Fast quantum noise in Landau-Zener transitions

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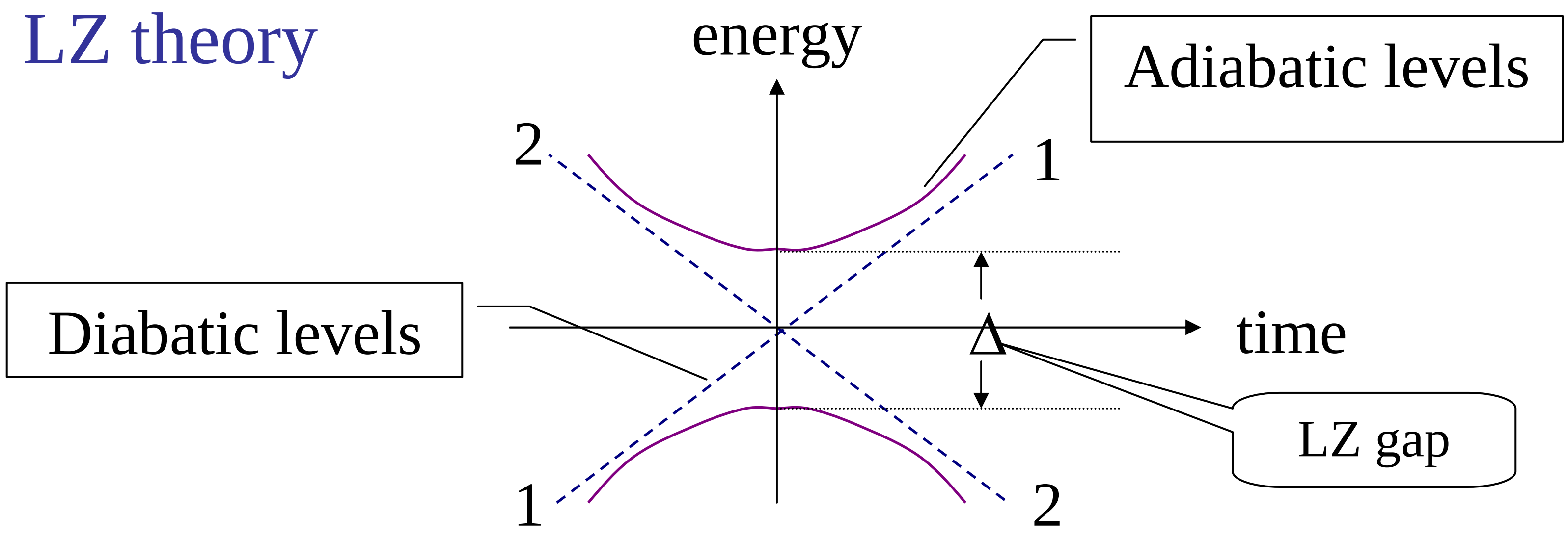
Cooled atoms, KITP, UCSB, May 2007

Outline

- Introduction and motivation
- Fast noise in 2-level systems: intuitive approach
- Quantum noise and its characterization
- Microscopic derivation of master equation
- Transitions produced by transverse noise
- Noise and regular transitions work together
- Zero temperature
- Noise in molecular magnets
- Conclusions

Introduction and motivation

LZ theory



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:

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

Center-of mass energy = 0

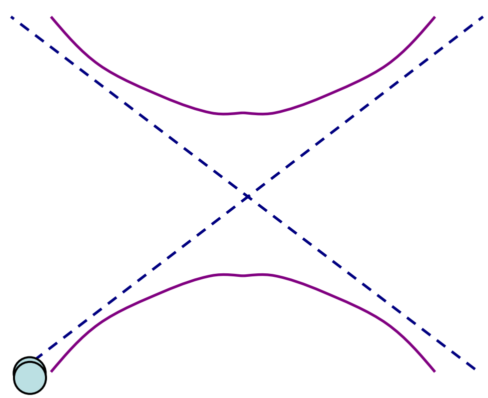
$$E_2 = -E_1 = \dot{\Omega} t / 2$$

LZ parameter:

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

γ □ 1

γ □ 1

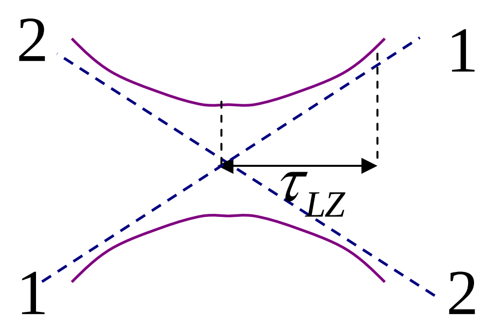


LZ transition matrix $U = \begin{pmatrix} \alpha & \beta \\ -\beta^* & \alpha^* \end{pmatrix}$ $|\alpha|^2 + |\beta|^2 = 1$

Amplitude to stay at the same diabatic level (surviving amplitude) $\alpha = e^{-\pi\gamma^2}$

Amplitude of transition $\beta = -\dfrac{\sqrt{2\pi}\exp\left(-\dfrac{\pi\gamma^2}{2} + i\dfrac{\pi}{4}\right)}{\gamma\Gamma(-i\gamma^2)}$

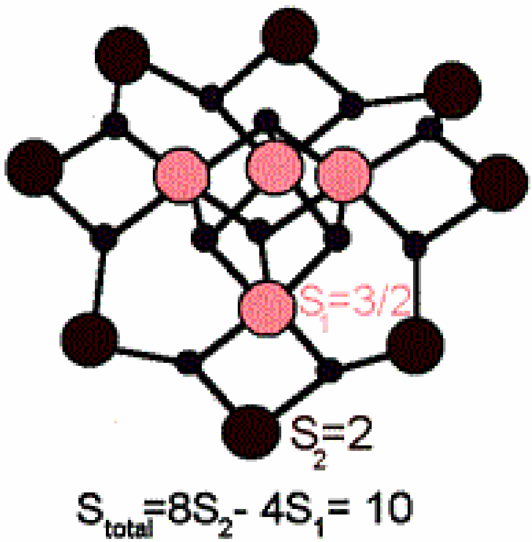
LZ transition time: $\tau_{LZ} = \dfrac{\Delta}{\dot{\Omega}}$



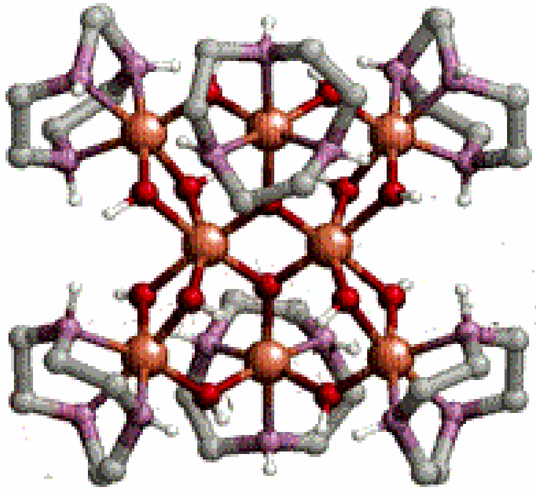
Condition of validity: $\tau_{LZ} \ll \tau_{sat} = \left|\dot{\Omega} / \ddot{\Omega}\right|$

Molecular magnets: Brief description

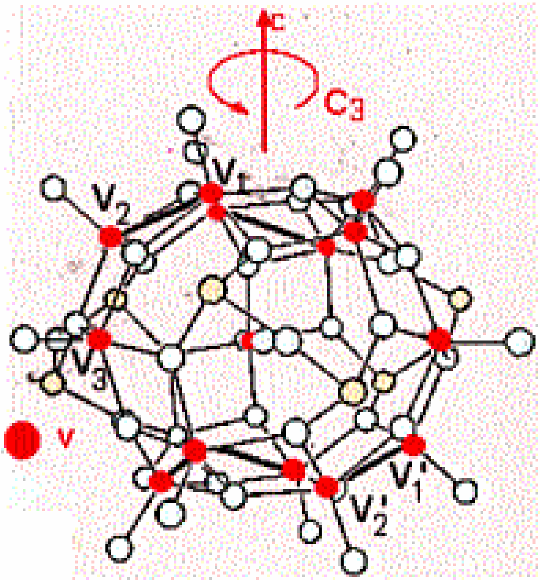
- $S = 10$: Mn_{12}, Fe_8. $S = 1/2$: V_{15}.



Mn_{12}

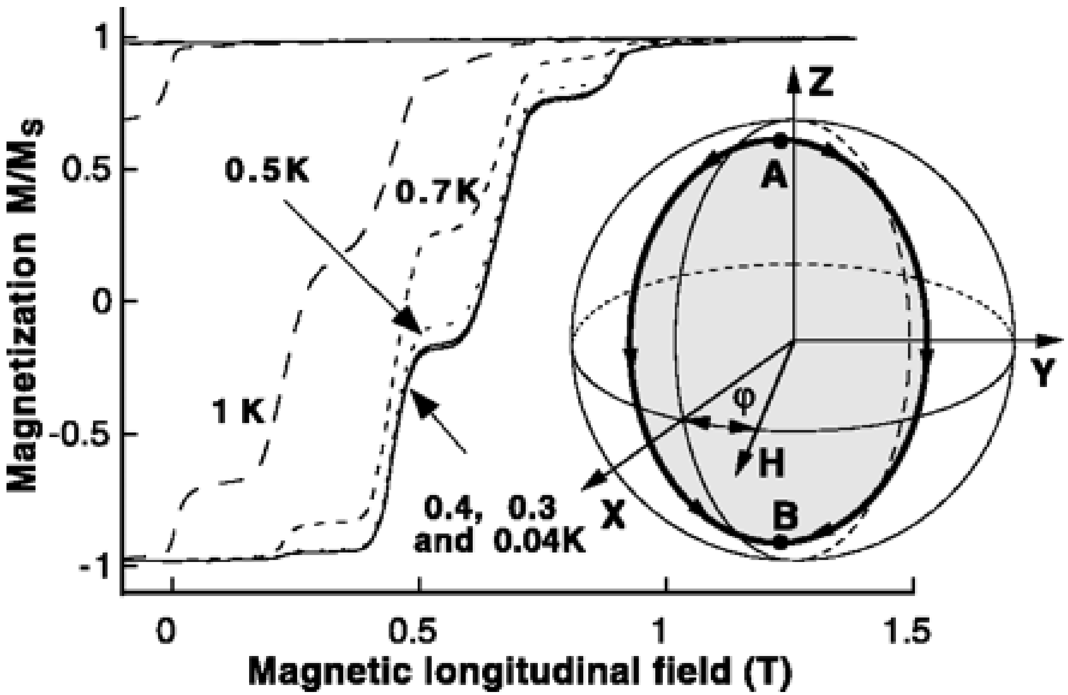


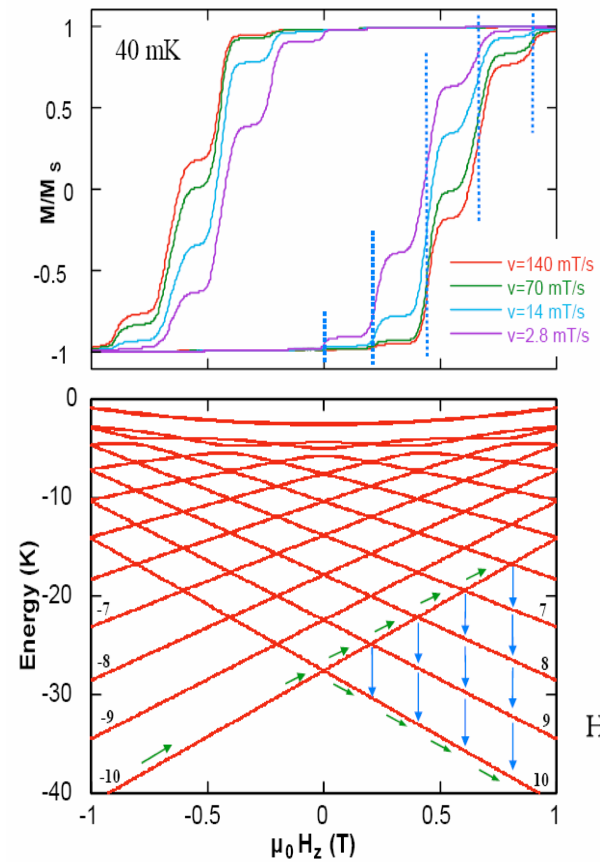
Fe_8



V_{15}

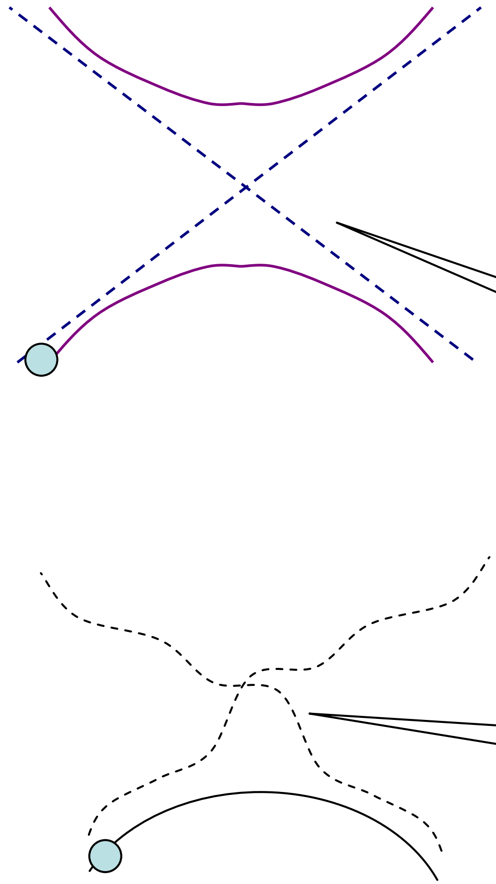
Spin reversal in nanomagnets





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

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)

C. Zener, Proc. Roy. Soc. A **137**, 696 (1932)

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

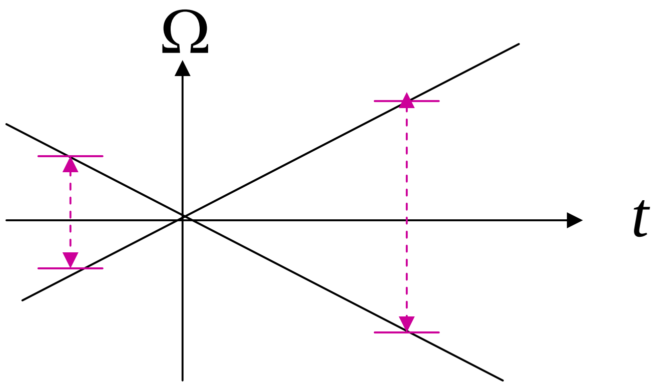
Y. Kayanuma, J. Phys. Soc. Jpn. **53**, 108 (1984)

V.L. Pokrovsky and N.A. Sinitsyn, Phys. Rev. B **67**, 144303 (2003).

V.L. Pokrovsky and S. Scheidl, Phys. Rev. B **70**, 014416 (2004).

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.

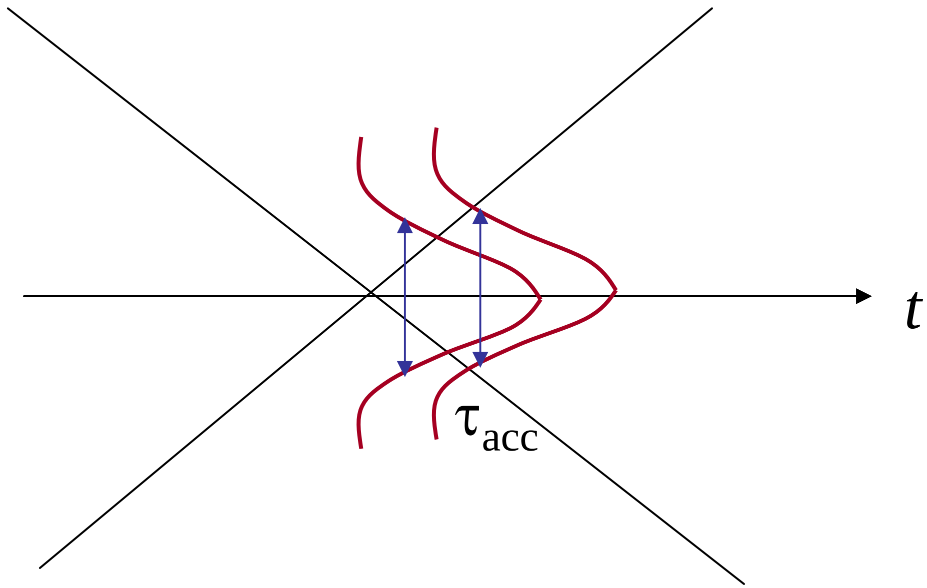


Transition probability measures the spectrum of noise

Master equation

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

Accumulation of transitions produced by transverse noise



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

Accumulation time: $\tau_{acc} = \frac{1}{\dot{\Omega}\,\tau_n} \square \tau_n$

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

Quantum noise and its characterization

Model of noise: phonons $$H_n = \sum_{\mathbf{k}} \omega_{\mathbf{k}} b_{\mathbf{k}}^{\dagger} b_{\mathbf{k}}$$

$$H_{\text{int}} = u_{\parallel} \sigma_z + u_{\perp} \sigma_x$$

$$u_{\alpha} = \eta_{\alpha} + \eta_{\alpha}^{\dagger};\ \eta_{\alpha} = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} g_{\alpha\mathbf{k}} b_{\mathbf{k}};\ \alpha = \parallel, \perp$$

Quantum noise: $$\langle \eta^{\dagger}(t)\eta(t') \rangle \neq \langle \eta(t')\eta^{\dagger}(t) \rangle$$

$$H_2 = \Omega(t)\sigma_z$$

$$H_{tot} = H_2 + H_n + H_{\text{int}}$$

$$\langle u(t)u(t')\rangle = \langle \eta(t)\eta^\dagger(t')\rangle + \langle \eta^\dagger(t)\eta(t')\rangle$$

$$\langle \eta(t)\eta^\dagger(t')\rangle = \frac{1}{V}\sum_{\mathbf{q}}\left(N_{\mathbf{q}}+1\right)\left|g_{\mathbf{q}}\right|^2 \exp\left[-i\omega_{\mathbf{q}}(t-t')\right]$$

Contains only positive frequencies. Induced and spontaneous transitions

$$\langle \eta^\dagger(t)\eta(t')\rangle = \frac{1}{V}\sum_{\mathbf{q}} N_{\mathbf{q}}\left|g_{\mathbf{q}}\right|^2 \exp\left[i\omega_{\mathbf{q}}(t-t')\right]$$

Contains only negative frequency. Only induced transitions

Time scales of the noise:

$$\tau_{ni} \sim T^{-1} \qquad\qquad \tau_{ns} \sim \omega_g^{-1}$$

Noise is fast if $T, \omega_g \gg \sqrt{\dot{\Omega}}\Delta$

Noise spectral power

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

$$\left\langle \eta\eta^{\dagger} \right\rangle_{\Omega} = \frac{1}{V} \sum_{\mathbf{q}} \left| g_{\mathbf{q}} \right|^{2} \left(N_{\mathbf{q}} + 1 \right) \delta\left(\Omega - \omega_{\mathbf{q}} \right)$$

Contains only positive frequencies
Induced and spontaneous emission

$$\left\langle \eta^{\dagger}\eta \right\rangle_{\Omega} = \int_{-\infty}^{\infty} \left\langle \eta^{\dagger}(t)\eta(0) \right\rangle e^{i\Omega t} dt = \frac{1}{V} \sum_{\mathbf{q}} \left| g_{\mathbf{q}} \right|^{2} N_{\mathbf{q}} \delta\left(\Omega + \omega_{\mathbf{q}} \right)$$

Contains only negative frequencies
Only induced emission

Equilibrium property:

$$\frac{\left\langle \eta\eta^{\dagger} \right\rangle_{\Omega}}{\left\langle \eta^{\dagger}\eta \right\rangle_{-\Omega}} = \frac{N(\Omega)+1}{N(\Omega)} = e^{\frac{\Omega}{T}}; \; \Omega > 0$$

Microscopic derivation of master equations

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

What to calculate?

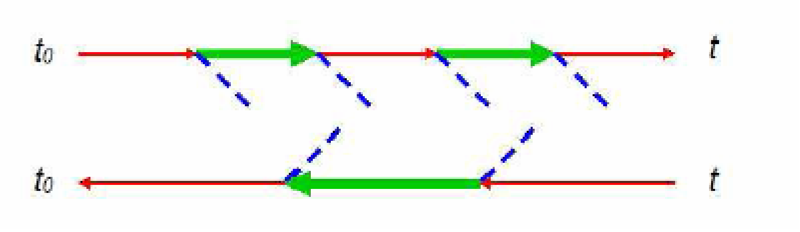
$$n_\alpha(t) = \mathrm{Tr}\left[\rho_n U_I^{-1}(t,-\infty)\left|\alpha\right\rangle\left\langle\alpha\right|U_I(t,-\infty)\right]$$

$$U_I(t,-\infty) = T\left[\exp\left(-i\int_{-\infty}^{t} V_I(t')\,dt'\right)\right];\ U_I^{-1}(t,-\infty) = \tilde{T}\left[\exp\left(i\int_{-\infty}^{t} V_I(t')\,dt'\right)\right]$$

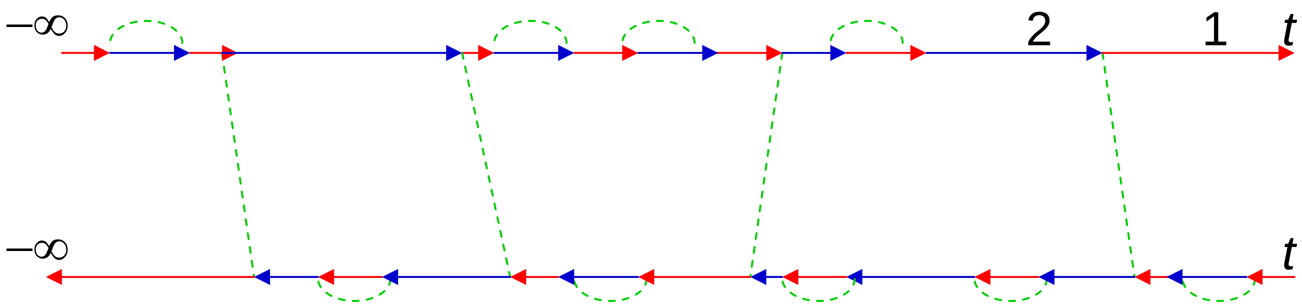
$$V_I(t) = \left[U_0(t,t_0)\right]^{-1} V U_0(t,t_0);$$

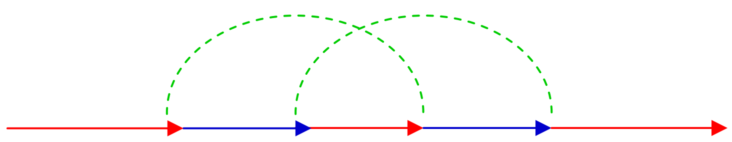
$$U_0(t,t_0) = \exp\left[-i\int_{t_0}^{t} H_0(\tau)\,d\tau\right];\ H_0(t) = \frac{\Omega(t)}{2}\sigma_z + H_n$$

Keldysh technique:



Essential graphs





Contains extra small factor

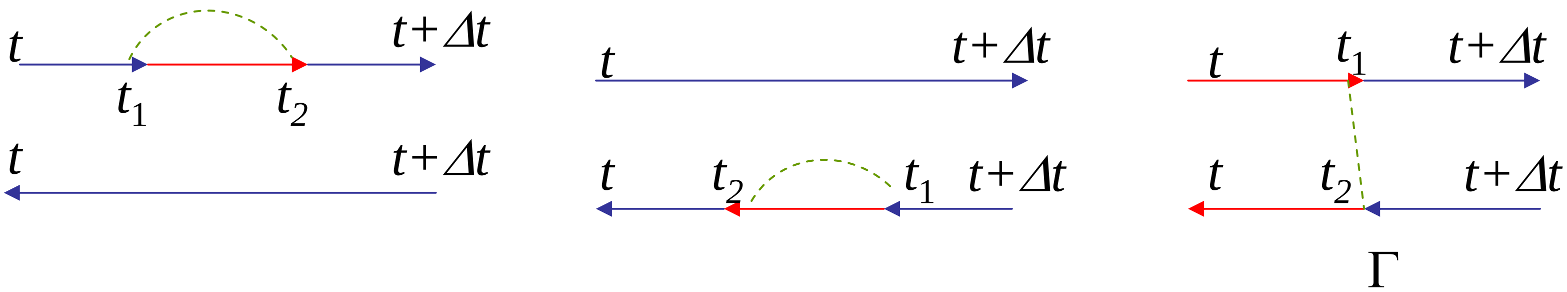
$$\left\langle u_\perp^2 \right\rangle \tau_n^2 \ll 1$$

Moderately strong noise

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

No multiphonon processes

Evaluation of elementary graphs



Coarse grain approach: $\tau_n \;\square\; \Delta t \;\square\; \left\langle u_\perp^2 \right\rangle^{-1}$

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

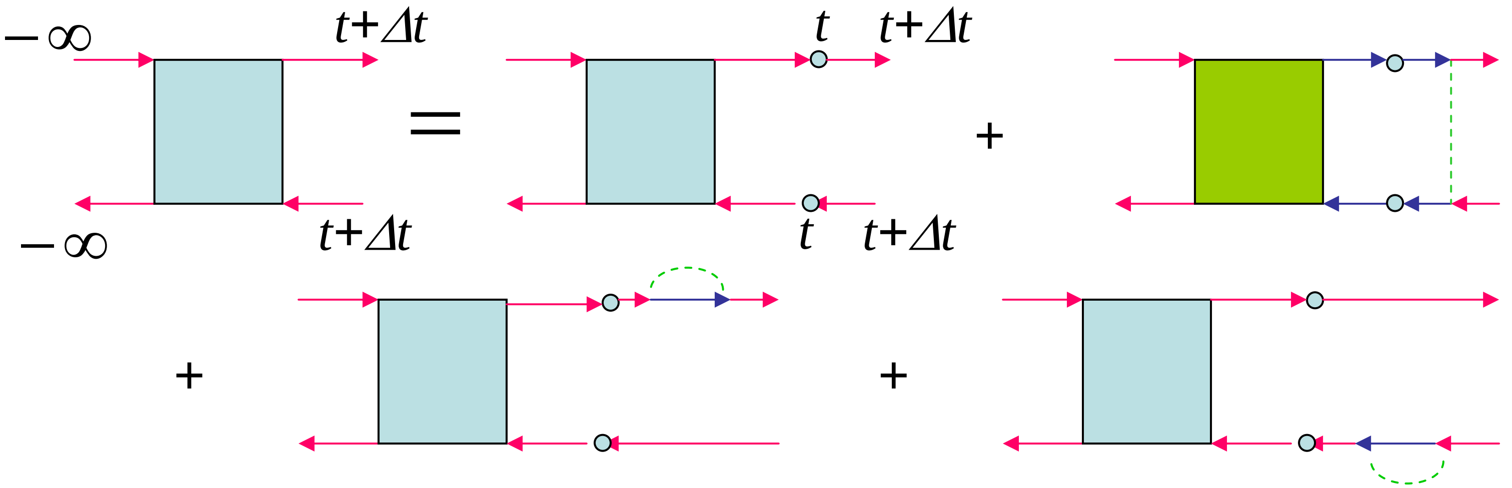
$$\left\langle AB \right\rangle_\Omega = \int_{-\infty}^{\infty} \left\langle A(\tau) B(0) \right\rangle e^{i\Omega\tau} d\tau$$

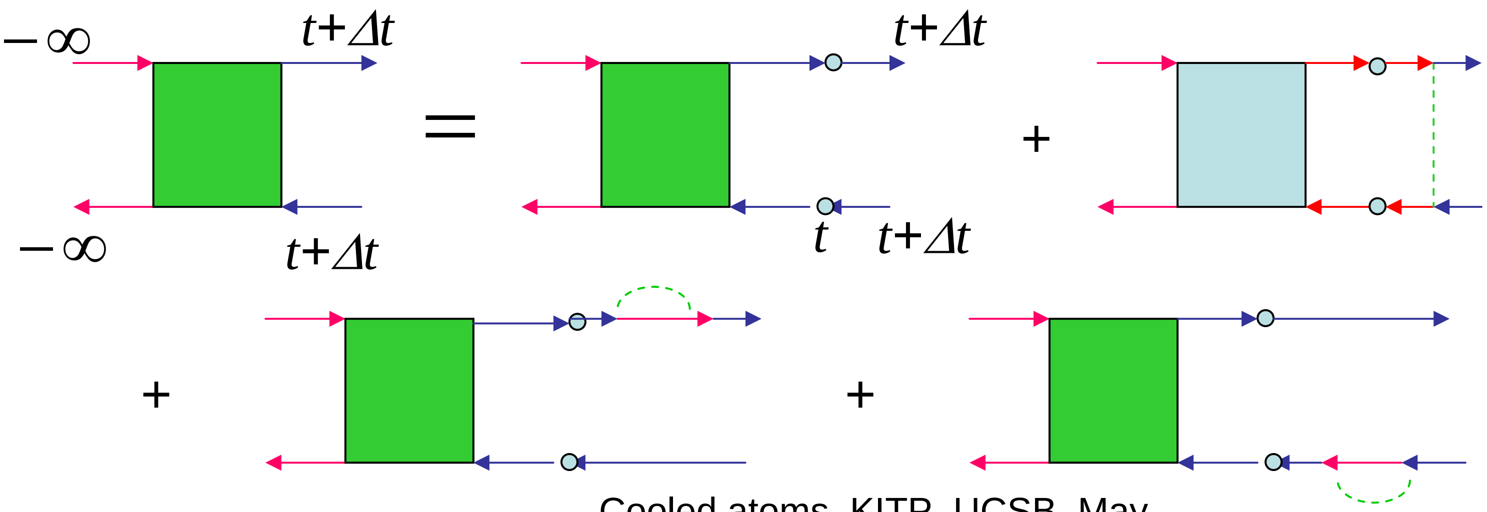
$$\int_{t_2}^{t_1} \Omega(\tau) d\tau \approx \Omega(t)(t_2 - t_1)$$

Contribution of two or more lines $\;\square\; \left\langle u_\perp^2 \right\rangle^2 \tau_n \cdot \Delta t$

Negligible for moderately strong noise

Equations of motion

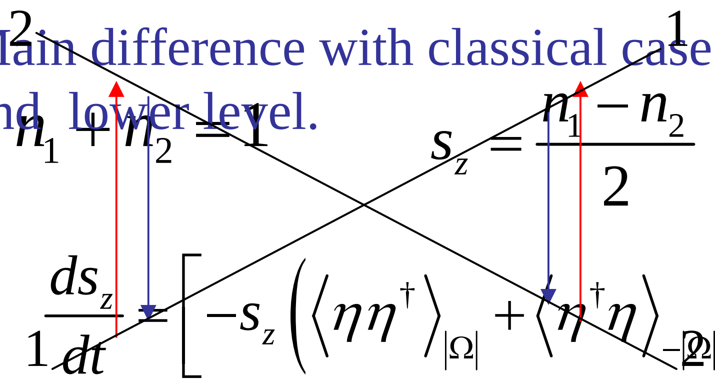




Master equation:

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

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



$$n_1 + n_2 = 1 \qquad s_z = \frac{n_1 - n_2}{2} \qquad n_{1,2} = \frac{1}{2} \pm s_z$$

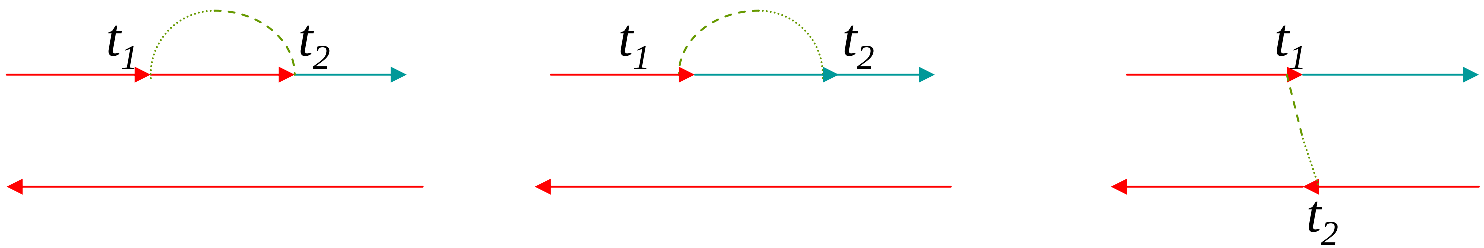
$$\frac{ds_z}{dt} = \left[-s_z\left(\left\langle \eta\eta^\dagger\right\rangle_{|\Omega|} + \left\langle \eta^\dagger\eta\right\rangle_{-|\Omega|}\right) + \operatorname{sign}(\Omega)\left(\left\langle \eta\eta^\dagger\right\rangle_{|\Omega|} - \left\langle \eta^\dagger\eta\right\rangle_{-|\Omega|}\right)\right]_{\Omega=\Omega(t)}$$

Classical limit: $\left\langle \eta\eta^\dagger\right\rangle_\Omega = \left\langle \eta^\dagger\eta\right\rangle_{-\Omega} \qquad (T=\infty)$

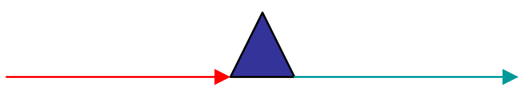
Adiabatic limit $s_z(t) = -\operatorname{sign}(\Omega)\dfrac{\left\langle \eta\eta^\dagger\right\rangle_{|\Omega|} - \left\langle \eta^\dagger\eta\right\rangle_{-|\Omega|}}{\left\langle \eta\eta^\dagger\right\rangle_{|\Omega|} + \left\langle \eta^\dagger\eta\right\rangle_{-|\Omega|}}$

Equilibrium: $s_z(t) = -\tanh\dfrac{\Omega(t)}{2T}$

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 Δ does.



$$\Delta \to \tilde{\Delta} = \Delta + i\int_0^{\infty} \left\langle \left[u_{\perp}(t), u_{\parallel}(0) \right] \right\rangle dt = \Delta - \frac{1}{V} \sum_{\mathbf{q}} \frac{g_{\perp}(\mathbf{q})\, g_{\parallel}(\mathbf{q})}{\omega_{\mathbf{q}}}$$

Renormalized gap does not depend on temperature.

Renormalization … experiments with

EUROPHYSICS LETTERS version of 15/ 2 / 2000
Europhys. Lett., ? (?), pp. ? (2000)

Nonadiabatic Landau Zener tunneling in Fe_8 molecular nanomagnets

Renormali … et al.)

W. Wernsdorfer[1], R. Sessoli[2], A. Caneschi[2], D. Gatteschi[2] and A. Cornia[3]
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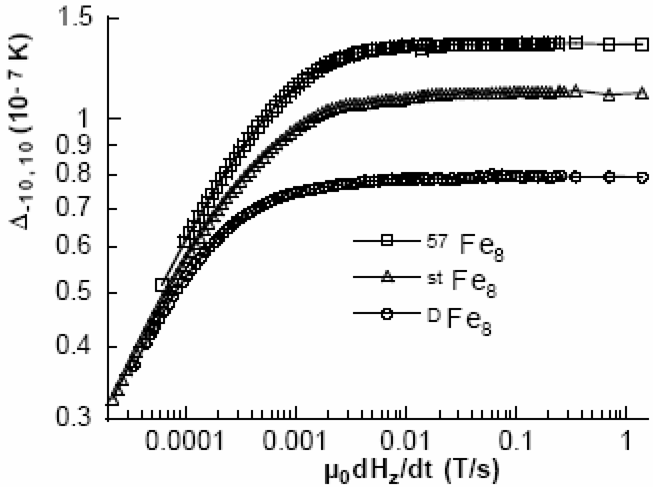
Noise-ind … zero

(received 28 Oct. 99; accepted)



Mc

Th … is allowed

Fig. 2. – Field sweeping rate dependence of the tunnel splitting $\Delta_{-10,10}$ measured by a Landau Zener method for three Fe_8 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.

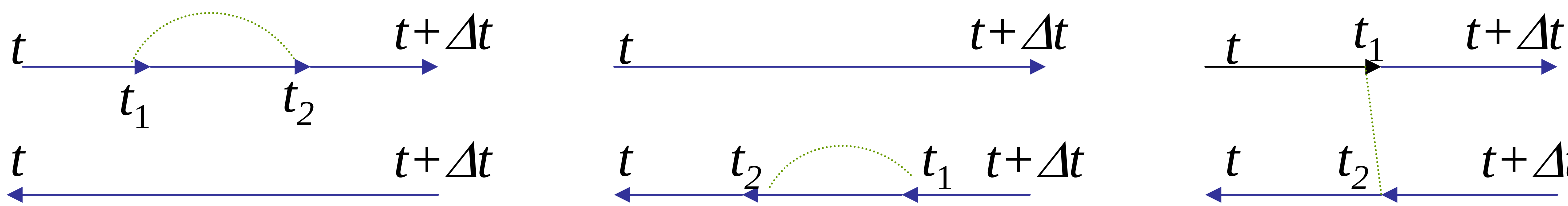
Ex … is allowed

Longitudinal noise (LN)

LN does not contribute to the Master Equation

$\tau_{LZ} \ll |t| \ll \tau_{acc}$ LZ gap Δ 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 $\Rightarrow$ **De**bye-Waller factor

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

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

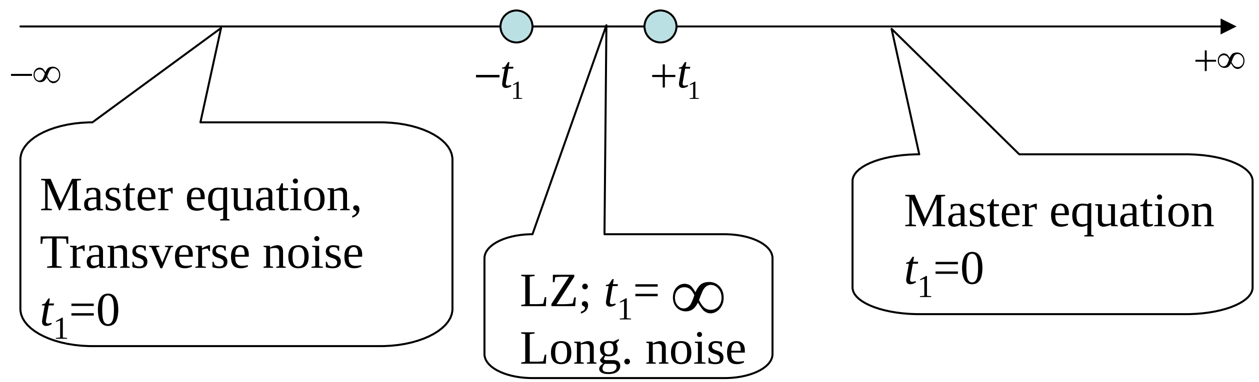
Produces significant effect if $\left\langle u_{\parallel}^2 \right\rangle \geq \left(\tau_n \tau_{LZ} \right)^{-1} = \dfrac{\dot{\Omega}}{\Delta \tau_n} \approx \dot{\Omega}$

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 $\tau_{LZ} \ll t_1 \ll \tau_{acc}$



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:

$$s_z(+\infty) = (\Lambda_1 + \Lambda_2)e^{-2\pi\gamma_\perp^2}s_z(-\infty) + \pi(\Lambda_1 - \Lambda_2)e^{-2\pi\gamma_\perp^2} +$$

$$\int_0^\infty \frac{d\Omega}{\dot{\Omega}} G(\Omega) e^{-2\pi\int_\Omega^\infty F(\omega)d\omega}\left[(\Lambda_1 + \Lambda_2)e^{-4\pi\int_0^\Omega F(\omega)d\omega} - 1\right]$$

Notations:

$$\gamma_\perp^2 = \frac{\langle u_\perp^2 \rangle}{\dot{\Omega}}$$

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

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

Survival probability:

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

Analysis: $\gamma_\perp$ □ 1 ⟹ Adiabatic limit

$\gamma_\perp$ □ 1 ⟹ LZ answer + noise correction □ $\gamma_\perp^2$

One more time scale: decoherence time $\tau_{dec} = \left(\left\langle u_\alpha^{\ 2}\right\rangle \tau_n\right)^{-1}$

For moderately strong noise τ_{dec} □ τ_n

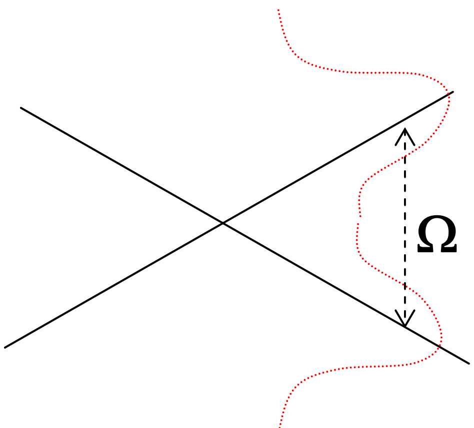
Can we say anything about strong noise $\langle u_\perp^2 \rangle \tau_n^2 \geq 1$?

It proceeds in deeply adiabatic regime $\gamma_\perp^2 = \dfrac{\langle u_\perp^2 \rangle}{\dot{\Omega}} \square \dfrac{1}{\dot{\Omega}\tau_n^2} \square \; 1$

Occupation numbers reach equilibrium.

Alternative treatment: the noise induced width level is $\Gamma \square \langle u_\perp^2 \rangle \tau_n$

For strong noise $\Gamma \geq \tau_n^{-1} \square \Omega$



Very strong noise: $\Gamma \square \; \Omega$

Two levels are not distinguishable:

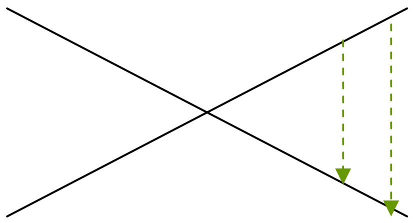
$n_1 = n_2 = 1/2$

Our equations give good interpolation between moderate and very strong noise

Zero temperature

Survival probability

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



Only spontaneous emission is allowed

$$\tilde{\gamma}^2 = \frac{\tilde{\Delta}^2}{\dot{\Omega}} \qquad \tilde{\Delta} = \Delta - \frac{1}{V}\sum_{\mathbf{q}} \frac{g_\perp(\mathbf{q})\, g_\parallel(\mathbf{q})}{\omega_{\mathbf{q}}}$$

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

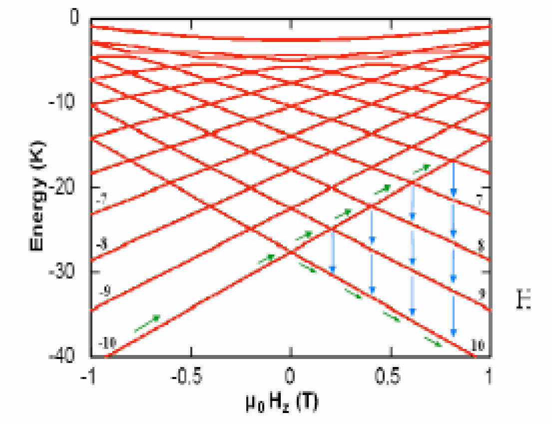
M. Wubs, K. Saito, S. Köhler, P. Hänggi, and Y.Kayanuma, Phys. Rev. Lett. **97**, 200404 (2006).

Noise in molecular magnets

Noise is fast: $\dot{\Omega} \square 10^{10} s^{-2}; \qquad \Delta \square 10^{-7} K \square 10^{4} s^{-1};$

$T \square 0.1 - 0.5K \square \ \Delta, \sqrt{\dot{\Omega}}$

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 ΔS_z become possible

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 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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