Fast quantum noise in Landau-Zener transitions

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Introduction and motivation

LZ theory

Diabatic levels

Adiabatic levels

Avoided level crossing (Wigner-Neumann theorem)

Schrödinger equations

\[ i\dot{a}_1 = E_1(t)a_1 + \Delta a_2 \]
\[ i\dot{a}_2 = \Delta^* a_1 + E_2(t)a_2 \]

\[ E_2(t) - E_1(t) = \Omega(t); \quad \hbar = 1 \]

\[ \Omega(t) = \dot{\Omega}t \]
Adiabatic levels:

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

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

Center-of-mass energy = 0

LZ parameter:

\[ \gamma = \frac{\Delta}{\hbar \sqrt{\dot{\Omega}}} \]

\[ \gamma \ll 1 \]

\[ \gamma \gg 1 \]

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LZ transition matrix

\[ U = \begin{pmatrix} \alpha & \beta \\ -\beta^* & \alpha^* \end{pmatrix} \quad |\alpha|^2 + |\beta|^2 = 1 \]

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

\[ \alpha = e^{-\pi \gamma^2} \]

Amplitude of transition

\[ \beta = -\frac{\sqrt{2\pi} \exp \left( -\frac{\pi \gamma^2}{2} + i \frac{\pi}{4} \right)}{\gamma \Gamma (-i \gamma^2)} \]

LZ transition time:

\[ \tau_{LZ} = \frac{\Delta}{\dot{\Omega}} \]

Condition of validity:

\[ \tau_{LZ} \ | \ \tau_{sat} = \left| \frac{\dot{\Omega}}{\ddot{\Omega}} \right| \]
Molecular magnets: Brief description

\[ S = 10 : \text{Mn}_{12}, \text{Fe}_8. \quad S = 1/2 : \text{V}_{15}. \]

\[ S_{\text{total}} = 8S_2 - 4S_1 = 10 \]

\( \text{Mn}_{12} \)

\( \text{Fe}_8 \)

\( \text{V}_{15} \)
Spin reversal in nanomagnets

Controllable switch between states for quantum computing:

The noise introduces mistakes to the switch work.

Transverse noise

Longitudinal noise creates decoherence
History

Pioneering works

L.D. Landau, Phys. Z. Sovietunion, 2, 46 (1932)

Longitudinal noise


Classical transverse noise

Fast transverse noise in 2-level systems: Intuitive approach

Transition is produced by that spectral component of noise, whose frequency is equal to its instantaneous value in the LZ 2-level system.

Master equation

\[ \dot{n}_1 = -\langle \eta_{-\Omega(t)}^\dagger \eta_{-\Omega(t)} \rangle n_1 + \langle \eta_{\Omega(t)} \eta_{\Omega(t)}^\dagger \rangle n_2 \]

\[ n_1 + n_2 = 1 \]
Accumulation of transitions produced by transverse noise

Noise produces transitions until \( \Omega(t) = \dot{\Omega} t \leq 1 / \tau_n \)

Accumulation time: \( \tau_{acc} = \frac{1}{\dot{\Omega} / \tau_n} \)

**Longitudinal noise** does not change occupation numbers beyond the time interval \( (-\tau_{LZ}, \tau_{LZ}) \)

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Quantum noise and its characterization

Model of noise: phonons

\[ H_n = \sum_k \omega_k b_k^\dagger b_k \]

\[ H_{\text{int}} = u_z \sigma_z + u_x \sigma_x \]

\[ u_\alpha = \eta_\alpha + \eta_\alpha^\dagger; \quad \eta_\alpha = \frac{1}{\sqrt{V}} \sum_k g_{\alpha k} b_k; \quad \alpha = \square, \perp \]

Quantum noise:

\[ \langle \eta^\dagger(t) \eta(t') \rangle \neq \langle \eta(t') \eta^\dagger(t) \rangle \]

\[ H_2 = \Omega(t) \sigma_z \]

\[ H_{\text{tot}} = H_2 + H_n + H_{\text{int}} \]
\[ \langle u(t)u(t') \rangle = \langle \eta(t)\eta^\dagger(t') \rangle + \langle \eta^\dagger(t)\eta(t') \rangle \]

\[ \langle \eta(t)\eta^\dagger(t') \rangle = \frac{1}{V} \sum_q (N_q + 1) |g_q|^2 \exp[-i\omega_q (t - t')] \]

Contains only positive frequencies. Induced and spontaneous transitions

\[ \langle \eta^\dagger(t)\eta(t') \rangle = \frac{1}{V} \sum_q N_q |g_q|^2 \exp[i\omega_q (t - t')] \]

Contains only negative frequency. Only induced transitions

**Time scales of the noise:**

\[ \tau_{ni} \propto T^{-1} \quad \tau_{ns} \propto \omega_g^{-1} \]

Noise is fast if \( T, \omega_g \propto \sqrt{\Omega} \Delta \)
Noise spectral power

\[ \langle \eta \eta^{\dagger} \rangle_{\Omega} = \int_{-\infty}^{\infty} \langle \eta (t) \eta^{\dagger} (0) \rangle e^{i\Omega t} dt \]

\[ \langle \eta \eta^{\dagger} \rangle_{\Omega} = \frac{1}{V} \sum_{q} |g_q|^2 (N_q + 1) \delta(\Omega - \omega_q) \]

Contains only positive frequencies
Induced and spontaneous emission

\[ \langle \eta^{\dagger} \eta \rangle_{\Omega} = \int_{-\infty}^{\infty} \langle \eta^{\dagger} (t) \eta (0) \rangle e^{i\Omega t} dt = \frac{1}{V} \sum_{q} |g_q|^2 N_q \delta(\Omega + \omega_q) \]

Contains only negative frequencies
Only induced emission

Equilibrium property:

\[ \frac{\langle \eta \eta^{\dagger} \rangle_{\Omega}}{\langle \eta^{\dagger} \eta \rangle_{-\Omega}} = \frac{N(\Omega) + 1}{N(\Omega)} = e^{\frac{\Omega}{T}} ; \quad \Omega > 0 \]
Microscopic derivation of master equations

Neglect $\Delta$, longitudinal noise beyond interval ($-\tau_{LZ}, \tau_{LZ}$)

What to calculate?

\[
n_{\alpha}(t) = \text{Tr} \left[ \rho_n U_I^{-1}(t, -\infty) | \alpha \rangle \langle \alpha | U_I(t, -\infty) \right] \\
U_I(t, -\infty) = T \left[ \exp \left( -i \int_{-\infty}^{t} V_I(t') dt' \right) \right]; U_I^{-1}(t, -\infty) = \tilde{T} \left[ \exp \left( i \int_{-\infty}^{t} V_I(t') dt' \right) \right] \\
V_I(t) = \left[ U_0(t, t_0) \right]^{-1} VU_0(t, t_0); \\
U_0(t, t_0) = \exp \left[ -i \int_{t_0}^{t} H_0(\tau) d\tau \right]; H_0(t) = \frac{\Omega(t)}{2} \sigma_z + H_n
\]

Keldysh technique:
Essential graphs

Contains extra small factor

Moderately strong noise

No multiphonon processes

But no limitations for $\langle u_\perp^2 \rangle / \dot{\Omega}$

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Evaluation of elementary graphs

Coarse grain approach: \[ \tau_n \parallel \Delta t \parallel \left\langle u_{\perp}^2 \right\rangle^{-1} \]

\[
\Gamma = \int_{t}^{t+\Delta t} dt_1 \int_{t}^{t+\Delta t} dt_2 \left\langle u_{\perp}(t_1) u_{\perp}(t_2) \right\rangle e^{i \int_{t_2}^{t_1} \Omega(\tau) d\tau} \approx 2\pi \left\langle u_{\perp} u_{\perp} \right\rangle_{\Omega(t)} \Delta t
\]

\[
\left\langle AB \right\rangle_{\Omega} = \int_{-\infty}^{\infty} \left\langle A(\tau) B(0) \right\rangle e^{i \Omega \tau} d\tau
\]

\[
\int_{t_2}^{t_1} \Omega(\tau) d\tau \approx \Omega(t) (t_2 - t_1)
\]

Contribution of two or more lines \( \parallel \left\langle u_{\perp}^2 \right\rangle \tau_n \cdot \Delta t \)

Negligible for moderately strong noise

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Equations of motion
Master equation:

\[ \frac{dn_1}{dt} = 2\pi \left[ -n_1 \left( \left[ \theta(-\Omega)\langle \eta^\dagger \eta \rangle_\Omega + \theta(\Omega)\langle \eta \eta^\dagger \rangle_\Omega \right] \right) + n_2 \left( \theta(-\Omega)\langle \eta \eta^\dagger - \Omega \rangle_\Omega + \theta(\Omega)\langle \eta^\dagger \eta \rangle_{-\Omega} \right) \right]_{\Omega=\Omega(t)} \]

Main difference with classical case: transition probabilities distinguish upper and lower level.

\[ n_{1,2} = \frac{1}{2} \pm s_z \]

Classical limit:

\[ \langle \eta \eta^\dagger \rangle_{\Omega} = \langle \eta^\dagger \eta \rangle_{-\Omega} \quad (T = \infty) \]

Adiabatic limit

\[ s_z(t) = -\text{sign}(\Omega) \frac{\langle \eta \eta^\dagger \rangle_{\Omega} - \langle \eta^\dagger \eta \rangle_{-|\Omega|}}{\langle \eta \eta^\dagger \rangle_{\Omega} + \langle \eta^\dagger \eta \rangle_{-|\Omega|}} \]

Equilibrium:

\[ s_z(t) = -\tanh \frac{\Omega(t)}{2T} \]

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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.

$$\Delta \rightarrow \tilde{\Delta} = \Delta + \left. i \int_{0}^{\infty} \langle [u_{\perp}(t), u_{\parallel}(0)] \rangle \right| dt = \Delta - \frac{1}{V} \sum_{q} \frac{g_{\perp}(q) g_{\parallel}(q)}{\omega_{q}}$$

Renormalized gap does not depend on temperature.
Nonadiabatic Landau Zener tunneling in Fe₈ molecular nanomagnets

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Fig. 2. – Field sweeping rate dependence of the tunnel splitting \( \Delta_{-10,10} \) measured by a Landau Zener method for three Fe₈ 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.
Longitudinal noise (LN)

LN does not contribute to the Master Equation

\[ \tau_{LZ} \quad |t| \quad \tau_{acc} \quad \text{LZ gap } \Delta \text{ can be neglected} \]

Evaluation of elementary graphs of Master Equation for LN

They are the same as in the absence of the transverse noise, i.e. zero.
Longitudinal noise (continuation)

Within the LZ time interval $|t| < \tau_{LZ}$

**Classical LN $\rightarrow$ Debye-Waller factor**

$$\left\langle \exp \left( i \int_{t_0}^{t} u_{\perp}(t) \, dt \right) \right\rangle = \exp \left[ -\frac{1}{2} \left\langle \left( \int_{t_0}^{t} u_{\perp}(t) \, dt \right)^2 \right\rangle \right]$$

$$\left\langle \left( \int_{t_0}^{t} u_{\perp}(t) \, dt \right)^2 \right\rangle = \int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \left\langle u_{\perp}(t_1) u_{\perp}(t_2) \right\rangle \left\langle u_{\perp}^2 \right\rangle \tau_n \tau_{LZ}$$

**Produces significant effect if**

$$\left\langle u_{\perp}^2 \right\rangle \geq \left( \tau_n \tau_{LZ} \right)^{-1}$$

For transverse noise this condition is more liberal: $\left\langle u_{\perp}^2 \right\rangle \geq \dot{\Omega}$

See references. **New equation for the fast LN.**
Noise and LZ gap work together

Separation in time: LZ gap and longitudinal noise are efficient within LZ time interval, transverse noise produces transitions within accumulation time interval. One can solve this two problem separately and match the solutions at some intermediate time \( t_1 \) such that \( \tau_{LZ} \par\par t_1 \par\par \tau_{acc} \).
Linear relation between elements of the initial and final density matrices for the LZ problem with the LN:

\[ \rho_{\alpha\beta}(+\infty) = \Lambda_{\alpha\beta,\gamma\delta}\rho_{\gamma\delta}(-\infty) \]

Relations between elements of \( \Lambda_{\alpha\beta,\gamma\delta} \):

\[ \rho_{\alpha\alpha}(-\infty) = \rho_{\alpha\alpha}(+\infty) = 1 \]

**Abbreviation:** \( \Lambda_{11,11} = \Lambda_1; \Lambda_{22,22} = \Lambda_2 \)

**Result:**

\[ s_z(+\infty) = (\Lambda_1 + \Lambda_2)e^{-2\pi\gamma^2_\perp} s_z(-\infty) + \pi(\Lambda_1 - \Lambda_2)e^{-2\pi\gamma^2_\perp} + \]

\[ \int_{\Omega}^\infty \frac{d\Omega}{\Omega} G(\Omega)e^{-2\pi\int_{\Omega}^\infty F(\omega)d\omega} \left[(\Lambda_1 + \Lambda_2)e^{-4\pi\int_{0}^\Omega F(\omega)d\omega} - 1 \right] \]

**Notations:**

\[ \gamma^2_\perp = \frac{\langle u^2_\perp \rangle}{\Omega} \]

\[ F(\Omega) = \langle \eta\eta^\dagger \rangle_\Omega + \langle \eta^\dagger\eta \rangle_{-\Omega}; G(\Omega) = \langle \eta\eta^\dagger \rangle_\Omega - \langle \eta^\dagger\eta \rangle_{-\Omega} \]

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LN is negligible: \[ \Lambda_1 = \Lambda_2 = e^{-2\gamma^2} - \frac{1}{2}; \quad \gamma^2 = \frac{\Delta^2}{\dot{\Omega}} \]

Survival probability:

\[
P_{1\rightarrow 1} = \frac{1}{2} \left[ 1 + e^{-2\gamma^2} \left( 2e^{-2\gamma^2} - 1 \right) \right] + \pi \int_0^{\infty} d\Omega G(\Omega) \left( \frac{2\pi}{\Omega} \int_0^\infty F(\omega) d\omega \right) \left( 2e^{-2\gamma^2} - 1 \right) e^{-\frac{4\pi}{\Omega} \int_0^\infty F(\omega) d\omega} - 1 \]

Analysis: \[ \gamma_\perp \nRightarrow 1 \quad \Rightarrow \quad \text{Adiabatic limit} \]
\[ \gamma_\perp \nRightarrow 1 \quad \Rightarrow \quad \text{LZ answer + noise correction} \quad \nRightarrow \gamma_\perp^2 \]

One more time scale: decoherence time

\[ \tau_{\text{dec}} = \left( \left\langle u^2 \right\rangle \tau_n \right)^{-1} \]

For moderately strong noise \[ \tau_{\text{dec}} \nRightarrow \tau_n \]
Can we say anything about strong noise \( \left< u_\perp^2 \right> \tau_n^2 \geq 1 \)?

It proceeds in deeply adiabatic regime

\[
\gamma_\perp^2 = \frac{\left< u_\perp^2 \right>}{\Omega} \frac{1}{\Omega \tau_n^2} \leq 1
\]

Occupation numbers reach equilibrium.

Alternative treatment: the noise induced width level is \( \Gamma \left< u_\perp^2 \right> \tau_n \)

For strong noise \( \Gamma \geq \tau_n^{-1} \Box \Omega \)

Very strong noise: \( \Gamma \Box \Omega \)

Two levels are not distinguishable:

\( n_1 = n_2 = 1/2 \)

Our equations give good interpolation between moderate and very strong noise.
Zero temperature

Survival probability

\[ P_{1 \rightarrow 1} = \exp \left[ -2\pi \left( \tilde{\gamma}^2 + \gamma_\perp^2 \right) \right] \]

\[ \tilde{\gamma}^2 = \frac{\Delta^2}{\Omega} \]

\[ \tilde{\gamma} = \Delta - \frac{1}{V} \sum_q \frac{g_\perp(q) g_\parallel(q)}{\omega_q} \]

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

Noise in molecular magnets

Noise is fast: $\dot{\Omega} \ll 10^{10} \, s^{-2}$; $\Delta \ll 10^{-7} \, K \ll 10^4 \, s^{-1}$; $T \ll 0.1 – 0.5 \, K \ll \Delta, \sqrt{\dot{\Omega}}$

What is the transverse noise?

$$H_{s-p} = \Lambda_{iklm} u_{ik} S_l S_m$$

$$\Delta S_z \leq 2$$

Need: $\Delta S_z = 20, 18…$

Solution: admixtures of other projections.

Transitions with odd $\Delta S_z$ become possible
Conclusions

- Transitions induced by transverse noise are accumulated during a long time $\tau_{\text{acc}} = (\dot{\Omega} \tau_n)^{-1}$
- The LZ gap induces transitions during a shorter time $\tau_{\text{LZ}} = \Delta / \dot{\Omega}$
- The longitudinal noise is effective during the same time.
- The coherence is destroyed during the longest time $\tau_{\text{dec}} = (\langle \dot{u}^2 \rangle \tau_n)^{-1}$
- Within the accumulation time the transition probability obeys the Master equations if noise is moderately strong.
- The correlation of longitudinal and transverse noise leads to renormalization of the LZ gap, which can explain its isotopic effect in molecular magnets and transitions between states with different parities of $S_z$.
- Quantum noise distinguishes upper and lower levels.
- When noise is strong, the system occurs in a deeply adiabatic regime.
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