Quantum Tunneling Time

with Applications to Point Mutations in DNA

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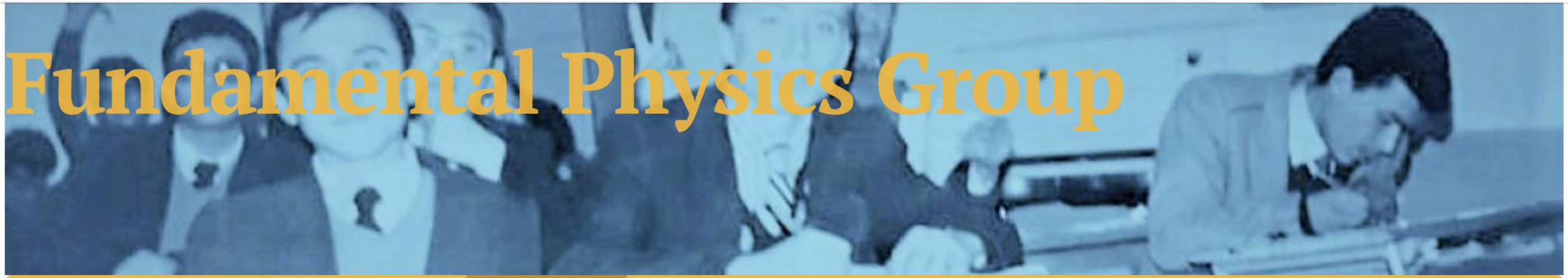
Sabancı Üniversitesi
FACULTY OF ENGINEERING AND NATURAL SCIENCES



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OUTLINE

- Tunneling Time: Which interpretation of the quantum theory is realized in nature?

- Tunneling Time: What is the true transmission time?

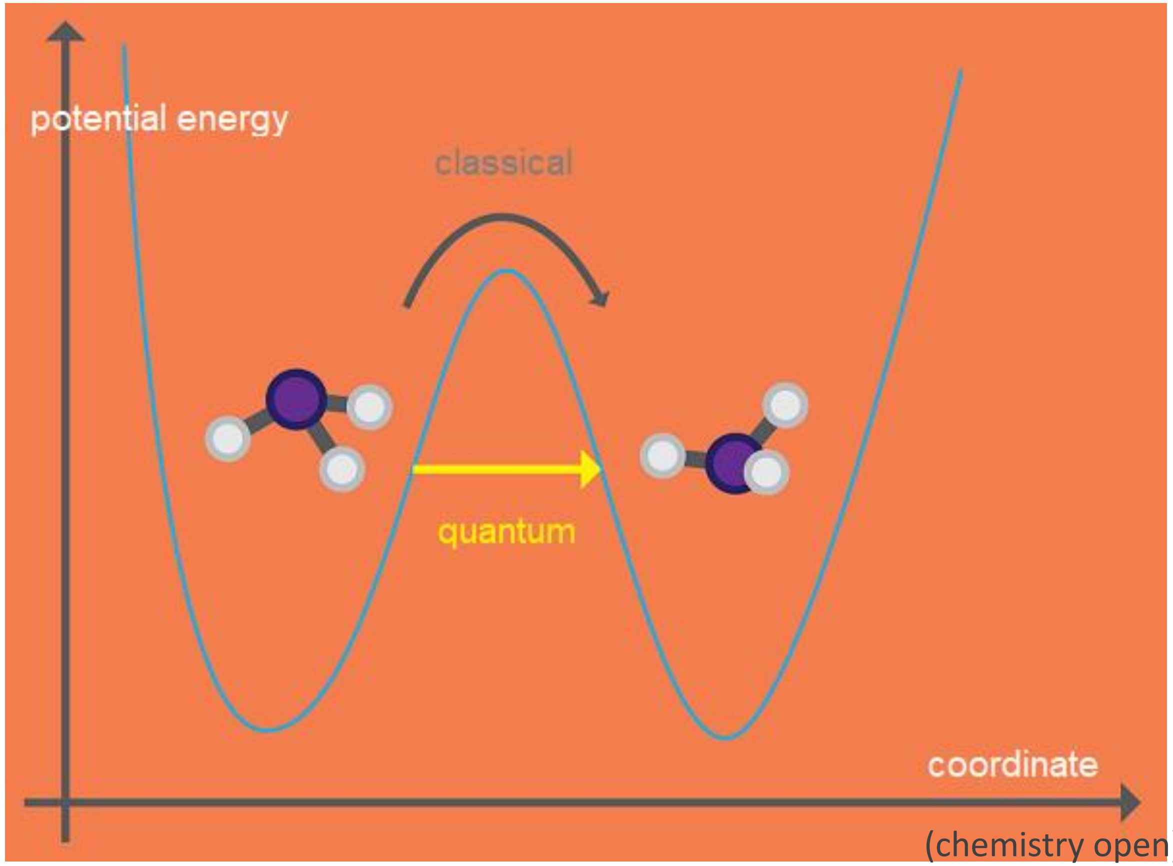
- Tunneling Time: Is there an entropic equivalent of the imaginary time under the barrier?

    - Entropic Proton Tunneling Time and Point Mutations in DNA

- Future Prospects

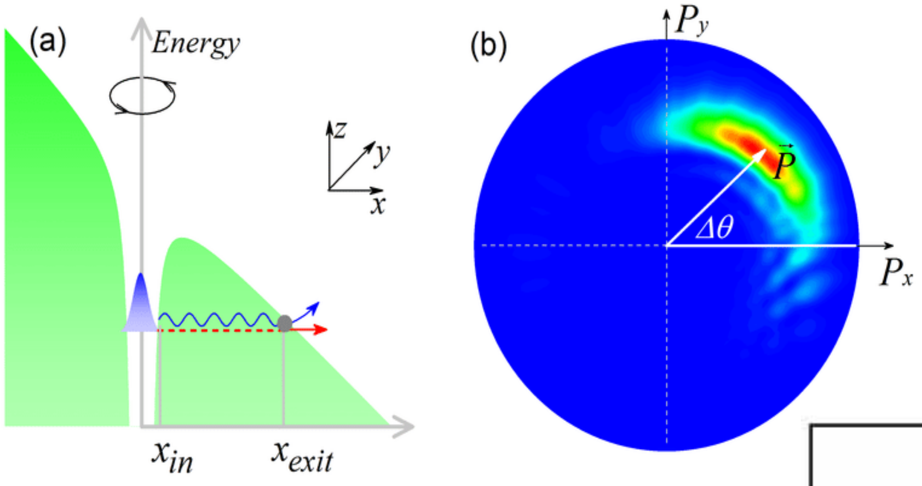
TUNNELING TIME: THEORETICAL AND EXPERIMENTAL STATUS

- Tunneling is a textbook topic, tunneling time is not.
- In quantum theory, time is not an observable so tunneling time needs be modeled by some additional methods/ideas.
- Experiments have already measured a finite tunneling time for quantum particles (electron, proton, atoms).
- Strong-field tunnel ionization experiments have sidelined most of the past tunneling time models.
- It is time to build more complete tunneling time models, test them with the experimental data, and make predictions for other phenomena.

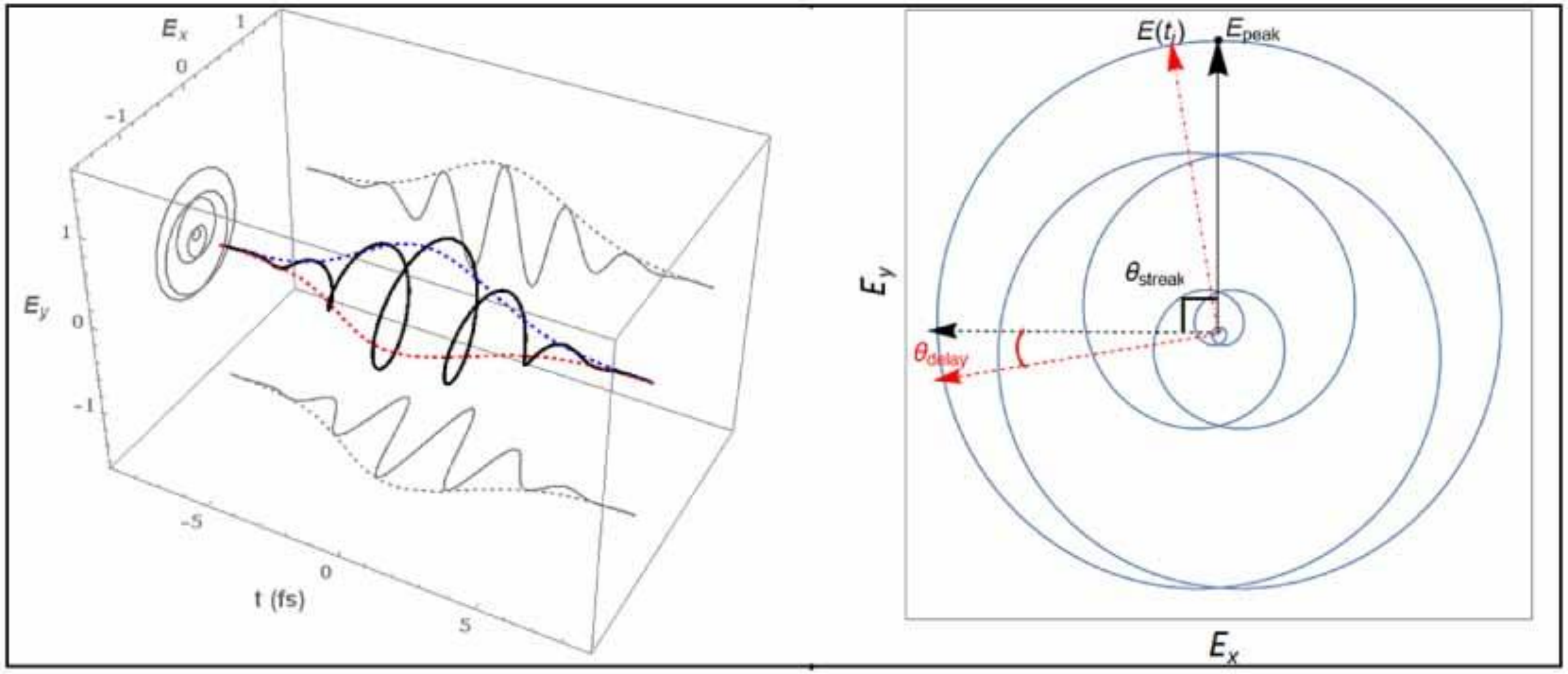


(chemistry open)

EXPERIMENTS: TUNNELING TAKES TIME



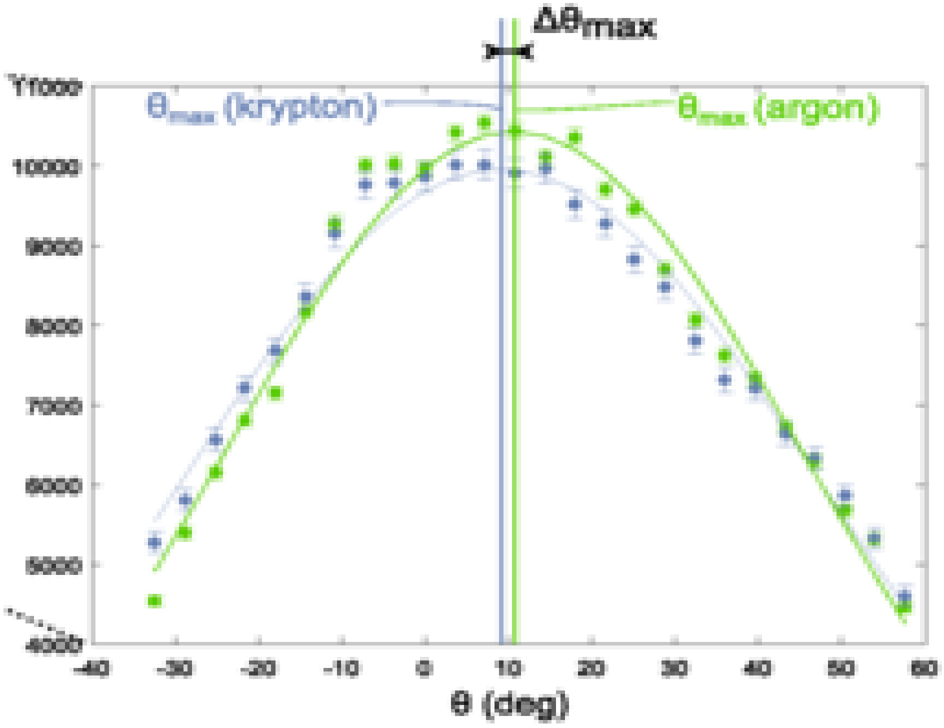
(M. Yuan, Optics Exp. 27 (2019) 6502)



U. Sainadh et al J. Phys. Photonics **2** (2020) 042002

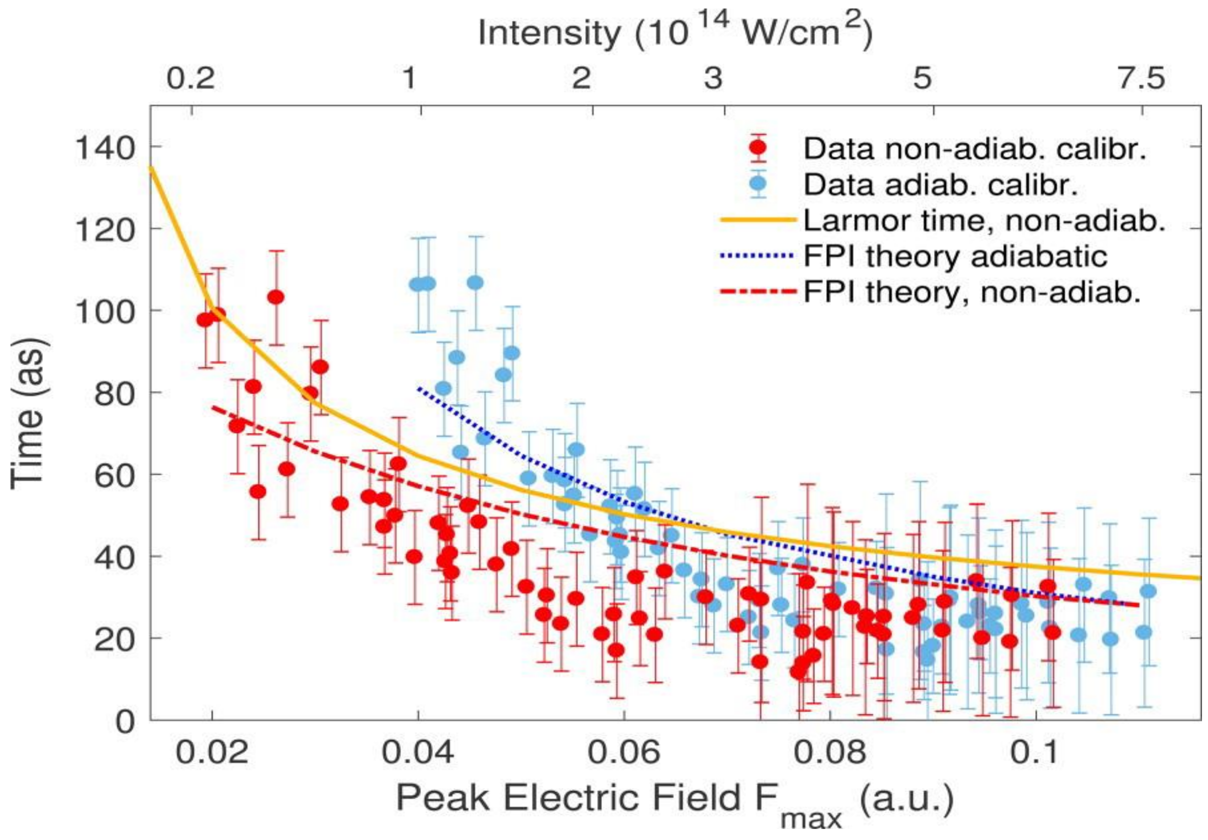
EXPERIMENTS: TUNNELING TAKES TIME

Ar vs Kr tunnel ionizations:



(N. Camus et al., PRL 119 (2017) 023201)

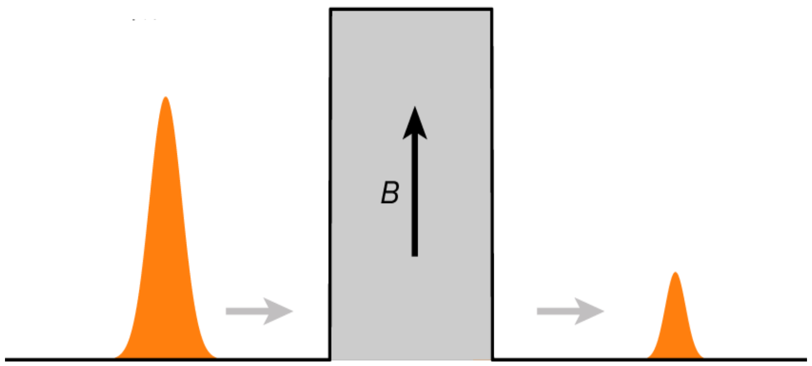
He tunnel ionization:

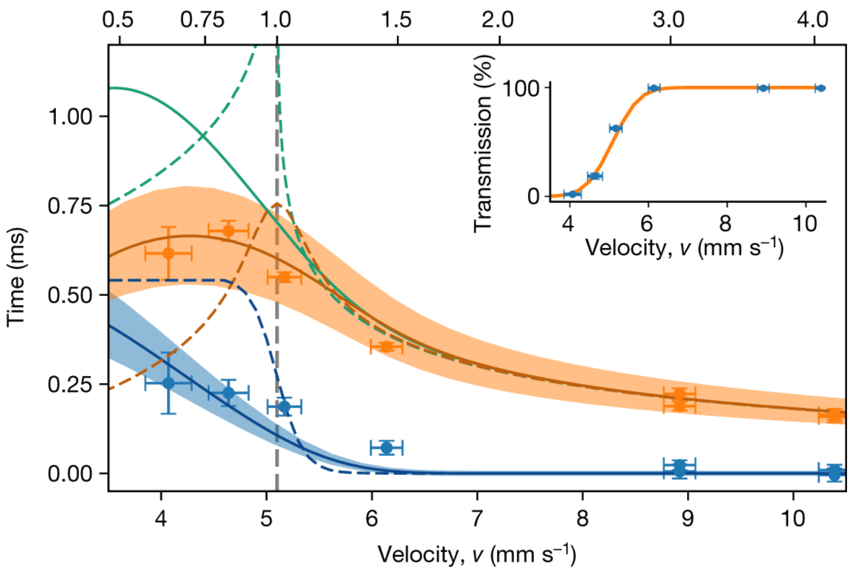


(C. Hoffmann et al., J. Mod. Optics 66 (2019) 1052)

EXPERIMENTS: TUNNELING TAKES TIME

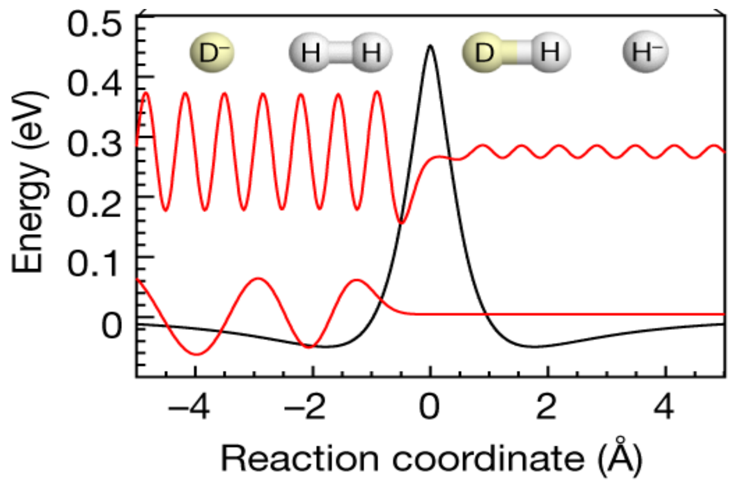
Rb atom tunneling across an optical potential:

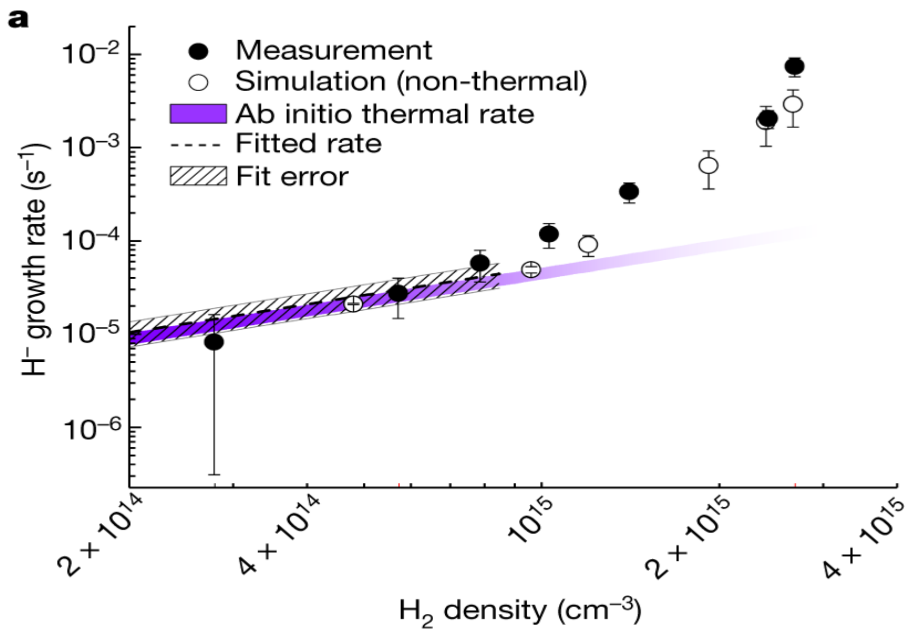




(R. Ramos et al., Nature 583 (2020) 569)

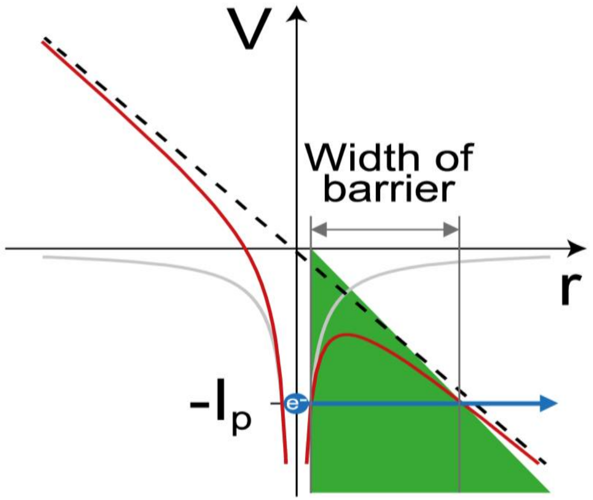
Proton tunneling in $H_2 + D^- \rightarrow H^- + HD$:

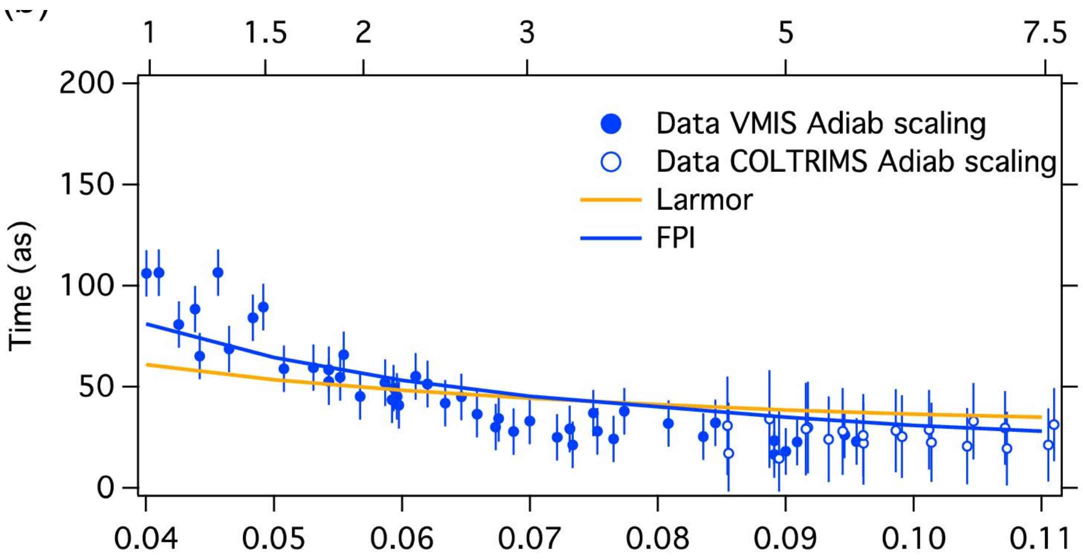




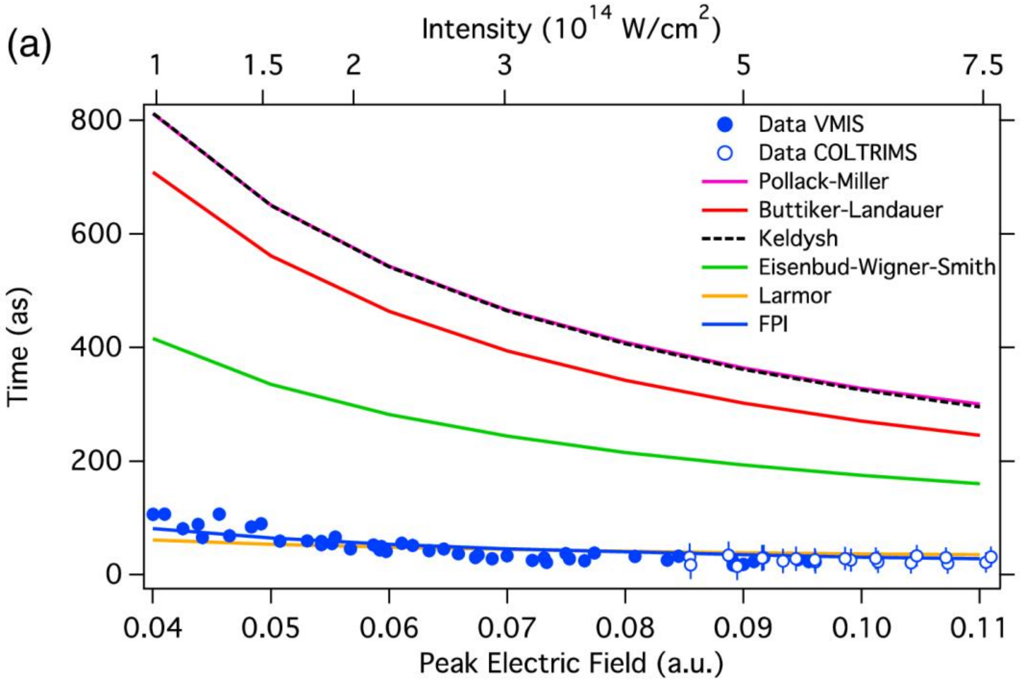
(R. Wild et al., Nature 615 (2023) 425)

KNOWN TIME MODELS DISAGREE WITH EXPERIMENT

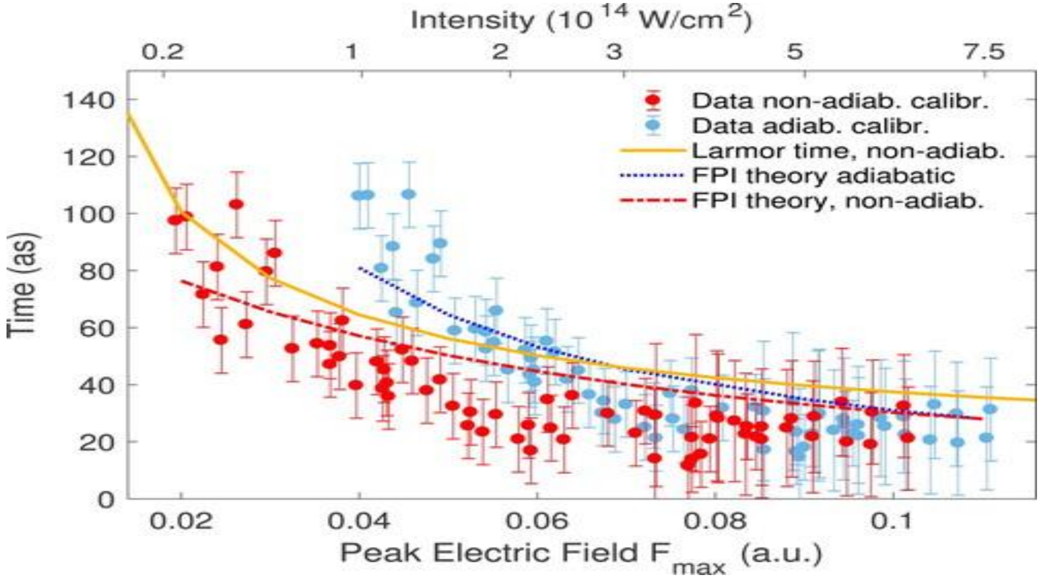




(A. Landsman et al., Optica 1 (2016) 343)



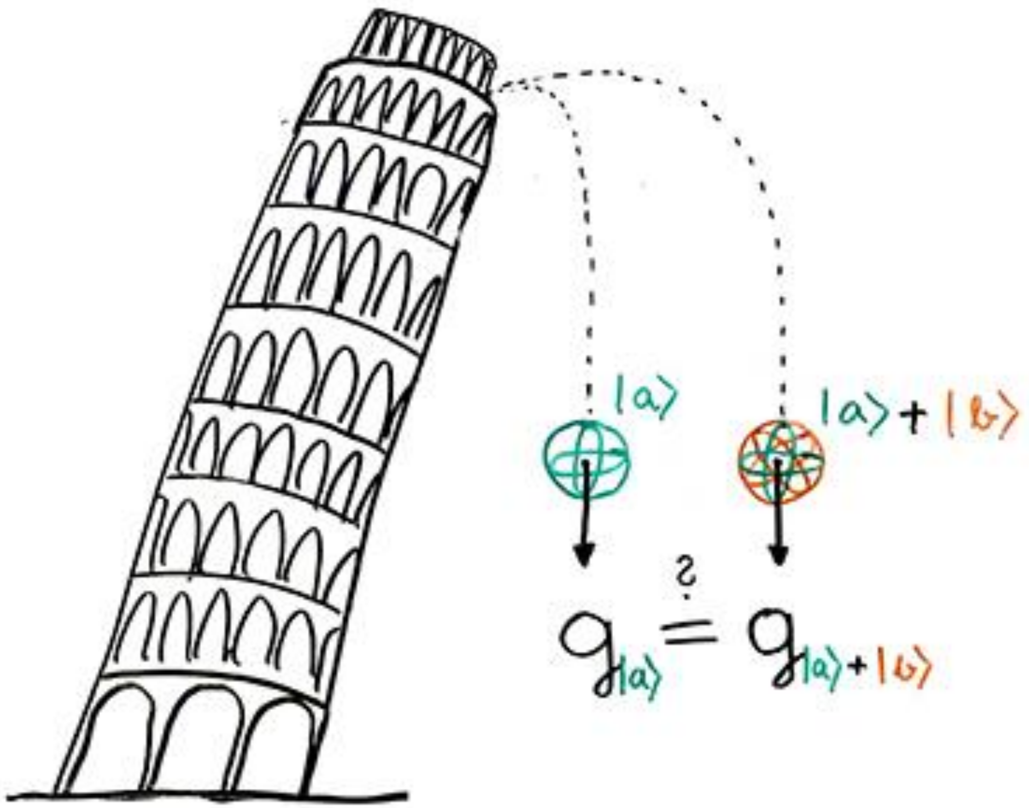
(A. Landsman et al., Optica 1 (2016) 343)



(C. Hoffmann et al., J. Mod. Optics 66 (2019) 1052)

WHICH INTERPRETATION OF THE QUANTUM THEORY ?

- Imagine an ultra-high vacuum (pressures about 10^{-5} Pa or mean free paths about 10^{5} m).
- Throw quantum particles upwards and measure their return time.
- This process enables us to answer two crucial questions:
  - Which interpretation of quantum theory is realized in nature? Copenhagen or Bohmian?
  - What is the tunneling time formula?

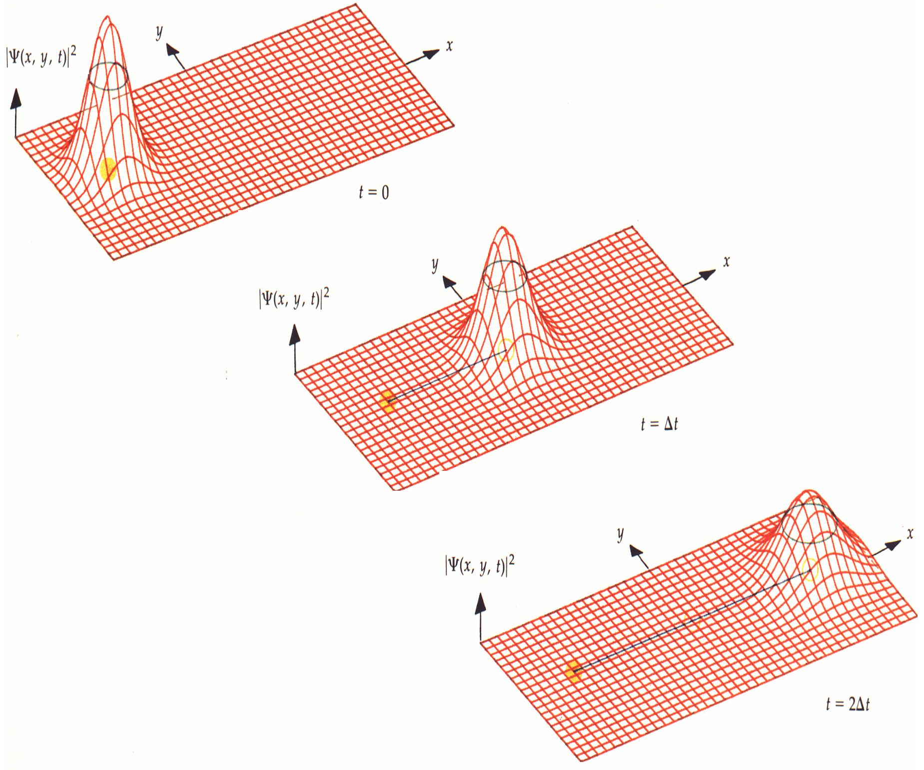


(taken from https://equs.org)

WHICH INTERPRETATION OF THE QUANTUM THEORY ?

- Imagine an ultra-high vacuum (pressures about 10^{-5} Pa or mean free paths about 10^{5} m).

- Model particles by a wavepacket of width d.



(taken from user42076 @ stack exchange)

	Copenhagen	Bohmian
particle trajectory	no	yes
probability backflow	yes	no

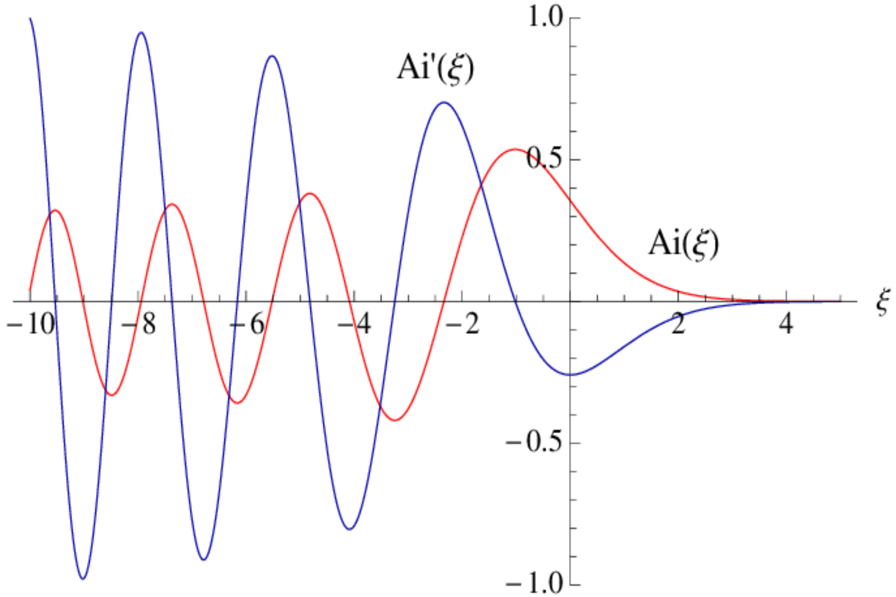
	Copenhagen	Bohmian
$\frac{(\Delta t)_q}{(\Delta t)_c}$	$1+\frac{\hbar^2}{4m^2d^2v_i^2}+\vartheta(\hbar^4)$	$1+\frac{\hbar}{m\sqrt{2gd^3}}+\vartheta(\hbar^2)$

(P. Flores et al., Phys. Rev. A99 (2019) 042113)

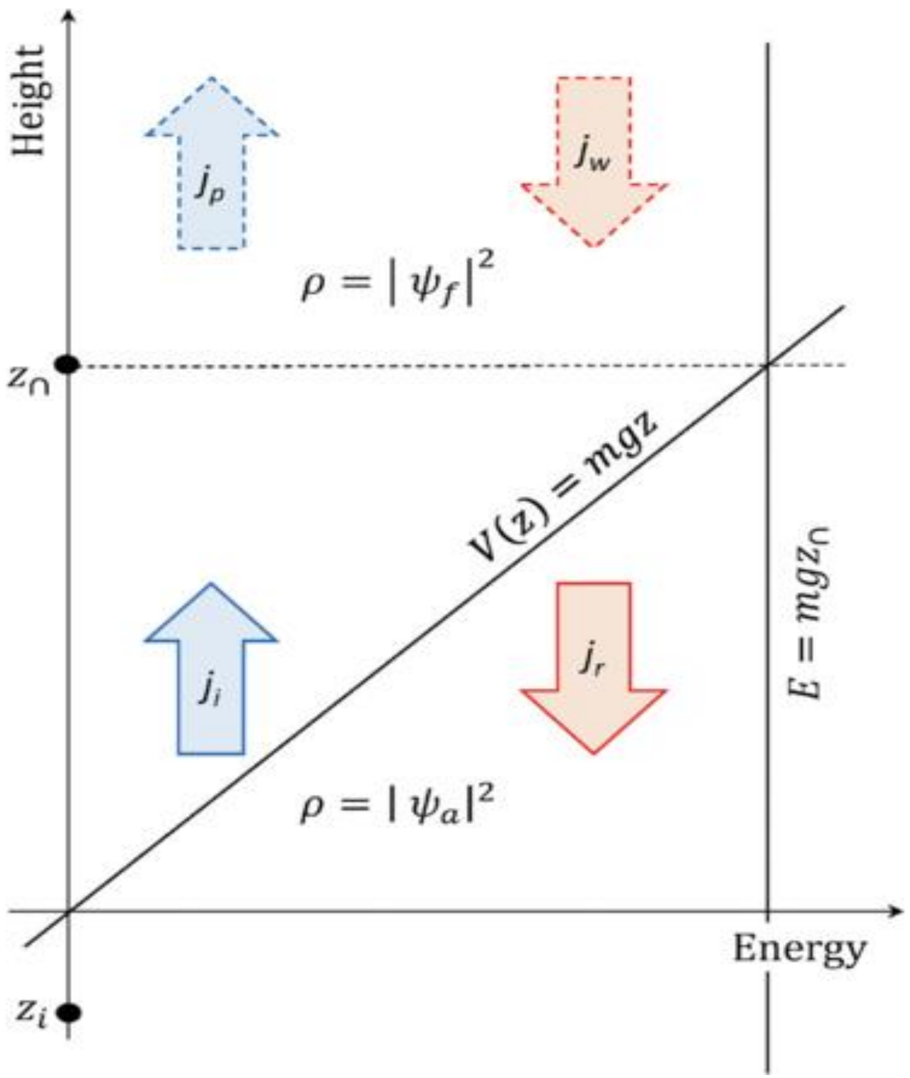
(DD, Phys. Rev. A106 (2022) 022215)

WHICH INTERPRETATION OF THE QUANTUM THEORY ?

- Imagine an ultra-high vacuum (pressures about 10^{-5} Pa or mean free paths about 10^5 m).
- Consider stationary-state mono-energetic particles (states with no classical analogue).



$$\zeta = \frac{2}{3}\left(\frac{|z - z_{\cap}|}{L_q}\right)^{\frac{3}{2}} \quad \text{with} \quad L_q = \left(\frac{\hbar^2}{2m^2 g}\right)^{\frac{1}{3}}$$



(DD, Phys. Rev. A106 (2022) 022215)

WHICH INTERPRETATION OF THE QUANTUM THEORY ?

$$\psi_f(z) = \psi_p(z) + \psi_w(z)$$

$$\psi_p(z) = Ni\zeta^{\frac{1}{3}}\left(e^{\frac{i\pi}{6}} I_{\frac{1}{3}}(\zeta) + e^{-\frac{i\pi}{6}} I_{-\frac{1}{3}}(\zeta)\right)$$

$$\psi_w(z) = -N\zeta^{\frac{1}{3}}\left(\left(1 - e^{-\frac{i\pi}{3}}\right) I_{\frac{1}{3}}(\zeta) - \left(1 - e^{\frac{i\pi}{3}}\right) I_{-\frac{1}{3}}(\zeta)\right)$$

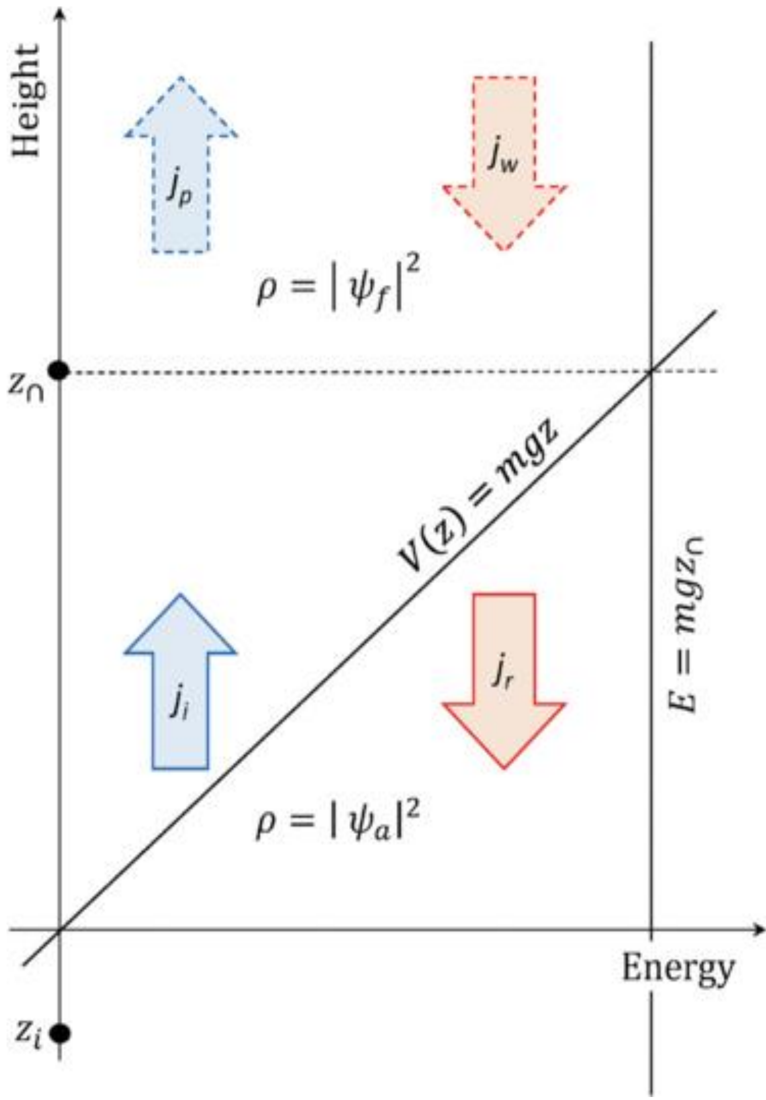
$$j_p = -j_w = \frac{3N^2}{2\pi}\left(\frac{3g\hbar}{m}\right)^{\frac{1}{3}}$$

$$\psi_a(z) = \psi_i(z) + \psi_r(z)$$

$$\psi_i(z) = N\zeta^{\frac{1}{3}}\left(e^{-\frac{i\pi}{3}} J_{\frac{1}{3}}(\zeta) + e^{\frac{i\pi}{3}} J_{-\frac{1}{3}}(\zeta)\right)$$

$$\psi_r(z) = N\zeta^{\frac{1}{3}}\left(\left(1 - e^{-\frac{i\pi}{3}}\right) J_{\frac{1}{3}}(\zeta) + \left(1 - e^{\frac{i\pi}{3}}\right) J_{-\frac{1}{3}}(\zeta)\right)$$

$$j_i = -j_r = \frac{3N^2}{2\pi}\left(\frac{3g\hbar}{m}\right)^{\frac{1}{3}}$$

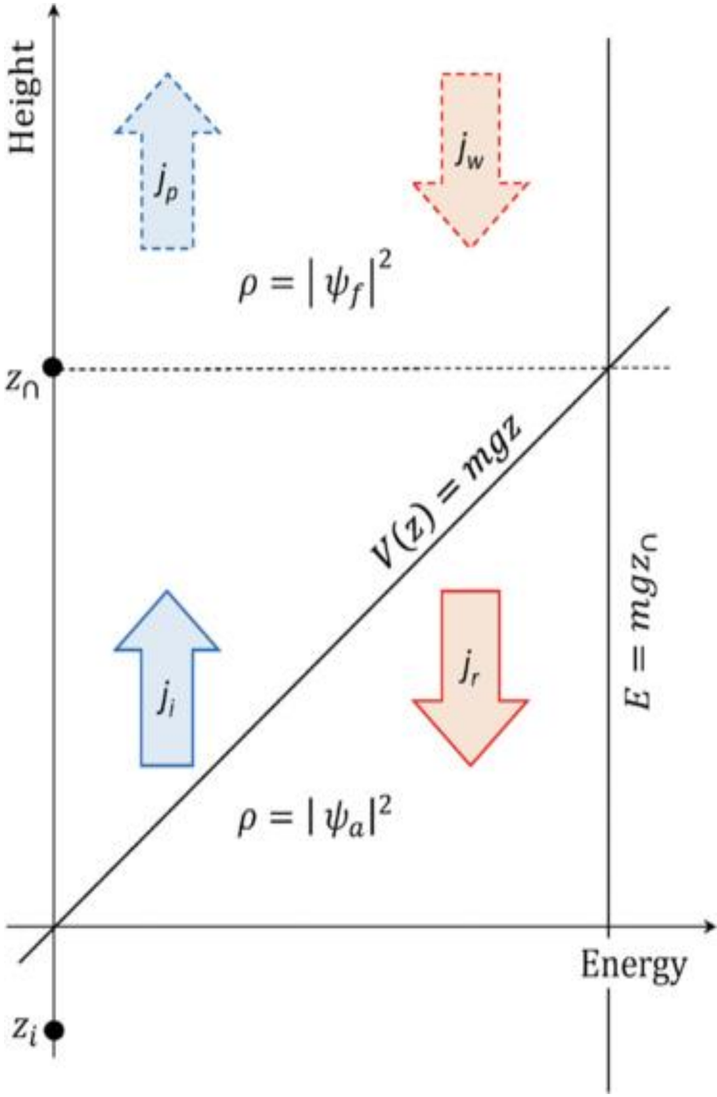


(DD, Phys. Rev. A106 (2022) 022215)

WHICH INTERPRETATION OF THE QUANTUM THEORY ?

$$(\Delta t)_q^{(penetrate)} = \int_{z_i}^{z_\cap} \frac{\left|\psi_f(z)\right|^2}{2j_p} dz = \frac{2\pi T_q}{\left[3^{\frac{1}{3}}\Gamma\left(\frac{1}{3}\right)\right]^2} = (\Delta t)_q^{(withdraw)}$$

$$(\Delta t)_q^{(rise)} = \int_{z_i}^{z_\cap} \frac{|\psi_a(z)|^2}{2j_i} dz = -\frac{2\pi T_q}{\left[3^{\frac{1}{3}}\Gamma\left(\frac{1}{3}\right)\right]^2} + 2\pi T_q \left(\beta_q\left[Ai(-\beta_q)\right]^2 + \left[Ai'(-\beta_q)\right]^2\right) = (\Delta t)_q^{(fall)}$$

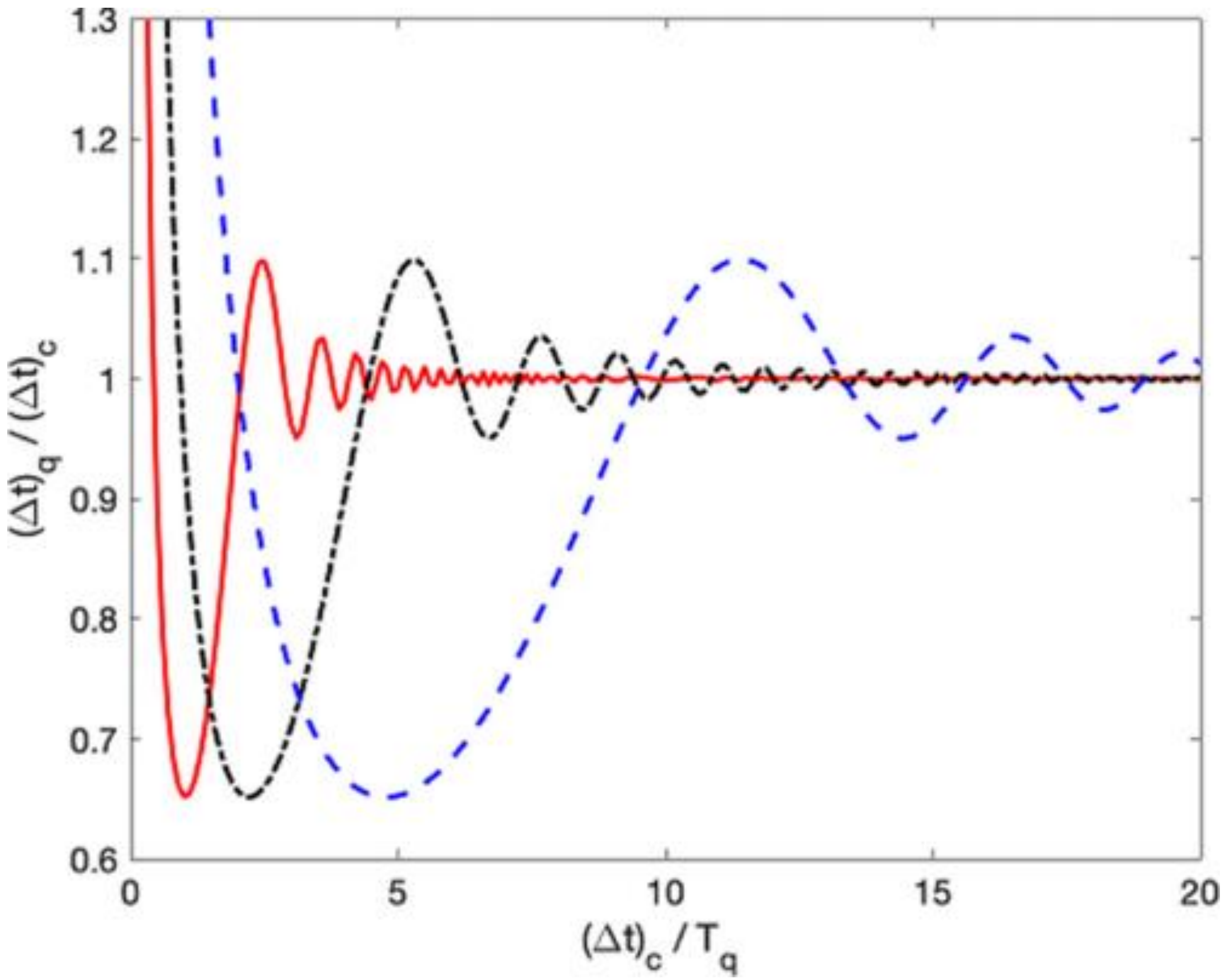


$$\beta_q = \left(\frac{(\Delta t)_c}{4T_q}\right)^2 \quad \text{with} \quad T_q = \left(\frac{\hbar}{4mg^2}\right)^{\frac{1}{3}}$$

(DD, Phys. Rev. A106 (2022) 022215)

WHICH INTERPRETATION OF THE QUANTUM THEORY ?

$$(\Delta t)_q = (\Delta t)_q^{(rise)} + (\Delta t)_q^{(penetrate)} + (\Delta t)_q^{(withdraw)} + (\Delta t)_q^{(fall)}$$



- Low $(\Delta t)_c$: $(\Delta t)_q$ fluctuates strongly. It could be smaller or larger than $(\Delta t)_c$.
- High $(\Delta t)_c$: $(\Delta t)_q$ relaxes in an oscillatory fashion towards $(\Delta t)_c$.
- Short-height flights can better extract quantum effects.
- Equivalence principle is attained for long-height flights.

(DD, Phys. Rev. A106 (2022) 022215)

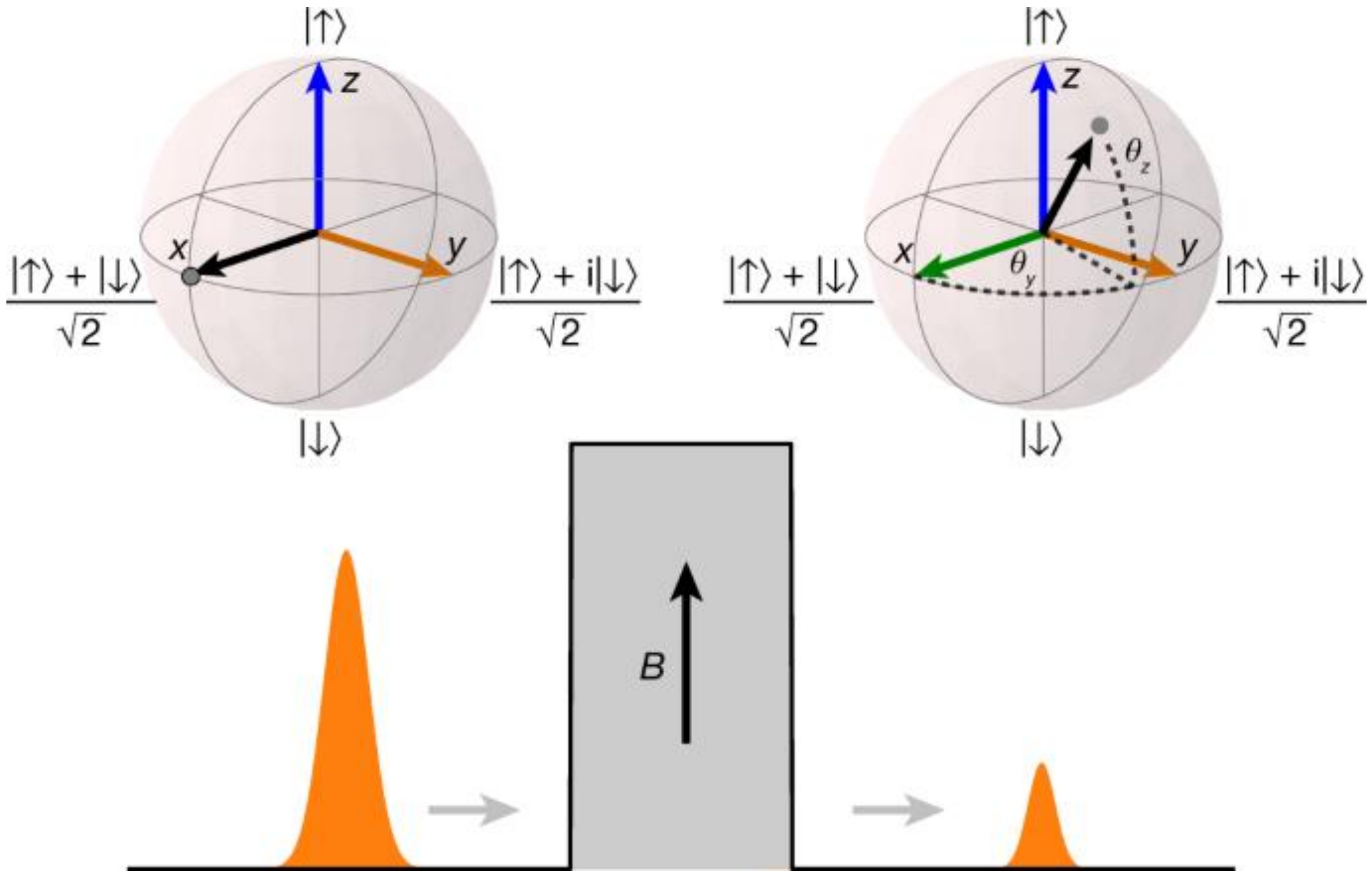
WHAT IS THE TRUE TRANSMISSION TIME?

- Particle spin precesses when passing through magnetic field regions.

- Given a barrier covered by a feeble magnetic field $\vec{B} = B\,\hat{z}$ and initial particle spin $\vec{S} = \frac{\hbar}{2}\,\hat{x}$:

  - Particle spin acquires a y-component, even when potential $= 0$!
  - Particle spin acquires a z-component only when potential $\neq 0$!
  - (Energy) state of the particle remains intact for feeble magnetic fields.

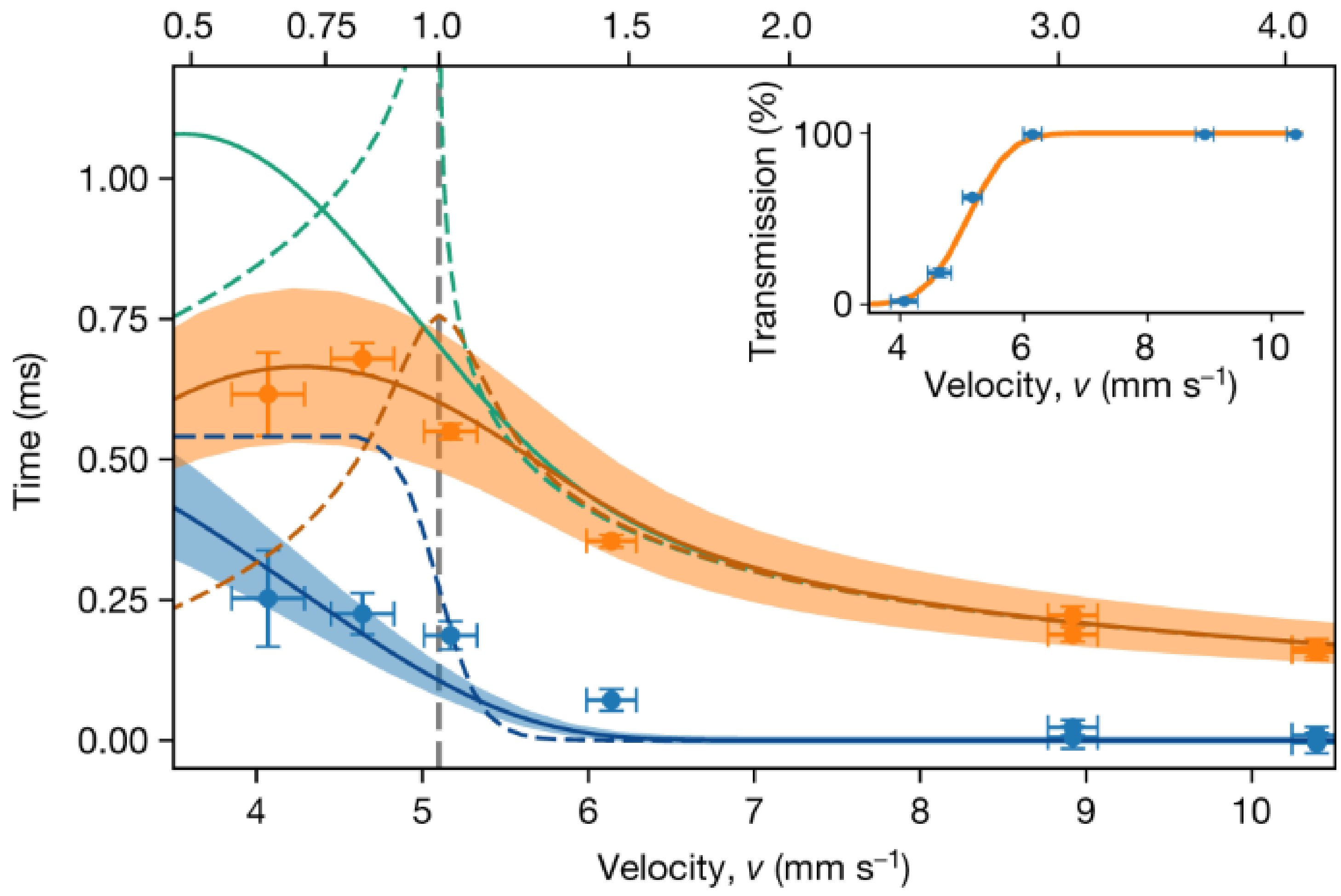
(M. Büttiker, Phys. Rev. B27 (1983) 6178)



(R. Ramos et al., Nature 583 (2020) 529)

WHAT IS THE TRUE TRANSMISSION TIME?

- There are two times:
  - τ_y for precession about y axis, and
  - τ_z for precession about z axis.
- Question: What is the actual tunneling time?
  - Büttiker: $(\mathrm{ATT})_B = \sqrt{\tau_y^2 + \tau_z^2}$
  - Steinberg: $(\mathrm{ATT})_S = \tau_y$



(M. Büttiker, Phys. Rev. B27 (1983) 6178)

(R. Ramos et al., Nature 583 (2020) 529)

WHAT IS THE TRUE TRANSMISSION TIME?

- Uncertainty product:

$$(\Delta S_x)^2 \left(\Delta S_y\right)^2 \geq \frac{\hbar^2}{4} \langle S_z \rangle^2$$

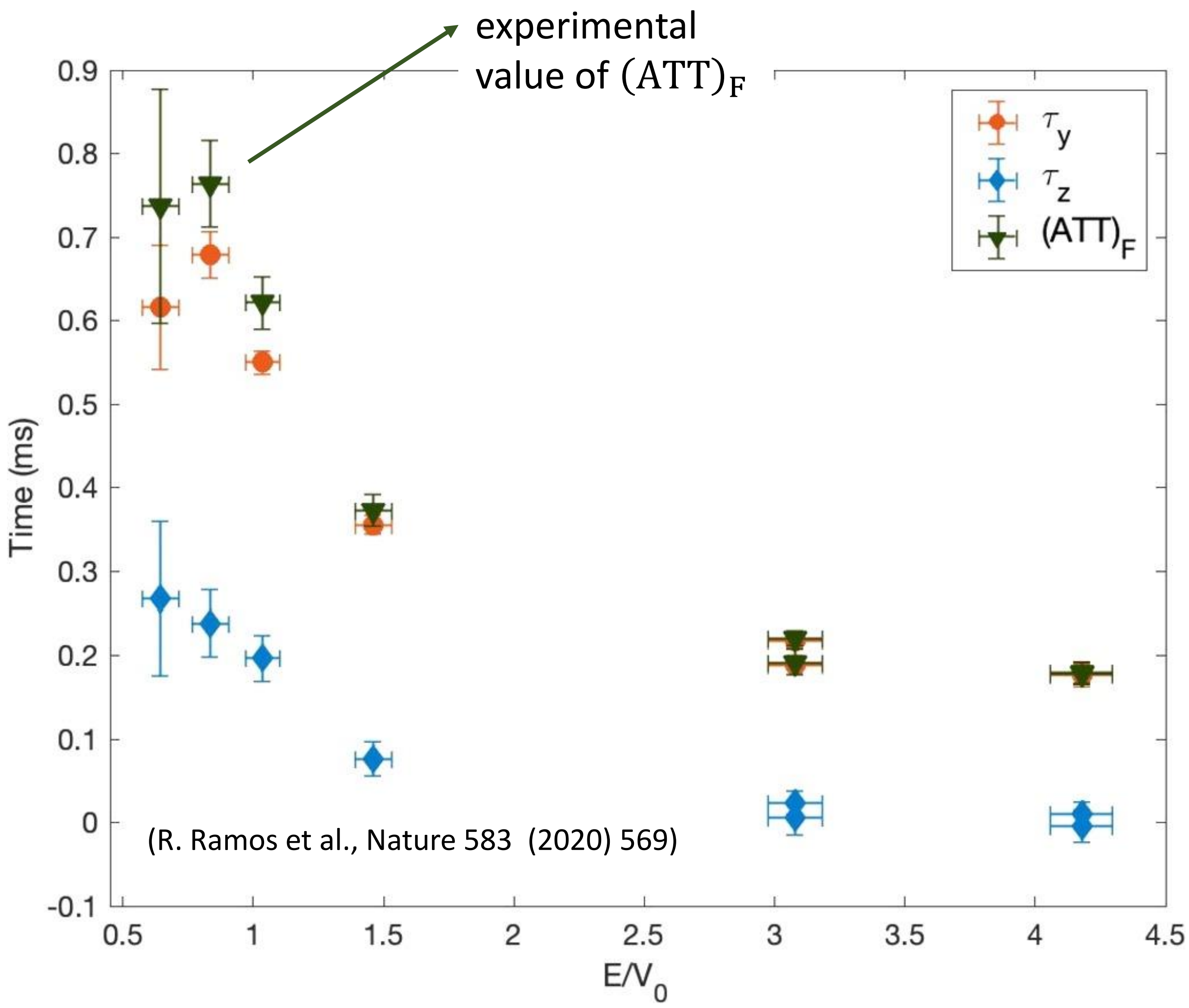
potential

- Fano factor $(\Delta S_x)^2 / \langle S_x \rangle$ = a measure of spin dispersion (Poisson, clustered, uniform).

- Use Fano factor to define the actual tunneling time:

$$(\mathrm{ATT})_F = \omega_L^{-1} \frac{(\Delta S_x)^2}{\frac{\hbar}{2}\langle S_x \rangle} \frac{\left(\Delta S_y\right)^2}{\frac{\hbar}{2}\langle S_y \rangle}$$

$$\Longrightarrow (\mathrm{ATT})_F = \tau_y + \frac{\tau_z^2}{\tau_y}$$



(DD, Phys. Lett. A448 (2022) 128321)

WHAT IS THE TRUE TRANSMISSION TIME?

- $(\mathrm{ATT})_\mathrm{F}$ proves to be a "physical transmission" time in all the relevant asymptotics.
- A genuine physical time that can be tested new materials to put a (hopefully) end to the question of what the actual tunneling time is.

Table 1: The three ATT candidates in the low-barrier, high-barrier, thick-barrier and classical dynamics limits.

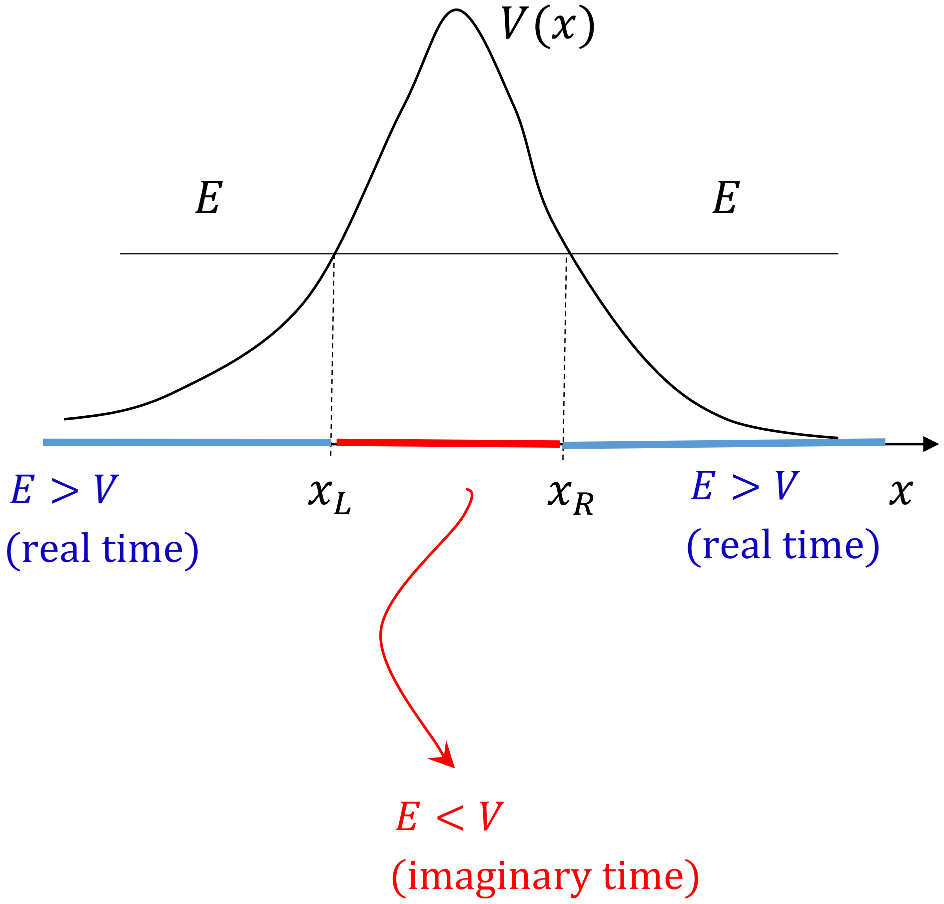
	τ_y	τ_z	$(\mathrm{ATT})_B$	$(\mathrm{ATT})_S$	$(\mathrm{ATT})_F$
low-barrier: $V_0 \ll E$ (fixed E)	$\tau_c(0,E)$	0	$\tau_c(0,E)$	$\tau_c(0,E)$	$\tau_c(0,E)$
high-barrier: $E \ll V_0$ (fixed V_0)	0	$\tau_c(V_0,0)$	$\tau_c(V_0,0)$	0	∞
thick-barrier: $L^2 \gg \frac{\hbar}{m}\tau_c(V_0,E)$ (fixed V_0, E)	$\frac{\hbar}{V_0}\frac{\tau_c(V_0,E)}{\tau_c(0,E)}$	∞	∞	$\frac{\hbar}{V_0}\frac{\tau_c(V_0,E)}{\tau_c(0,E)}$	∞
classical dynamics: $\hbar \to 0$ (fixed V_0, E, L)	0	$\tau_c(V_0,E)$	$\tau_c(V_0,E)$	0	∞

(DD, Phys. Lett. A448 (2022) 128321)

ENTROPIC TUNNELING TIME

- Time is imaginary in tunneling region (classical dynamics).
- Imaginary time is equivalent to inverse temperature (QM ≡ eq. Stat Mech.)
- Energy in quantum fluctuations (no real propagation) should pertain to (useless) entropic energy.
- Uncertainty product with thermal energy sets the time scale of the tunneling transition.
- Entropic tunneling time:

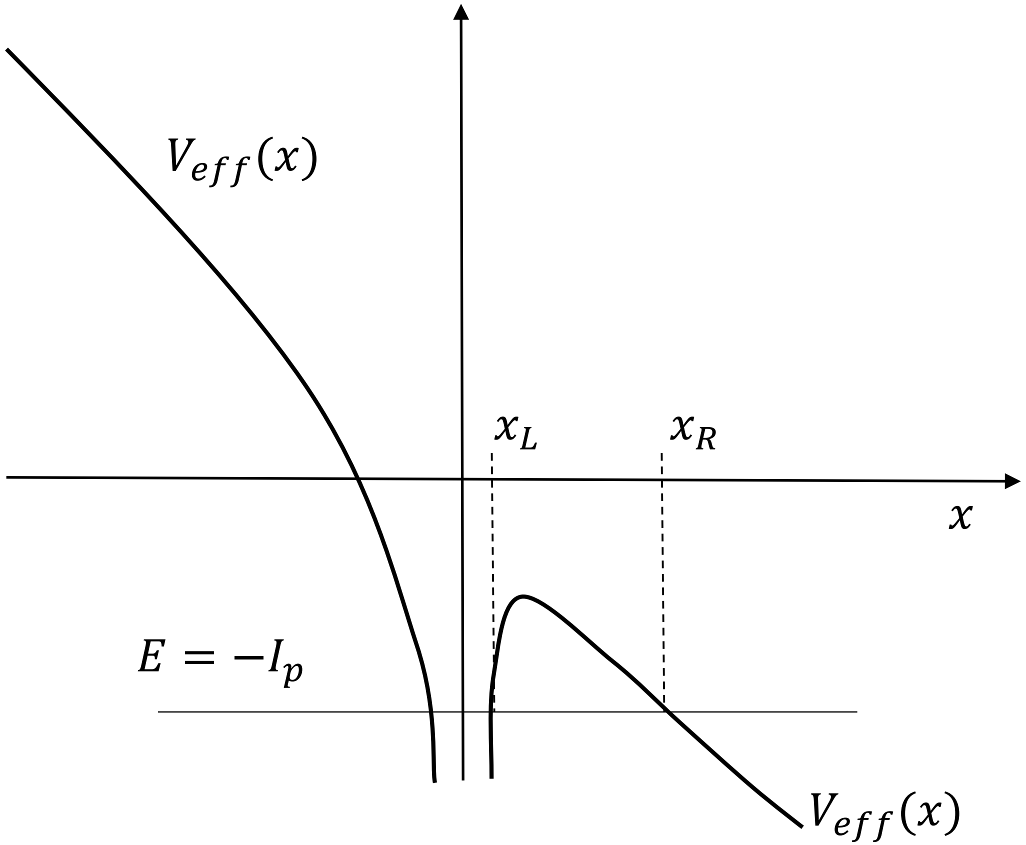
$$(\Delta t)_{ETT} \equiv \frac{k_B \tau_c}{S}$$



- $\tau_c = \int_{x_L}^{x_R} \frac{m\,dx}{\sqrt{2m\,(V(x) - E}}$
- $S \equiv -k_B P \log P$
- $P \equiv \int_{x_L}^{x_R} \psi^\star(x)\psi(x)dx$

ENTROPIC TUNNELING TIME

He tunnel ionization:



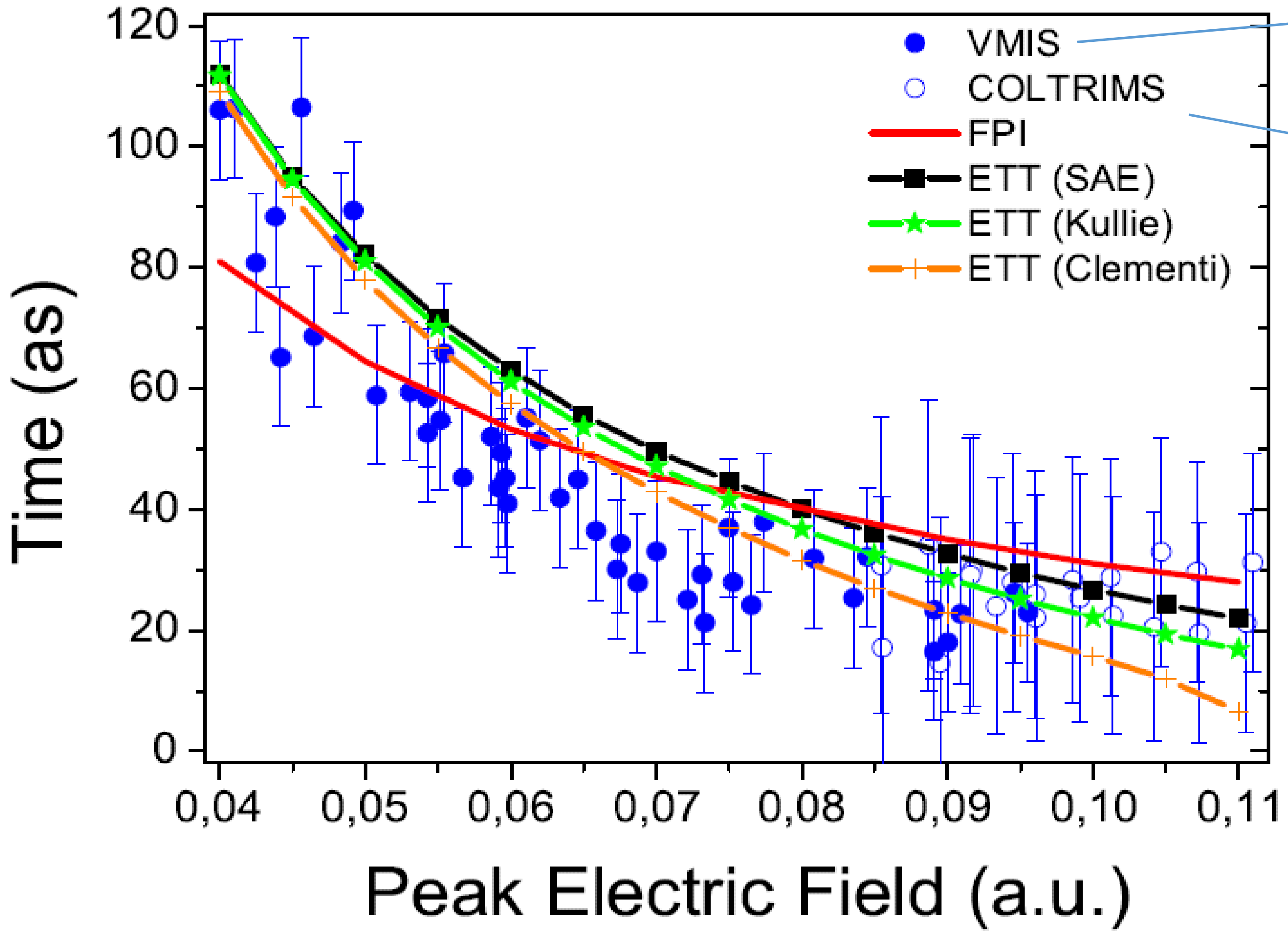
Effective potential at a radius x from the He^+ ion:

$$V_{eff}(x) = -\frac{Z_{eff}(x)}{x} - \mathcal{E}\,x$$

- $Z_{eff}(\text{SAE}) = 1 + 1.231\,e^{-0.662x} - 1.325\,e^{-1.236x} - 0.231\,e^{-0.48x}$
- $Z_{eff}(\text{Kullie}) = 1.375$
- $Z_{eff}(\text{Clementi}) = 1.687$

(SAE: X. Tong et al., J. Phys. B 38 (2005) 2593)
(Kullie: O. Kullie, J. Phys. B 49 (2016) 095601)
(Clementi: E. Clementi et al., J. Chem. Phys. 49 (1963) 2686)

ENTROPIC TUNNELING TIME



velocity map spectrometer (VMIS)

momentum spectrometer (COLTRIMS)

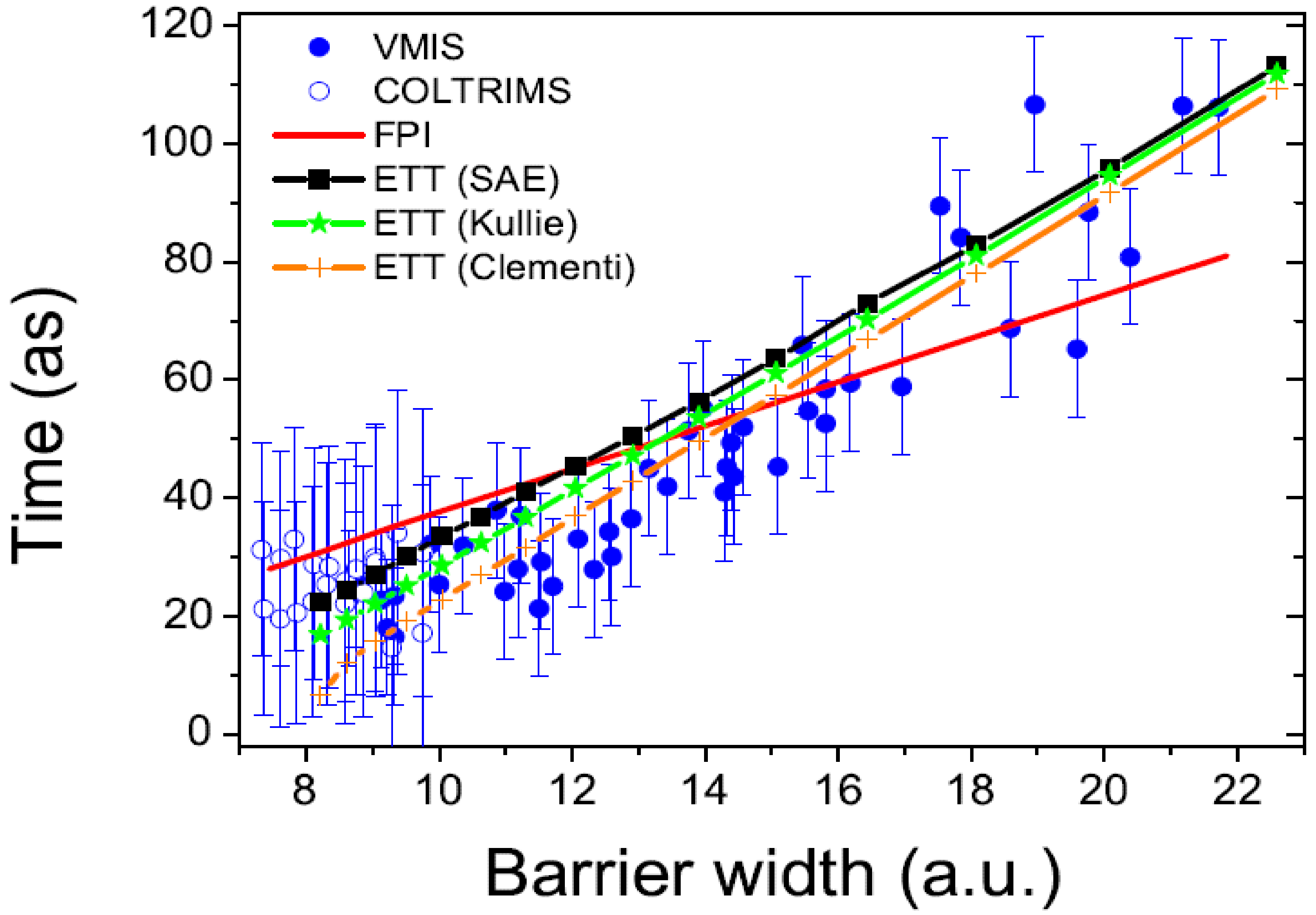
Experiment:

(A. Landsman et al, Optica 1 (2016) 343)

Model:

(DD & T. Güner, Annals of Physics 386 (2017) 291)

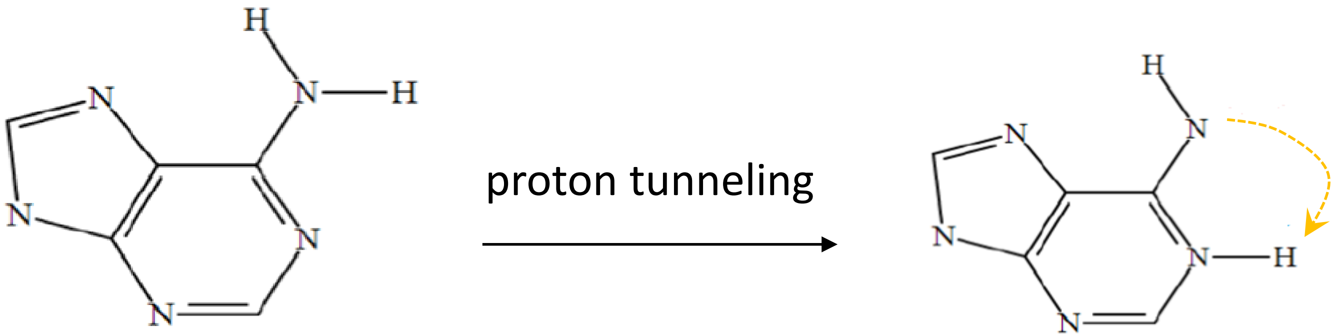
ENTROPIC TUNNELING TIME



Experiment: (A. Landsman et al., Optica 1 (2016) 343)

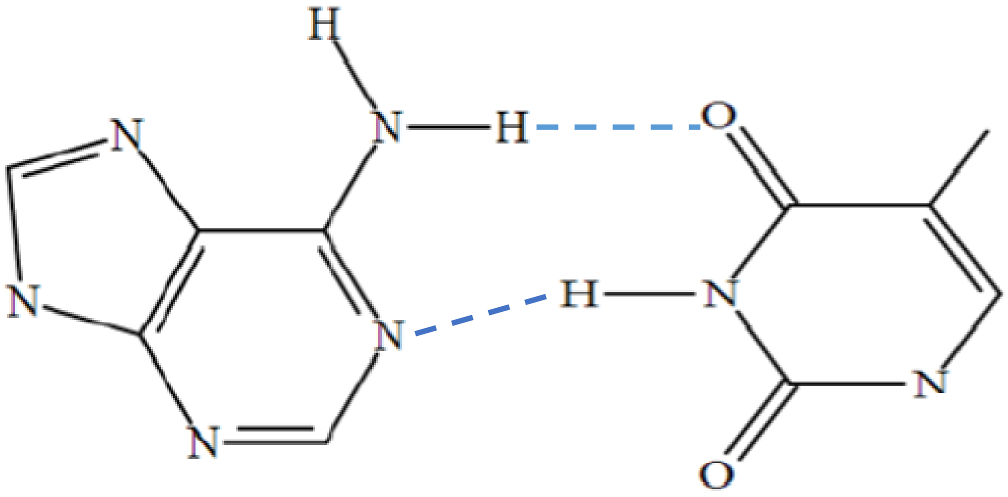
Model: (DD & T. Güner, Annals of Physics 386 (2017) 291)

ENTROPIC TUNNELING TIME: DNA MUTATION



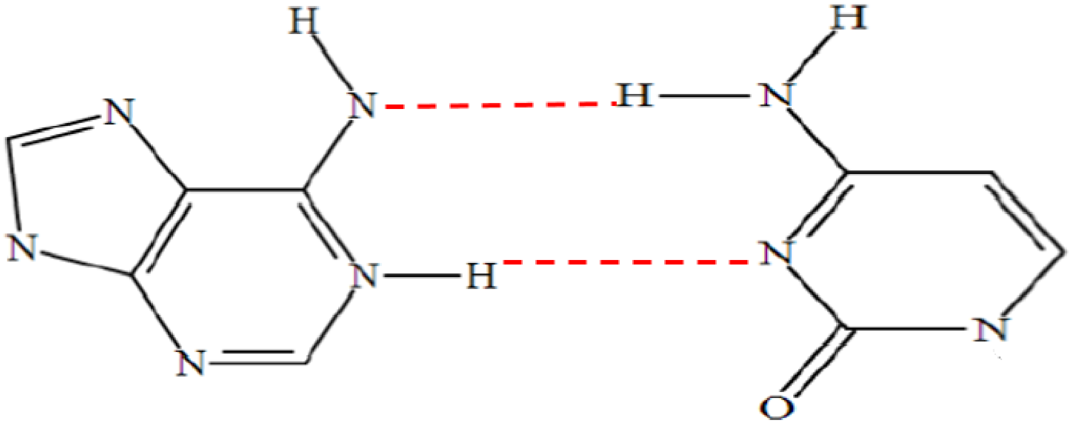
Adenine

Adenine*



Adenine

Thymine



Adenine*

Cytosine

A | C

T | G

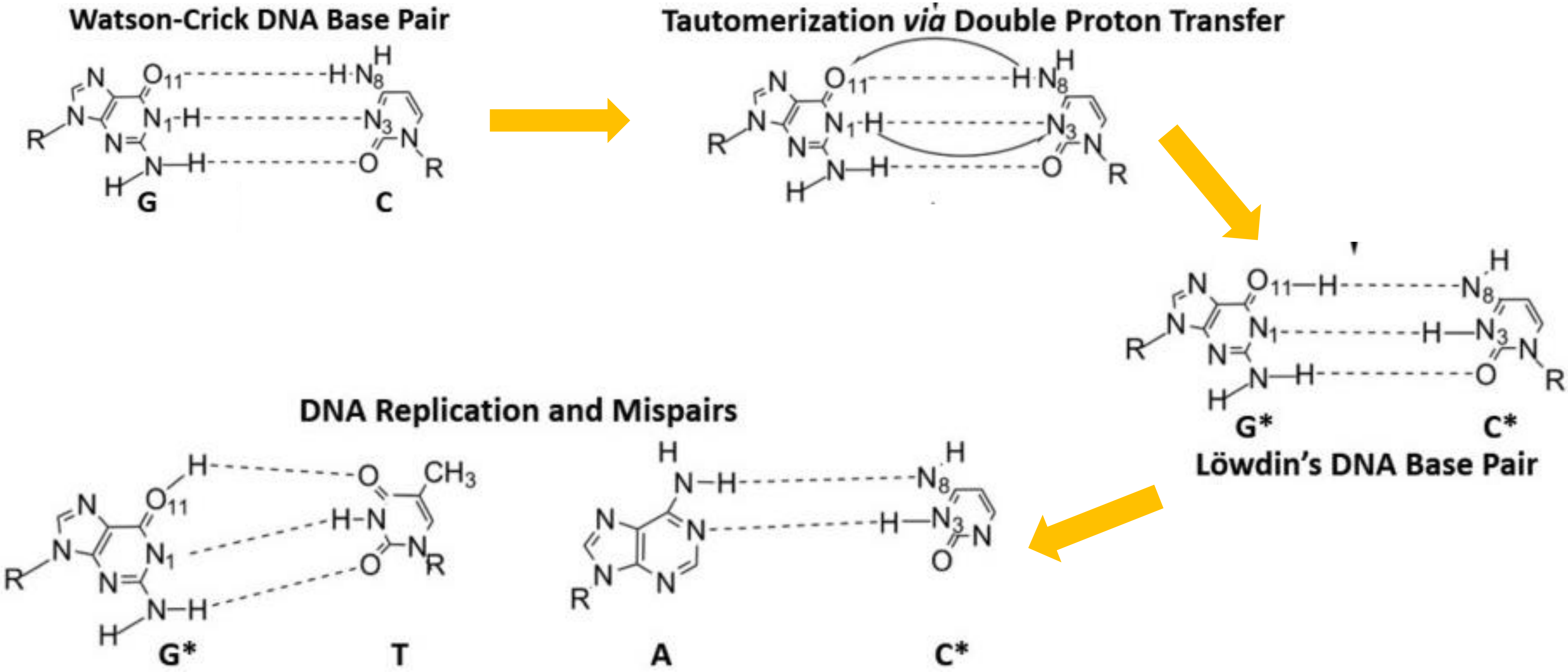
A* — C

T — G*

(P. Löwdin, Rev. Mod. Phys. 35 (1963) 724)

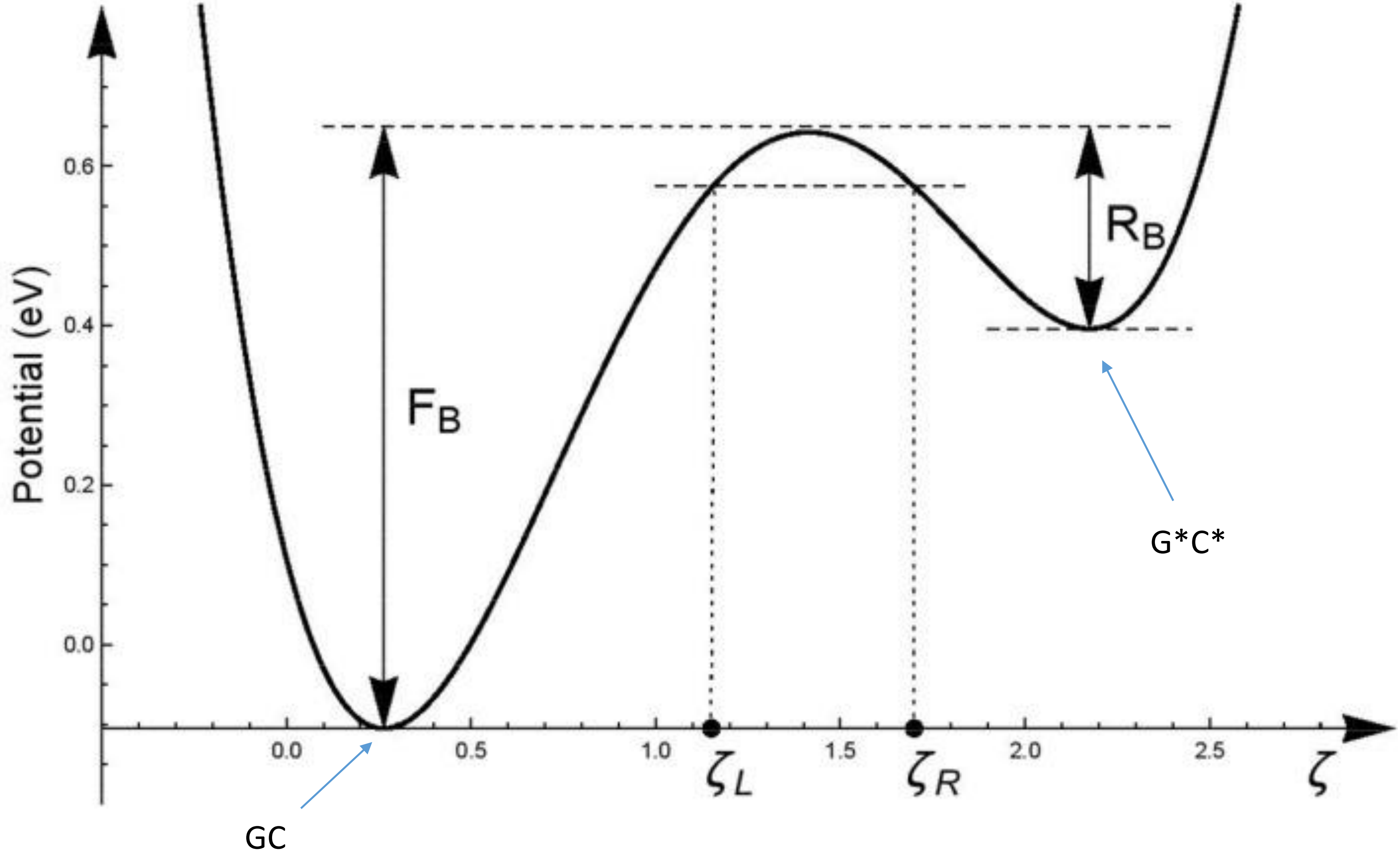
ENTROPIC TUNNELING TIME: DNA MUTATION

Inter-base proton tunneling:



(G. Çelebi, E. Özçelik, E. Vardar, DD, Prog. Biophysics and Molecular Biology 167 (2021) 96)

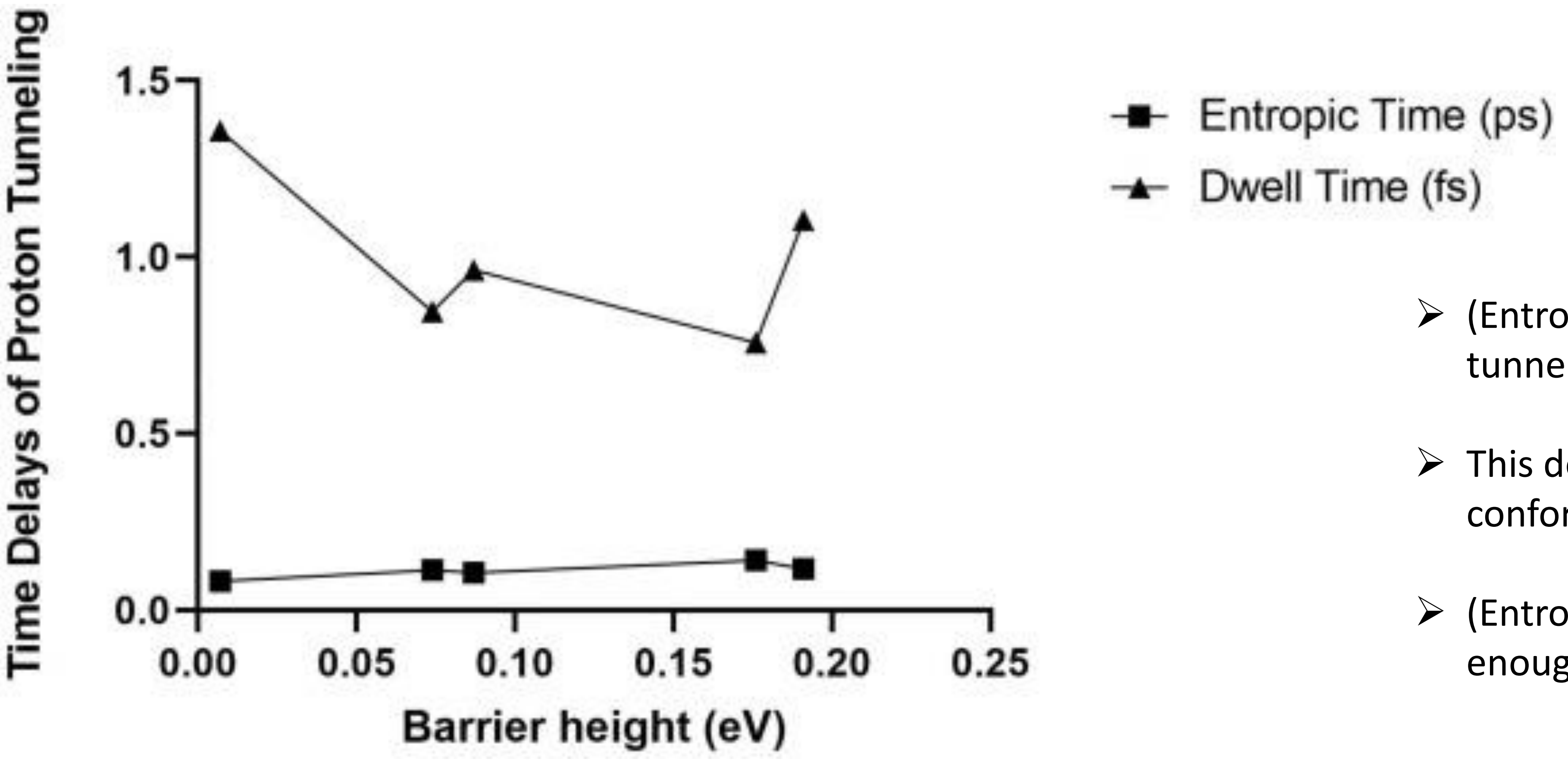
ENTROPIC TUNNELING TIME: DNA MUTATION



(D. Soler-Polo et al., J. Chem. Theor. Comput. 15 (2019) 6984)

ENTROPIC TUNNELING TIME: DNA MUTATION

Inter-base proton tunneling:

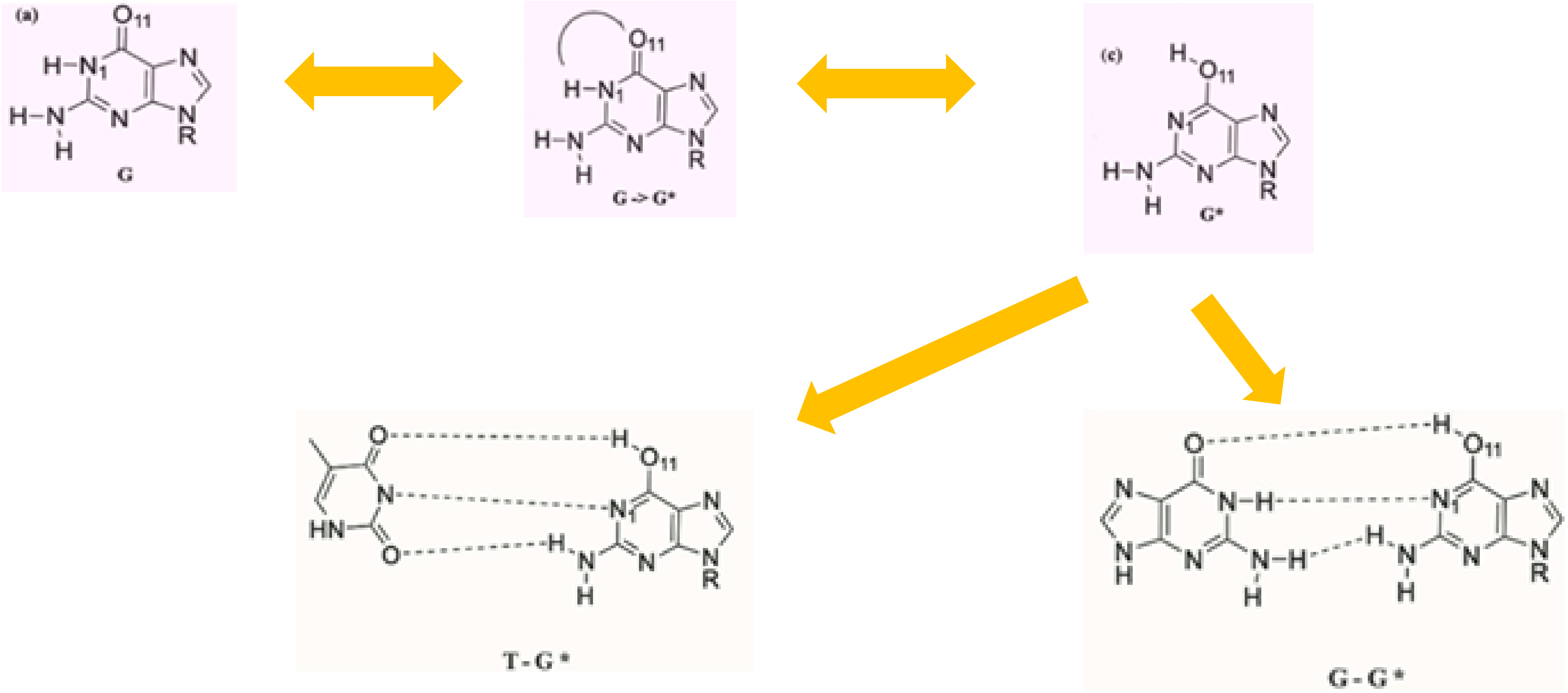


- (Entropic) time delay during the proton tunneling is about picoseconds.
- This delay is close to the time scale of conformational changes in biosystems.
- (Entropic) time delay could be long enough to start DNA point mutations.

(G. Çelebi, E. Özçelik, E. Vardar, DD, Prog. Biophysics and Molecular Biology 167 (2021) 96)

ENTROPIC TUNNELING TIME: DNA MUTATION

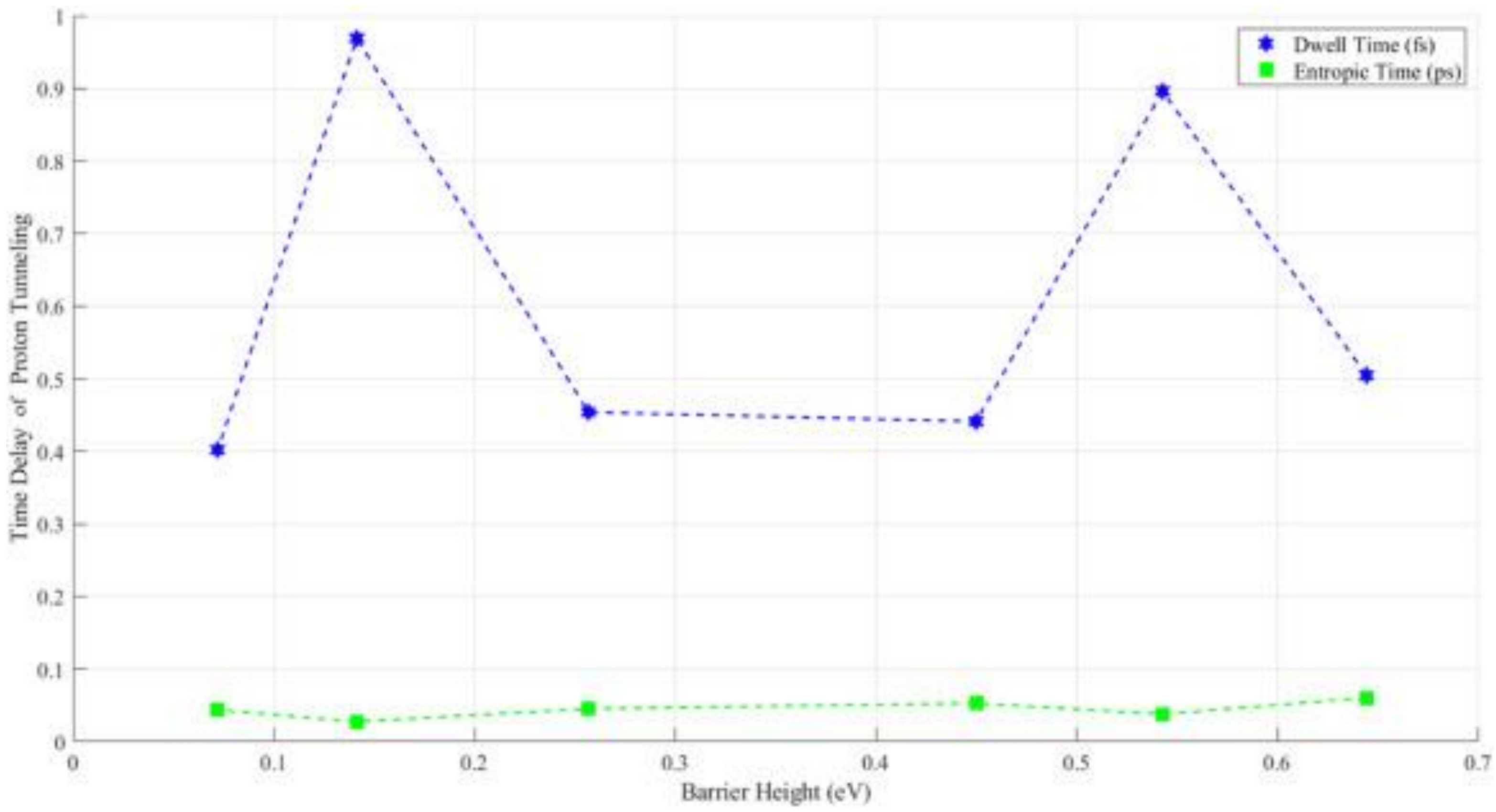
Intra-base proton tunneling:



(E. Özçelik, E. Akar, S. Zaman, DD, Prog. Biophysics and Molecular Biology 173 (2023) 4)

ENTROPIC TUNNELING TIME: DNA MUTATION

Intra-base proton tunneling:



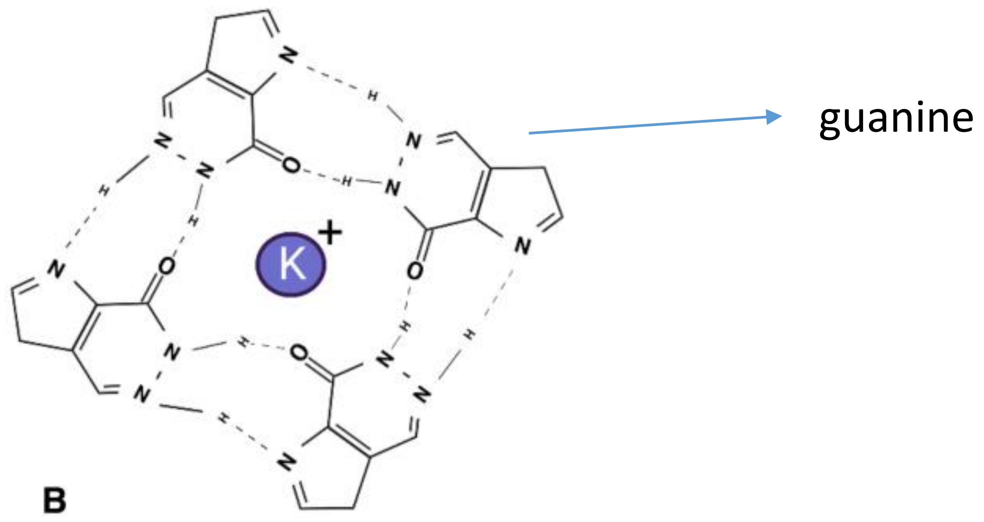
- (Entropic) time delay during the proton tunneling is about tenth of picoseconds.
- This delay is close to the time scale of conformational changes in biosystems.
- (Entropic) time delay could be long enough to start DNA point mutations.

(E. Özçelik, E. Akar, S. Zaman, DD, Prog. Biophysics and Molecular Biology 173 (2023) 4)

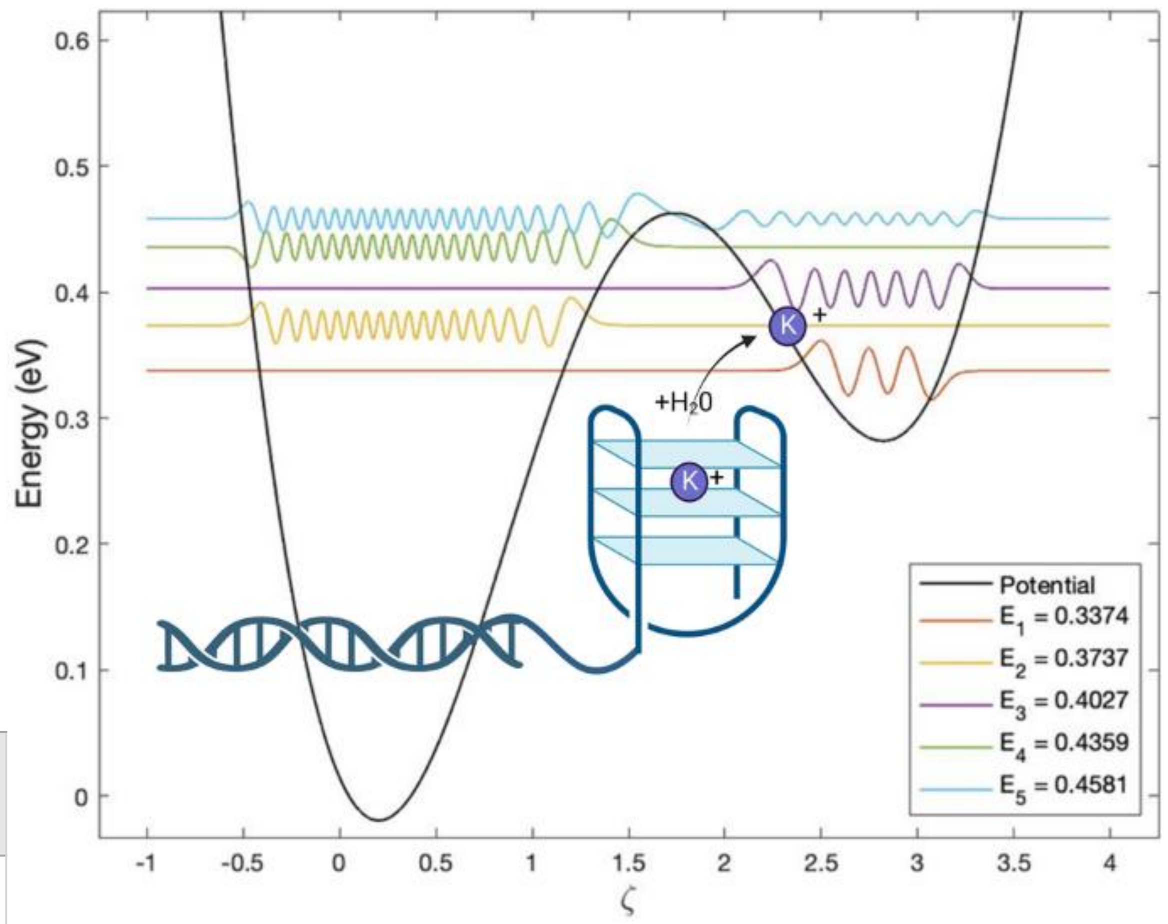
Entropic tunneling time applied to epilepsy: L. Al-Husinat et al., NeuroQuantology 20 (2022) 7292.

ENTROPIC TUNNELING TIME: GUANINE QUADRUPLEX

Potassium ion transfer in G-quadruplex systems:



Barrier height (eV)	Dwell entrance rate (mA)	Entropic entrance rate (pA)
0.1254	27.7	423.12
0.0891	38.4	352.35
0.0601	32.9	436.45
0.0268	31.9	482.23
0.0046	27.4	576.60



(G. Çelebi, G. Demir, DD,
J. Biological Inorganic Chemistry, 28 (2023) 213)

FUTURE PROSPECTS

Quantum Biology (DNA, enzymes, quadruplexes, …)

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GENETICS

Quantum Tunneling Makes DNA More Unstable

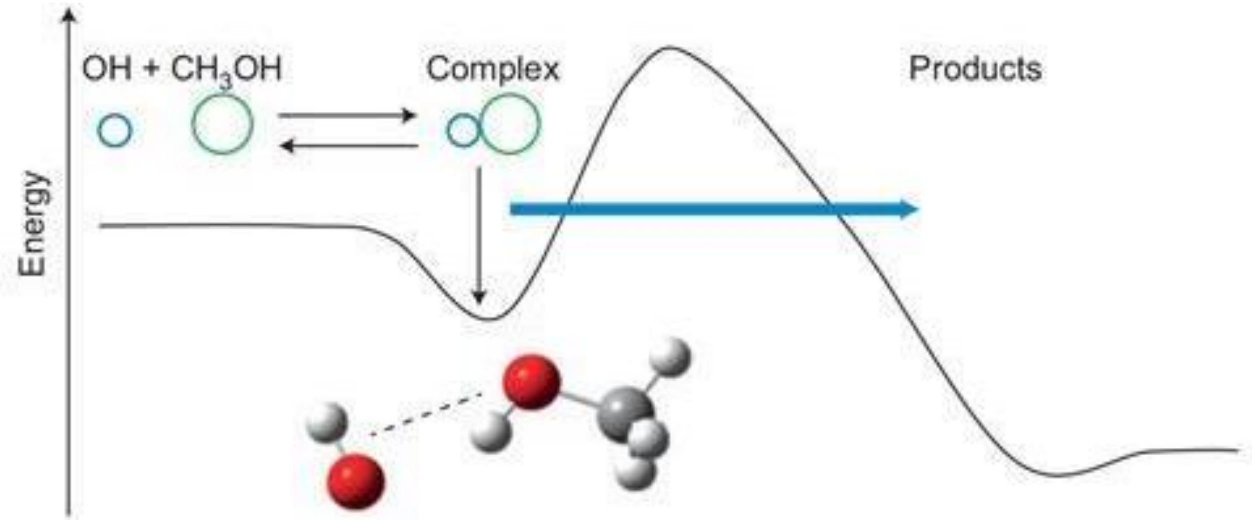
The freaky physics phenomenon of quantum tunneling may mutate genes

By Lars Fischer, Gary Stix on September 1, 2022

(Demir Group @ Sabancı and Al-Khalili Group @ Surrey)

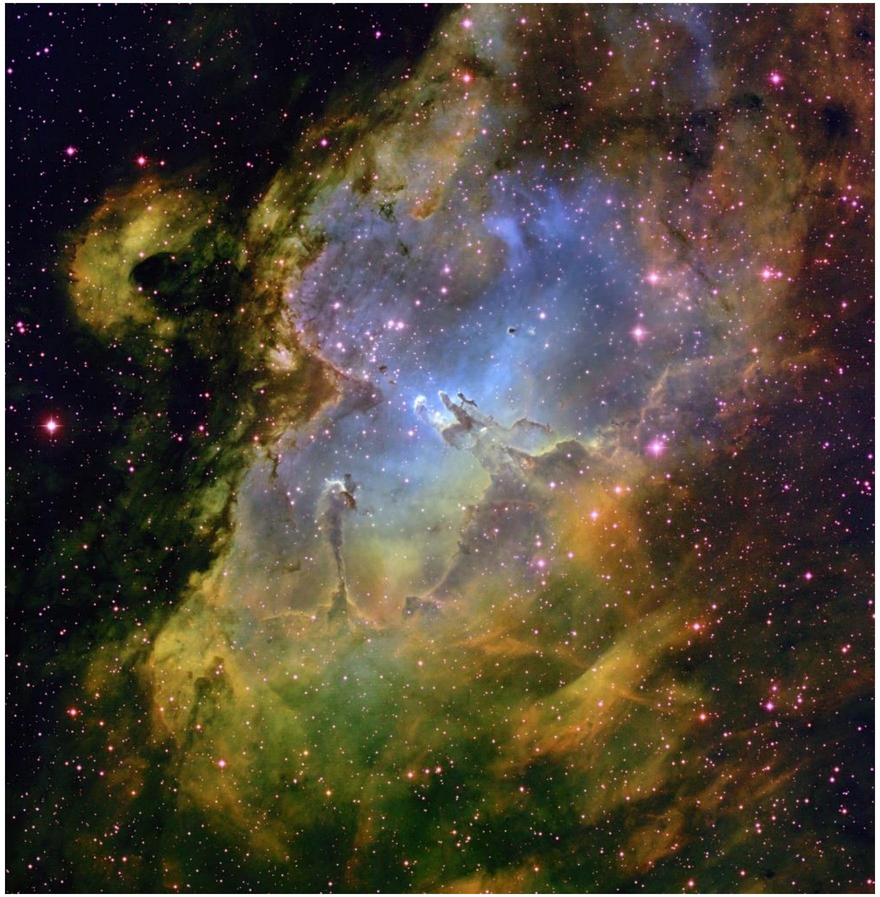
FUTURE PROSPECTS

Quantum Chemistry (reaction rates, interstellar chemistry, …):



Hydroxyl + Methanol → Products
(much faster @ 63 K than at 200 K)

(P. Schreiner et al., Nature 453 (2008) 906)

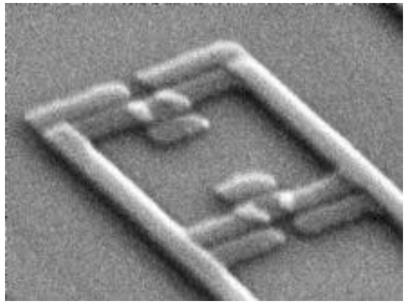


(Eagle Nebula – interstellar chemistry)

(M. Kara and DD, work in progress)

FUTURE PROSPECTS

Quantum Physics (annealing quantum computers, black holes, fusion, …):



- ”flux qubit”
- More than 1 million Josephson junctions
- Even a picosecond delay at each junction leads to nanosecond delays in total $\Longrightarrow$ An important obstacle for future realistic computations.
- Entropic and Bohmian time formulae could lead to a testable framework.

(O. Sargın and DD, work in progress)

THANK YOU !