Exploring Quantum Tunnelling in the ammonia molecule

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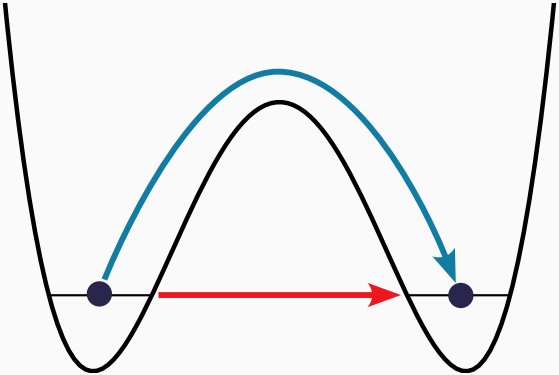
Tunnelling effect: penetration and transmission of molecules through a potential energy barrier.

- Classic *vs* Quantum
- Quantum phenomena
- Probabilistic nature
- Decreases with:

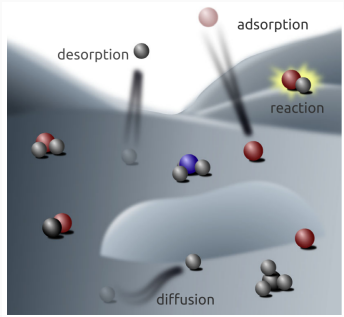
  $\uparrow m$

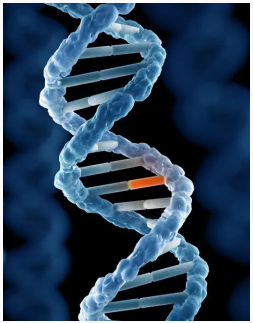
  $\uparrow$ height and width

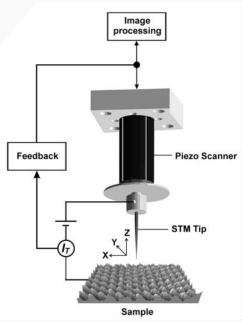


Scientific and technological fields:

- **Chemistry:** astrochemistry, electrochemistry, catalysis, radioactive, ...
- Biology: proteins and DNA mutations, ...
- Tehcnology: STM, quantum computing, ...







Ammonia MASER

Objective $\Longrightarrow$ study and simulate quantum tunnelling in realistic example

- First **MASER** $\Longrightarrow$ Nobel Prize Physics 1964

"for fundamental work in the field of quantum electronics, which has led to the construction of oscillators and amplifiers based on the maser-laser principle"

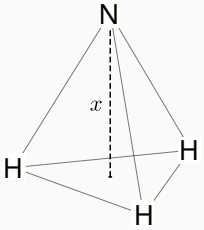
Charles Hard Townes

Nicolay Gennadiyevich Basov

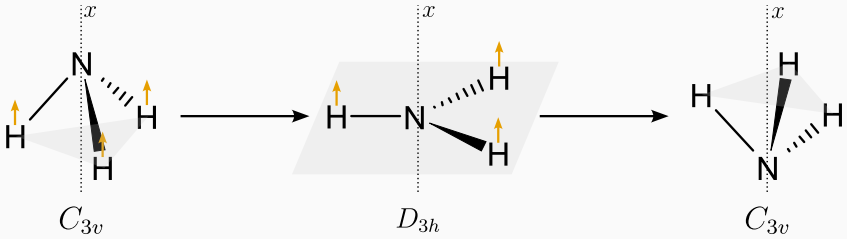
Aleksandr Mikhailovich Prokhorov

Inversion motion of NH_3

Inversion coordinate

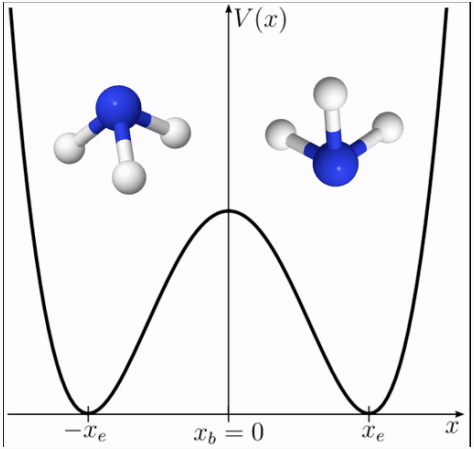


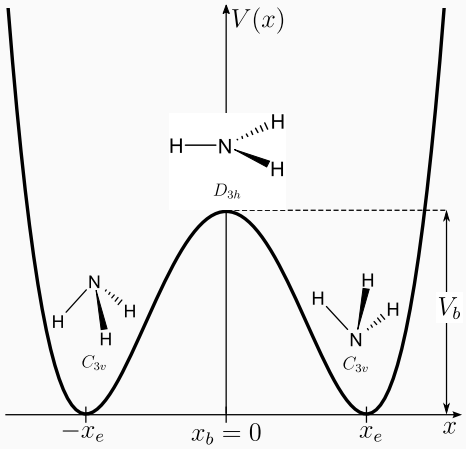
Umbrella type vibrational motion $\Longrightarrow$ symmetric angular mode



Double well potential

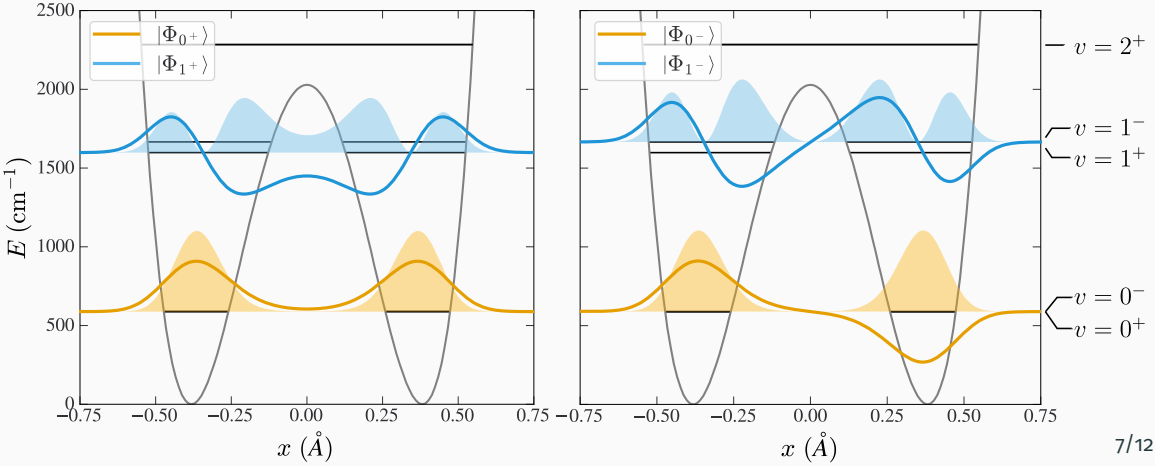
$$\hat{H} = -\frac{\hbar^2}{2\mu}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{V_b}{x_e^4}x^4 - \frac{2V_b}{x_e^2}x^2 + V_b$$





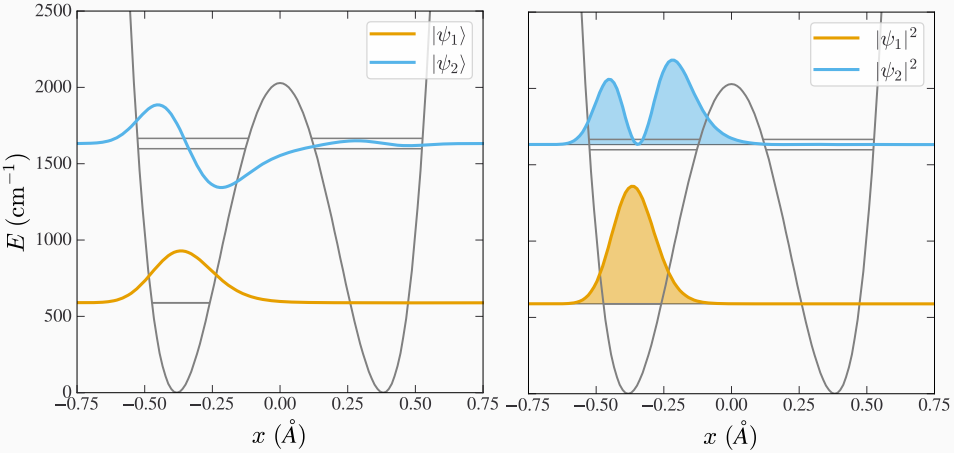
Energy levels & Stationary states

- Pseudo-degeneracy
- Symmetrically delocalized

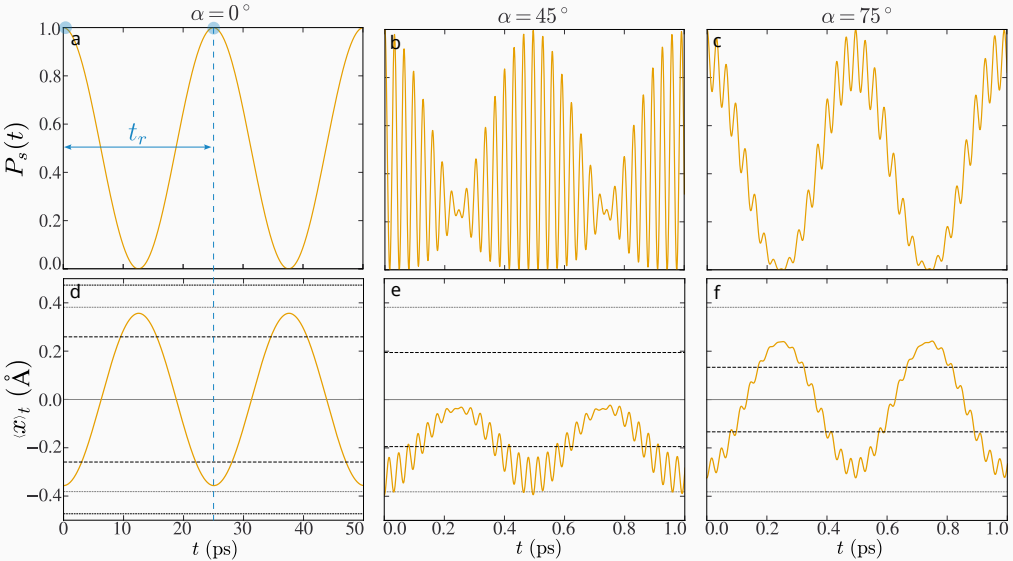


Non-stationary states

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

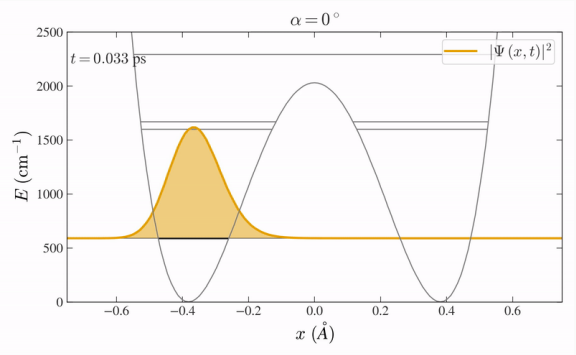


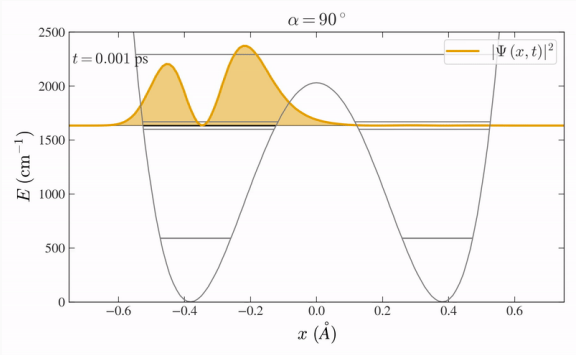
Time Dynamics of NS: Survival Probability, ⟨Position⟩ & Recurrence Time



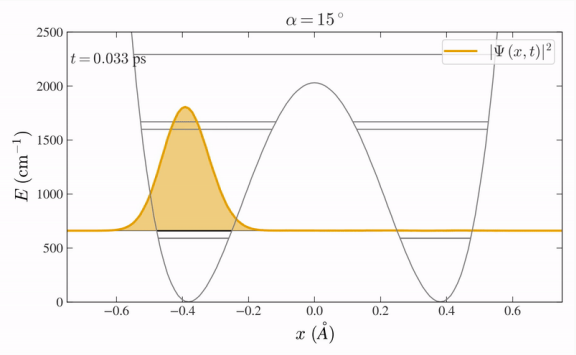
Animations

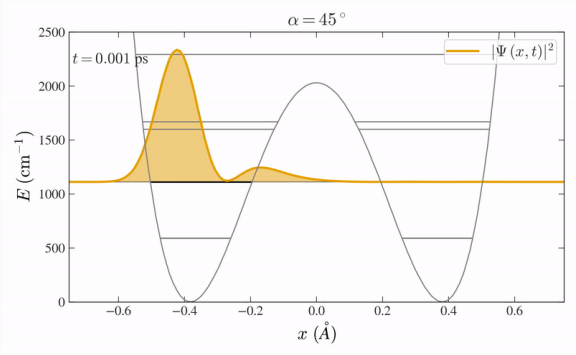
Limit non-stationary states





Intermediate non-stationary states





Conclusions

1. System can be described by NS $\rightarrow$ **spectroscopy**
2. Expectation values of eigenfunctions do not vary with $t \rightarrow$ **NS**
3. Observe tunnelling $\rightarrow$ QM time evolution of **localized NS**
4. Localized NS evolve over t crossing the barrier by **tunnelling**
5. Tunnelling is
   - **Regular** $\rightarrow$ initial NS of 2 SS $\implies \uparrow \boldsymbol{P_T}$
   - **Irregular** $\rightarrow$ NS of more than 2 SS in superposition $\implies \downarrow \boldsymbol{P_T}$