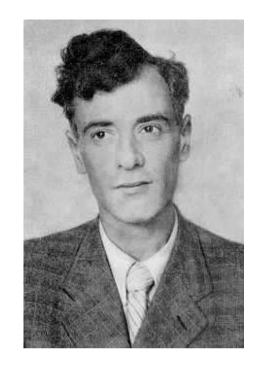
Landau-Zener Transitions in a Noisy Environment

Переходы Ландау-Зинера в шумящей среде



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# **Outline**

- Introduction to Landau-Zener transitions
- Some applications of the Landau-Zener theory
- Why and when noise is substantial
- Description of noise
- Transitions in the presence of fast noise
- Interaction of the transverse and longitudinal noise
- Conclusions

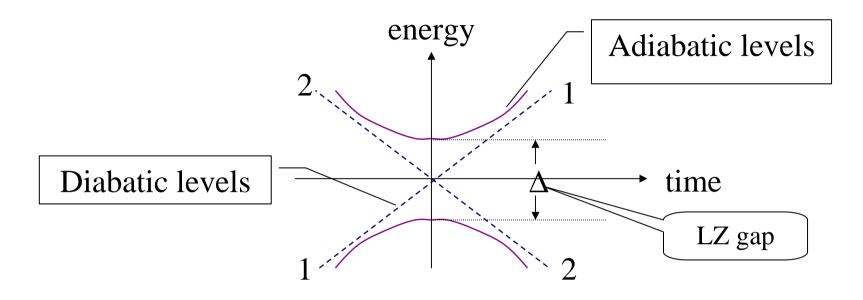
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L.D. Landau, Phys. Z. Sowietunion, 2, 46 (1932)
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C. Zener, Proc. R. Soc. A137, 696 (1932)

E.C.G. Stückelberg, Helv. Phys. Acta 5, 369 (1932)

E. Majorana, Nuovo Cimento 9, 43 (1932)

## **Introduction:** LZ theory



Avoided level crossing (Wigner-Neumann theorem)

### Schrödinger equations

$$i\dot{a}_1 = E_1(t)a_1 + \Delta a_2 \qquad E_2(t) - E_1(t) = \Omega(t); \quad \hbar = 1$$

$$i\dot{a}_2 = \Delta^* a_1 + E_2(t)a_2 \qquad \Omega(t) = \dot{\Omega}t$$

Diabatic levels:

$$E_2 = -E_1 = \dot{\Omega}t/2$$

Adiabatic levels:

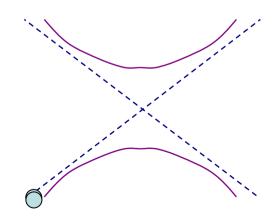
$$E_{\pm} = \pm \sqrt{\left(\frac{E_1 - E_2}{2}\right)^2 + \left|\Delta\right|^2}$$

LZ parameter:

$$\gamma = \frac{\Delta}{\hbar \sqrt{\dot{\Omega}}}$$

$$\gamma \Box 1$$





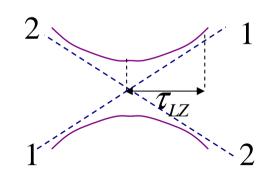
LZ transition matrix 
$$U = \begin{pmatrix} \alpha & \beta \\ -\beta^* & \alpha^* \end{pmatrix}$$
  $|\alpha|^2 + |\beta|^2 = 1$ 

Amplitude to stay at the same diabatic level (surviving amplitude)

$$\alpha = e^{-\pi \gamma^2}$$

Amplitude of transition 
$$\beta = -\frac{\sqrt{2 \pi} e \times p \left(-\frac{\pi \gamma^2}{2} + i \frac{\pi}{4}\right)}{\gamma \Gamma (-i \gamma^2)}$$

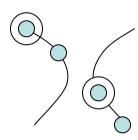
LZ transition time: 
$$\tau_{LZ} = \frac{\Delta}{\dot{\Omega}}$$



### Some applications of the Landau-Zener theory

#### Electronic transitions at atomic collisions

B.M. Smirnov, Physics of Atoms and Ions, Springer, 2003.



Proc. Natl. Acad. Sci. USA Vol. 77, No. 6, pp. 3105-3109, June 1980 Chemistry

#### Role of the chlorophyll dimer in bacterial photosynthesis

(electron transfer/charge separation/light energy storage)

ARIEH WARSHEL

Department of Chemistry, University of Southern California, Los Angeles, California 90007

Communicated by Martin D. Kamen, March 18, 1980

ABSTRACT The role of a special dimer (D) of bacteriochlorophyll molecules in bacterial photosynthesis was examined by calculations of the rates of electron transfer reactions in a system of the dimer and a bacteriopheophytin (BPh) molecule. It was found that the dependence of the potential surfaces of D on the distance between the monomers allows a fast lightinduced electron transfer from D to BPh but only a slow back reaction (reduction of D+ by BPh-). The same potential surfaces allow efficient reduction of D+ by cytochrome c. Possible advantages of greatly different values of the electronic matrix elements for the forward and back reactions are pointed out. It is suggested that the electrostatic interaction between D+ and an ionized group of the protein might play an important role in the photosynthetic reaction. classical trajectory approach of ref. 8. For small  $\sigma_{AB}$ , when the diabatic approximation is valid this gives essentially the Landau–Zener transition probability (8) which, when substituted into the rate expression in transition rate theory, gives exactly the same expression as Eq. 2.

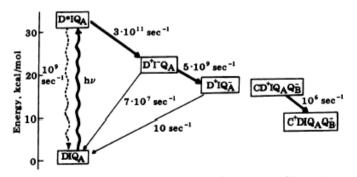
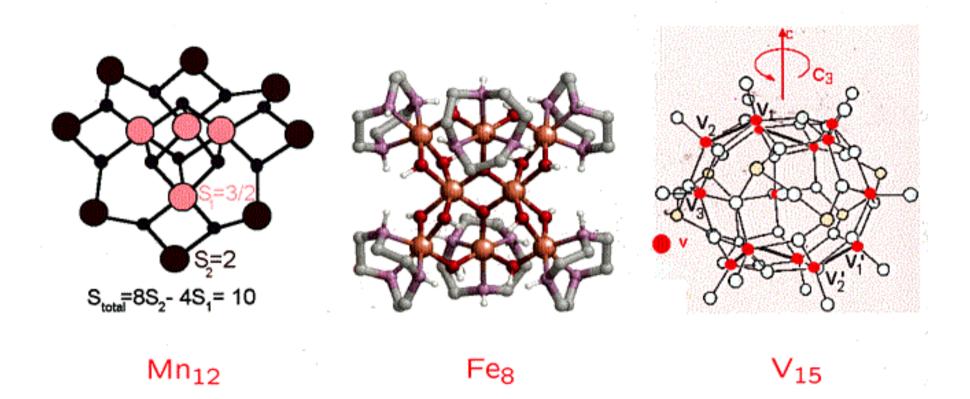


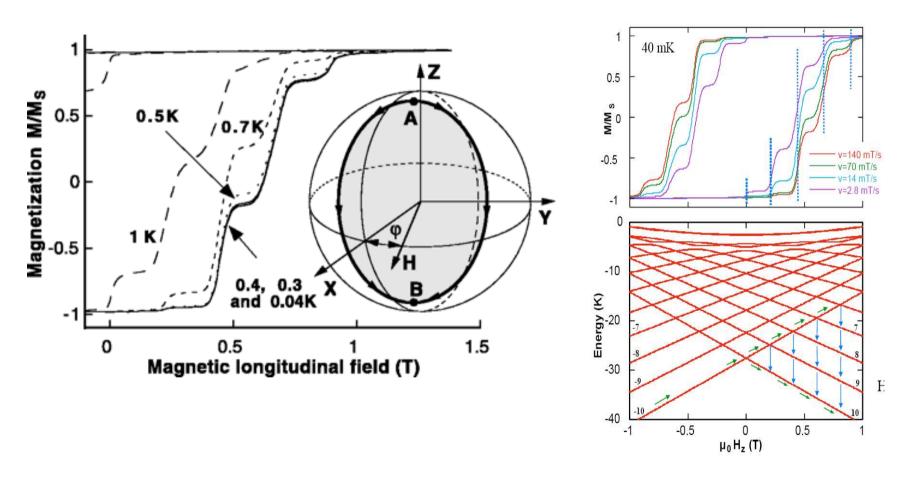
Fig. 1. Rates of electron transfer along different possible reaction

### **Molecular magnets**

▶ S = 10: Mn<sub>12</sub>, Fe<sub>8</sub>. S = 1/2: V<sub>15</sub>.



## Spin reversal in nanomagnets

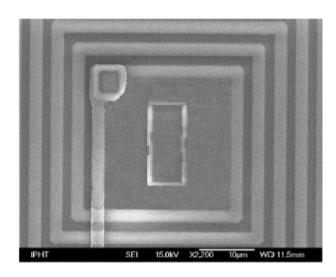


W. Wernsdorfer and R. Sessoli, Science 284, 133 (1999)

### Observation of macroscopic Landau–Zener transitions in a superconducting device

A. IZMALKOV<sup>1,2</sup>, M. GRAJCAR<sup>1,3</sup>, E. IL'ICHEV<sup>1</sup>(\*), N. OUKHANSKI<sup>1</sup>, TH. WAGNER<sup>1</sup>, H.-G. MEYER<sup>1</sup>, W. KRECH<sup>4</sup>, M. H. S. AMIN<sup>5</sup>, ALEC MAASSEN VAN DEN BRINK<sup>5</sup> and A. M. ZAGOSKIN<sup>5,6</sup>

<sup>&</sup>lt;sup>6</sup> Physics and Astronomy Dept., The University of British Columbia, 6224 Agricultural Rd., Vancouver, B.C., V6T 1Z1 Canada



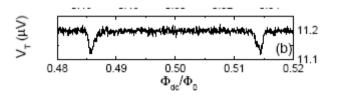


Fig. 2 - Electron micrograph of the qubit at the centre of the tank coil.

Institute for Physical High Technology, P.O. Box 100239, D-07702 Jena, Germany

<sup>&</sup>lt;sup>2</sup> Moscow Engineering Physics Institute (State University), Kashirskoe shosse 31, 115409 Moscow, Russia

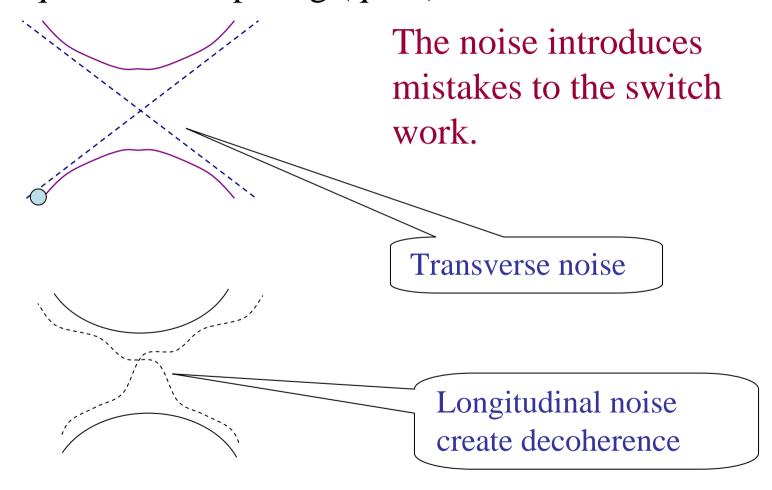
<sup>&</sup>lt;sup>3</sup> Department of Solid State Physics, Comenius University, SK-84248 Bratislava, Slovakia

<sup>&</sup>lt;sup>4</sup> Friedrich Schiller University, Institute of Solid State Physics, D-07743 Jena, Germany

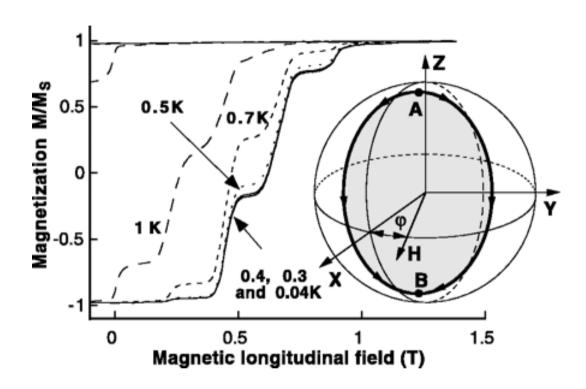
D-Wave Systems Inc., 320-1985 West Broadway, Vancouver, B.C., V6J 4Y3 Canada

### Why and when noise is substantial?

Controllable switch between states for quantum computing (qubit):



### Molecular magnets



Thernal noise changes the hysteresis loop at T>0.5 K

### **History**

### Longitudinal noise

- Y. Kayanuma, J. Phys. Soc. Jpn. **54**, 2087 (1985)
- Y. Gefen, E. Ben-Jacob, and A.O. Caldeira, Phys. Rev B 36, 2770 (1987)
- P. Ao and J. Rammer, Phys. Rev. B 43, 5397 (1991)
- Y. Kayanuma and H. Nakamura, Phys. Rev. B **57**, 13099 (1998)

#### Classical transverse noise

- Y. Kayanuma, J. Phys. Soc. Jpn. **53**, 108 (1984)
- V.L. Pokrovsky and N.A. Sinitsyn, Phys. Rev. B 67, 144303 (2003).

### Quantum fast noise

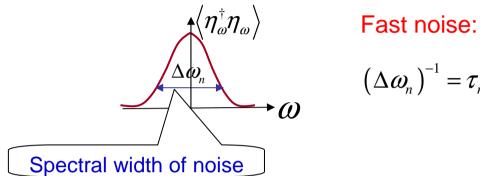
V.L. Pokrovsky and D. Sun, Phys. Rev. B **76**, 024310 (2007).

## Description of noise

Transverse or longitudinal

$$\eta(t) = \eta_l(t)\sigma_z + \eta_t(t)\sigma_x$$

Fast or slow



$$\left(\Delta \omega_{_{\!n}}
ight)^{\!-1} = au_{_{\!n}} \, \Box \, \, \, au_{_{\!L\!Z}}$$

Strong or weak

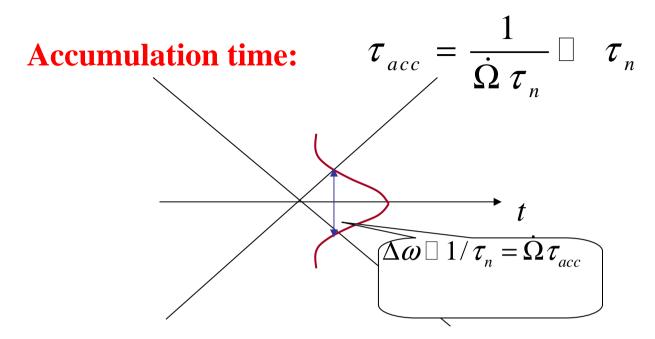
Strong noise: 
$$\left\langle \eta_{l,t}^{2}(t) \right
angle \Box \hbar^{2}\dot{\Omega}$$

Quantum or classical

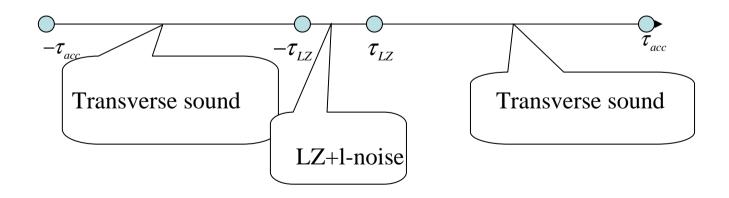
Quantum noise: 
$$\langle \eta_{\alpha}(t) \eta_{\beta}(t') \rangle \neq \langle \eta_{\beta}(t') \eta_{\alpha}(t) \rangle$$

Thermal or non-thermal

Thermal noise: 
$$\left\langle \eta_{\omega}^{\dagger} \eta_{\omega} \right\rangle = e^{-\hbar \omega / T} \left\langle \eta_{\omega} \eta_{\omega}^{\dagger} \right\rangle$$

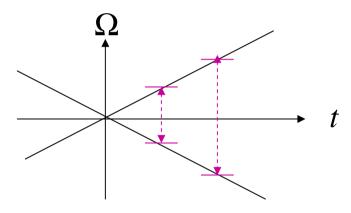


Time separation of LZ and transverse-noise-induced transitions



## Fast transverse noise in 2-level systems:

Transition is produced by that spectral component of noise, whose frequency is in resonance with instantaneous frequency of the LZ 2-level system.



Transition probability measures the spectrum of noise

Master equation

$$\dot{n}_1 = -\left\langle \eta_{-\Omega(t)}^{\dagger} \eta_{-\Omega(t)} \right\rangle n_1 + \left\langle \eta_{\Omega(t)} \eta_{\Omega(t)}^{\dagger} \right\rangle n_2 \qquad n_1 + n_2 = 1$$

### Master equation:

$$n_{1} + n_{2} = 1 \qquad s_{z} = \frac{n_{1} - n_{2}}{2} \qquad n_{1,2} = \frac{1}{2} \pm s_{z}$$

$$\frac{ds_{z}}{dt} = \left[ -s_{z} \left( \left\langle \eta \eta^{\dagger} \right\rangle_{|\Omega|} + \left\langle \eta^{\dagger} \eta \right\rangle_{-|\Omega|} \right) + \operatorname{sign}(\Omega) \left( \left\langle \eta \eta^{\dagger} \right\rangle_{|\Omega|} - \left\langle \eta^{\dagger} \eta \right\rangle_{-|\Omega|} \right) \right]_{\Omega = \Omega(t)}$$

$$\text{Classical limit:} \qquad \left\langle \eta \eta^{\dagger} \right\rangle_{\Omega} = \left\langle \eta^{\dagger} \eta \right\rangle_{-\Omega}$$

$$\text{Adiabatic limit} \qquad s_{z}(t) = -\operatorname{sign}(\Omega) \frac{\left\langle \eta \eta^{\dagger} \right\rangle_{|\Omega|} - \left\langle \eta^{\dagger} \eta \right\rangle_{-|\Omega|}}{\left\langle \eta \eta^{\dagger} \right\rangle_{|\Omega|} + \left\langle \eta^{\dagger} \eta \right\rangle_{-|\Omega|}}$$

$$\text{Equilibrium:} \qquad s_{z}(t) = -\tanh \frac{\Omega(t)}{2T}$$

New dimensional parameter: 
$$\gamma_t^2 = \frac{\langle \eta_t^2 \rangle}{\dot{\Omega}}$$

 $\gamma_t \square 1$  adiabatic regime for noise transitions

$$s_{z}(t) = -\operatorname{sign}(\Omega) \frac{\left\langle \eta \eta^{\dagger} \right\rangle_{|\Omega|} - \left\langle \eta^{\dagger} \eta \right\rangle_{-|\Omega|}}{\left\langle \eta \eta^{\dagger} \right\rangle_{|\Omega|} + \left\langle \eta^{\dagger} \eta \right\rangle_{-|\Omega|}}$$

 $\gamma_t \ \square \ 1$  moise transitions are negligible – pure LZ transition

New time scale: decoherence time:  $au_{dec} = \left(\left\langle \eta_{\alpha}^{2} \right\rangle au_{n} \right)^{-1}$ 

Survival probability:

$$P_{1\to 1} = \frac{1}{2} \left[ 1 + e^{-2\pi\gamma_t^2} \left( 2e^{-2\pi\gamma^2} - 1 \right) \right] + \frac{\pi}{\dot{\Omega}} \int_{0}^{\infty} d\Omega G(\Omega) e^{-\frac{2\pi}{\dot{\Omega}} \int_{\Omega}^{\infty} F(\omega) d\omega} \left[ \left( 2e^{-2\pi\gamma^2} - 1 \right) e^{-\frac{4\pi}{\dot{\Omega}} \int_{0}^{\Omega} F(\omega) d\omega} - 1 \right]$$

$$F(\Omega) = \left\langle \eta \eta^{\dagger} \right\rangle_{\Omega} + \left\langle \eta^{\dagger} \eta \right\rangle_{-\Omega}; G(\Omega) = \left\langle \eta \eta^{\dagger} \right\rangle_{\Omega} - \left\langle \eta^{\dagger} \eta \right\rangle_{-\Omega}$$

### Renormalization of the LZ gap

Correlated transverse and longitudinal sound produces almost instantaneous transition between the states of the 2-state system exactly as LZ gap  $\Delta$  does.



$$\Delta \to \tilde{\Delta} = \Delta + i \int_{0}^{\infty} \langle \left[ u_{\perp}(t), u_{\square}(0) \right] \rangle dt$$

Renormalized gap does not depend on temperature.

Renormalization is isotopically sensitive (Wernsdorfer et al.)

### Nonadiabatic Landau Zener tunneling in Fe<sub>8</sub> molecular nanomagnets

W. Wernsdorfer<sup>1</sup>, R. Sessoli<sup>2</sup>, A. Caneschi<sup>2</sup>, D. Gatteschi<sup>2</sup> and A. Cornia<sup>3</sup>

(received 28 Oct. 99; accepted )

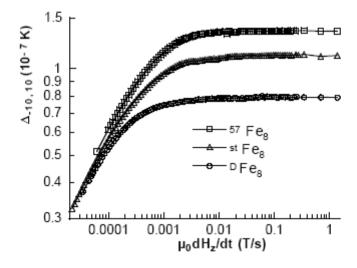


Fig. 2. – Field sweeping rate dependence of the tunnel splitting  $\Delta_{-10,10}$  measured by a Landau Zener method for three Fe<sub>8</sub> samples, for  $H_x=0$ . The Landau Zener method works in the region of high sweeping rates where  $\Delta_{-10,10}$  is sweeping rate independent. Note that the differences of  $\Delta_{-10,10}$  between the three samples are rather small in comparison to the oscillations in Fig. 3.

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<sup>&</sup>lt;sup>2</sup> Dept. of Chemistry, Univ. of Florence, Via Maragliano 77, 50144 Firenze, Italy

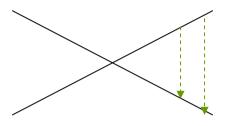
<sup>&</sup>lt;sup>3</sup> Dept. of Chemistry, Univ. of Modena, Via G. Campi 183, 41100 Modena, Italy

### **Zero temperature**

Survival probability

$$P_{1\to 1} = \exp\left[-2\pi\left(\tilde{\gamma}^2 + \gamma_t^2\right)\right]$$

$$\tilde{\gamma}^2 = \frac{\tilde{\Delta}^2}{\dot{\Omega}}$$



Only spontaneous emission is allowed

**Exact calculation: no assumptions on strength of noise and short correlation time** 

M. Wubs, K. Saito, S. Köhler, P. Hänggi, and Y.Kayanuma, Phys. Rev. Lett. **97**, 200404 (2006).

# Conclusions

- Transitions induced by transverse noise are accumulated during a long time  $\tau_{acc} = (\dot{\Omega}\tau_n)^{-1}$
- The LZ gap induces transitions during a shorter time  $\tau_{LZ} = \Delta/\dot{\Omega}$
- The longitudinal noise is effective during the same time
- The coherence is destroyed during the longest time  $\tau_{dec} = (\langle u^2 \rangle \tau_n)^{-1}$
- Within the accumulation time the transition probability obey the Master equations if noise is moderately strong
- The correlation of longitudinal and transverse noise leads to renormalization of the LZ gap, which explains its isotopic variation and violation of selection rule in molecular magnets