

# Quantum Tunneling Time: New Approaches and Potential Applications

Durmuş A. Demir

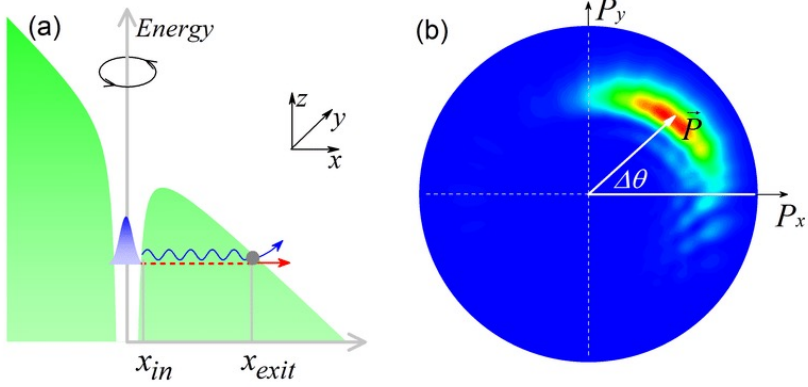
Sabancı University, İstanbul

---

YMF-İstanbul (İstanbul University, 26-27 September 2022)

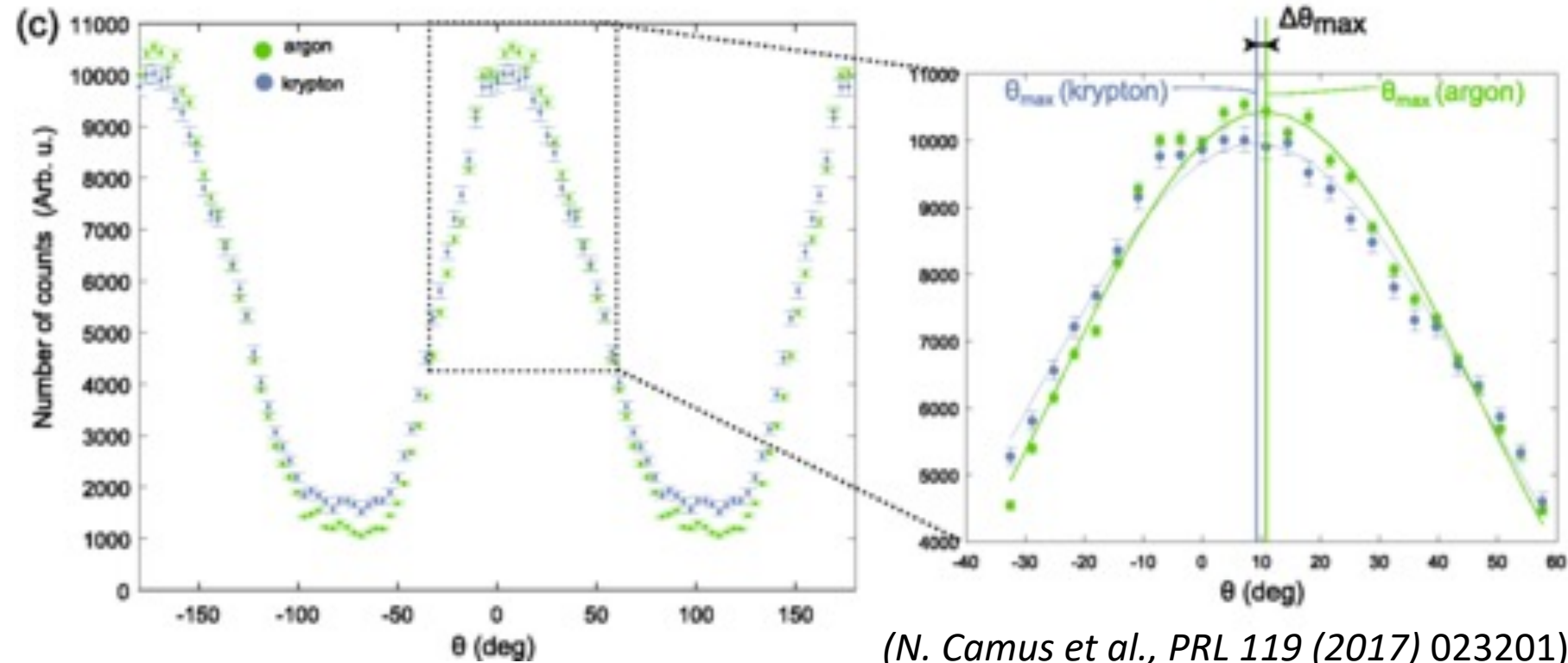
- Tunneling is a textbook topic, tunneling time is not.
  - In quantum theory time is not an operator so time, more specifically, tunneling time needs be modeled from the scratch.
    - Experiments give a finite tunneling time for quantum particles (atoms).
      - Strong-field tunnel ionization experiments have sidelined most of the past tunneling time models.
    - Statistical and Bohmian approaches to tunneling time happen to yield new testable time models.
  - These time models give realistic predictions for tunnel ionization of atoms, DNA point mutation, and free-fall time.
- Tunneling time, in general, can have important implications for physical, biological, chemical and technological processes. Annealing quantum computer is one clear example.

# TUNNELING TIME IS NONZERO



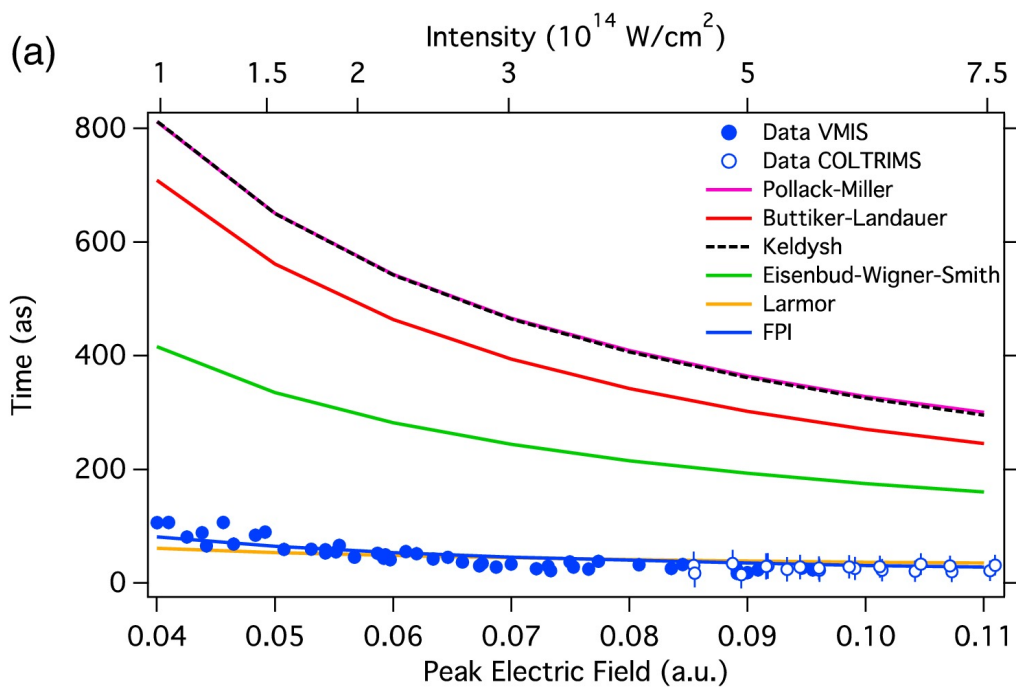
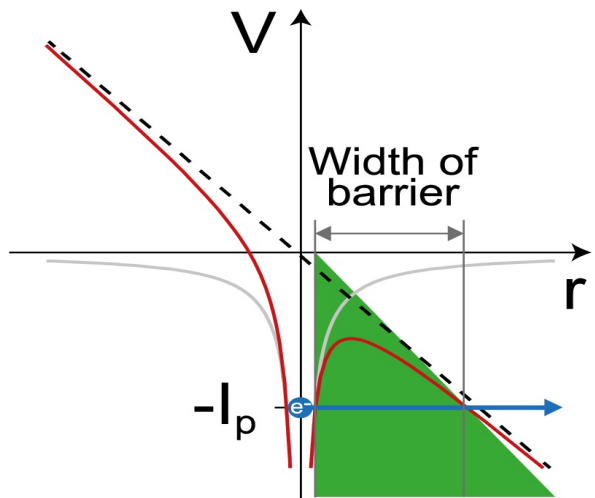
(M. Yuan, *Optics Express* 27 (2019) 6502)

Ar vs Kr tunnel ionization times:

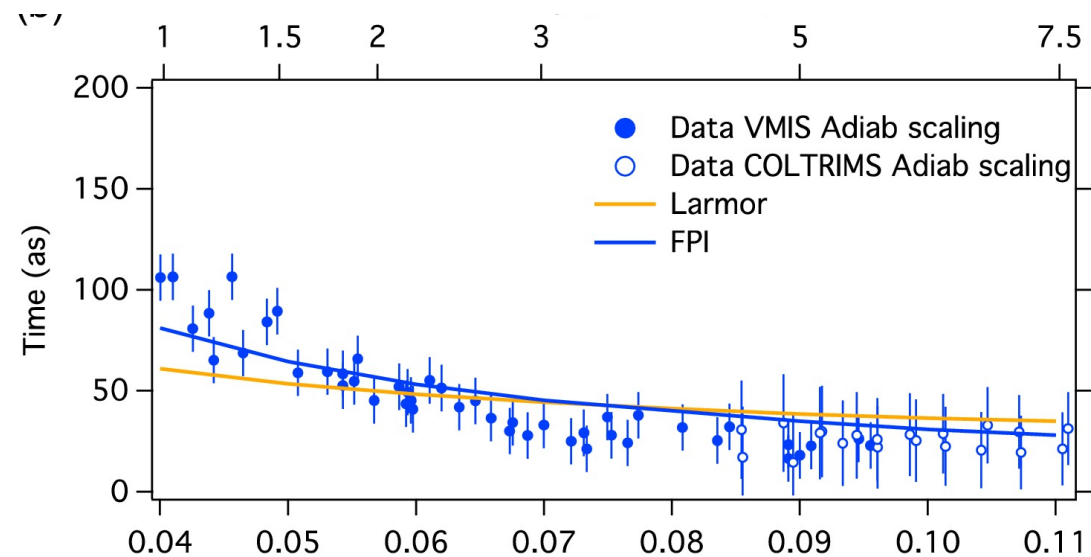


(N. Camus et al., *PRL* 119 (2017) 023201)

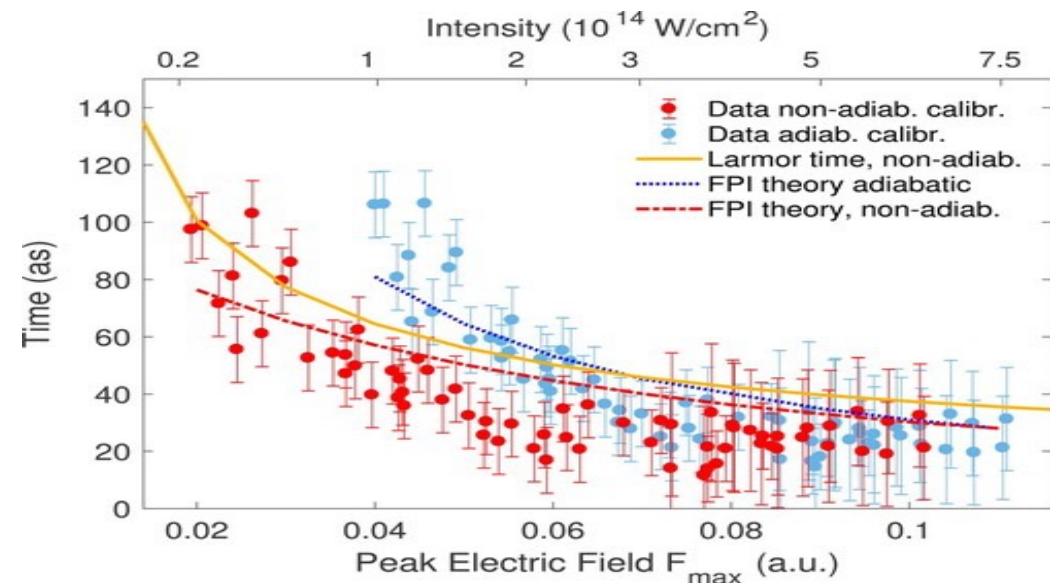
# KNOWN TIME MODELS DISAGREE WITH EXPERIMENT



(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)

# ENTROPIC TUNNELING TIME

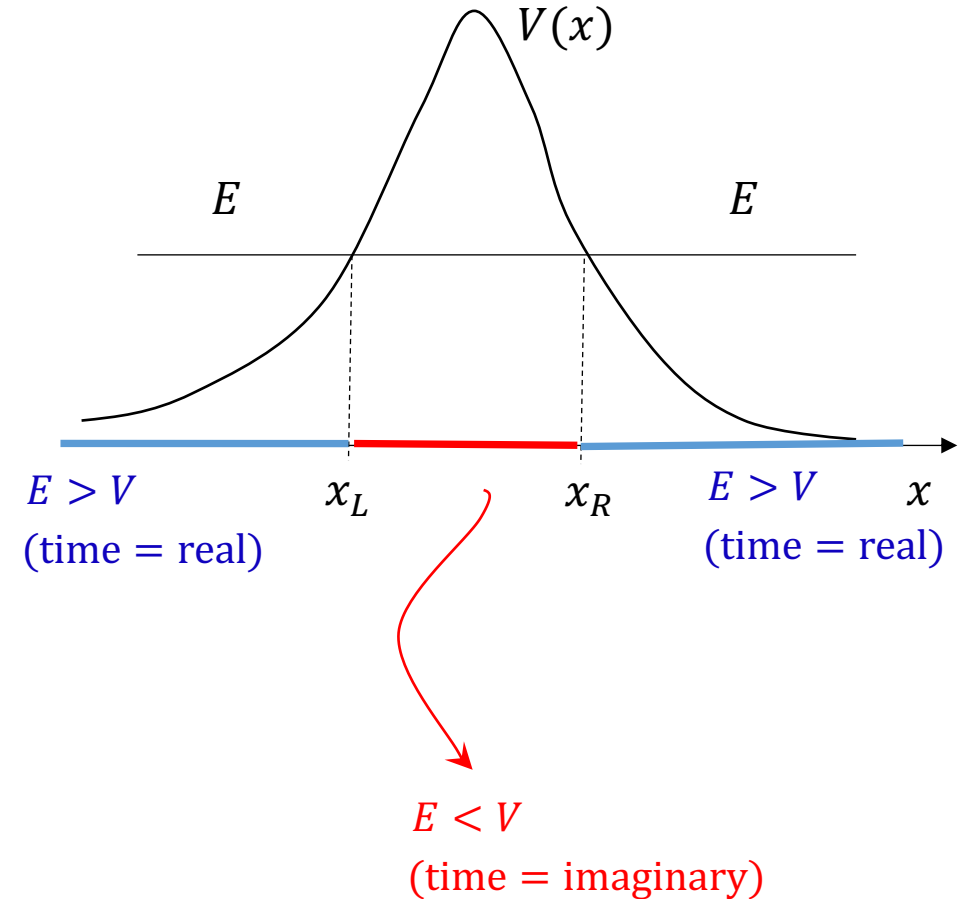
- Time is imaginary in tunneling region (classical dynamics).
- Imaginary time is equivalent to inverse temperature (QM  $\equiv$  eq. Stat Mech.)
- Energy in quantum fluctuations (no real propagation) should pertain to (useless) entropic energy.
- Uncertainty product with thermal sets the time scale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

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

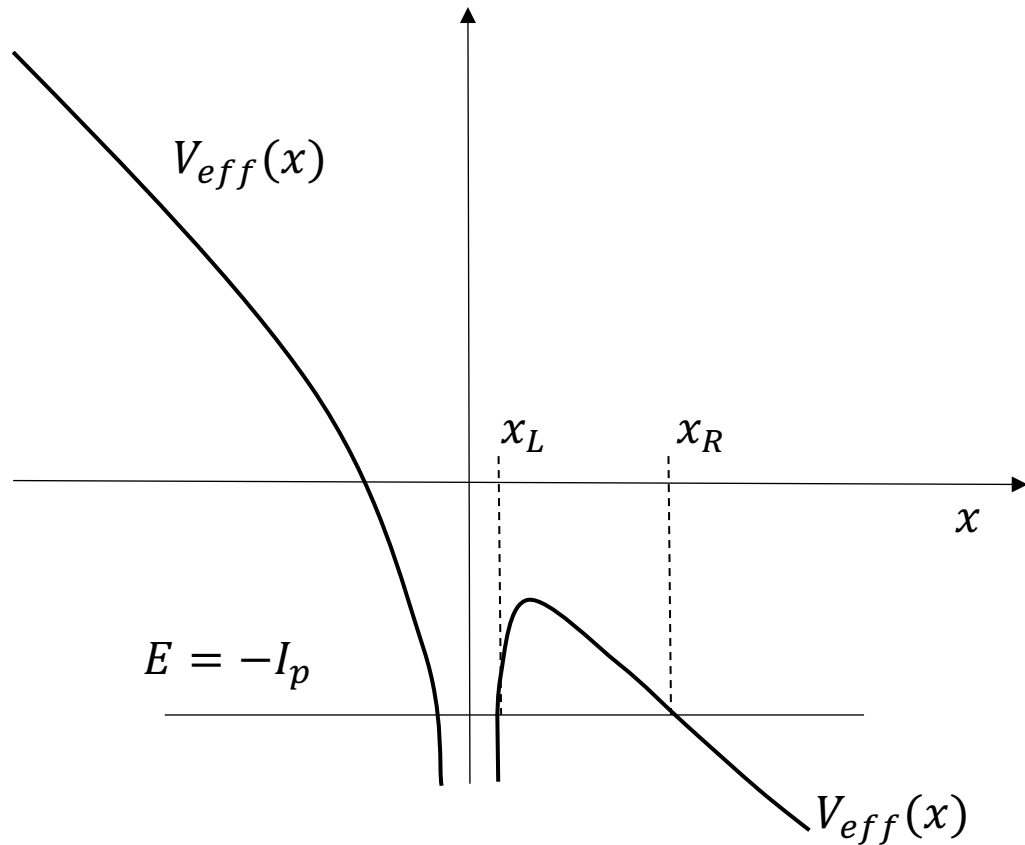
$$\tau_c = \int_{x_L}^{x_R} \frac{m dx}{\sqrt{2m(V(x)-E)}}$$

$$S \equiv -k_B P \log P$$

$$P \equiv \int_{x_L}^{x_R} \psi^*(x)\psi(x)dx$$



## ENTROPIC TUNNELING TIME: He IONIZATION



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

$$V_{eff}(x) = -\frac{Z_{eff}(x)}{x} - \varepsilon x$$

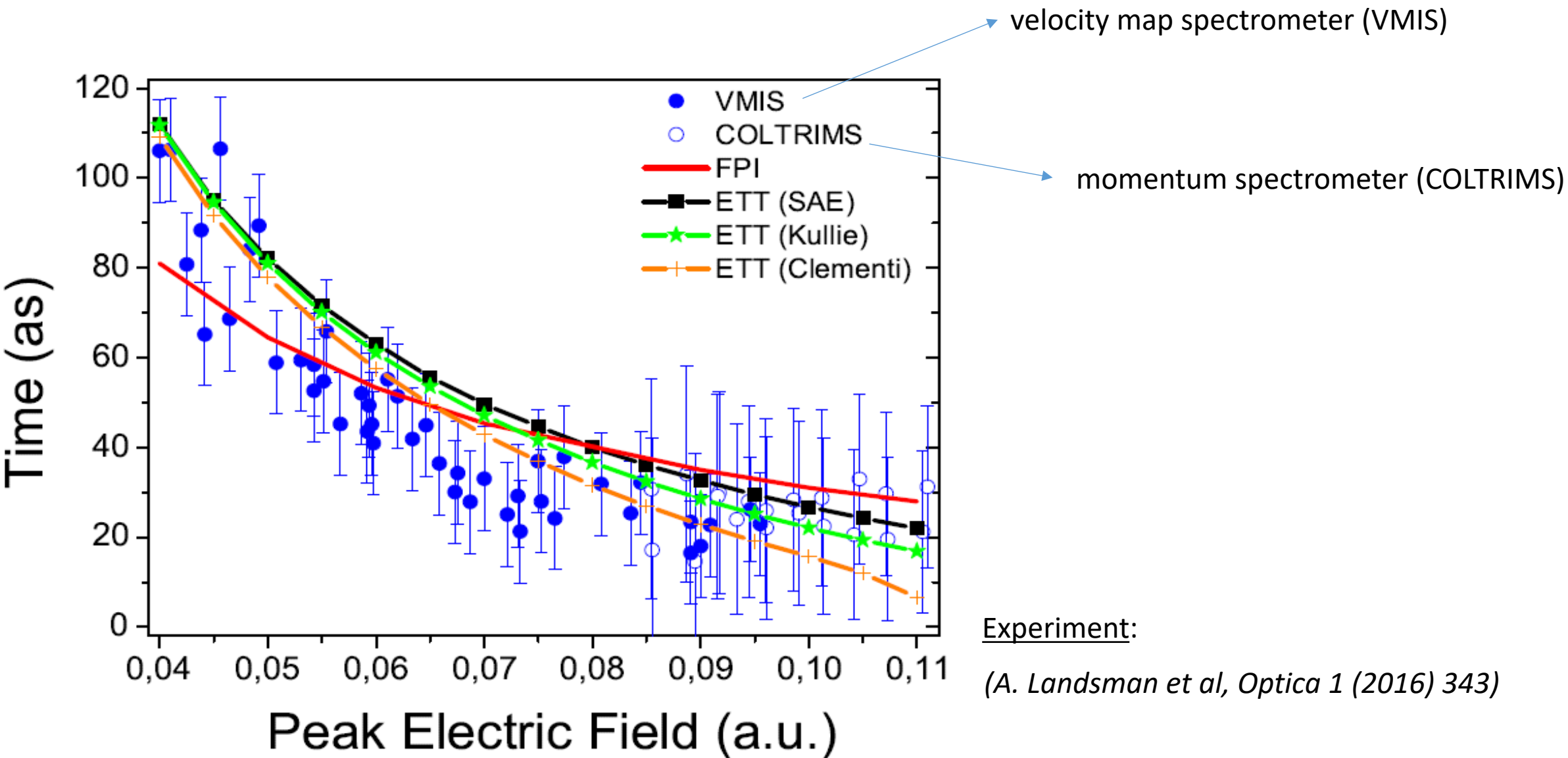
- $Z_{eff}(\text{SAE}) = 1 + 1.231 e^{-0.662x} - 1.325 e^{-1.236x} - 0.231 e^{-0.48x}$
- $Z_{eff}(\text{Kullie}) = 1.375$
- $Z_{eff}(\text{Clementi}) = 1.6875$

(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: He IONIZATION



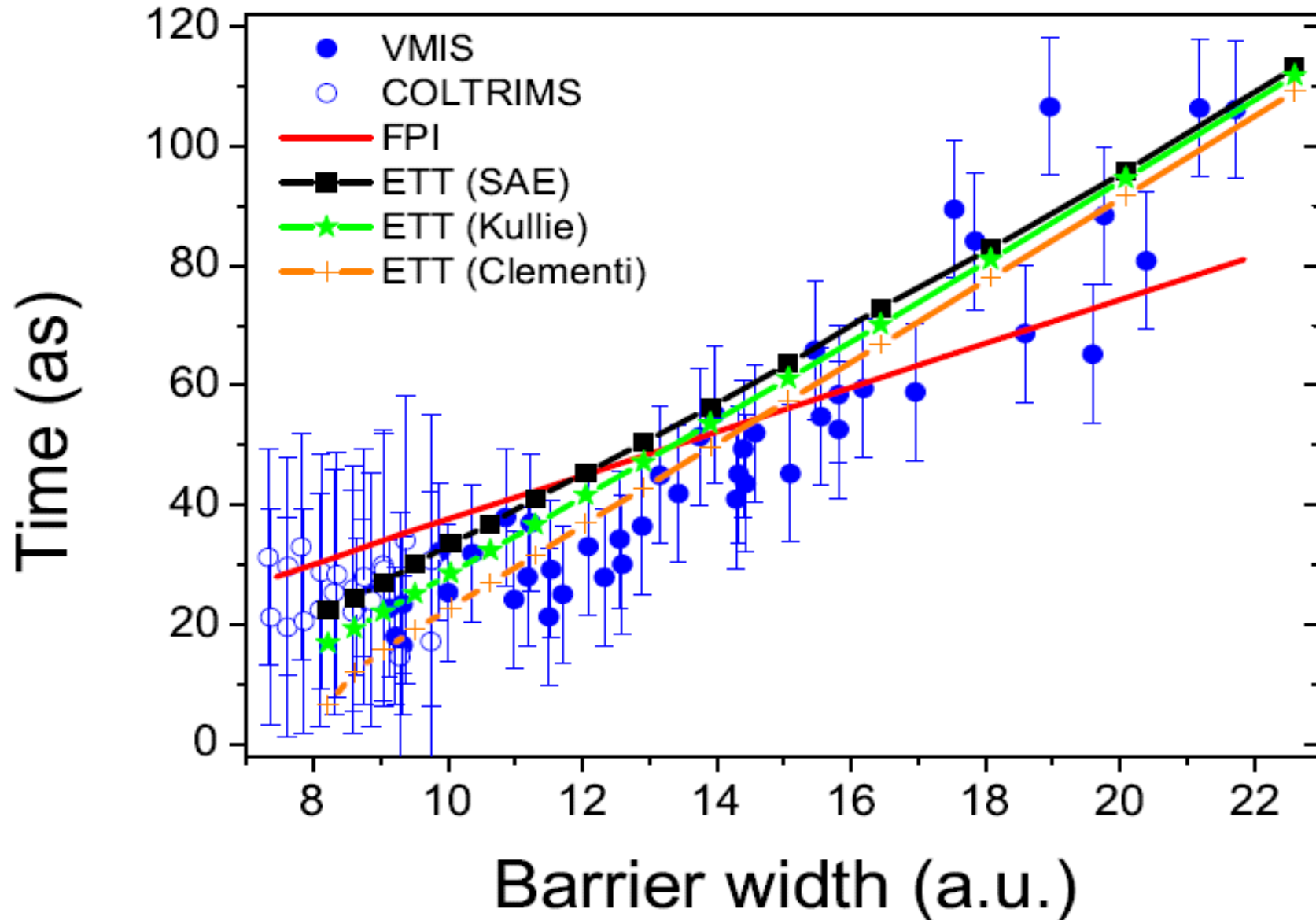
Experiment:

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

Model:

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

# ENTROPIC TUNNELING TIME: He IONIZATION

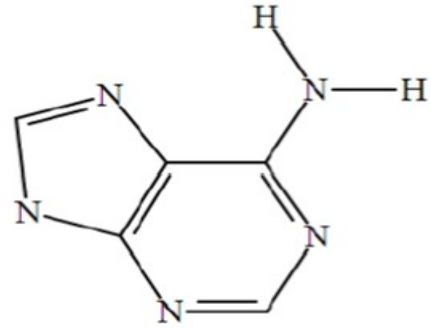


Experiment: (A. Landsman et al., *Optica* 1 (2016) 343)

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

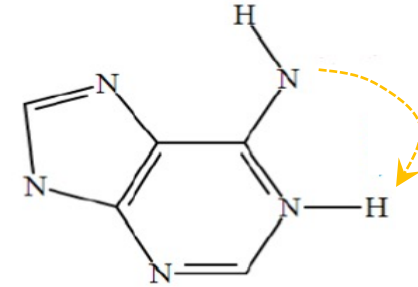
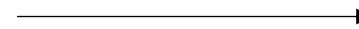


# ENTROPIC TUNNELING TIME: DNA MUTATION

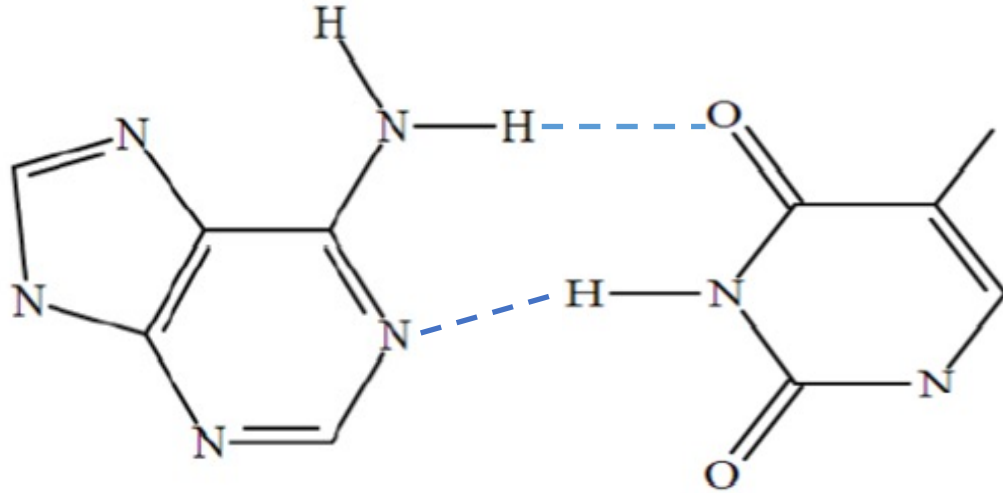


Adenine

proton tunneling

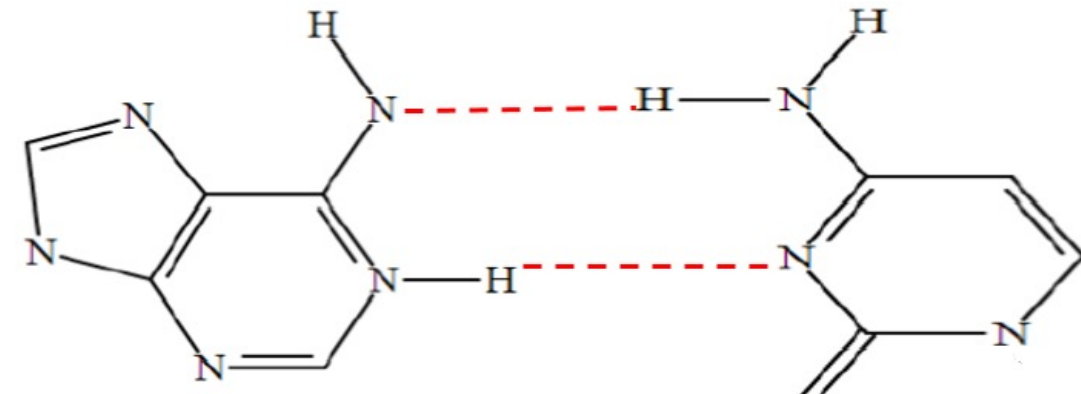


Adenine\*



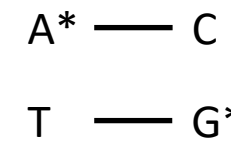
Adenine

Thymine



Adenine\*

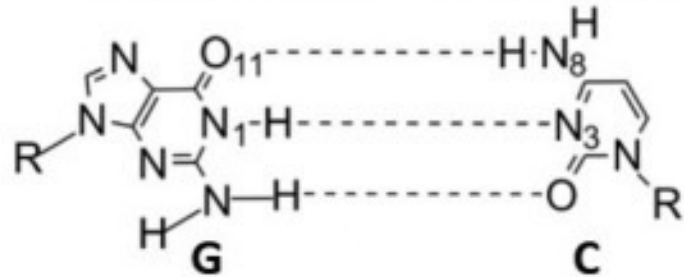
Cytosine



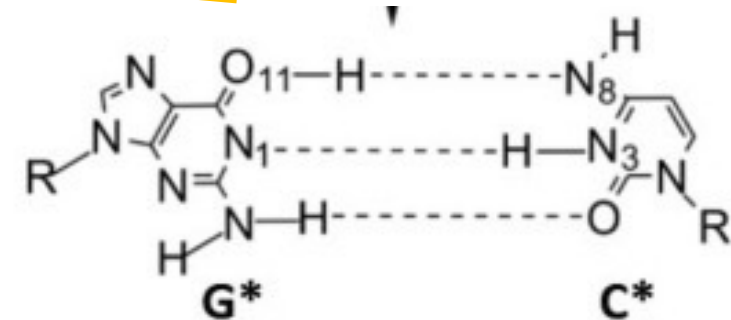
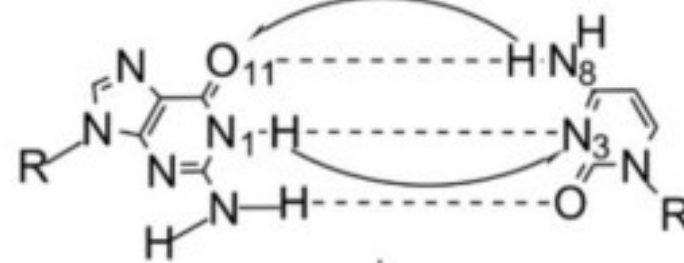
# ENTROPIC TUNNELING TIME: DNA MUTATION

Inter-base proton tunneling:

**Watson-Crick DNA Base Pair**

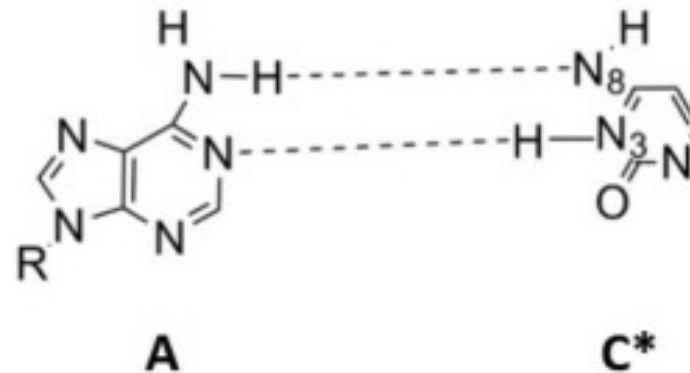
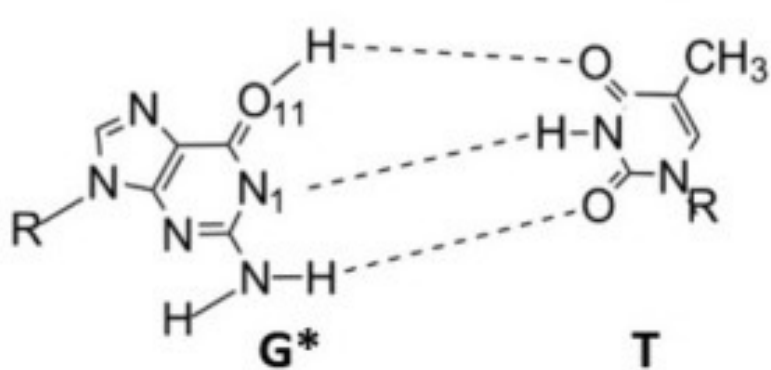


**Tautomerization via Double Proton Transfer**

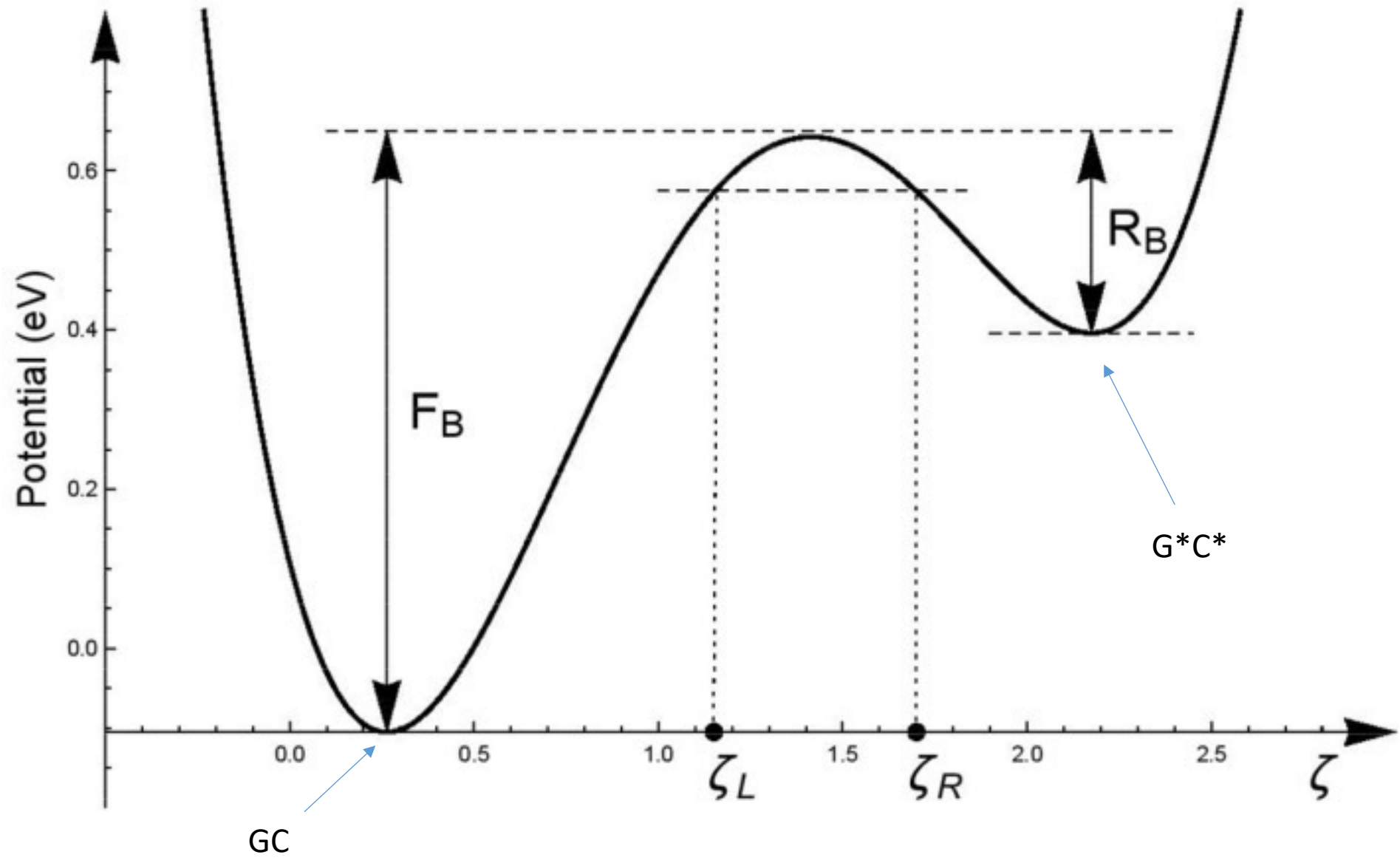


**Löwdin's DNA Base Pair**

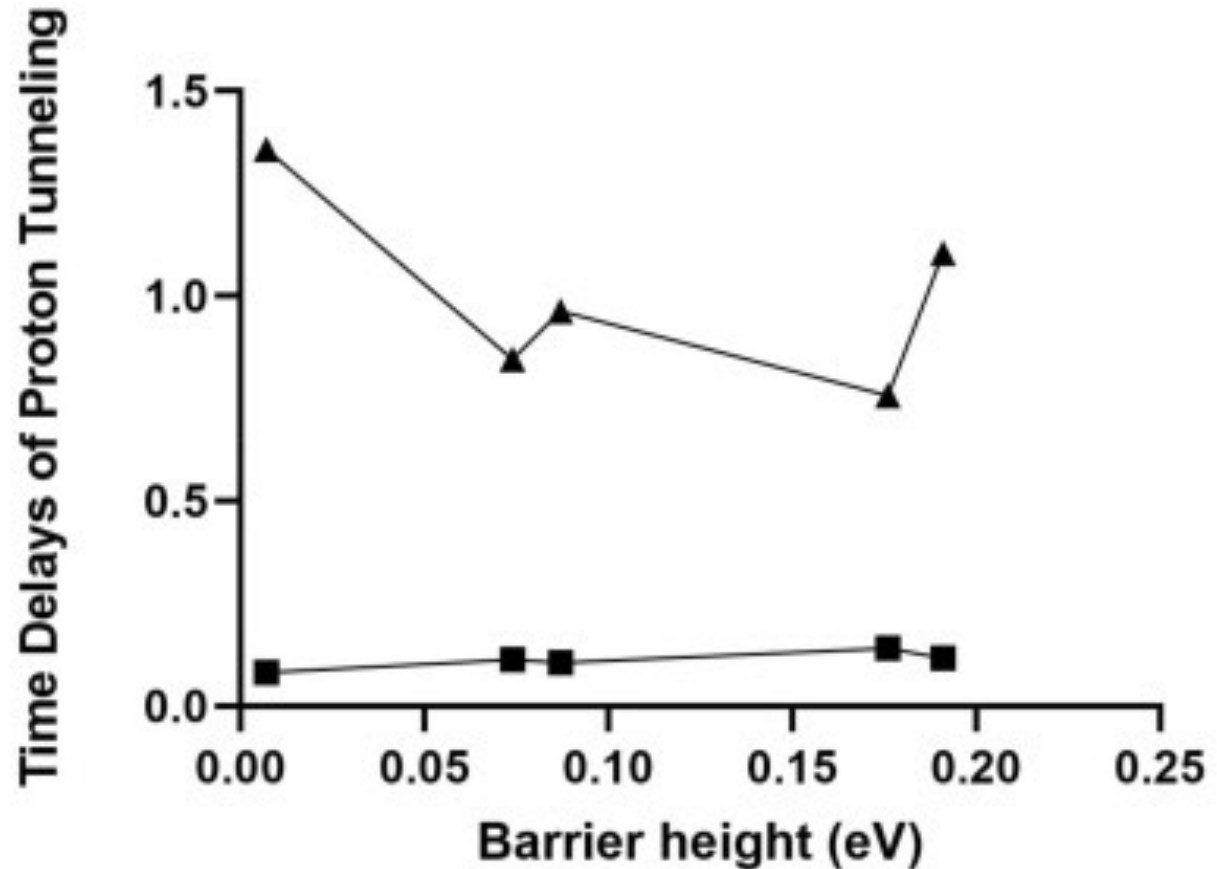
**DNA Replication and Mispairs**



# ENTROPIC TUNNELING TIME: DNA MUTATION



## Inter-base proton tunneling:



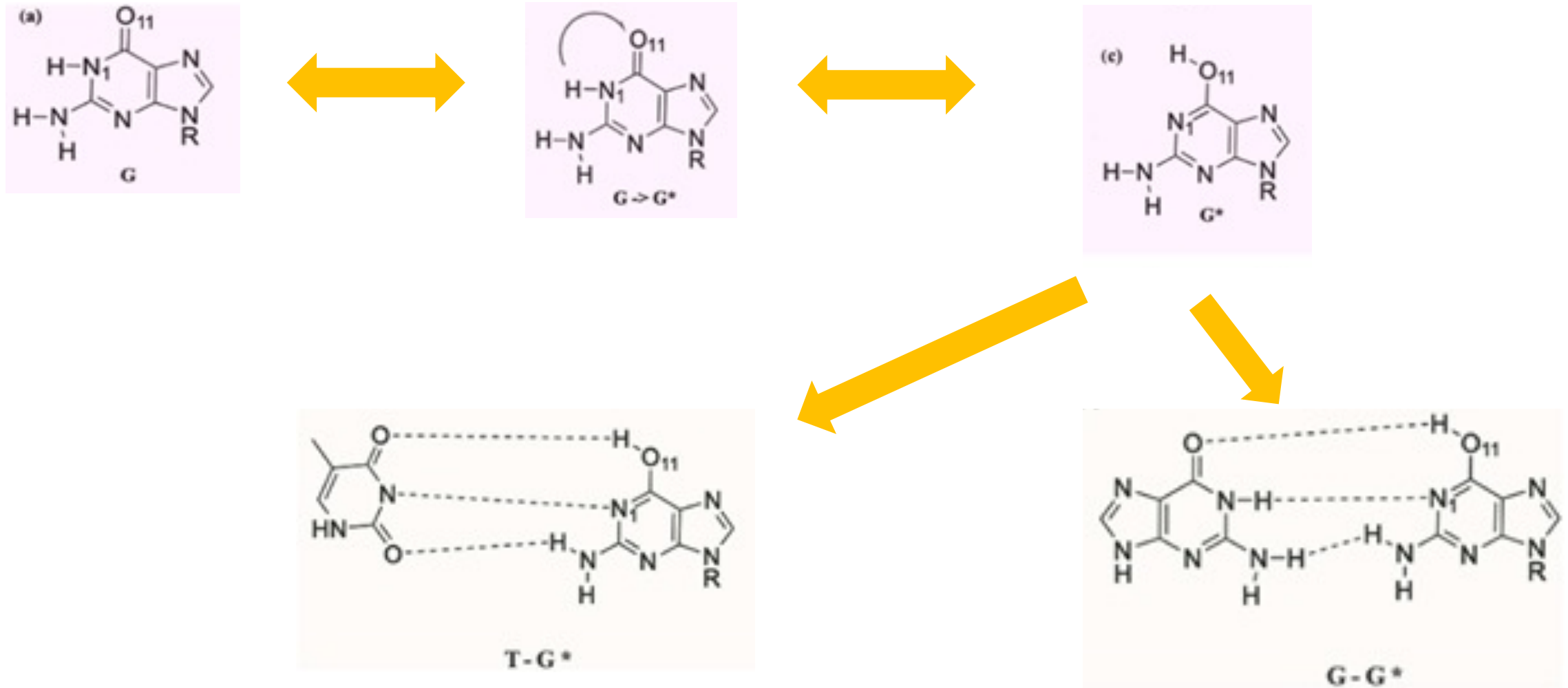
■ Entropic Time (ps)

▲ Dwell Time (fs)

- (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.

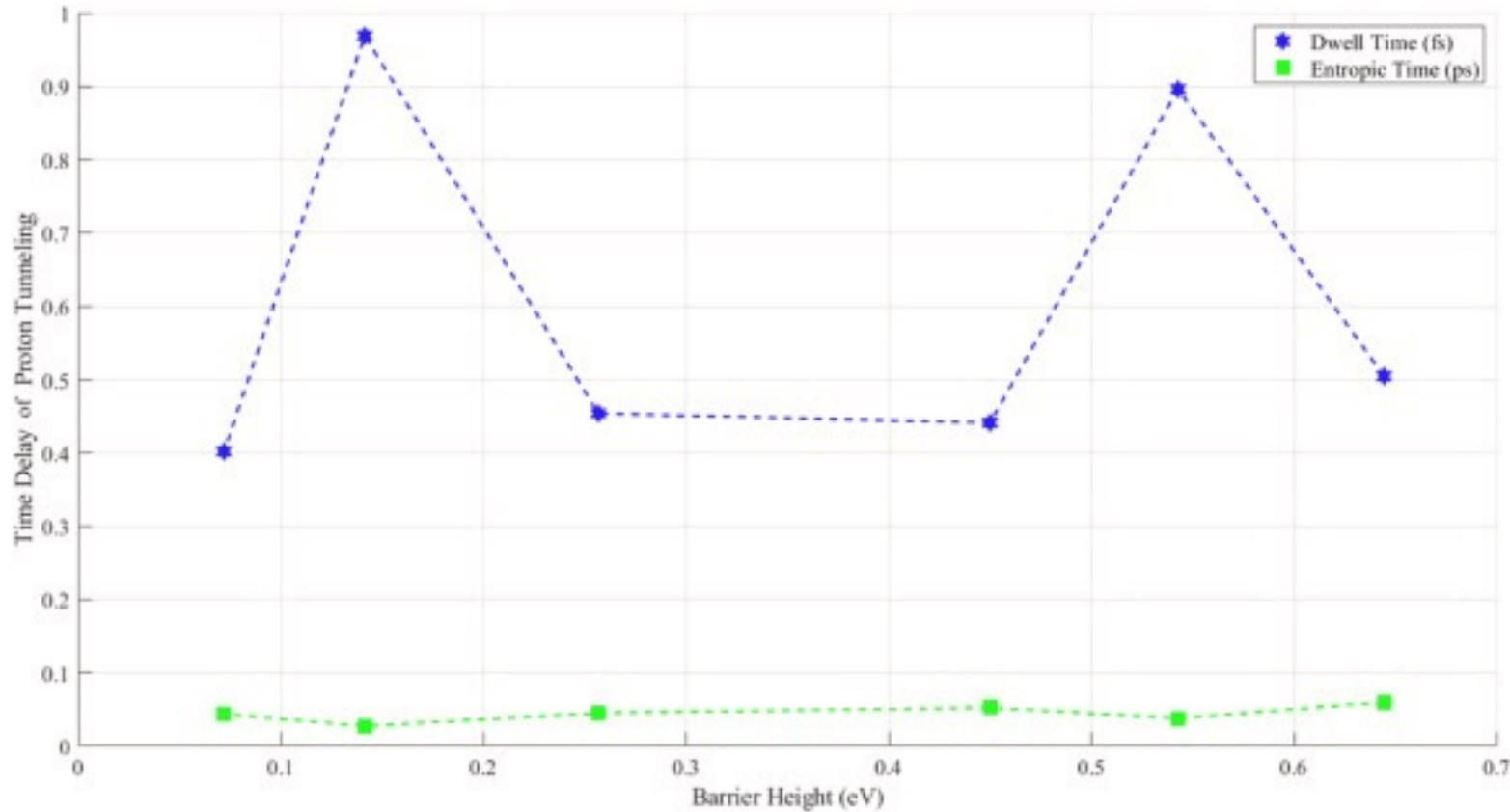
# ENTROPIC TUNNELING TIME: DNA MUTATION

Intra-base proton tunneling:



# ENTROPIC TUNNELING TIME: DNA MUTATION

## Intra-base proton tunneling:



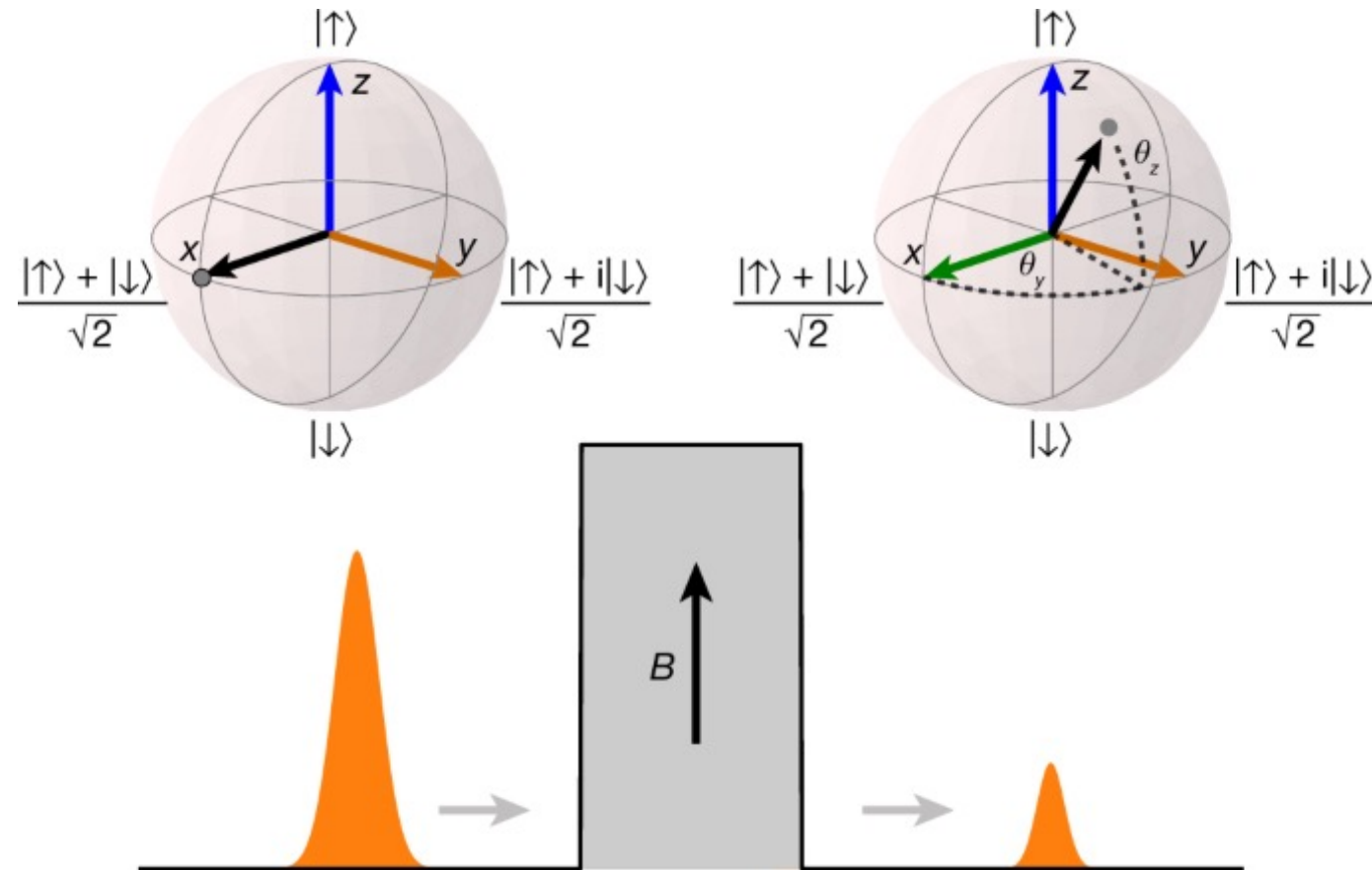
- (Entropic) time delay during the proton tunneling is about tenth of picoseconds.
- This delay is close to the time scale of conformational changes in biosystems.
- (Entropic) time delay could be long enough to start DNA point mutations.

*(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.*

# ACTUAL TUNNELING TIME BY LARMOR CLOCK

- Particle spin precesses when passing through magnetic field regions.
- Given a barrier spanned by 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.



# ACTUAL TUNNELING TIME BY LARMOR CLOCK

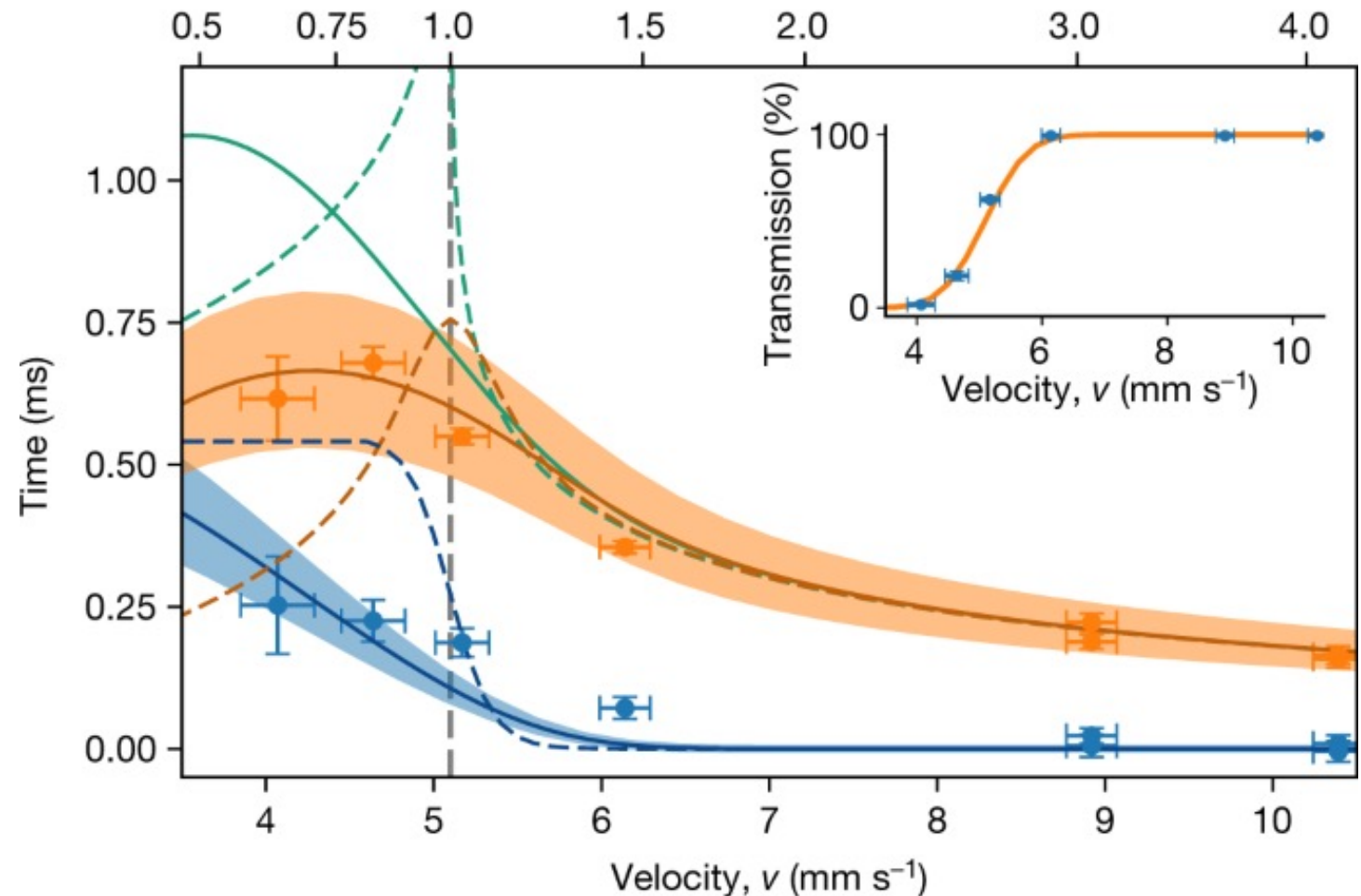
➤ There are two times:

- ❑  $\tau_y$  for precession about  $y$  axis, and
- ❑  $\tau_z$  for precession about  $z$  axis.

➤ Question: What is the actual tunneling time?

❑ Büttiker:  $(ATT)_B = \sqrt{\tau_y^2 + \tau_z^2}$

❑ Steinberg:  $(ATT)_S = \tau_y$





# ACTUAL TUNNELING TIME BY LARMOR CLOCK

- Uncertainty product:

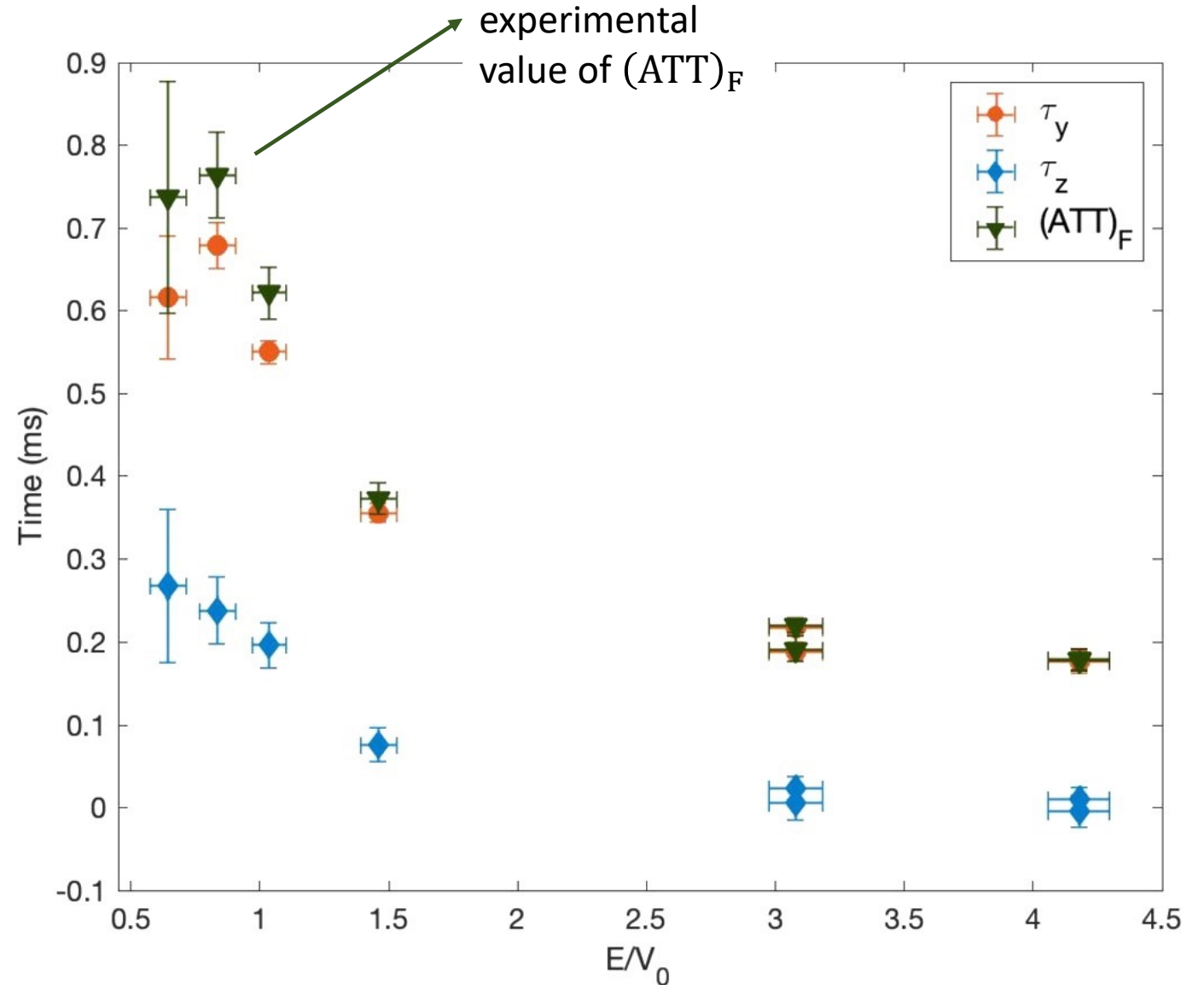
$$(\Delta S_x)^2 (\Delta S_y)^2 \geq \frac{\hbar^2}{4} \langle S_z \rangle^2$$

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:

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

$$\Rightarrow (\text{ATT})_F = \tau_y + \frac{\tau_z^2}{\tau_y}$$



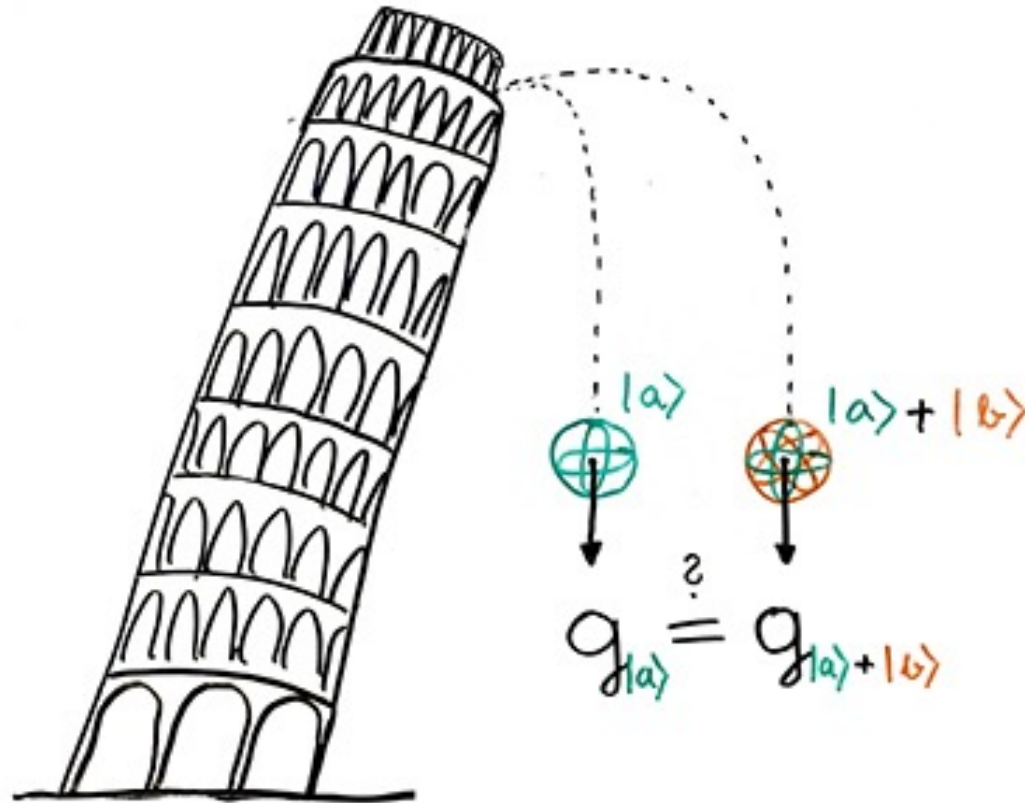
- $(ATT)_F$  proves to be a “physical transmission” time in all the relevant asymptotics.
- A genuine physical time that can be tested new materials to put a (hopefully) end to the question of what the actual tunneling time is.

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

	$\tau_y$	$\tau_z$	$(ATT)_B$	$(ATT)_S$	$(ATT)_F$
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	$\infty$
thick-barrier: $L^2 \gg \frac{\hbar}{m} \tau_c(V_0, E)$ (fixed $V_0, E$ )	$\frac{\hbar}{V_0} \frac{\tau_c(V_0, E)}{\tau_c(0, E)}$	$\infty$	$\infty$	$\frac{\hbar}{V_0} \frac{\tau_c(V_0, E)}{\tau_c(0, E)}$	$\infty$
classical dynamics: $\hbar \rightarrow 0$ (fixed $V_0, E, L$ )	0	$\tau_c(V_0, E)$	$\tau_c(V_0, E)$	0	$\infty$

## TUNNELING TIME FROM FREE-FALL

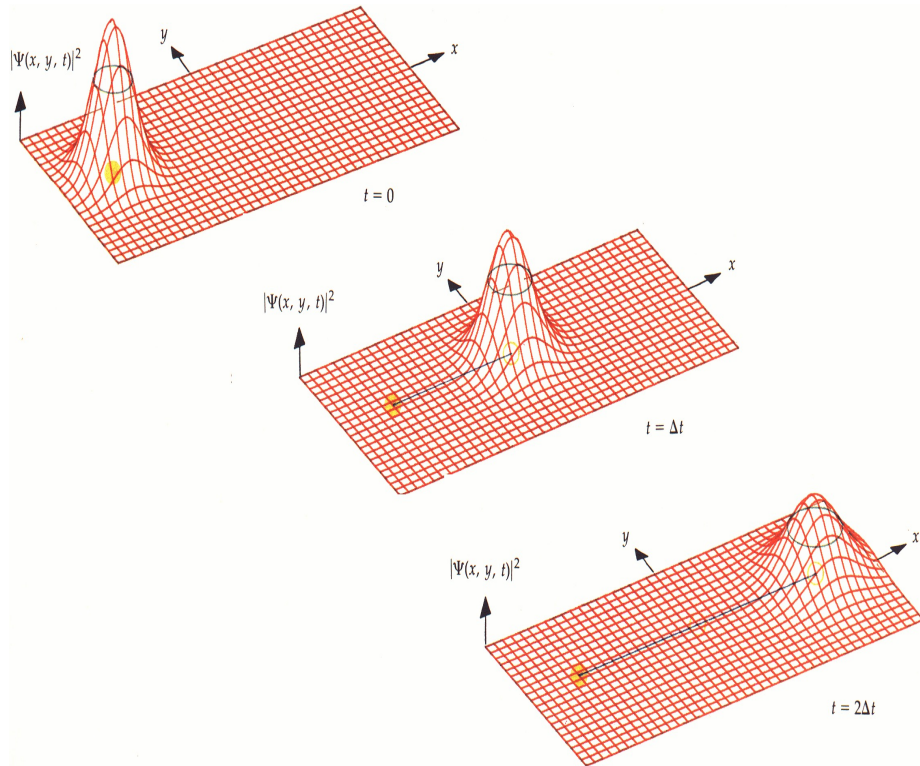
- Imagine an ultra-high vacuum (pressures about  $10^{-5}$  Pa or mean free paths about  $10^5$  m).
- Throw quantum particles upwards and measure their return time.
- This process enables us to answer two crucial questions:
  - Which interpretation of quantum theory is realized in nature? Copenhagen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



(taken from <https://equis.org>)

# TUNNELING TIME FROM FREE-FALL

- 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

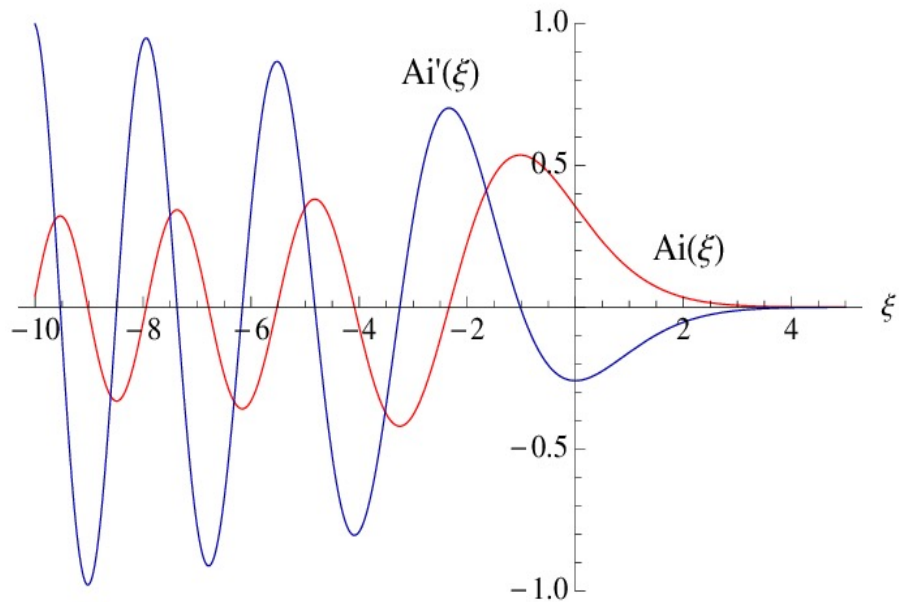
	Copenhagen	Bohmian
$\frac{(\Delta t)_q}{(\Delta t)_c}$	$1 + \frac{\hbar^2}{4m^2 d^2 v_i^2} + \mathcal{O}(\hbar^4)$	$1 + \frac{\hbar}{m\sqrt{2gd^3}} + \mathcal{O}(\hbar^2)$

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

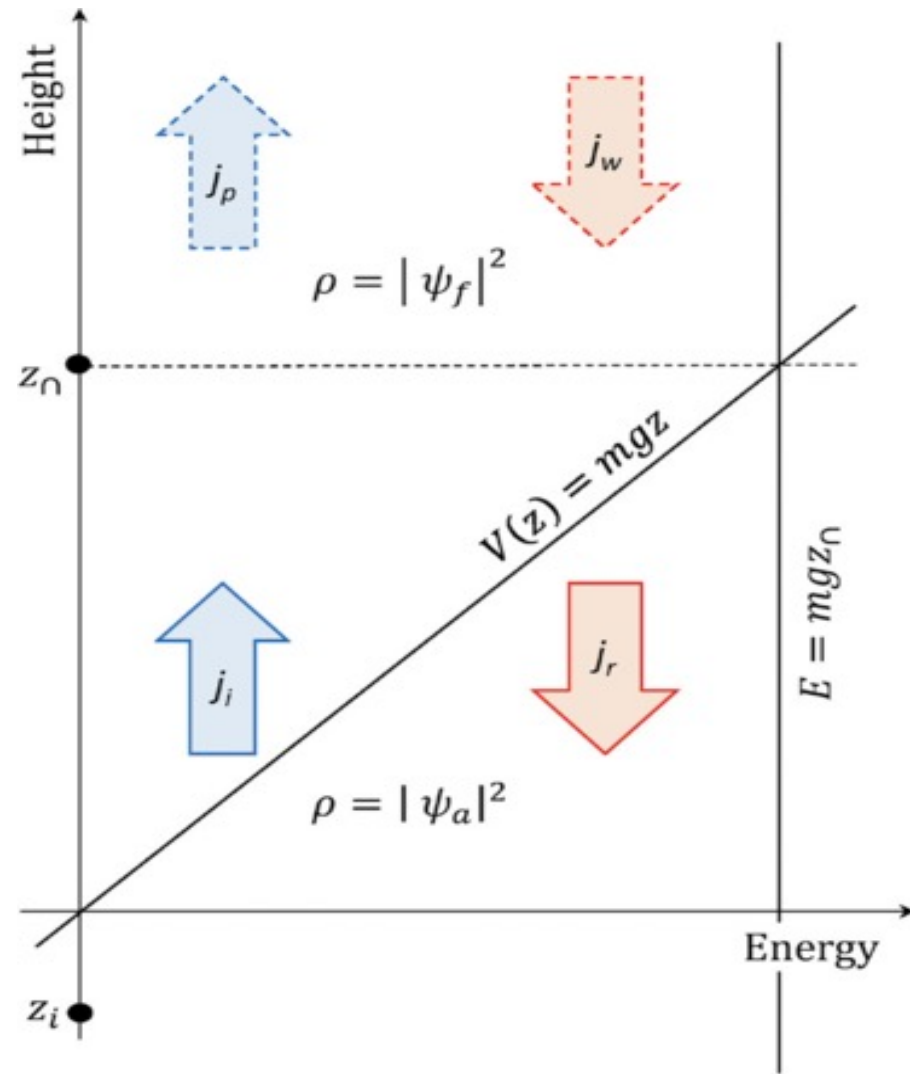
(DD, Phys. Rev. A106 (2022) 022215)

# TUNNELING TIME FROM FREE-FALL

- 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).



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



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

# TUNNELING TIME FROM FREE-FALL

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

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

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

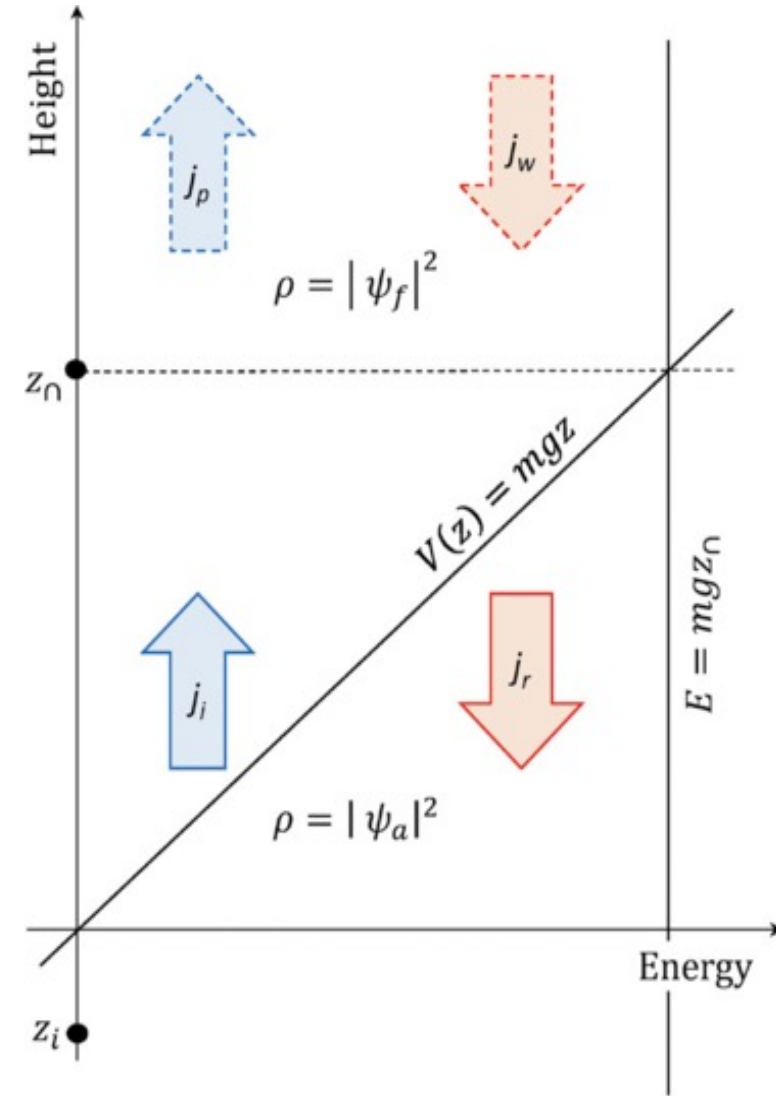
$$j_p = -j_w = \frac{3N^2}{2\pi} \left( \frac{3g\hbar}{m} \right)^{\frac{1}{3}}$$

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

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

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

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

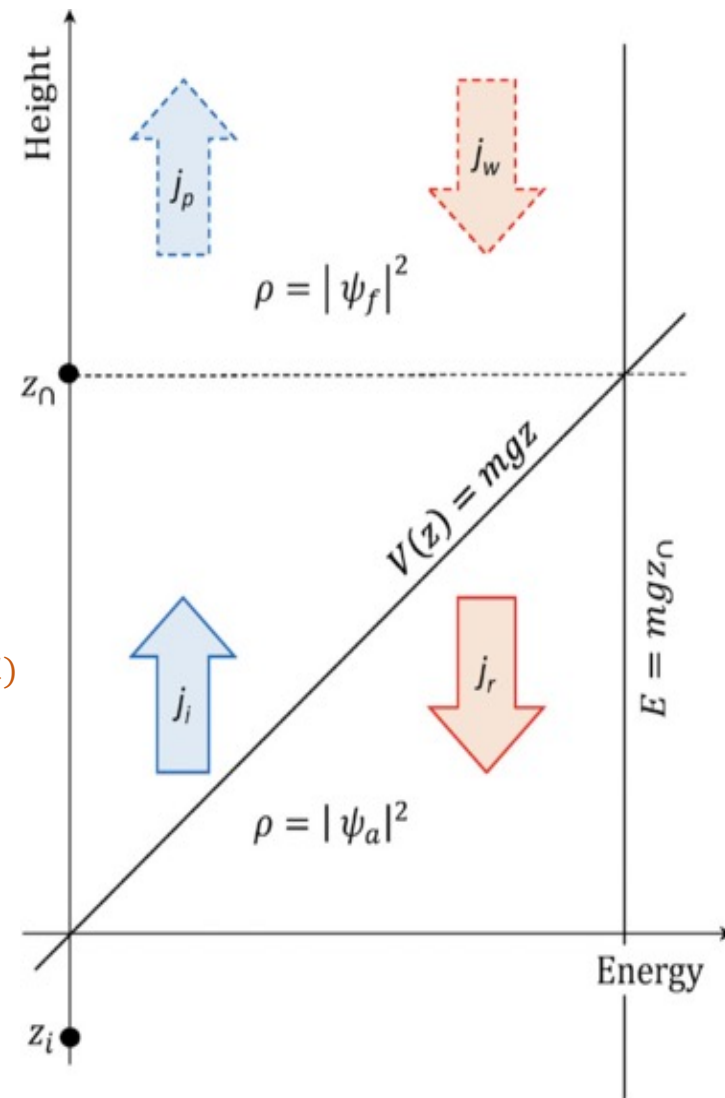


# TUNNELING TIME FROM FREE-FALL

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

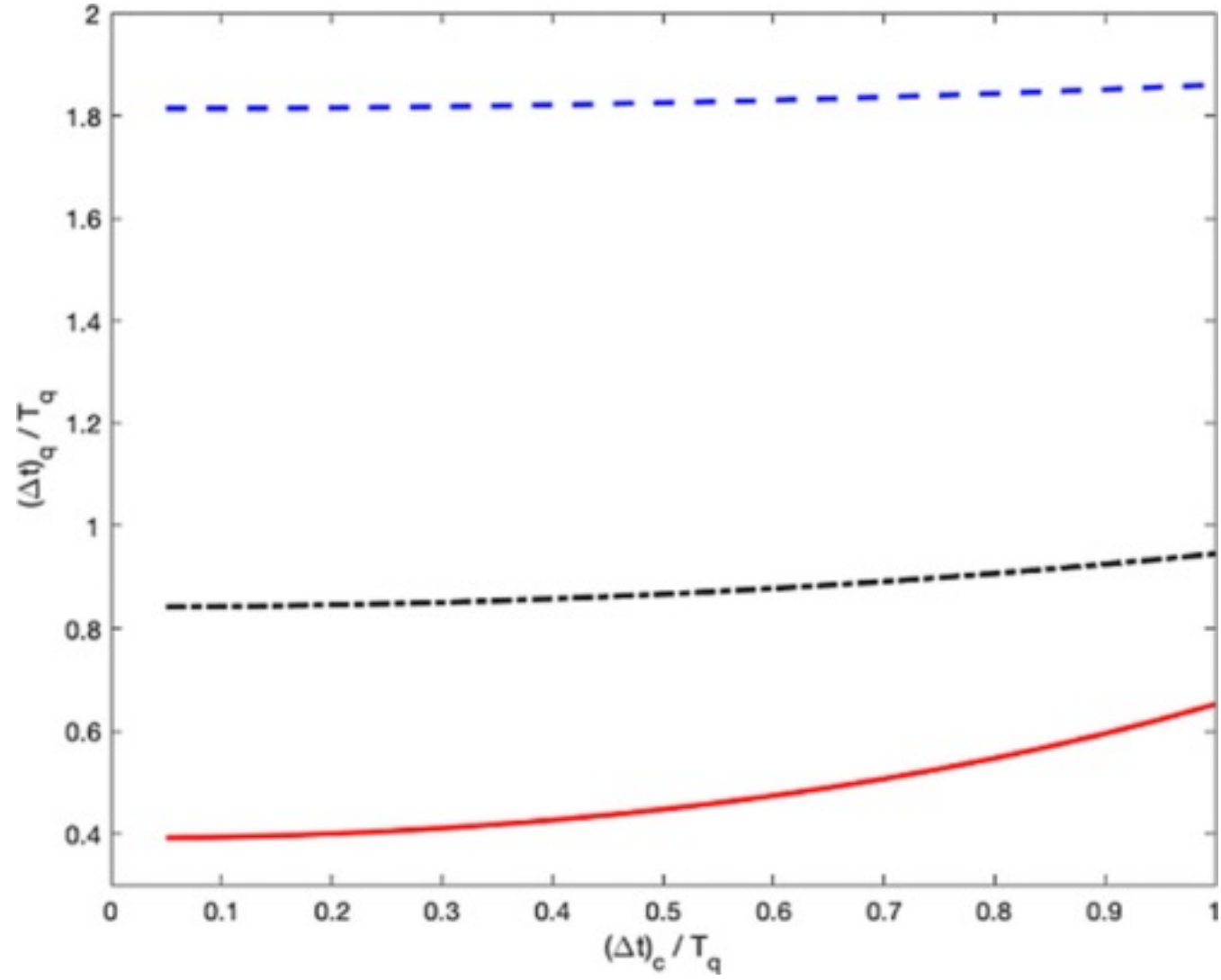
$$(\Delta t)_q^{(rise)} = \int_{z_i}^{z_n} \frac{|\psi_a(z)|^2}{2j_i} dz = -\frac{2\pi T_q}{\left[3^{\frac{1}{3}}\Gamma\left(\frac{1}{3}\right)\right]^2} + 2\pi T_q \left( \beta_q [Ai(-\beta_q)]^2 + [Ai'(-\beta_q)]^2 \right) = (\Delta t)_q^{(fall)}$$

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



# TUNNELING TIME FROM FREE-FALL

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



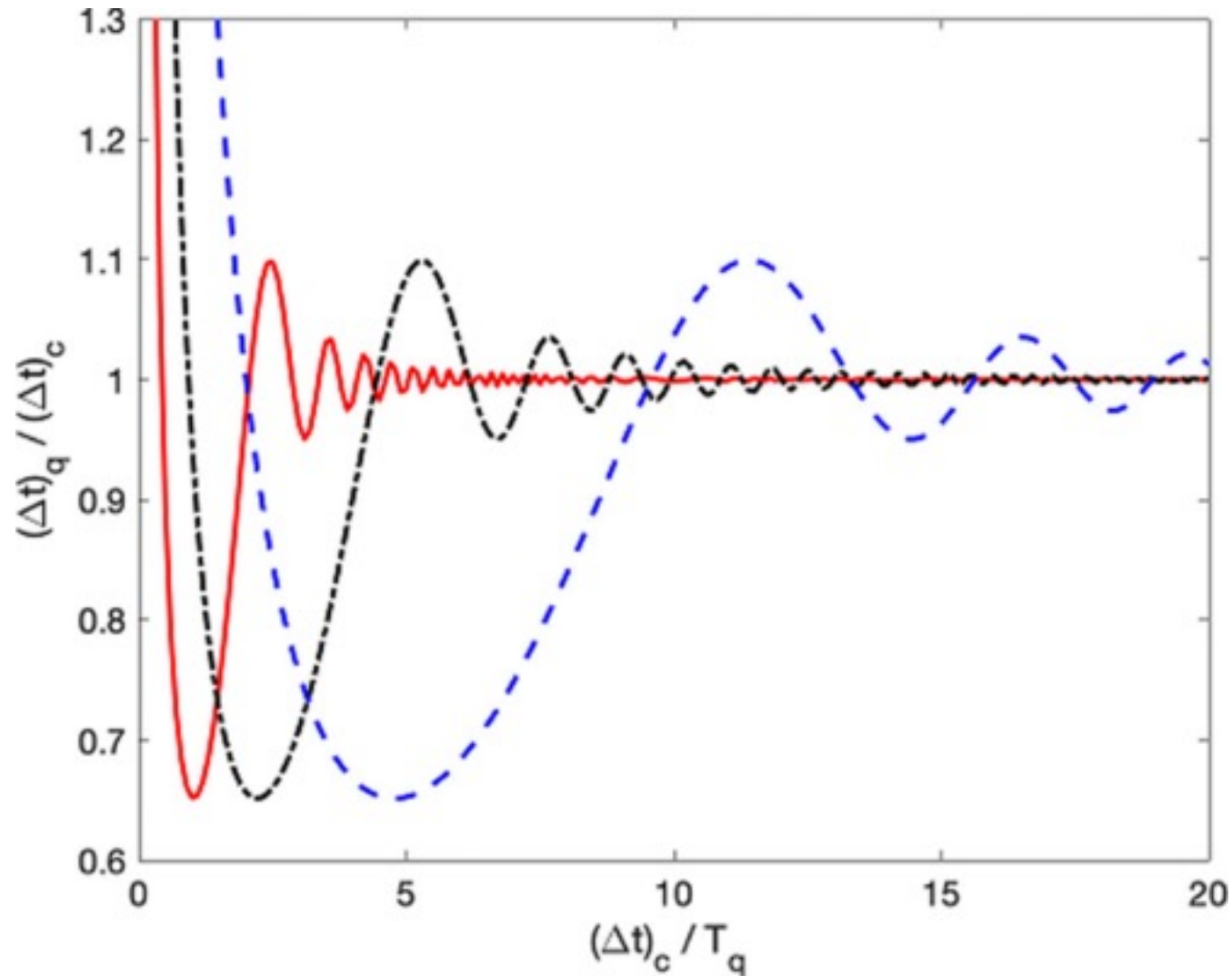
➤  $z_\cap = z_i \Rightarrow (\Delta t)_c = 0$

➤  $z_\cap = z_i$  but  $(\Delta t)_q \neq 0$



## TUNNELING TIME FROM FREE-FALL

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



- 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.

Quantum Biology (DNA, enzymes, Quadruplexes, ...)

Subscribe

Latest Issues

SCIENTIFIC  
AMERICAN®

Cart 0

Sign In | Newsletters

Coronavirus

Health

Mind & Brain

Environment

Technology

Space & Physics

Video

Podcasts

Opinion

Store



Fall Flash Sale. Save 20%

Subscribe

GENETICS

# Quantum Tunneling Makes DNA More Unstable

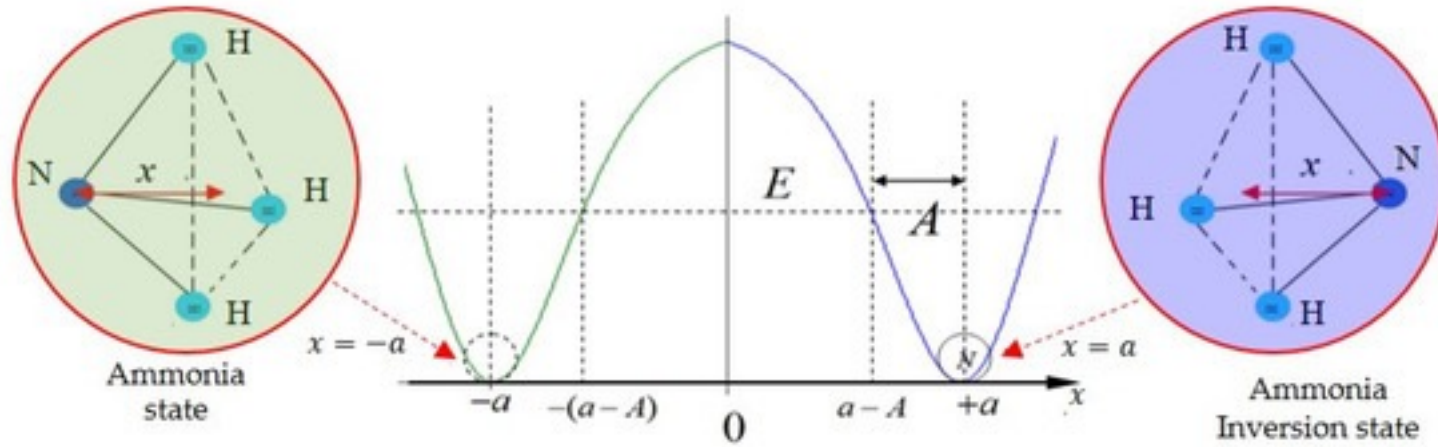
The freaky physics phenomenon of quantum tunneling may mutate genes

---

By Lars Fischer, Gary Stix on September 1, 2022

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

Quantum Chemistry (reaction rates, ammonia inversion, ...):

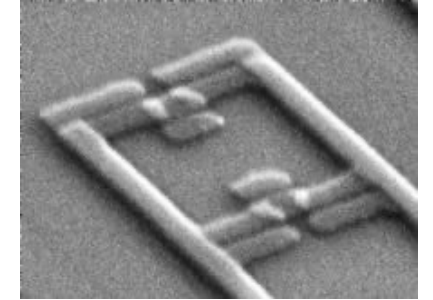


(C. Yang et al., *Int. J. Mol. Sci.* 22 (2021) 8282)

(M. Kara and DD, work in progress)

## CONCLUSION AND 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  $\Rightarrow$  An important obstacle for future realistic computations.
- Entropic and Bohmian time formulae could lead to a testable framework.

*(O. Sargin, A. Hayreter, DD, work in progress)*

**THANK YOU!**