- Tunnelling is
 - Uniform** for initial NS of 2 SS $\Rightarrow \uparrow P_T$ tunnelling probability
 - Irregular** for NS of more than 2 SS in superposition $\Rightarrow \downarrow P_T$

Animations



References

- Trixler, F Quantum Tunnelling to the Origin and Evolution of Life., *Current Organic Chemistry* **2013**, 17, 1758–1770.
- Nobel Prize in Physics 1964 awarded to Charles Hard Townes, Nicolay Gennadiyevich Basov and Aleksandr Mikhailovich Prokhorov.,