YKIS2007 Kyoto
29 Nov. 2007

Quantum dynamics in low dimensional spin systems

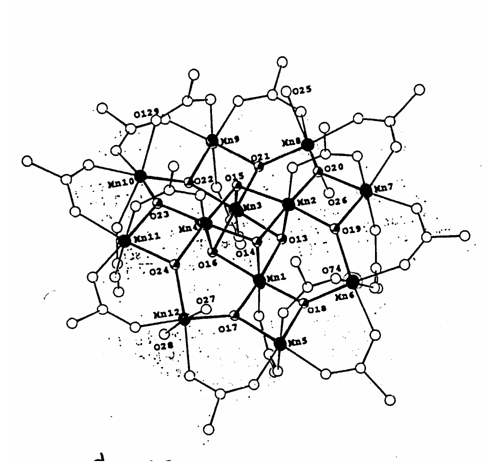
University of Tokyo
Seiji MIYASHITA

Topics

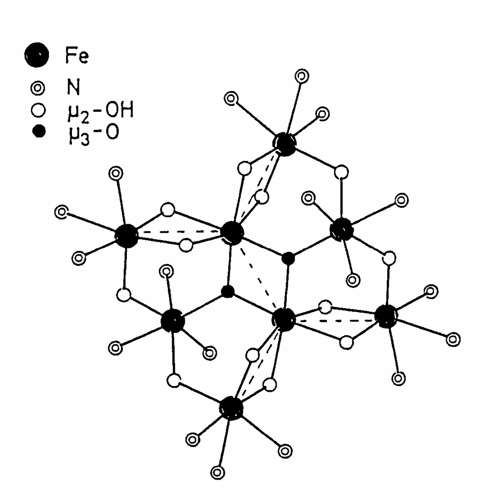
- **Quantum dynamics under time-dependent fields**
  - Quantum hysteresis in single molecular magnets
    - Landau-Zener process + Magnetic Foehn effects (Sweep)
  - Nontrivial Resonance and Coherent Destruction of Tunneling (AC)
  - Quantum mechanical reentrant phenomena
  - Quantum annealing
- **Quantum dynamics between macroscopic states**
  - Quantum spinodal phenomena of quantum phase transition
  - Nagaoka magnetism
- **Quantum Response**
  - ESR in pure quantum dynamic
  - ESR in dissipative dynamics
- **Related topics**
  - Origin of the energy gap and Gap control
  - Potential trap

Quantum dynamics of magnetization

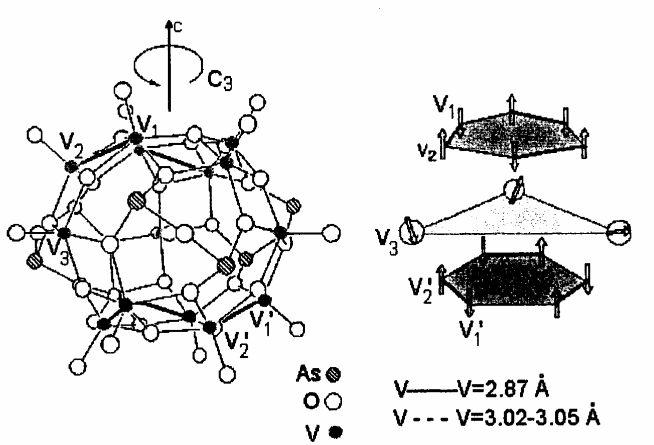
Molecular magnets



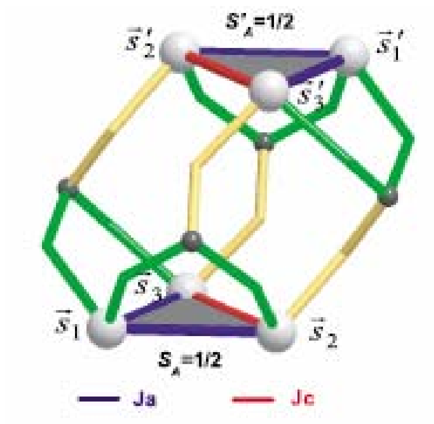
Mn12



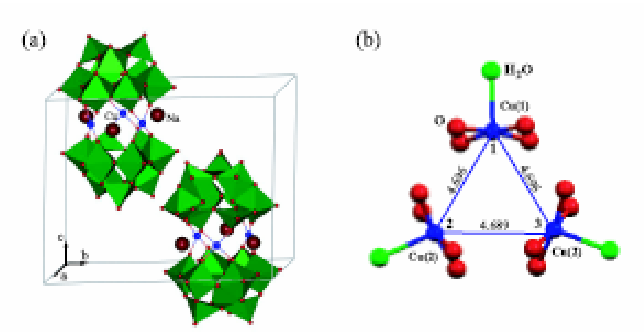
Fe8



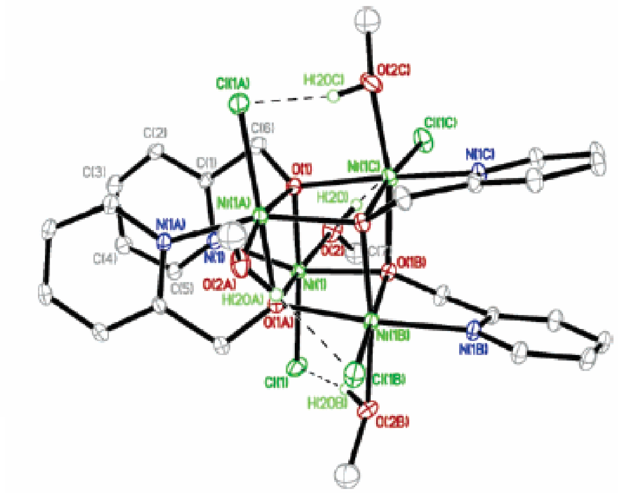
V15



V6



Cu3



Ni4

Temperature dependence

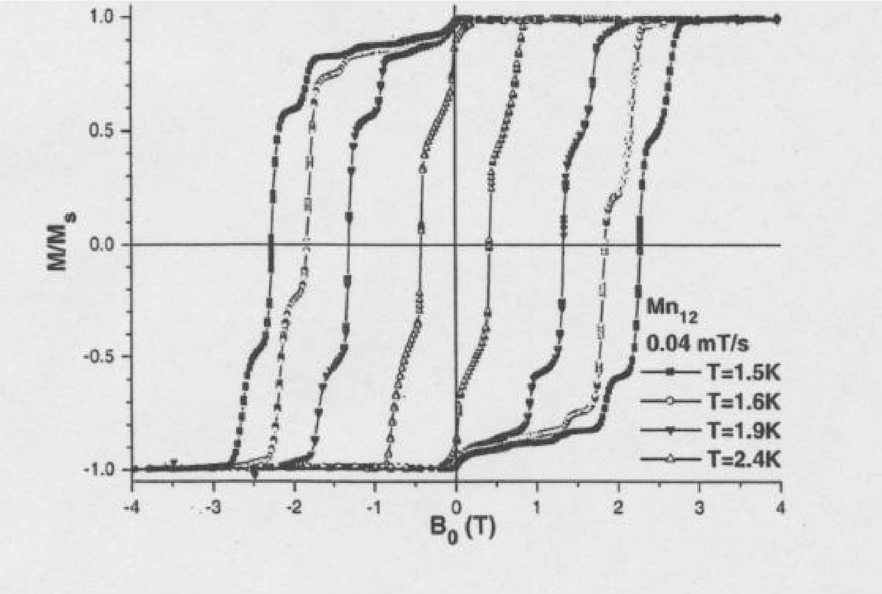
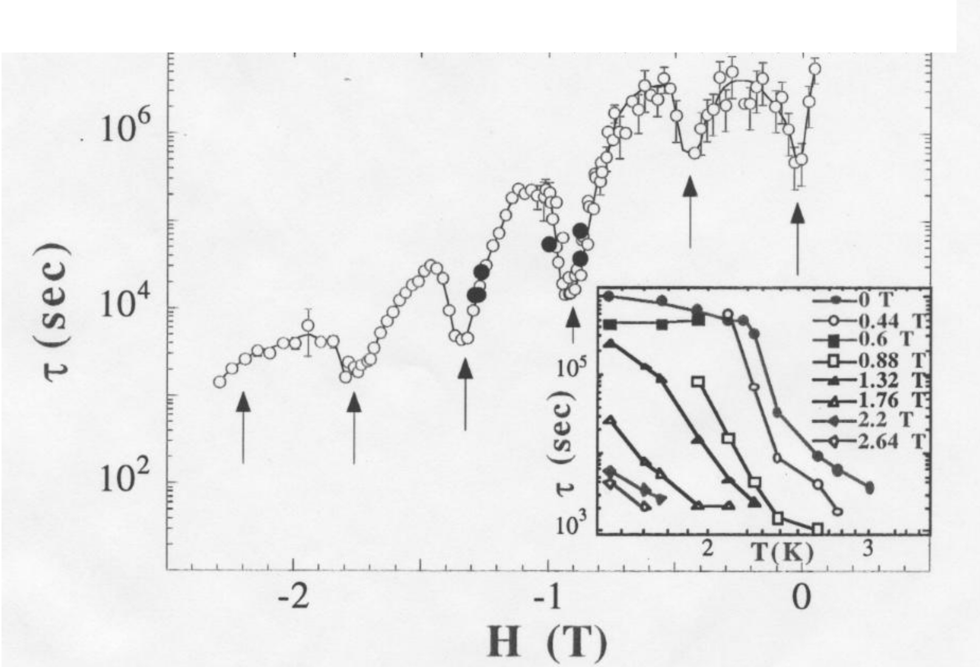
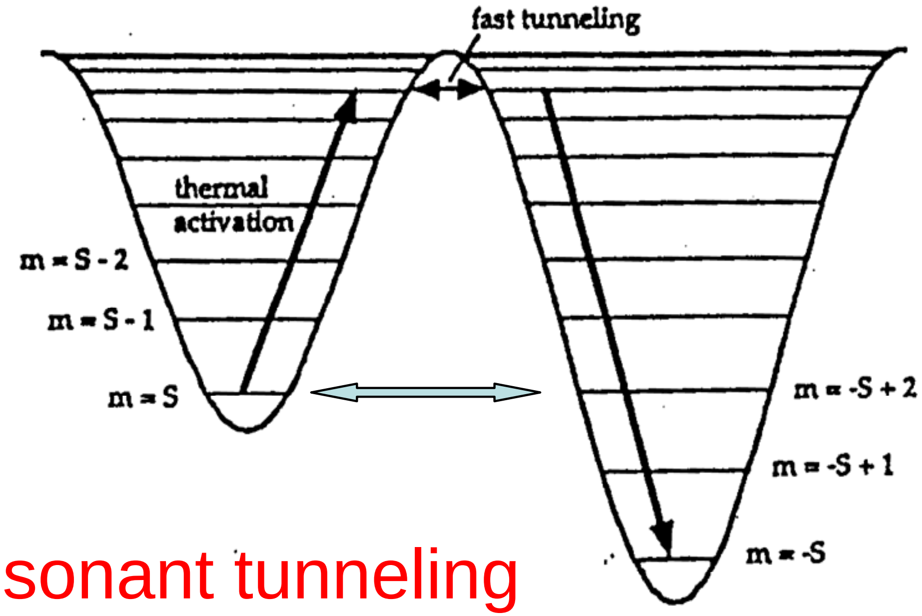


Fig. 1. Hysteresis loops of Mn$_{12}$-ac, with the field along the c−axis. Alternations of plateaus and steps suggest a "macroscopic quantization" of the longitudinal magnetization component. This in fact simply reminiscent of the quantization of S_z of individual molecules + tunneling in the presence of a complex environment.



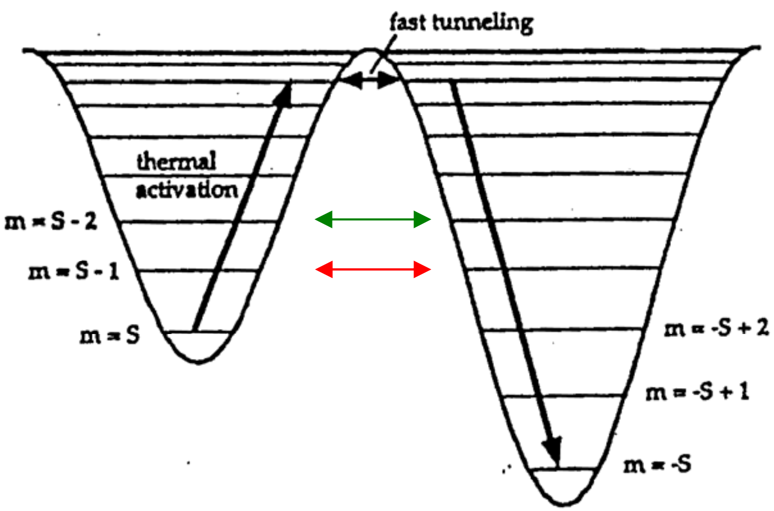
Quantum tunneling
+
Thermal effects

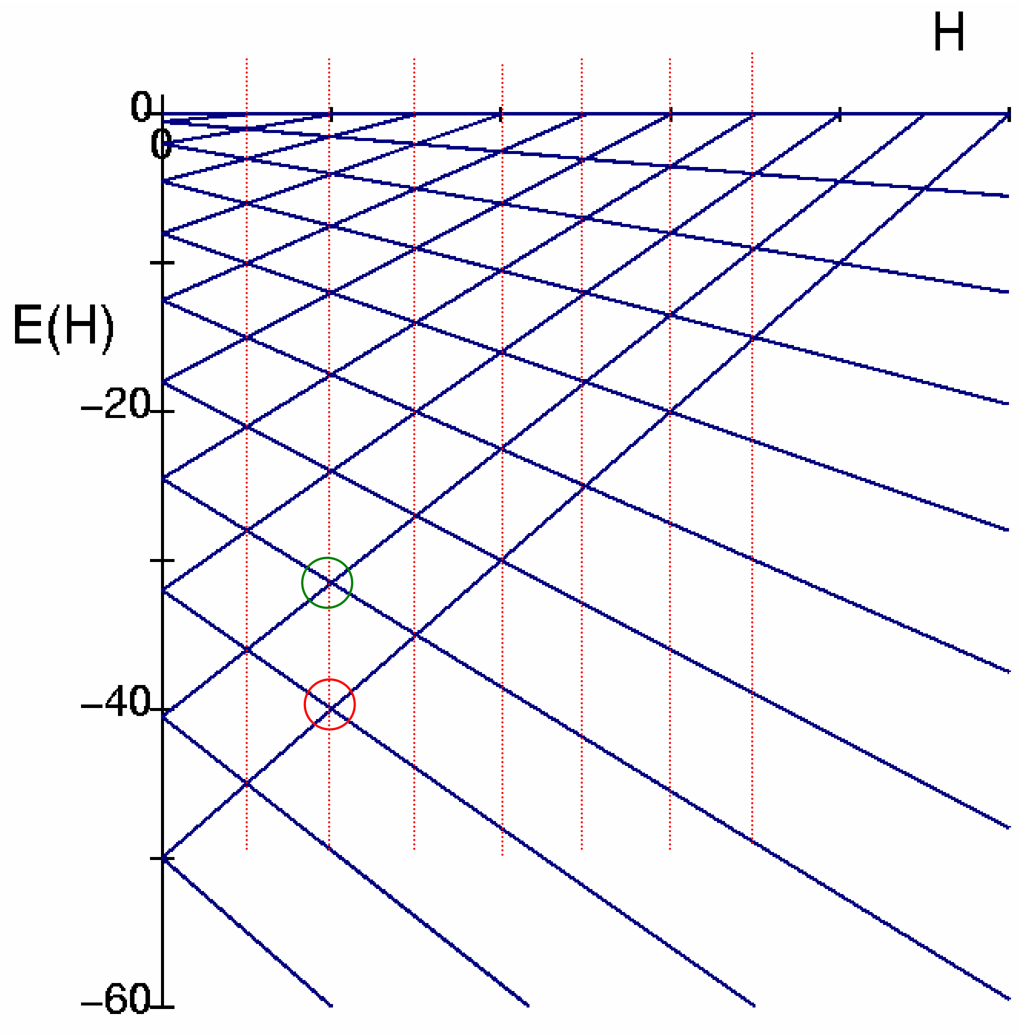


L. Thomas, et al.
Nature 383 (1996) 167.

Resonant tunneling

Resonance tunneling



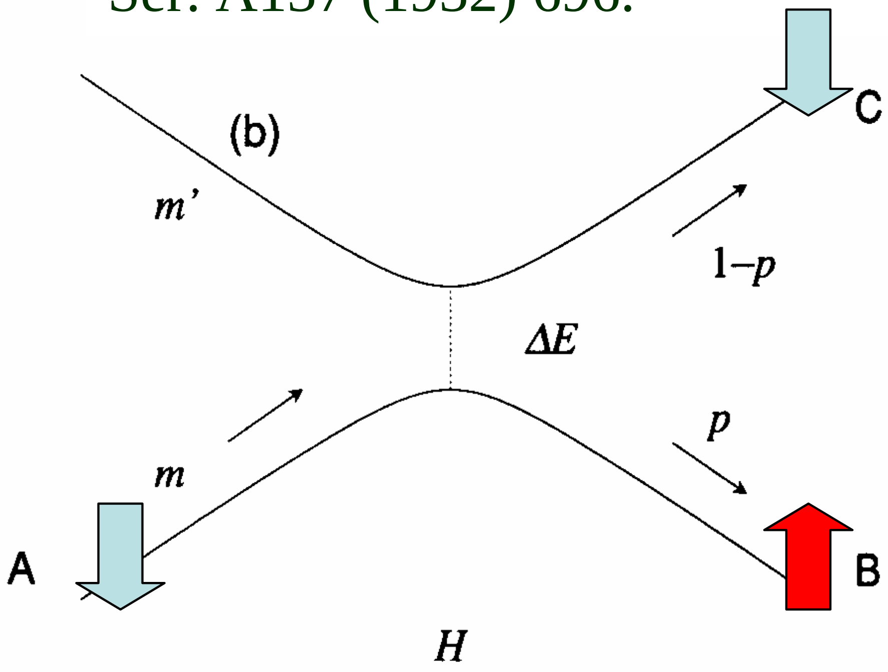


Control of quantum states in Discrete energy structure

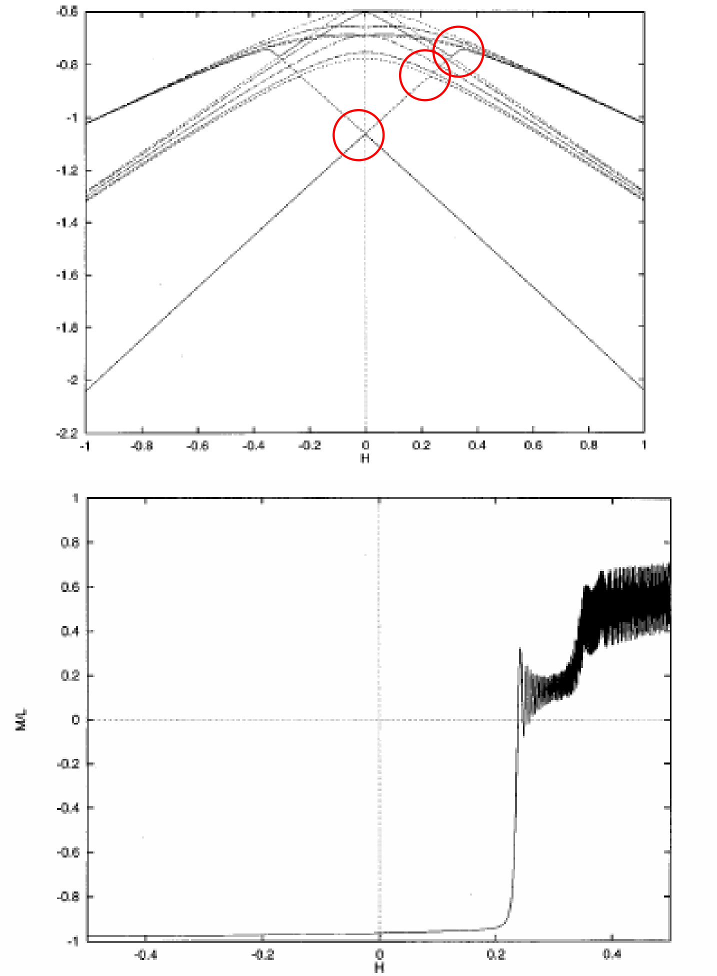
(Non)-adiabatic transition

Landau-Zener-Stueckelberg Mechanism

C. Zener, Proc. R. Soc. (London) Ser. A137 (1932) 696.

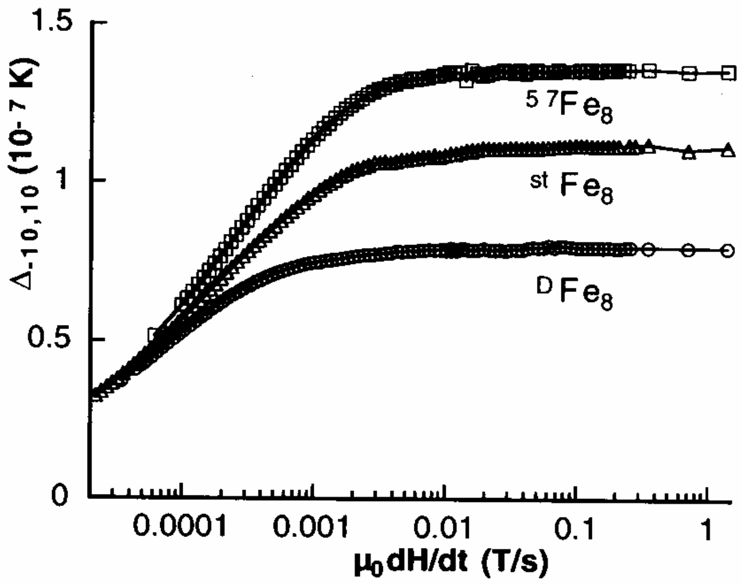


$$p = 1 - \exp\left(-\frac{\pi (\Delta E)^2}{2\left| M_{\rm in} - M_{\rm out} \right| v} \right)$$



SM, JPSJ 64(1995) 3207, 65(1996) 2734.
H. De Raedt et al, PRB56 (1997) 2734

Sweeping velocity dependence

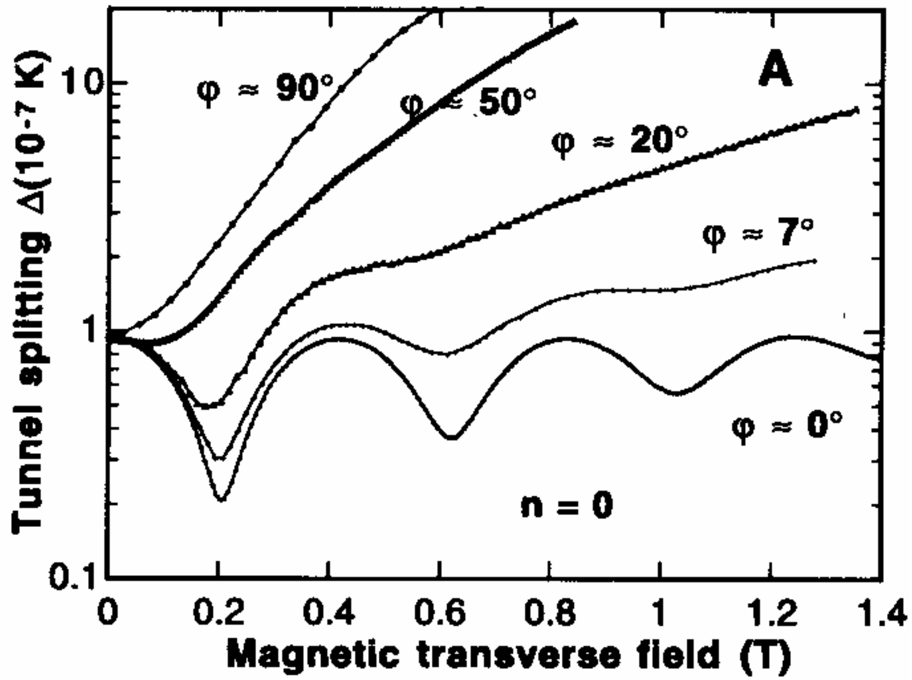


W. Wernsdorfer et al. EPL 50 (2000) 552
JPSJ 69 Suppl. 375.

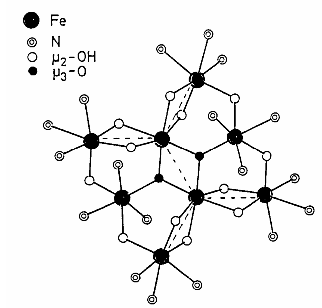
Quantum interference

Berry phase

W.Wernsdorfer & R. Sessoli:
Science 284 (1999) 133



NMR (H) measurement on Fe8 Effect on the resonant tunneling



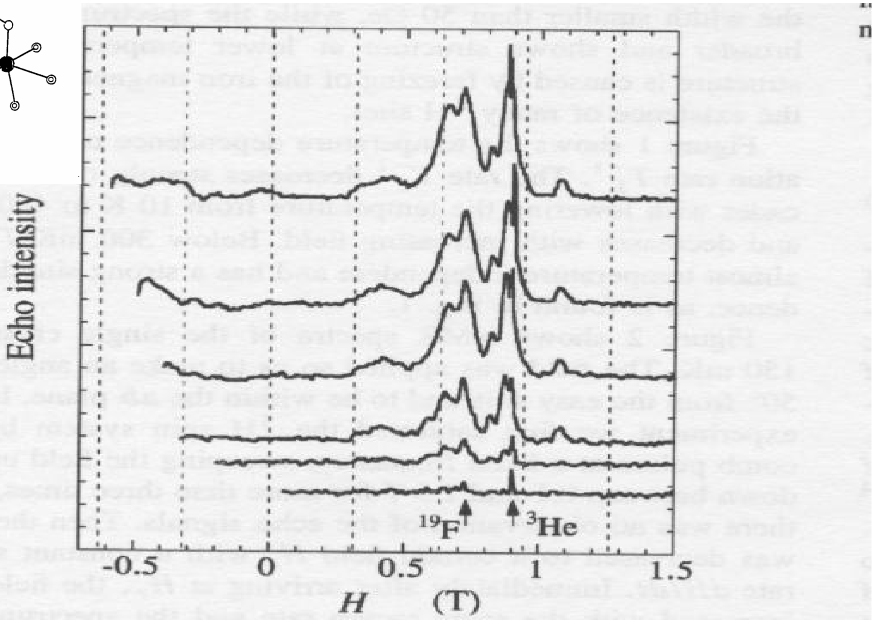
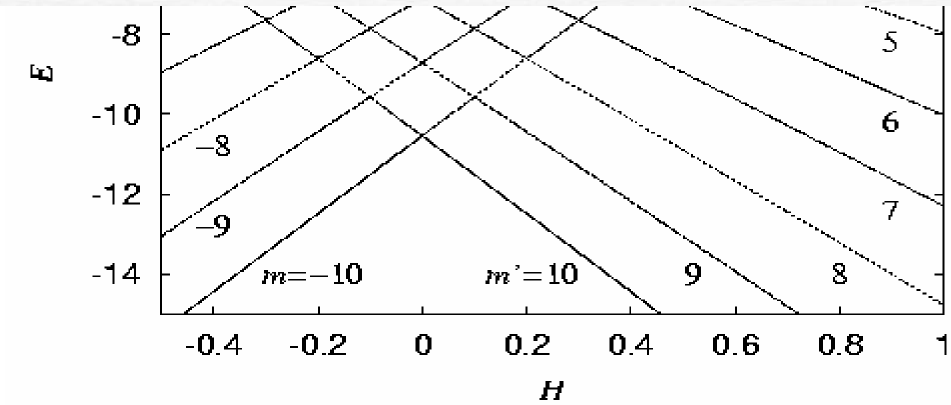
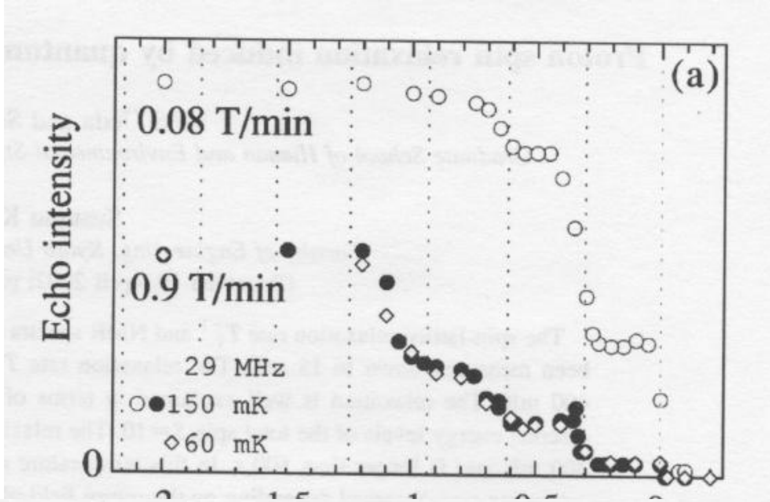
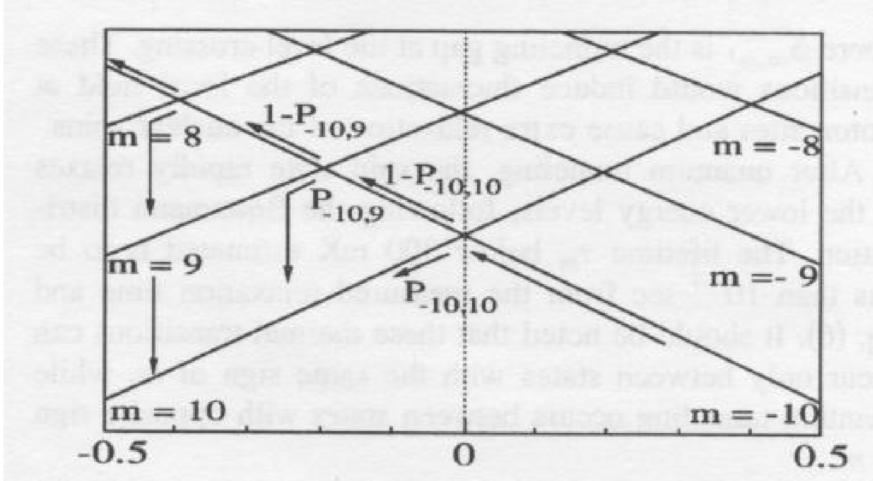


FIG. 2. NMR spectra of single crystal Fe8, which were taken with increasing the field from H, after the saturation. $T=150$ mK, $f=29$ MHz, $dH/dt=0.9$ T/min, and $\theta=50°$. Broken lines show the level crossing fields.







$$p = 1 - \exp\left(-\frac{\pi(\Delta E)^2}{2\left|M_{in} - M_{out}\right| v}\right)$$

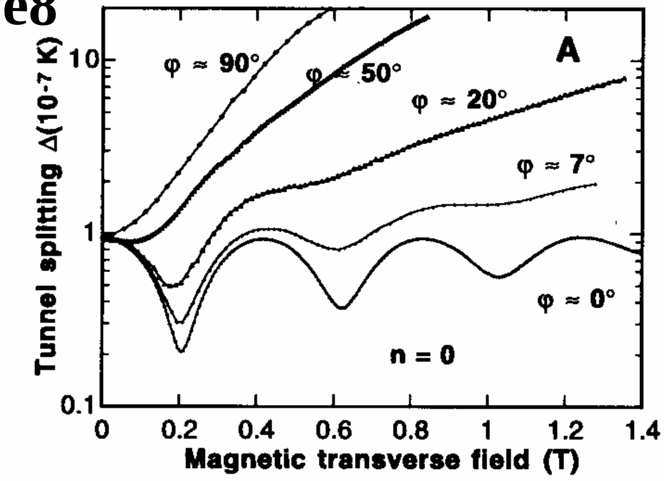
$$\Delta_{-10,10} = 3.52\times10^{-7}\,\mathrm{K}$$

$$\Delta_{-10,9} = 9.66\times10^{-7}\,\mathrm{K}$$

M. Ueda, S. Maegawa and S. Kitagawa: Phys. Rev. B66 (2002) 073309

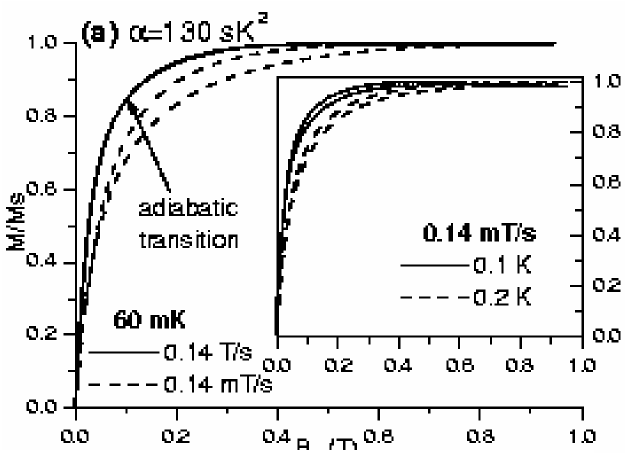
Landau-Zener transitions in magnetization process

Fe8



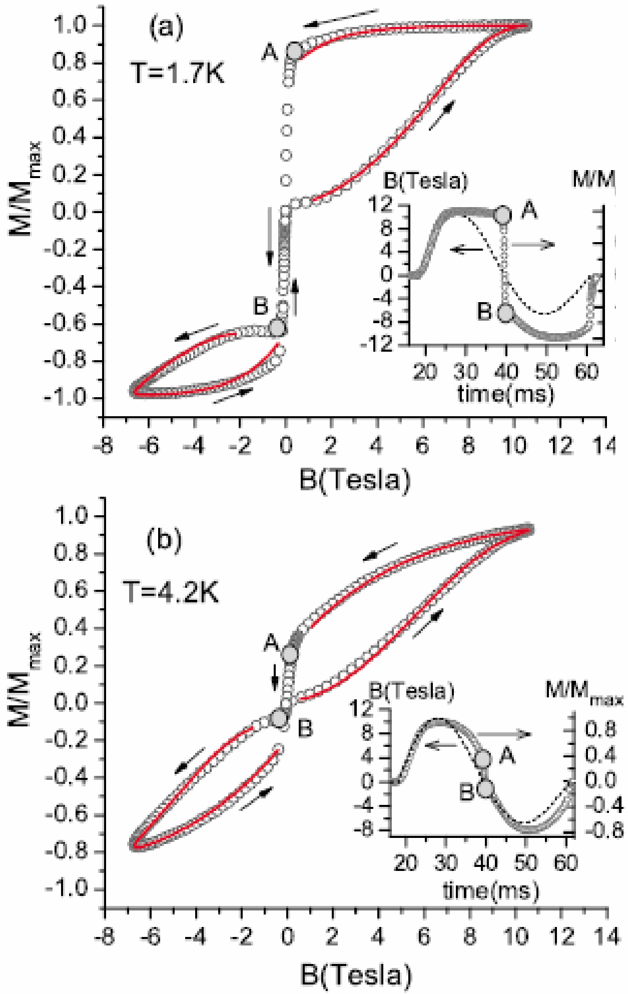
W.Wernsdorfer & R. Sessoli: Science 284 (1999) 133

V15



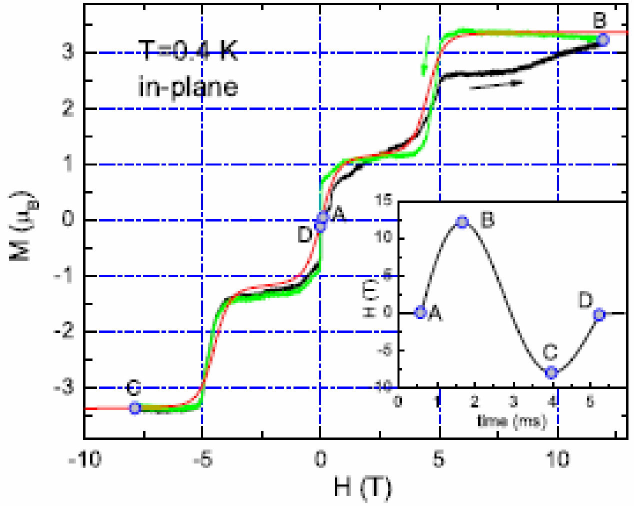
I. Chiorescu, et al Phys. Rev. Lett. 84 (2000) 3454.

V6



I. Rousouchazakis, et al. PRL 94 (2005) 147204

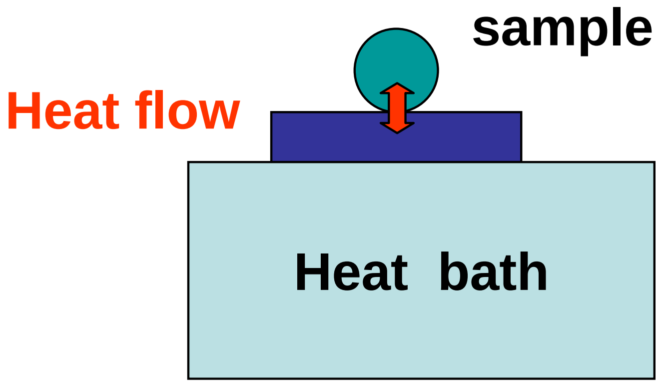
Cu3

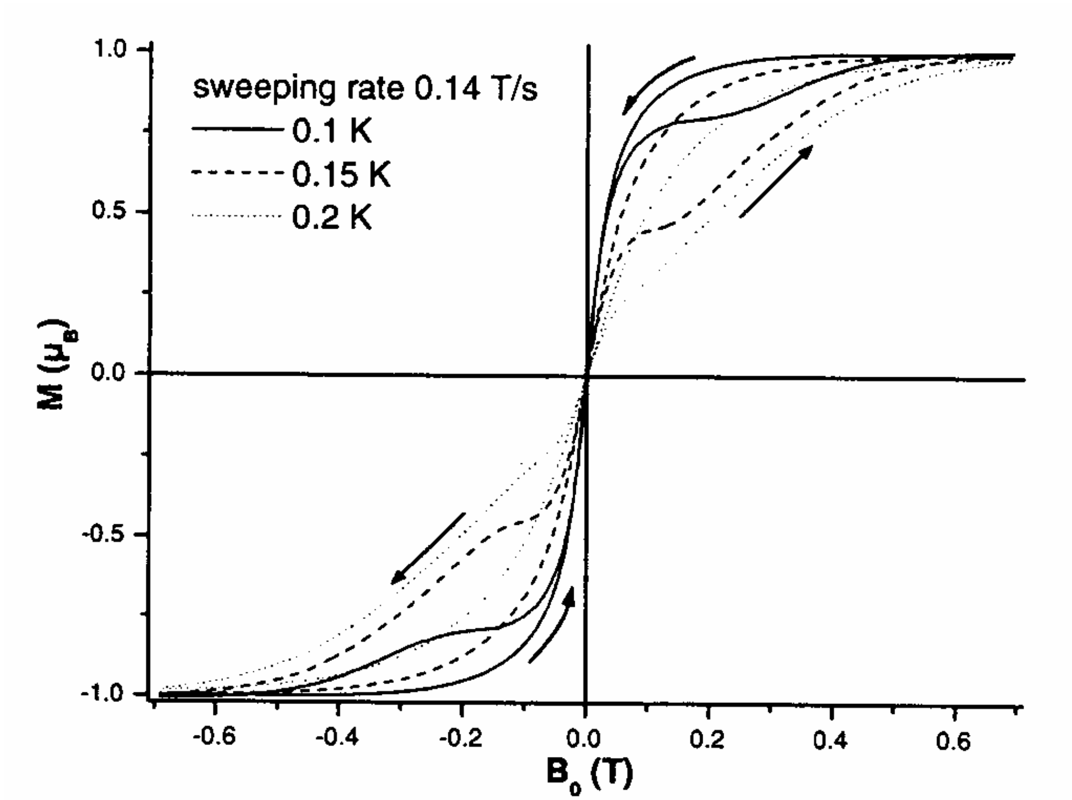


K.Y. Choi, et al. PRL 96 (2006) 107202

Phonon Bottleneck phenomena in V15

Plateau induced by thermal effect





Chiorescu, W. Wernsdorfer,
A. Mueller, H. Boegge, B. Barbara,
Phys. Rev. Lett. 84 (2000) 3454.

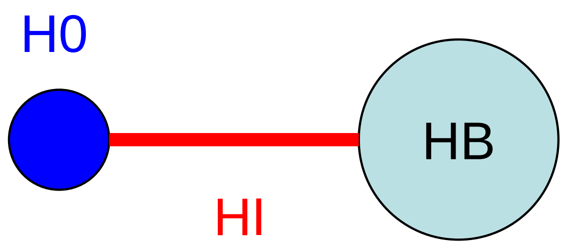
Quantum Master Equation

$$\frac{\partial}{\partial t}\rho = iL\rho = \frac{1}{i\eta}\left[H_0 + H_\mathrm{I} + H_\mathrm{B}, \rho\right]$$

$$H = H_0 + H_\mathrm{I} + H_\mathrm{B},$$

$$H_\mathrm{I} = \sum_k \lambda_k \left(b_k^+ + b_k\right)X,$$

$$H_\mathrm{B} = \sum_k \omega_\kappa b_k^+ b_k$$



Reduction of environment

$$\sigma = \mathrm{p}\rho = \rho_\mathrm{eq}\mathrm{Tr_B}\rho, \qquad \rho_\mathrm{eq} = \mathrm{e}^{-\beta H_0} / \mathrm{Tr_B}\mathrm{e}^{-\beta H_0}$$

$$\frac{\partial}{\partial t}\sigma = i\mathrm{p}L\sigma + \mathrm{p}iL\int_0^t \mathrm{e}^{(t-s)(1-\mathrm{p})\mathrm{iL}}(1-\mathrm{p})iL\mathrm{p}\rho(t)ds \quad + \quad \mathrm{p}iL\mathrm{e}^{(t-s)(1-\mathrm{p})\mathrm{iL}}(1-\mathrm{p})\rho(0)$$

e.g. Photon dissipation and pumping :

(SM., H. Ezaki, and E. Hanamura PRA 57 (1998) 2046)

$$\frac{\partial\sigma}{\partial t} = \frac{1}{i\eta}\left[H_0, \sigma\right] - \kappa\left(b^+ b\sigma - 2b\sigma b^+ + \sigma b^+ b\right)$$

Lindblad form ➔ Stochastic Schrodinger Equation (antibunching, squeezing photo emission)

General formulation

$$\frac{d\rho}{dt} = \frac{1}{i\eta}[H,\rho]$$

$$-\frac{\lambda^2}{\eta^2}\int_0^t ds \int_{-\infty}^{\infty} d\omega e^{i\omega t}\Phi(\omega)\{XX(-s)\rho(t) - e^{\beta\eta\omega}X\rho(t)X(-s)$$

$$+ e^{\beta\eta\omega}\rho(t)X(-s)X - X(-s)\rho(t)X \}$$

time correlation function of the reservoie's operators $\Phi(t)$

$$\Phi(\omega) = \int_{-\infty}^{\infty} dt e^{-i\omega t}\Phi(t) = \eta\gamma(\omega)^2 \frac{D(\omega) - D(-\omega)}{e^{\beta\eta\omega} - 1}$$

$I(\omega) = \gamma(\omega)^2 D(\omega) = I_0\omega^\alpha \quad \omega > 0:$ the spectral density

$$\langle k|R|m\rangle = \zeta\left(\frac{E_k - E_m}{\eta}\right) n_\beta(E_k - E_m)\langle k|X|m\rangle,$$

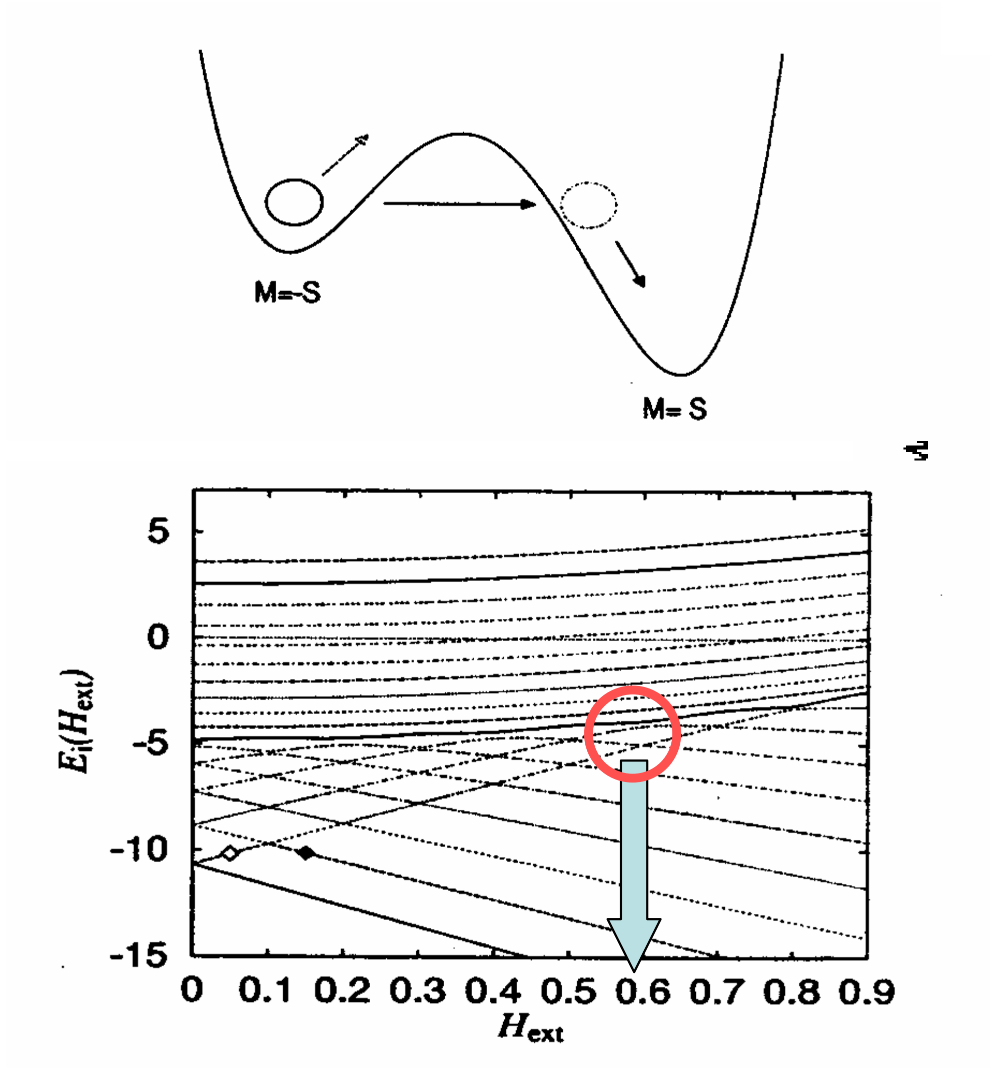
$$\zeta(\omega) = I(\omega) - I(-\omega)$$

$$\frac{d\rho}{dt} = -i[H,\rho] - \lambda\left([X, R\rho] + [X, R\rho]^{+}\right)$$

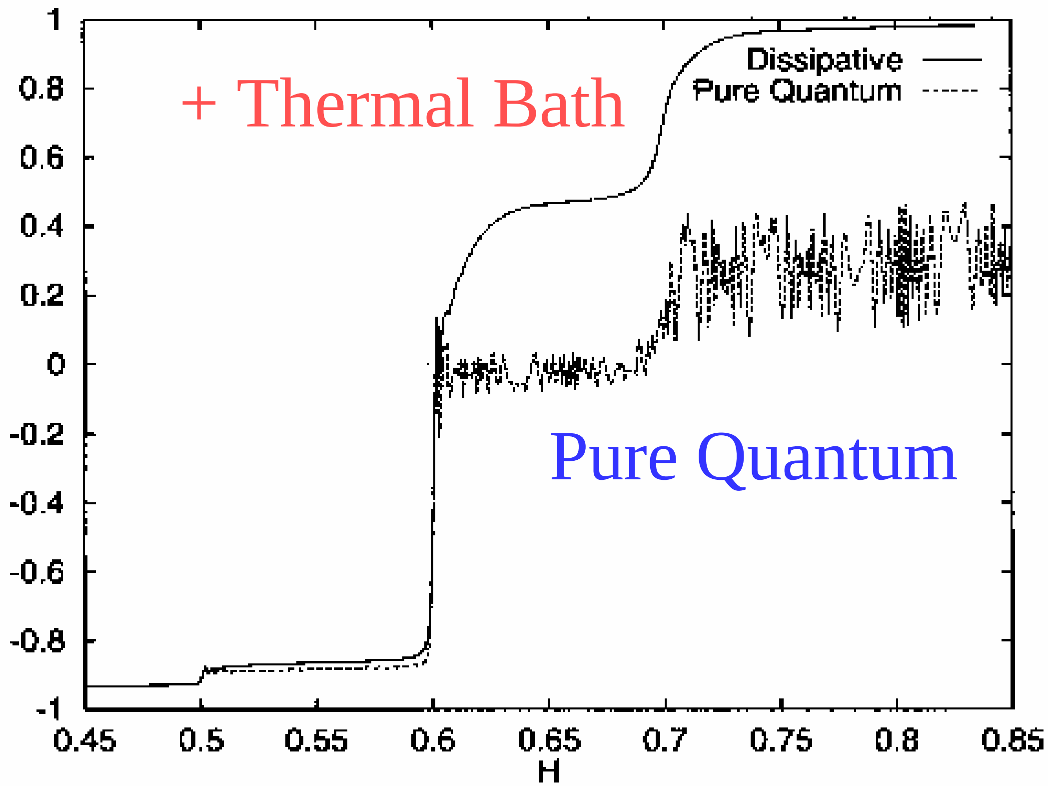
No feedback effects

K. Saito, S. Takesue and SM. Phys. Rev. B61 (2000) 2397

Adiabatic transition and Relaxation



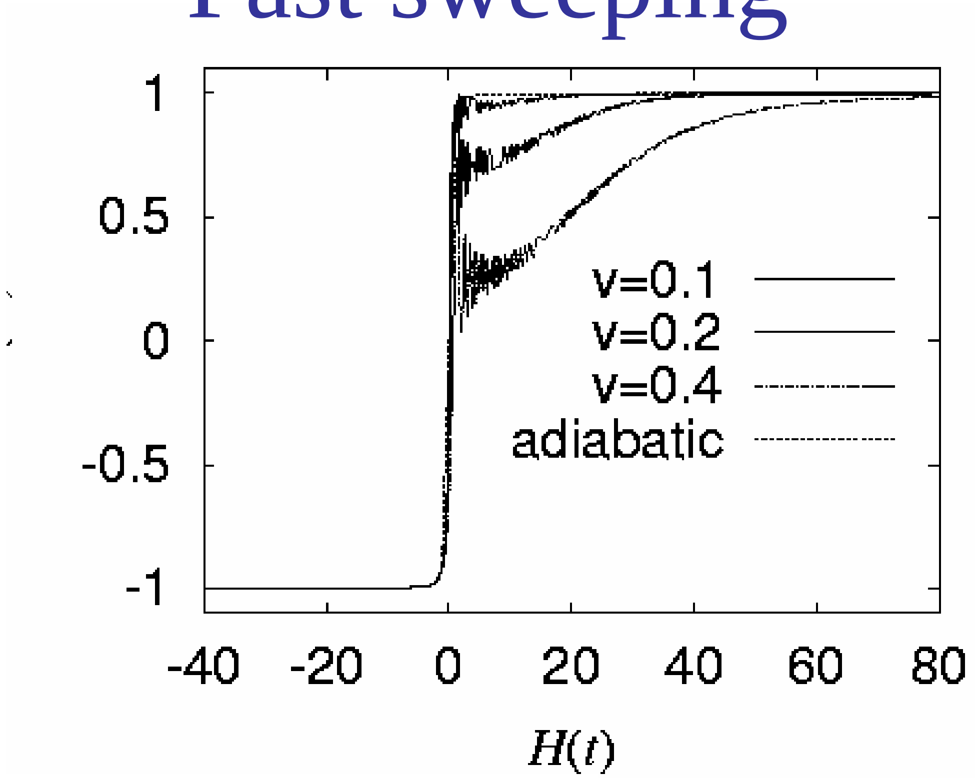
$T \to 0$



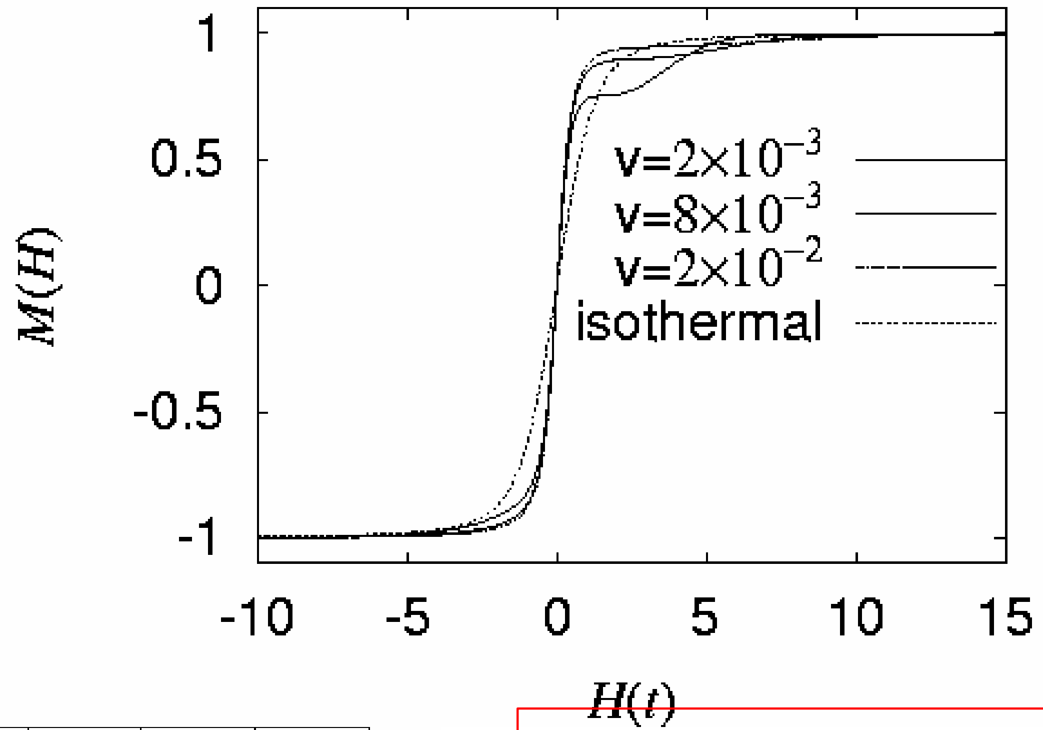
K. Saito, SM, H.de Raedt,
Phys. Rev. B60 (1999) 14553

Field sweeping with thermal bath

Fast sweeping

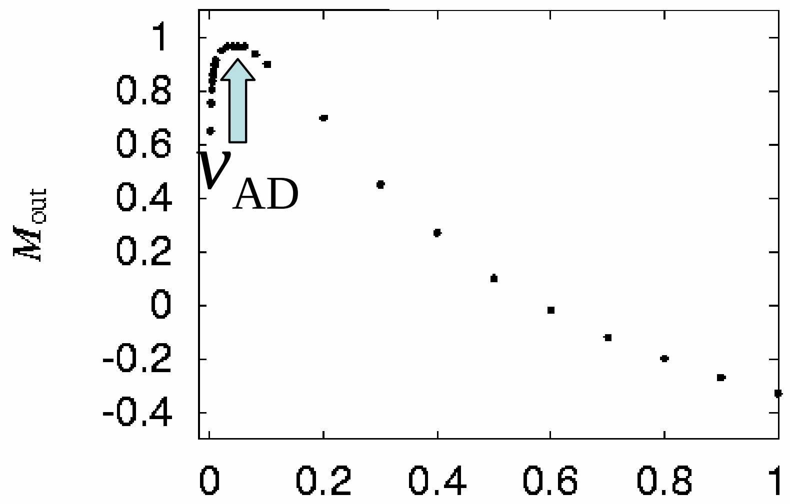


Slow sweeping



$v_{AD} < v$

LZS

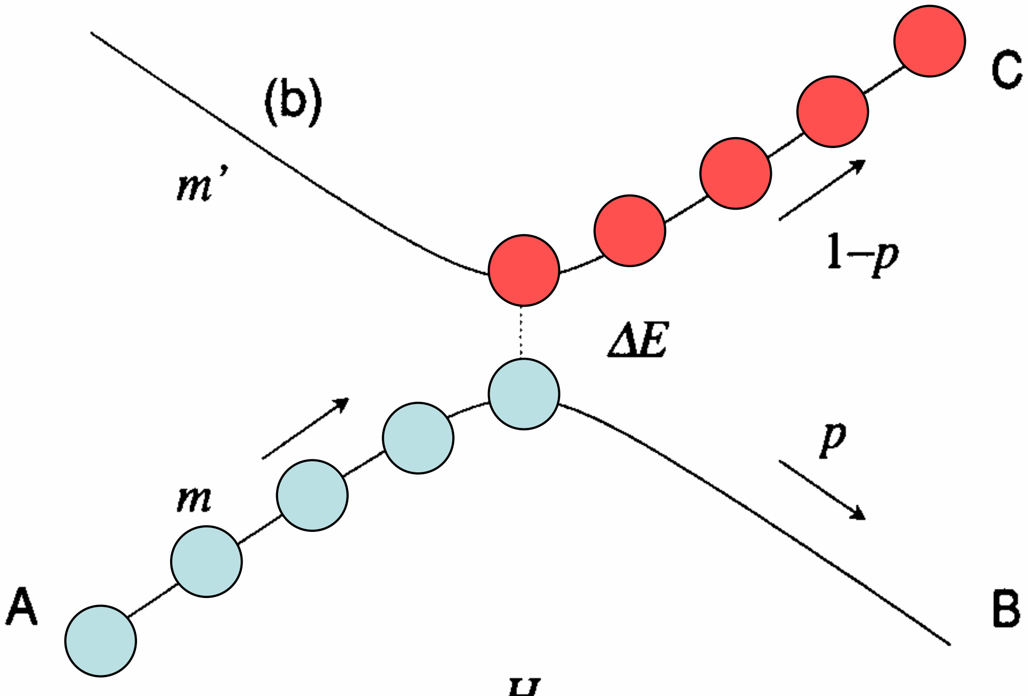


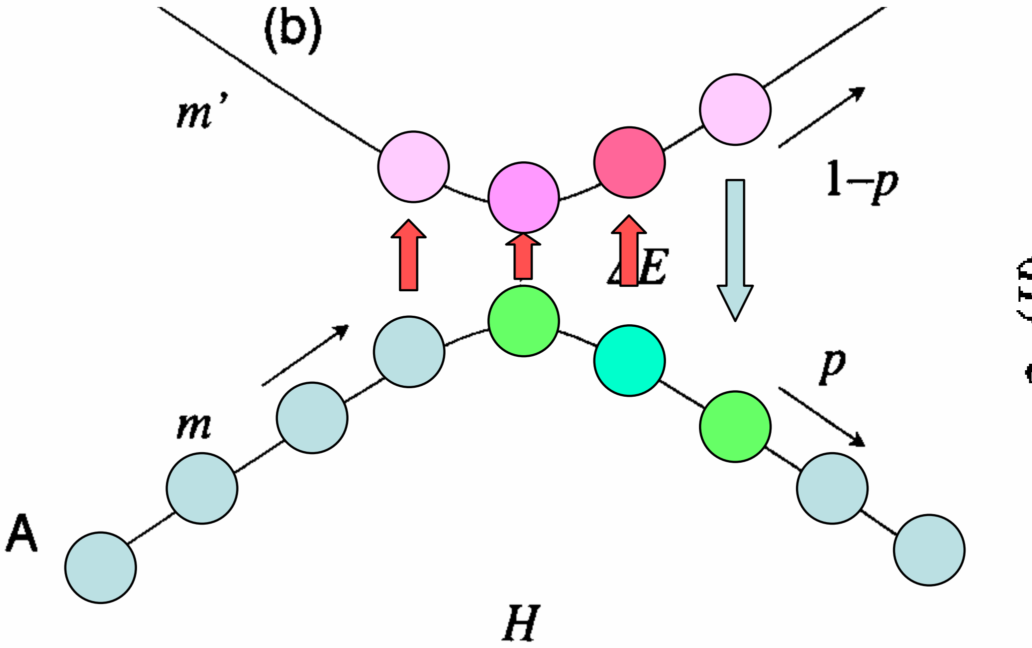
$v_{TH} < v < v_{AD}$

Magnetic Foehn Effect

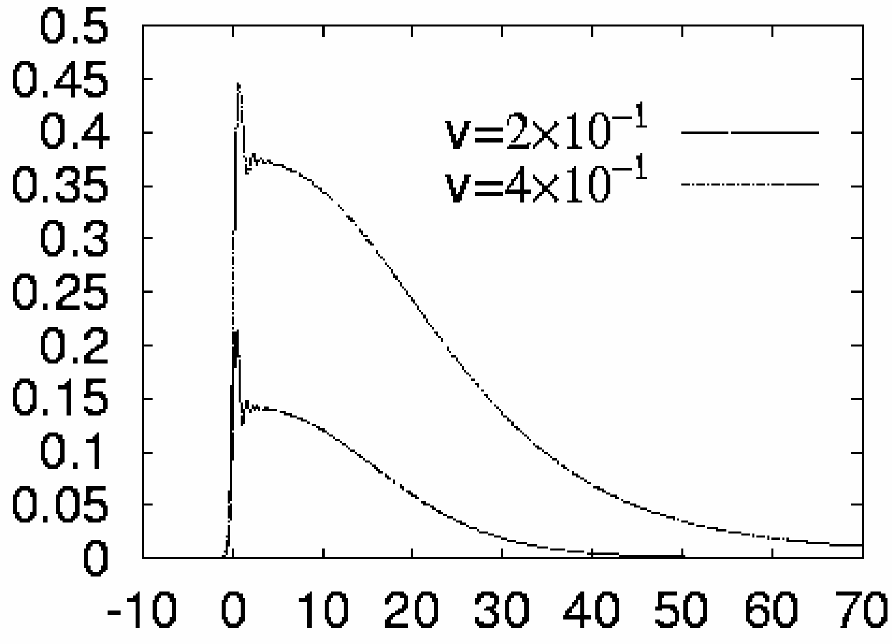
K. Saito & SM. JPSJ (2001) 3385.

Nonadiabatic Tr. & Heat-inflow

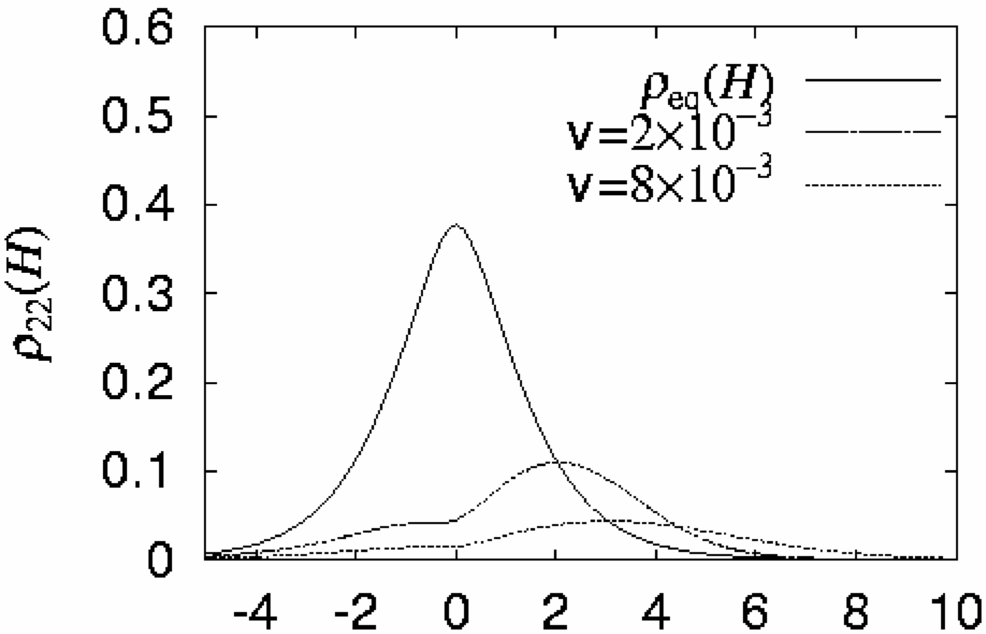




LZ transition



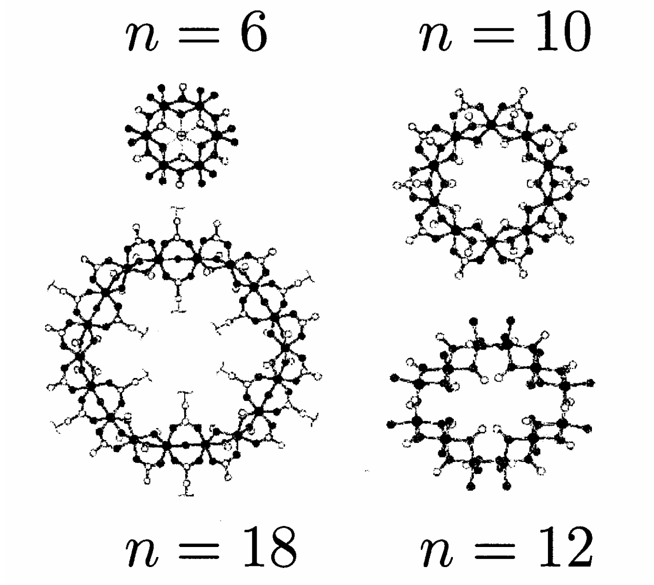
Magnetic Foehn Effect

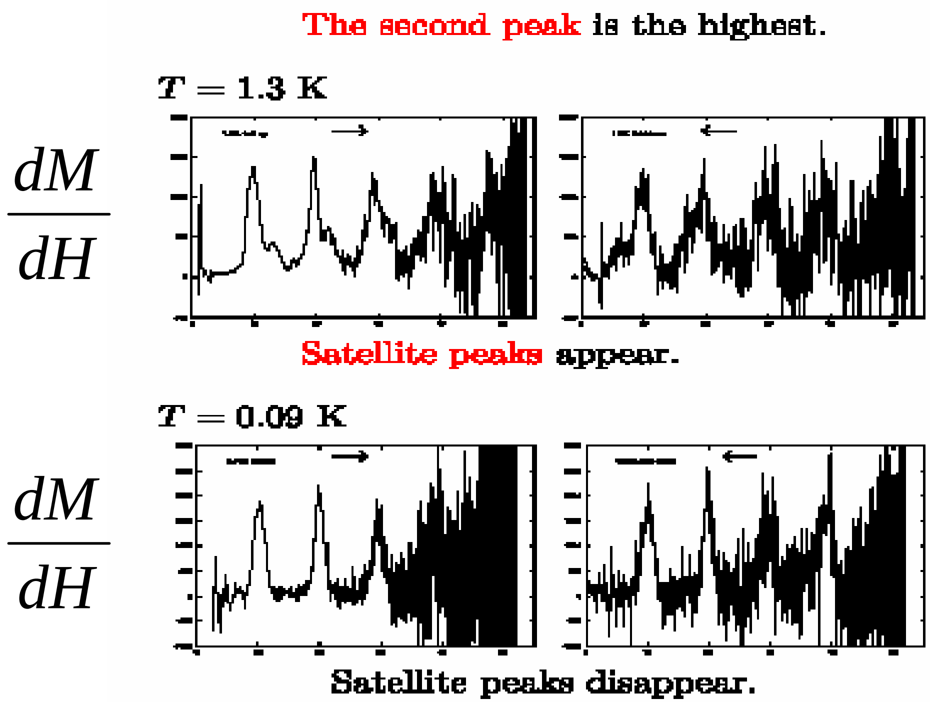


Fe2

Fe-rings

Y. Shapira, et al PRB59 (1999) 1046

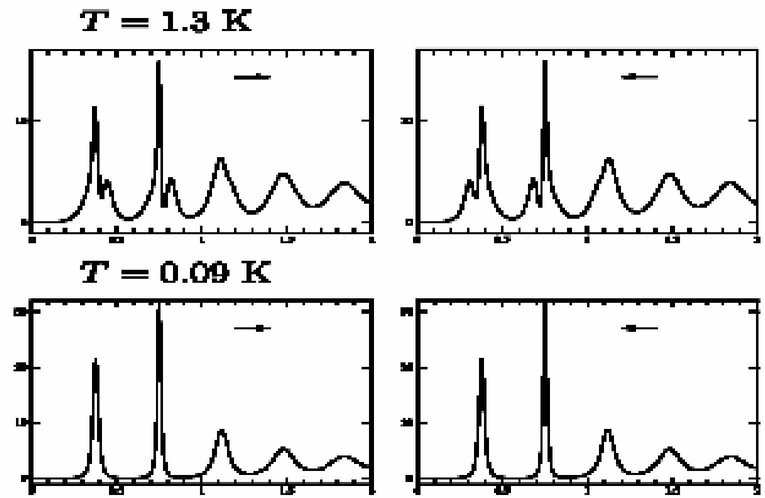




Y. Ajiro & Y. Inagaki

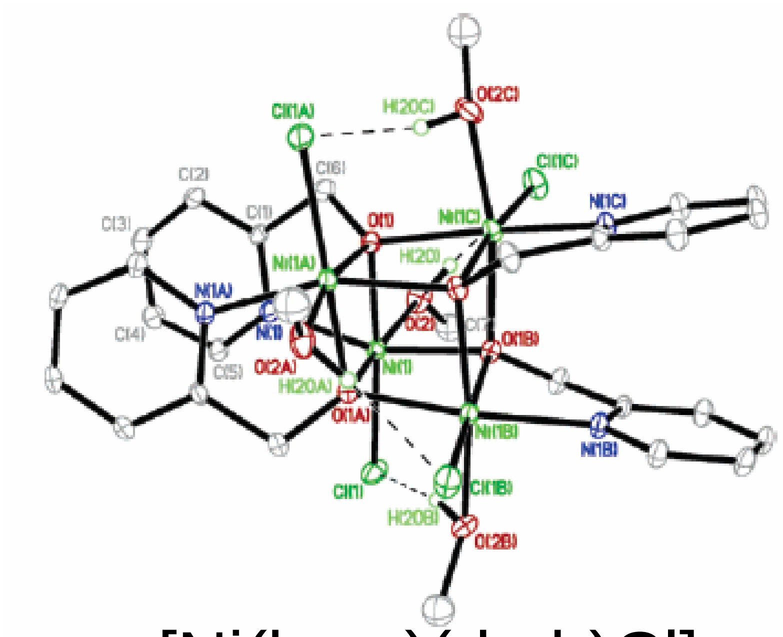
Y. Narumi & K. Kindo

H. Nakano & SM, JPSJ 70(2001) 2151

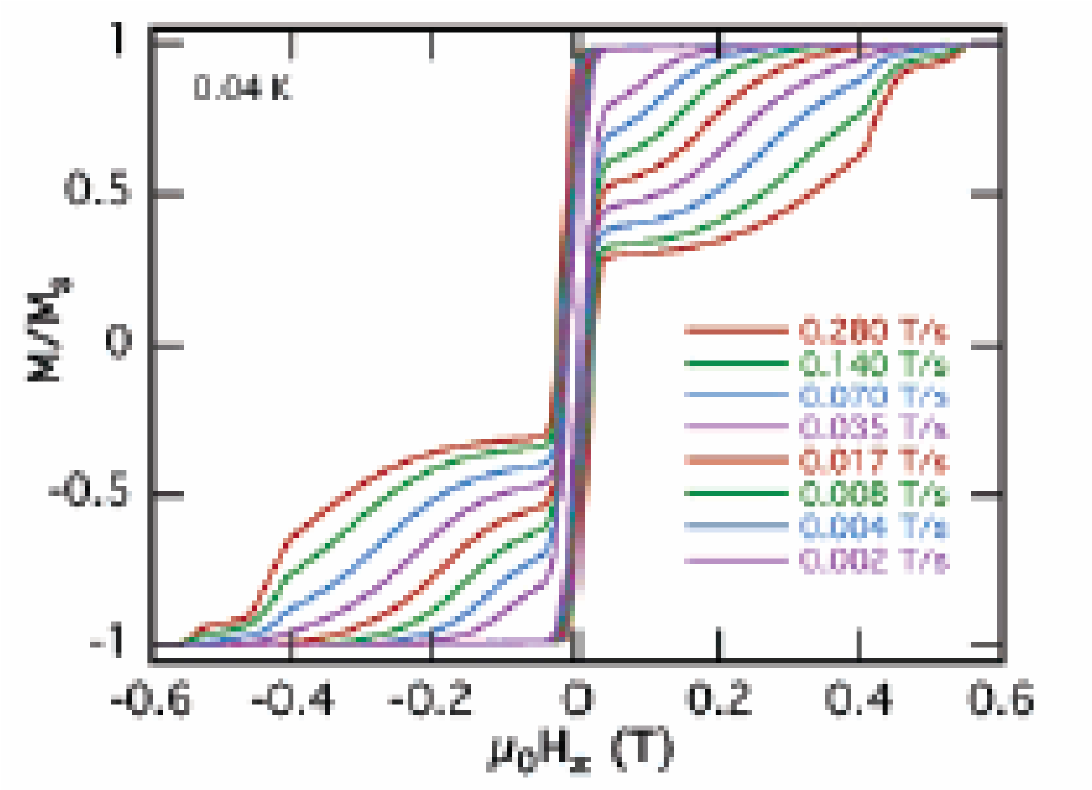


Fast Magnetization Tunneling in Tetranicke(II) SMM

En-Che Yang,et al: Inorg. Chem. 45 (2006) 529



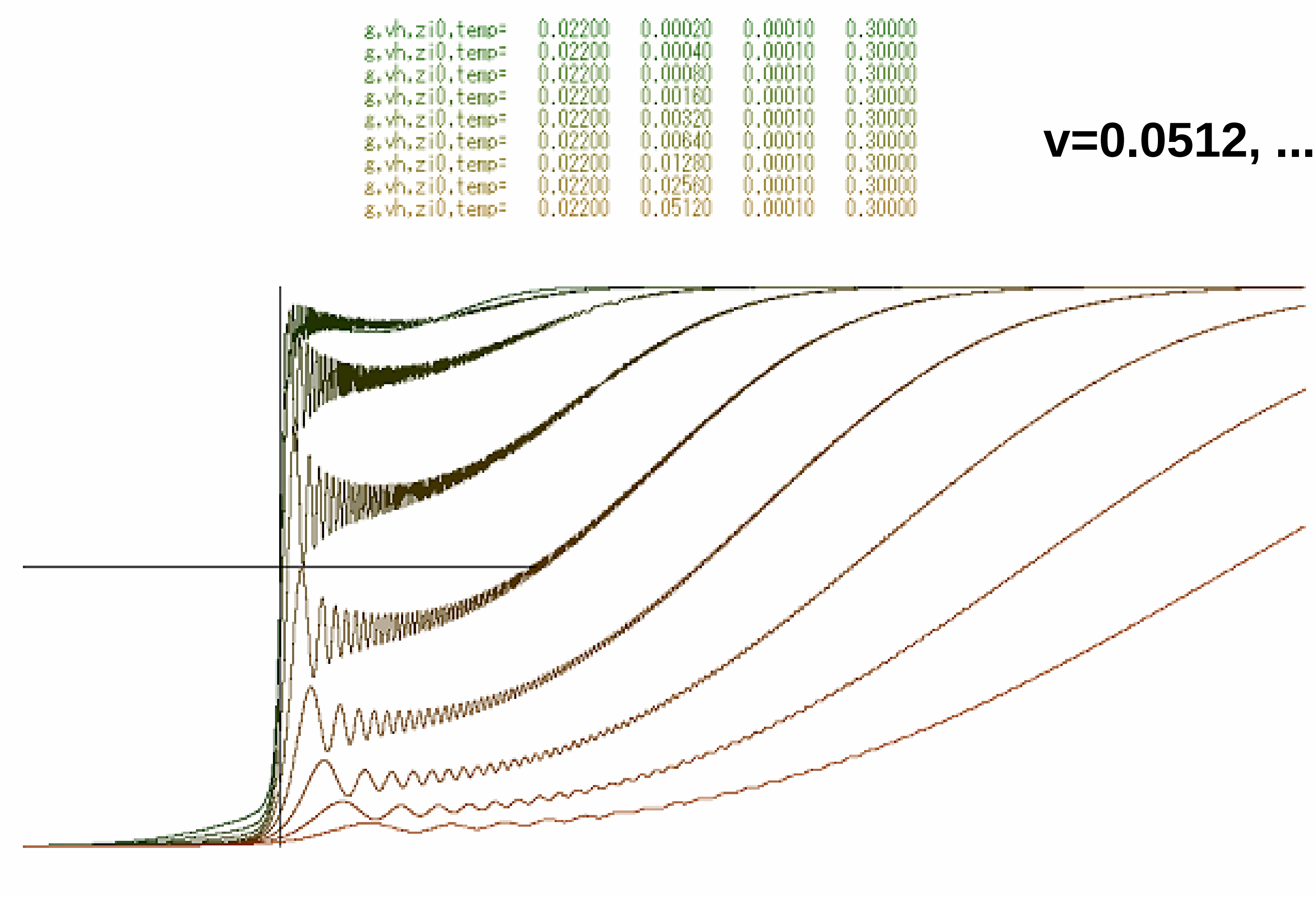
[Ni(hmp)(dmb)Cl]4



V=0.002, ... , 0.28T/s

LZ transition + Thermal relaxation + MFE

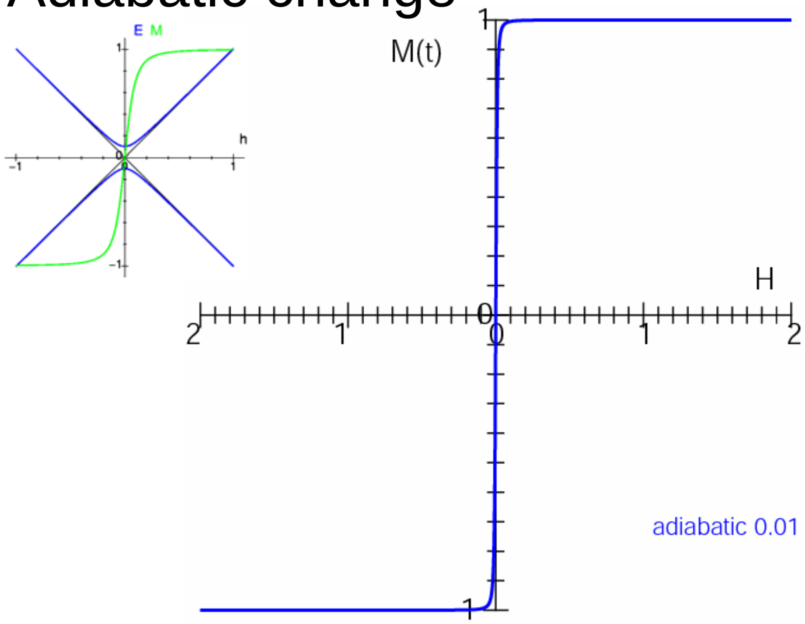
$$\frac{d\rho}{dt} = -i[H, \rho] - z\left([X, R\rho] + [X, R\rho]^{+}\right)$$



v=0.0512, ..., 0.0002

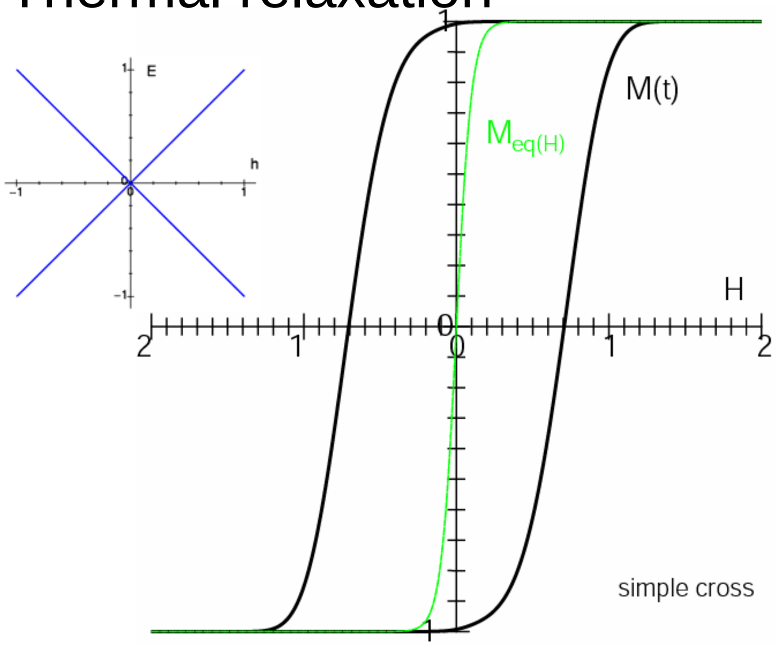
Two different types of sites ?

Adiabatic change

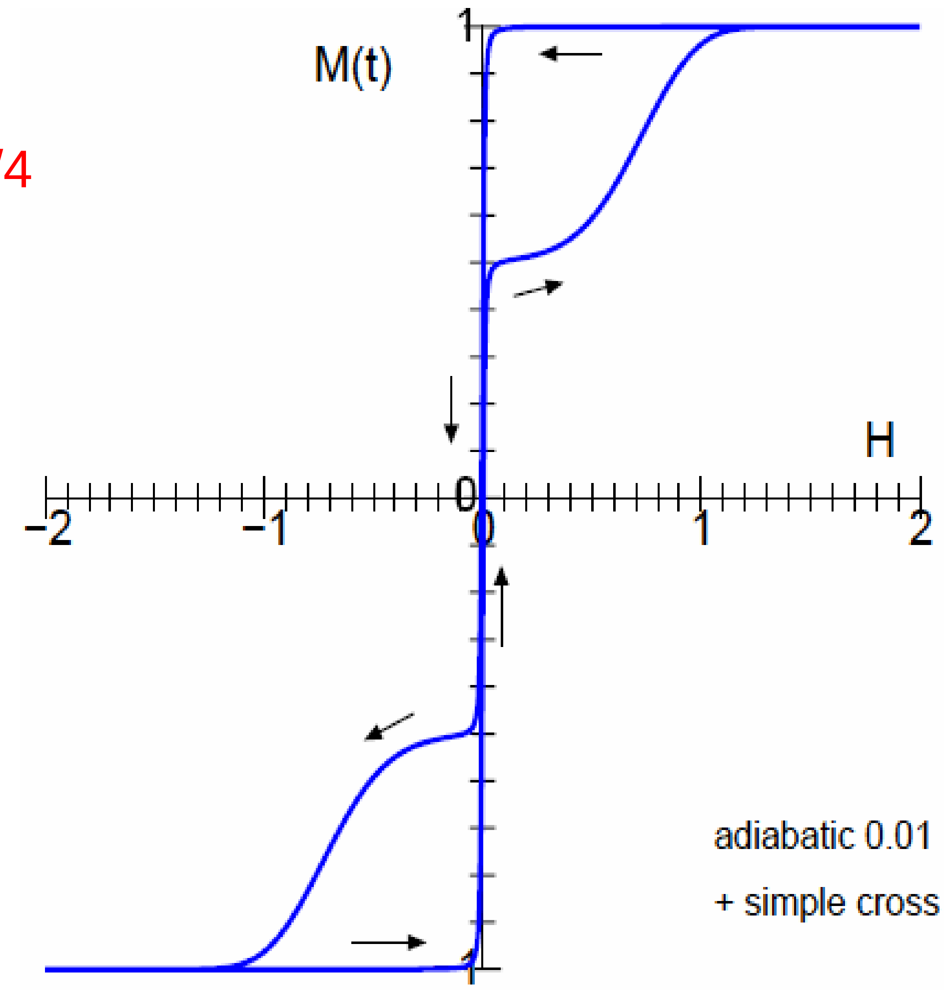


x 3/4

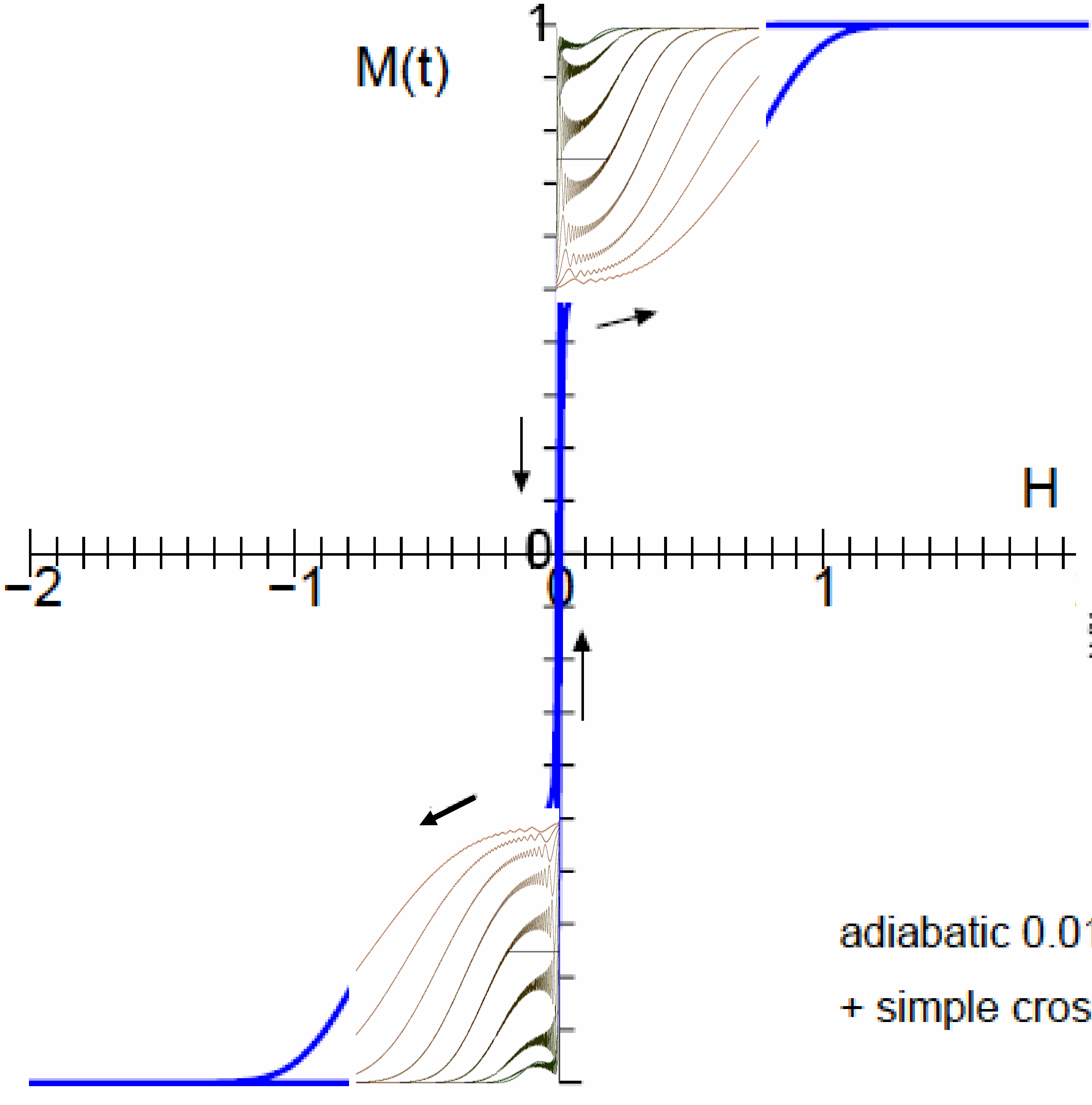
Thermal relaxation

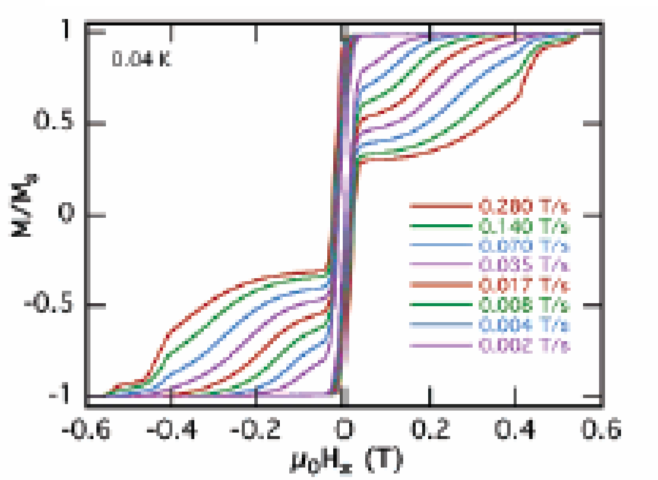


x 1/4



Possible magnetic process



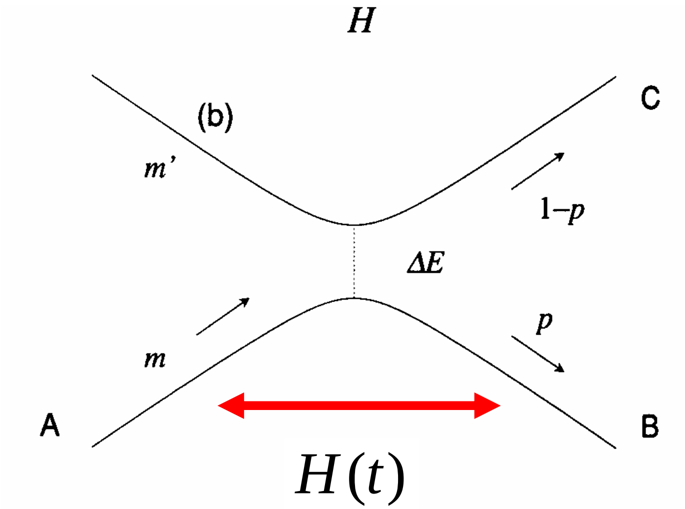


adiabatic 0.01

+ simple cross

Quantum dynamics under an AC field
Non-trivial Resonance

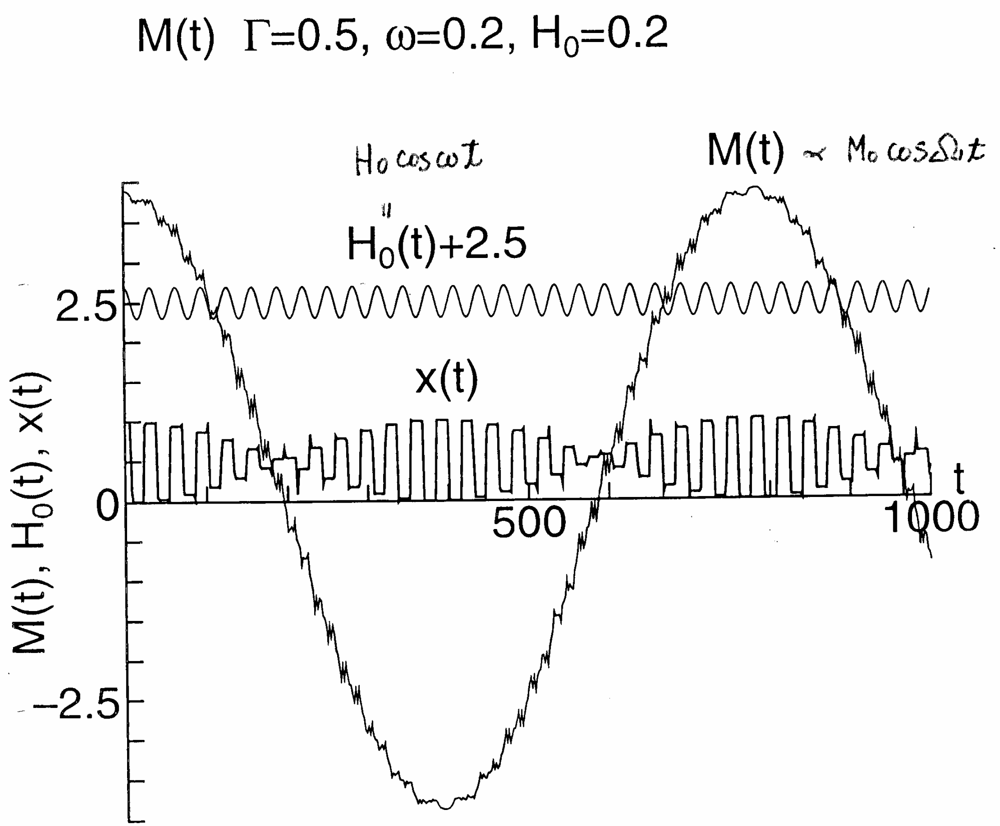
$$H(t) = -h_W \cos(\omega t)\sum_i S_i^z$$



$$M(t) = M_0 \cos(\Omega t + \delta),$$

$$\Omega = \frac{\omega}{\pi}\sqrt{2p(1-\cos\alpha)}$$

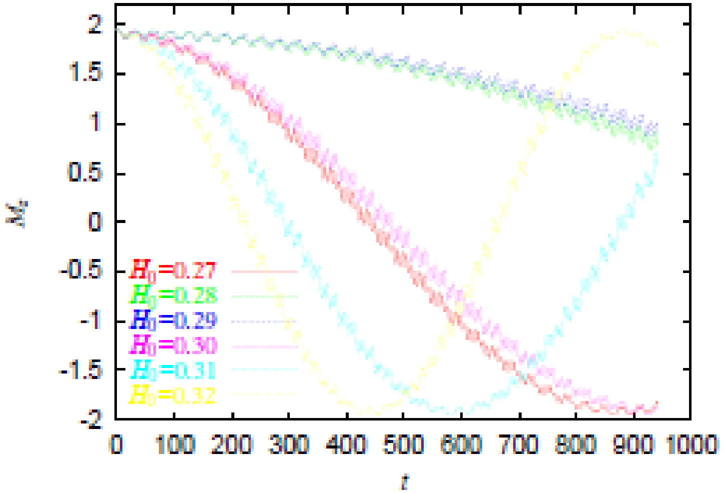
$$p = 1 - \exp\left(-\frac{\pi(\Delta E)^2}{4c\Delta M}\right)$$

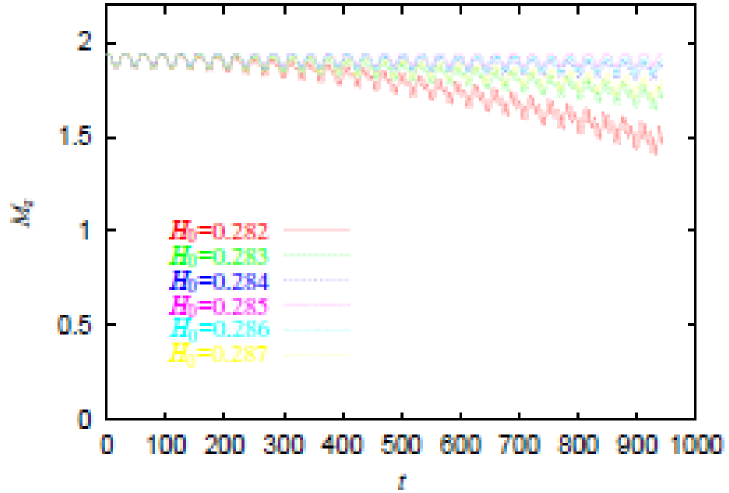


$$T = \begin{pmatrix} t_{11}, & t_{12} \\ t_{21}, & t_{22} \end{pmatrix} = \begin{pmatrix} e^{i\theta}\sqrt{p}, & e^{i\phi}\sqrt{1-p} \\ \sqrt{1-p}, & -e^{i(-\theta+\phi)}\sqrt{p} \end{pmatrix}$$

SM, K. Saito, H. De Daedt,
Phys. Rev. Lett. 80 (1998) 1525.

Amplitude dependence (Coherent destruction of tunneling)

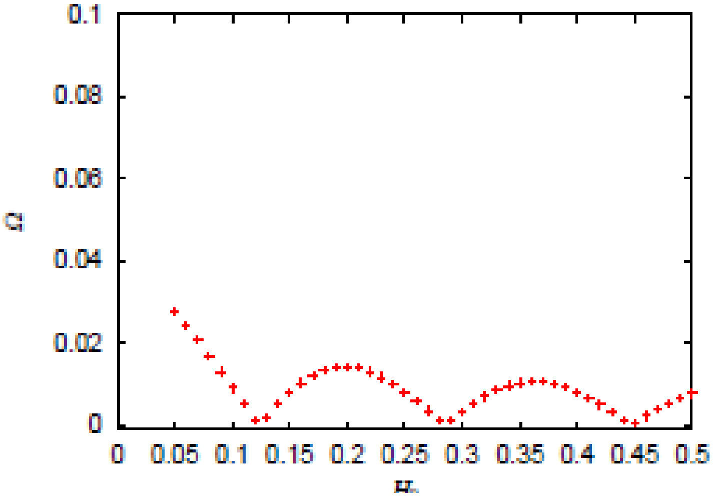




Fitting function of magnetization

$$M_z = A\cos(\Omega t)$$

$\Omega \Rightarrow$



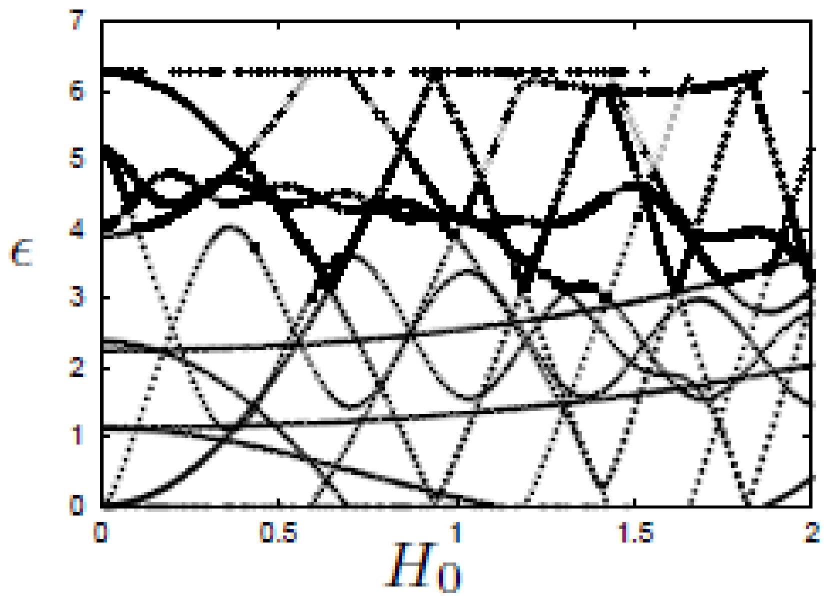
F. Grossman, et al. Phys. Rev. Lett. 67 (1991) 516.

Y. Kayamuma, PRB 47 (1993) 9940.

SM, K. Saito, H. De Daedt, Phys. Rev. Lett. 80 (1998) 1525.

Eigenstates of Floquet operator and Hamiltonian

Floquet energy

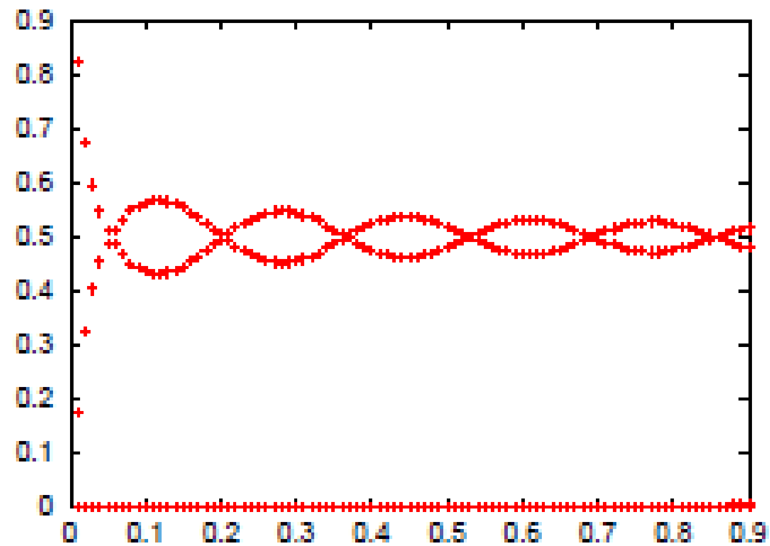


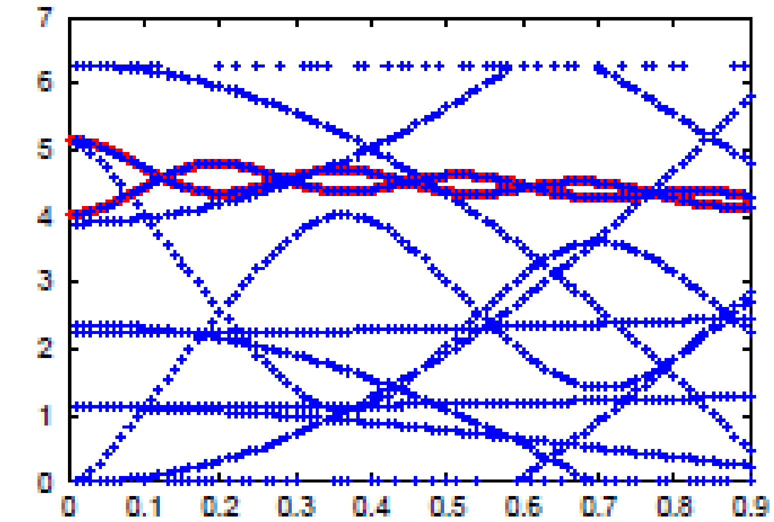
$$F = \mathrm{T}\exp\left(-i\int_0^{2\pi/\omega} H(s)ds\right)$$

$$F\left|\Psi_j(T)\right\rangle = e^{-i\varepsilon_j}\left|\Psi_j(T)\right\rangle$$

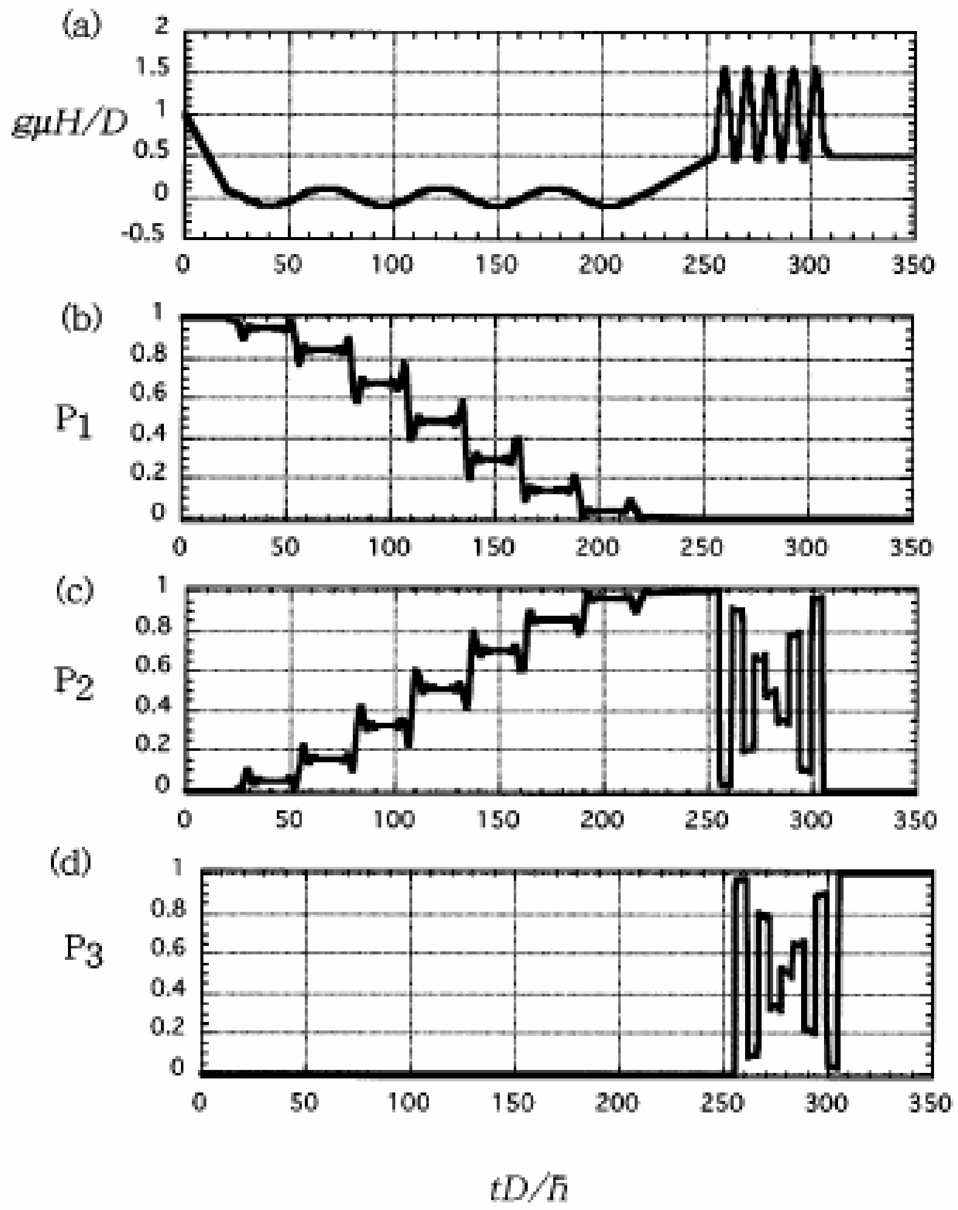
$$H\left|\phi_j\right\rangle = E_j\left|\phi_j\right\rangle$$

Fractions $|\langle\phi_i|\,\Psi(T)\rangle|^2$



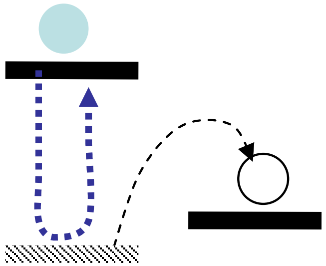


Switching by AC field



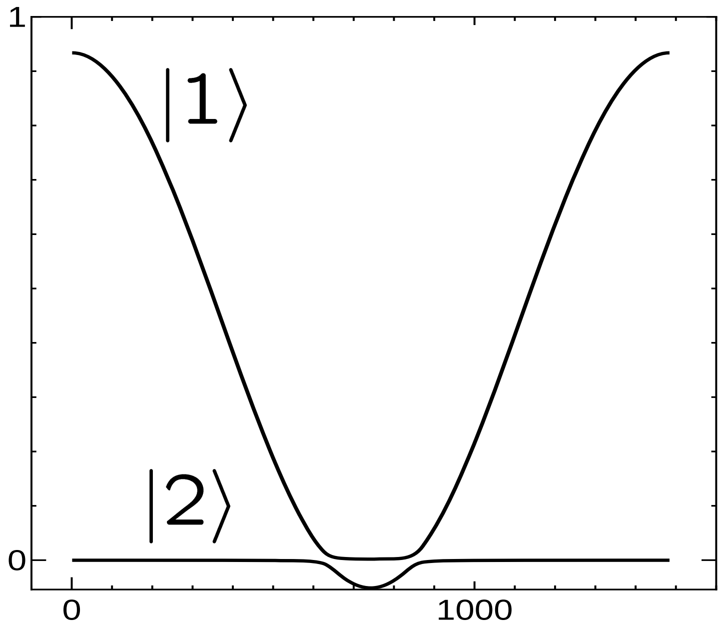
Y.Teranishi and H. Nakamura: PRL81(1998) 2032

With appropriate oscillation,
We may change the state by
a single operation.

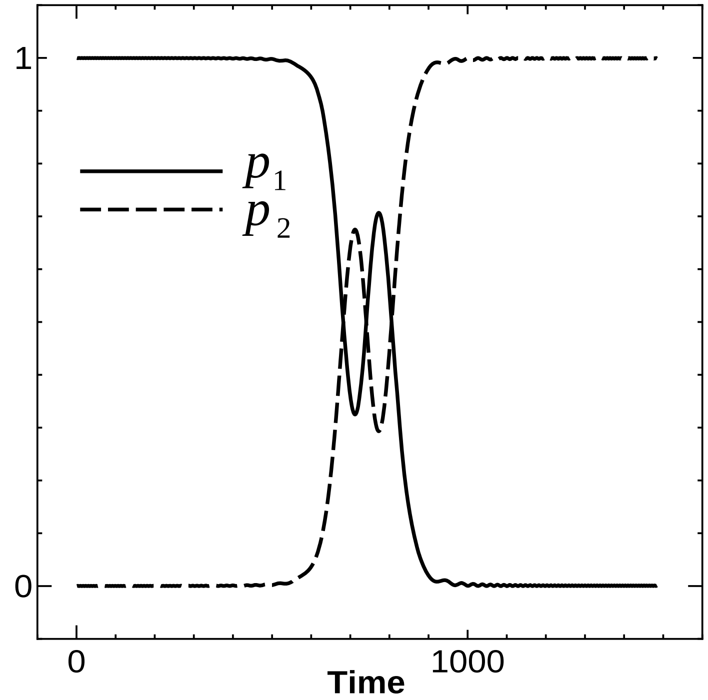


K.Saito and Y. Kayanuma
PRB 70 201304(R) (2004)

Energy level as a function of time



Probability of the Level k P_k

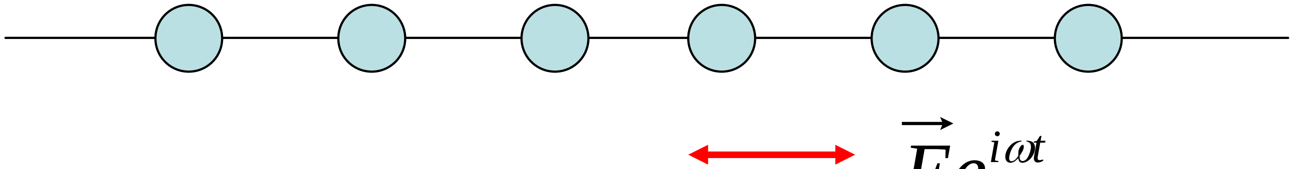


AC field trap by Coherent Destruction of Tunneling (CDT)

$$H = -t\sum_{ij} c_i^+ c_j - Ee^{i\omega t}\sum_i x_i n_i$$

E=0 **diffusion**

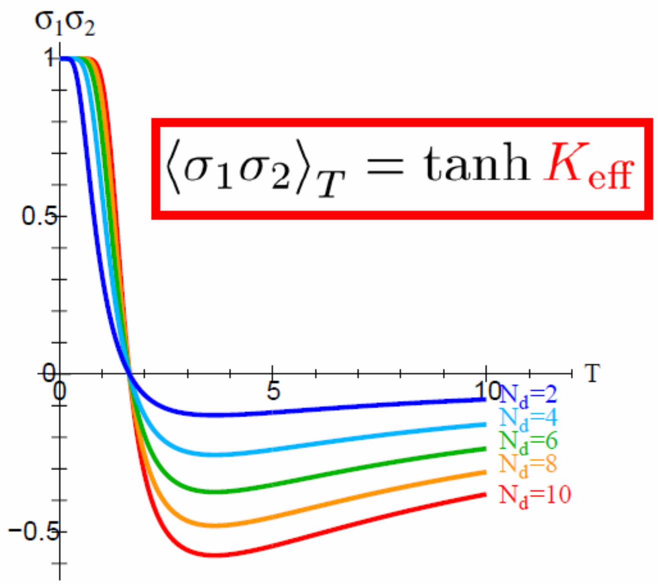
CDT localization



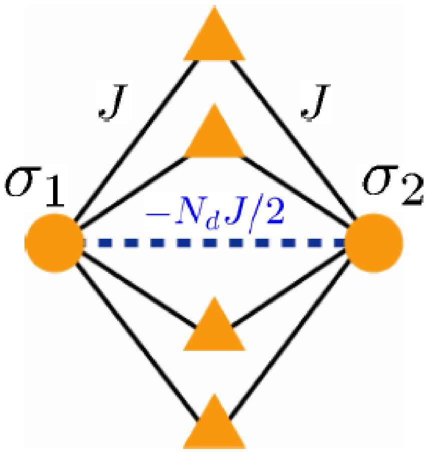
$\vec{E}e^{i\omega t}$

Y. Kayanuma and K. Saito: arXiv:0708.3570

Reentrant behavior in quantum fluctuation



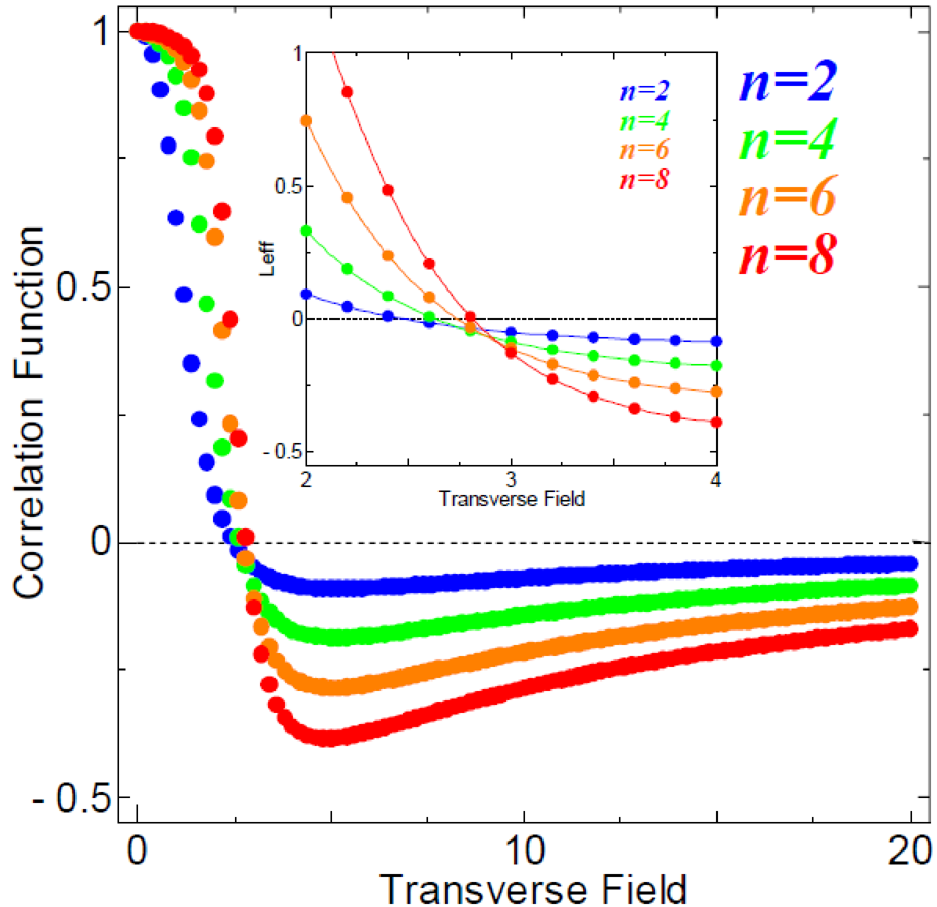
decorated bond system $\mathcal{H} = \mathcal{H}_{\mathrm{classical}} - \Gamma \sum_i \sigma_i^x$



● system spin σ_1, σ_2

▲ decorated spin s_i

number of ▲ spins: N_d



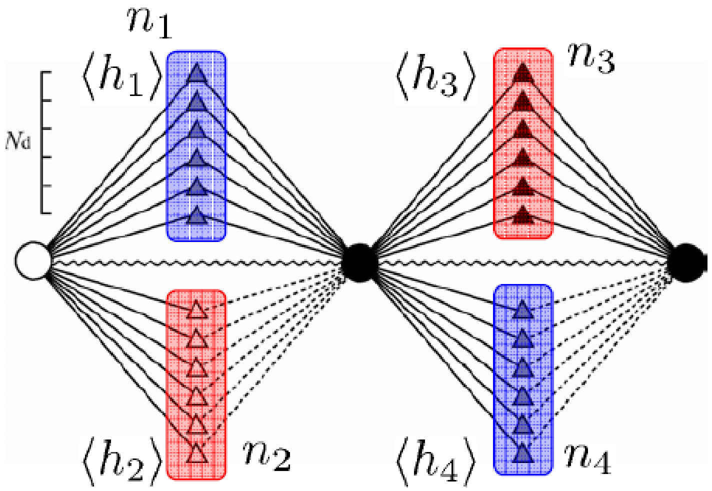
Ground state search: Quantum annealing

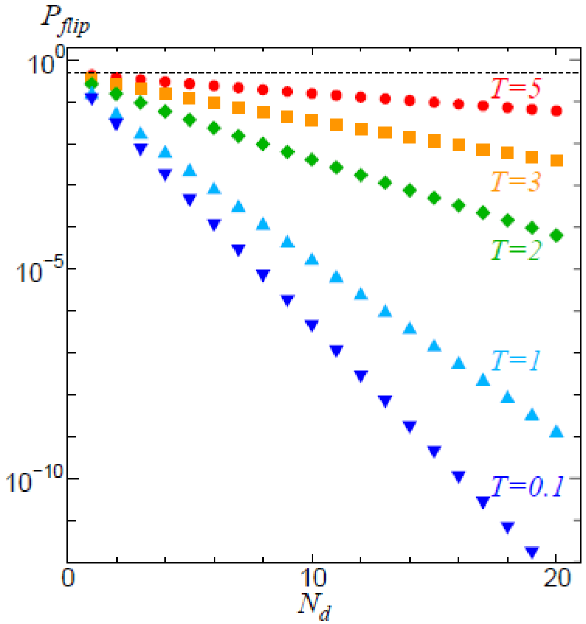
$$\mathcal{H}_0 = -J'\sigma_1^z\sigma_2^z - J\sigma_1\sum_{i=1}^{N} S_i^z - J\sigma_2\left(\sum_{i=1}^{N/2} S_i^z - \sum_{i=N/2+1}^{N} S_i^z\right)$$

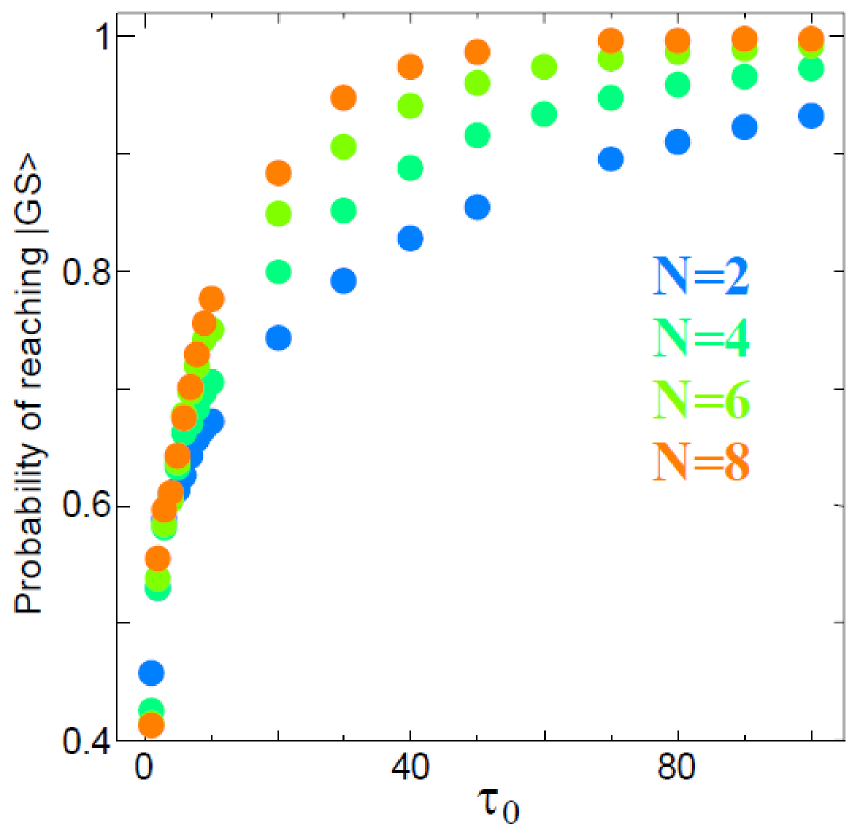
$$\mathcal{H}_t(t) = -\Gamma(t)\left(\sigma_1^x + \sigma_2^x + \sum_{i=1}^{N} S_i^x\right)$$

$$\Gamma(t) = \Gamma_0\left(1 - t/\tau_0\right)$$

$|GS\rangle$: ground state at $\Gamma(\tau_0) = 0$







Quantum dynamics in TI model

$$H = -J\sum_i \sigma_i^{\ z}\sigma^{z}{}_{i+1} - h(t)\sum_i \sigma^{z}{}_i - \Gamma(t)\sum_i \sigma^{x}{}_i$$

$$i\eta\frac{d\psi}{dt} = H(t)\psi$$

$$\left[\sigma_i^{\ z},\sigma_i^{\ x}\right] \neq 0, \quad \left[M, H\right] \neq 0,$$

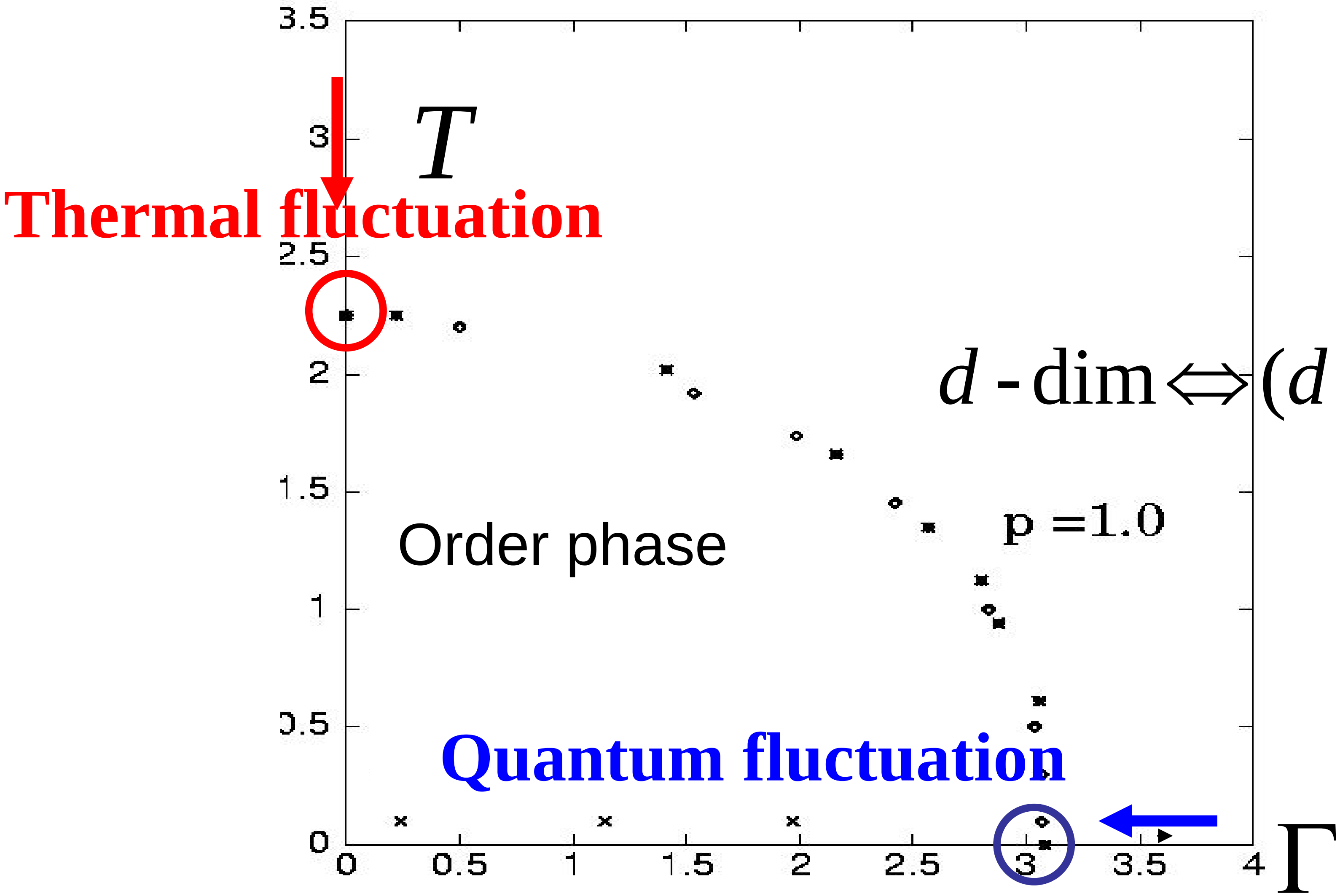
$$\Gamma = H_X$$

Quantum fluctuation

quantum tunneling: LZ in TI model
quantum nucleation
quantum spinodal decomposition?
collective motion?

Ground state Phase transition

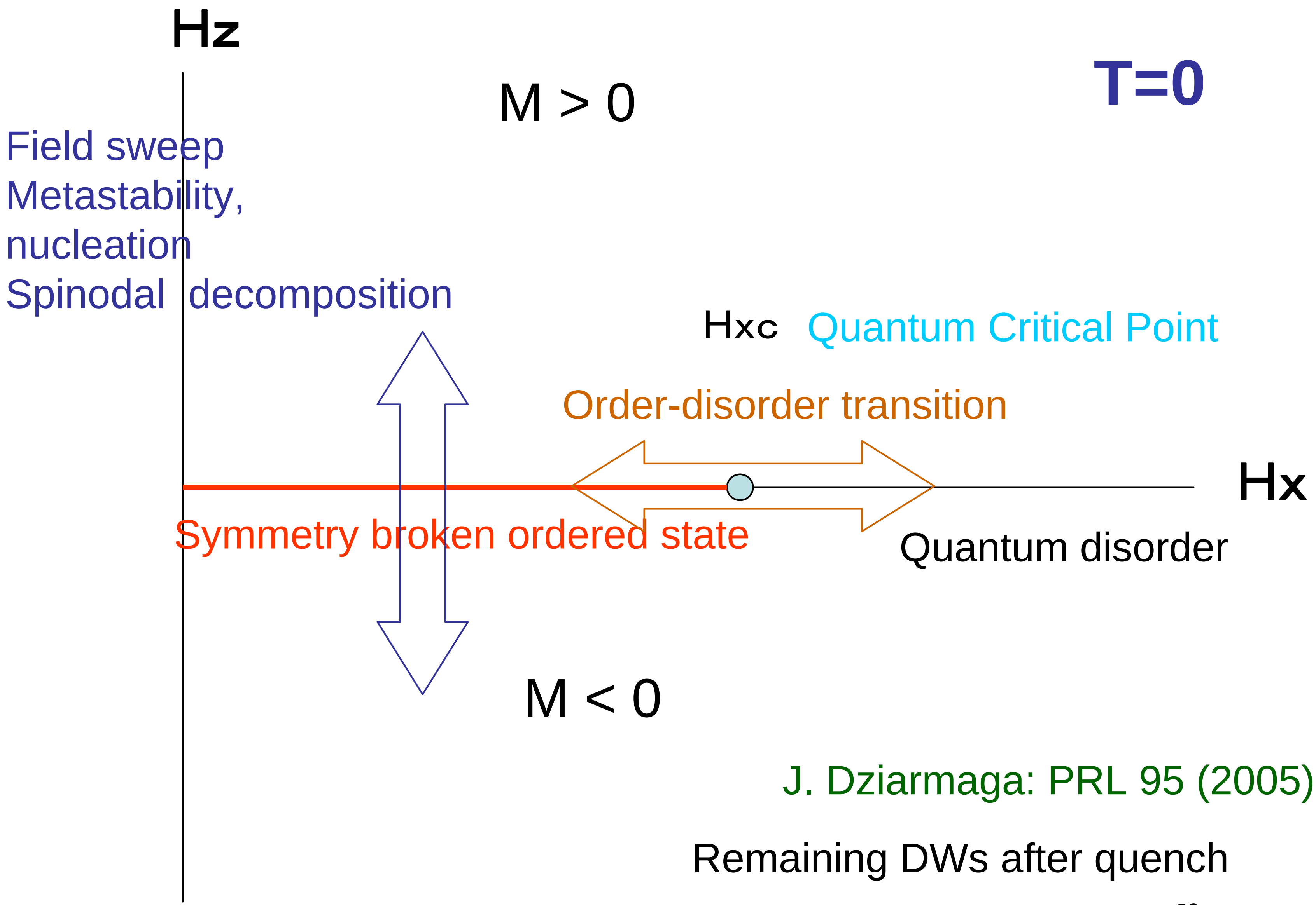
$$H = -J\sum \sigma_i^z \sigma_j^z - \Gamma \sum \sigma_i^x$$



$$d\text{-dim} \Leftrightarrow (d+1)\text{-dim}$$

T. Ikegami, SM, H. Rieger: JPSJ 67 (1998) 2671

Phase diagram of Transverse Ising model

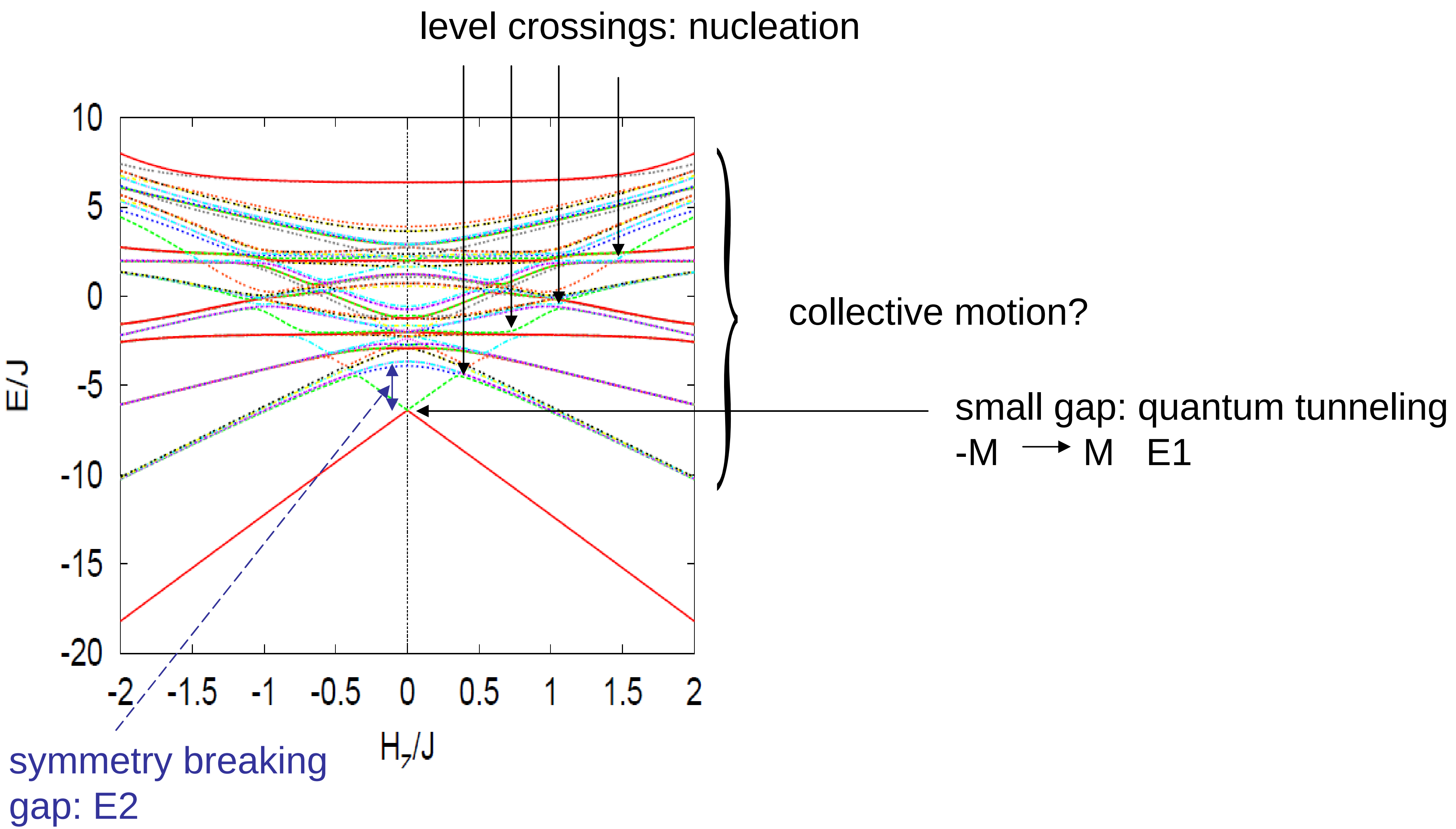


J. Dziarmaga: PRL 95 (2005) 245701

Remaining DWs after quench

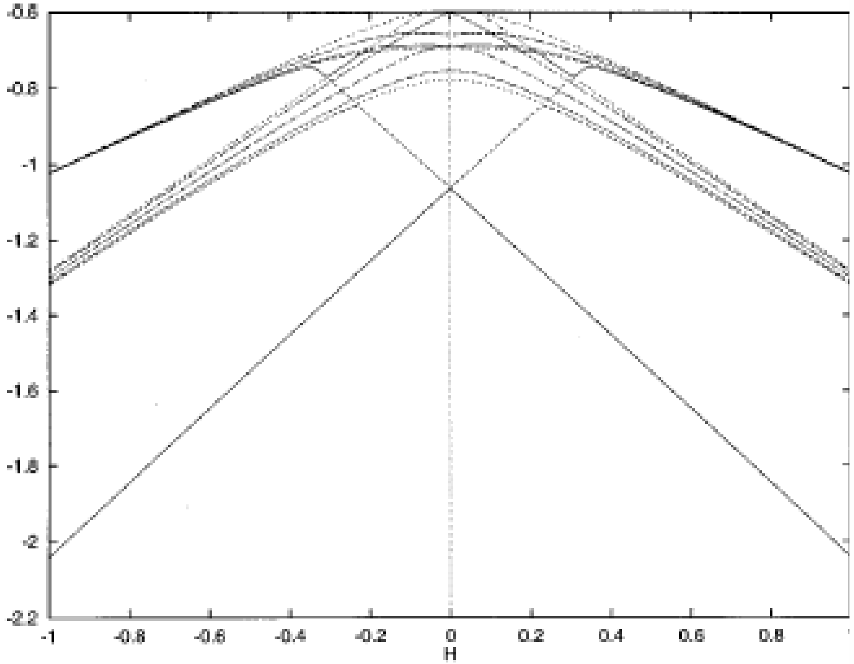
$$n = \frac{1}{2\pi\sqrt{2J\tau/\eta}}$$

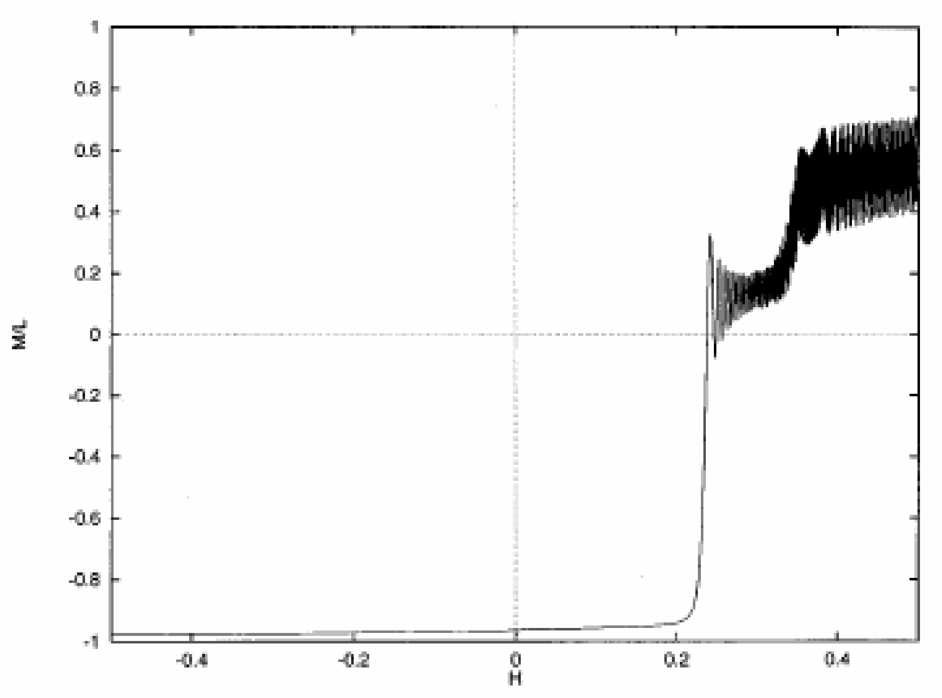
Critical phenomena in Energy spectrum E(H)



Landau-Zener-Stueckerberg scattering at each crossings

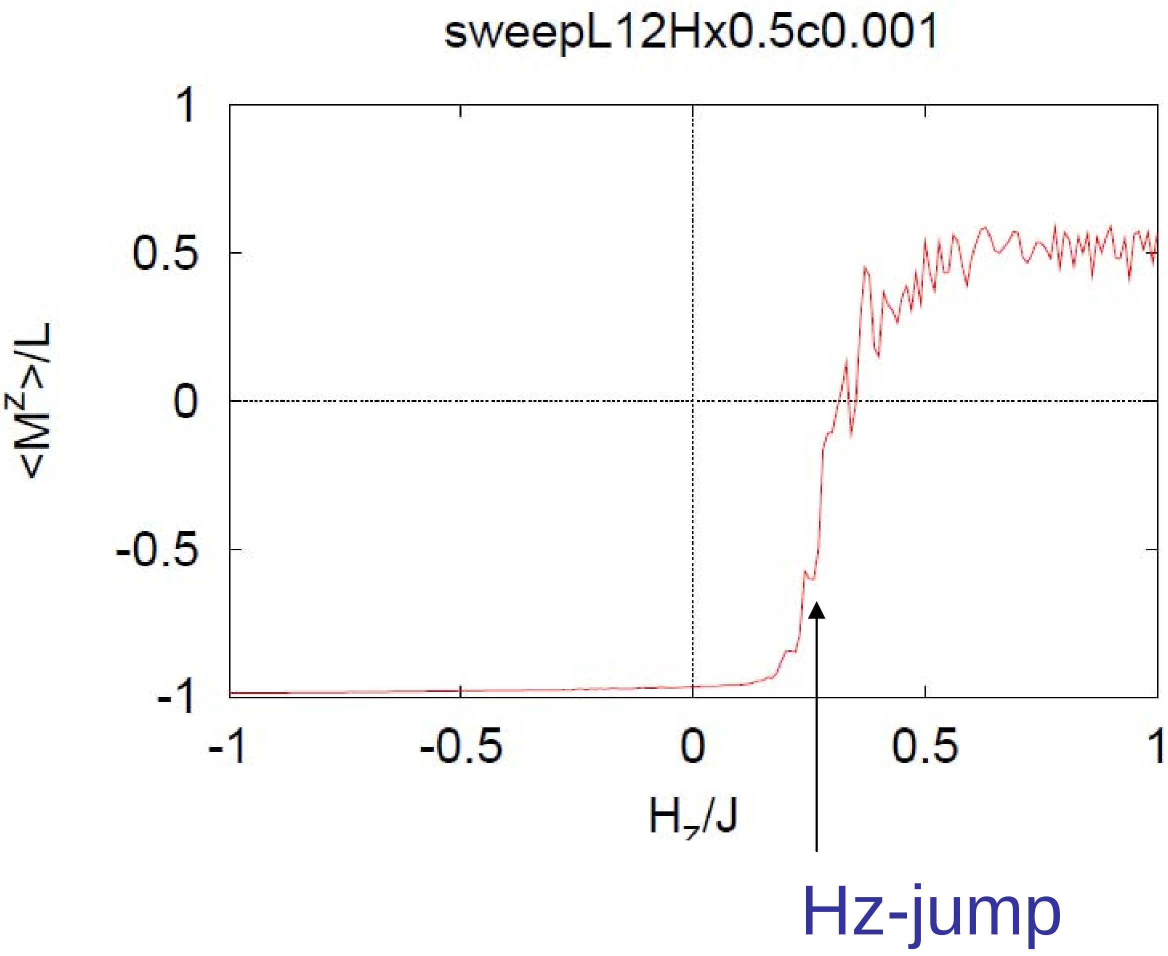
Non-adiabatic transition at the avoided level crossing points



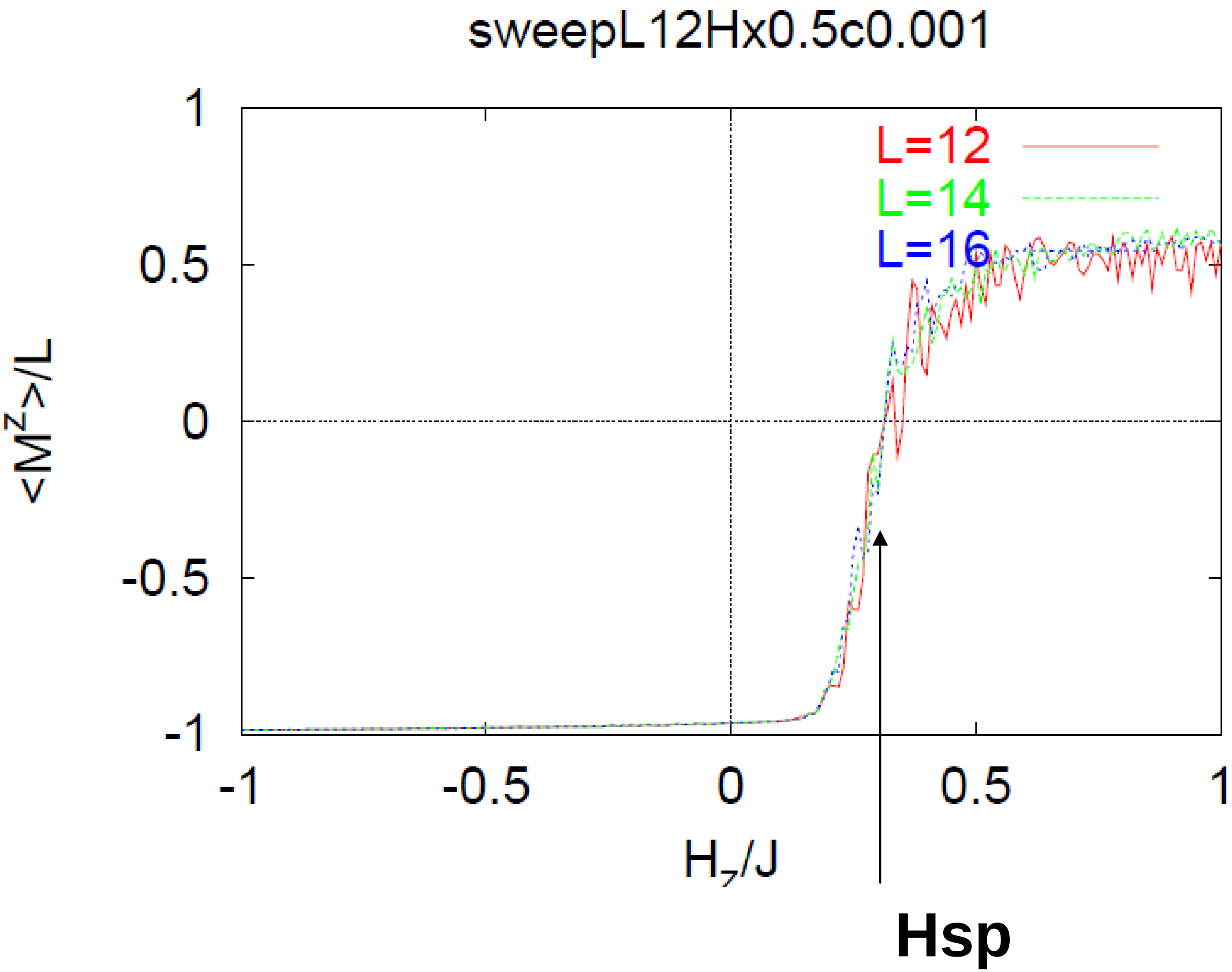


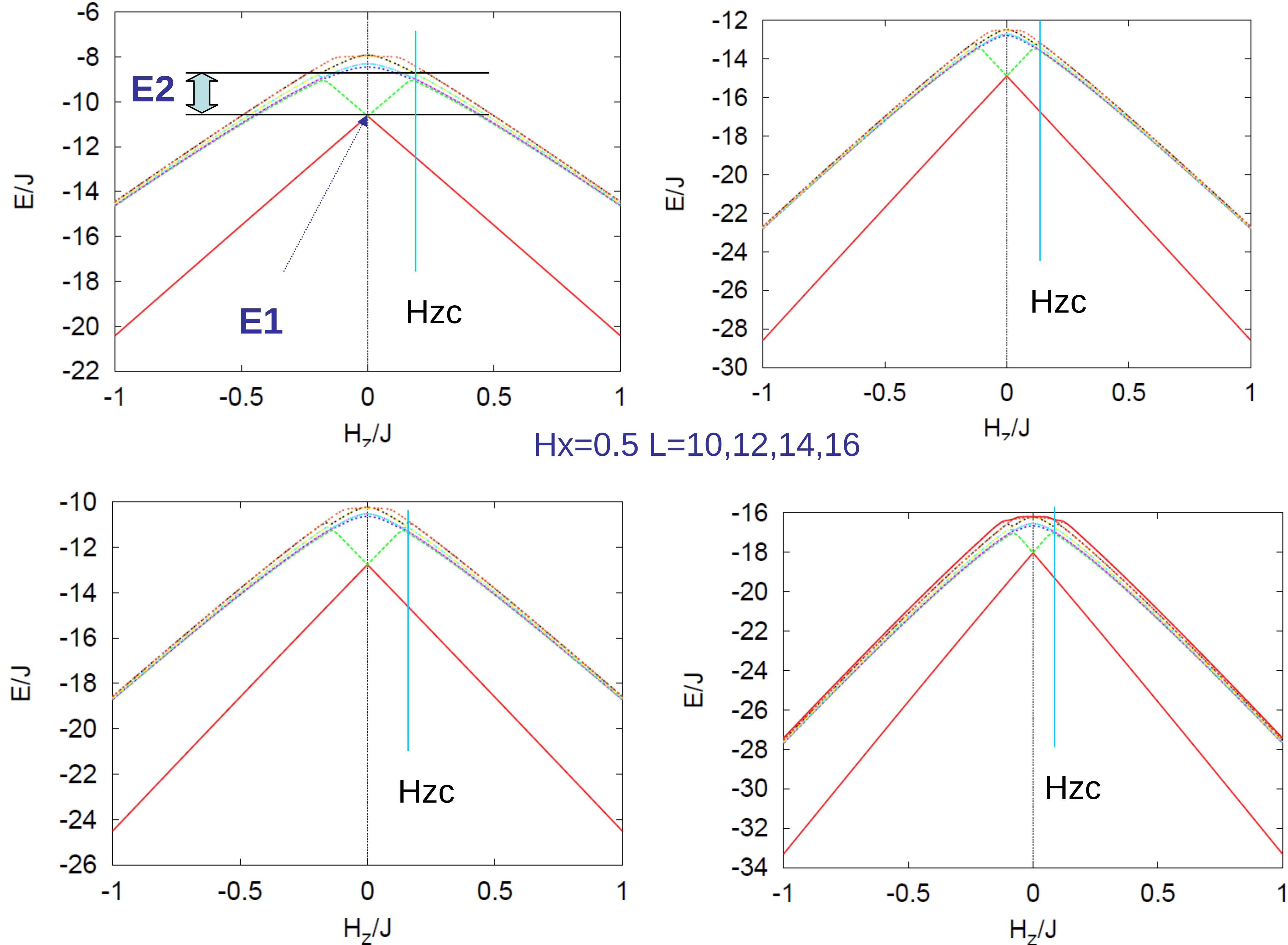
H. De Raedt, S. Miyashita, K. Saito, D. Garcia-Pablos and N. Garcia: Phys. Rev. B56 (1997) 11761

Field sweep



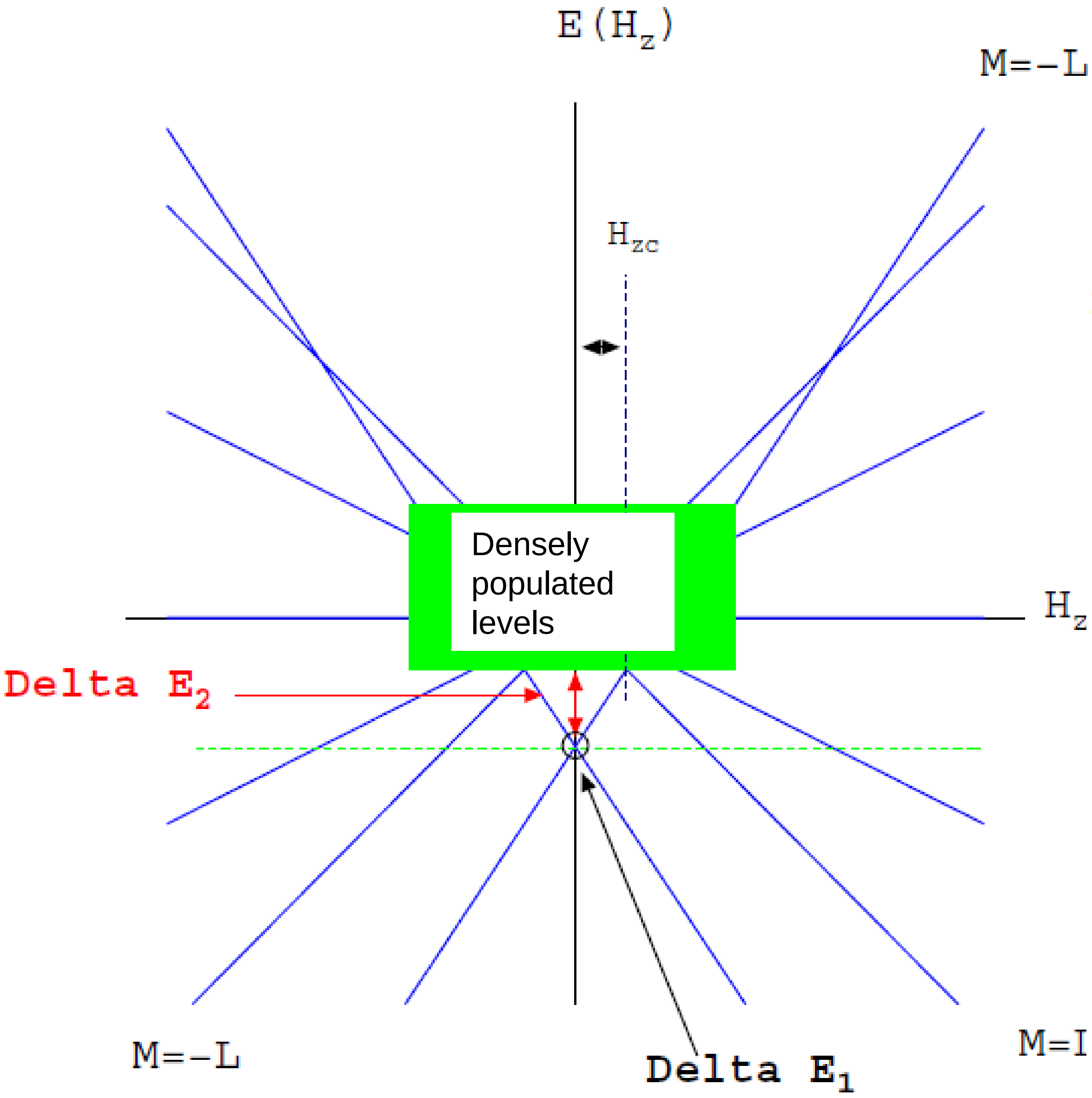
Size-independent phenomena a kind of collective motion(?)

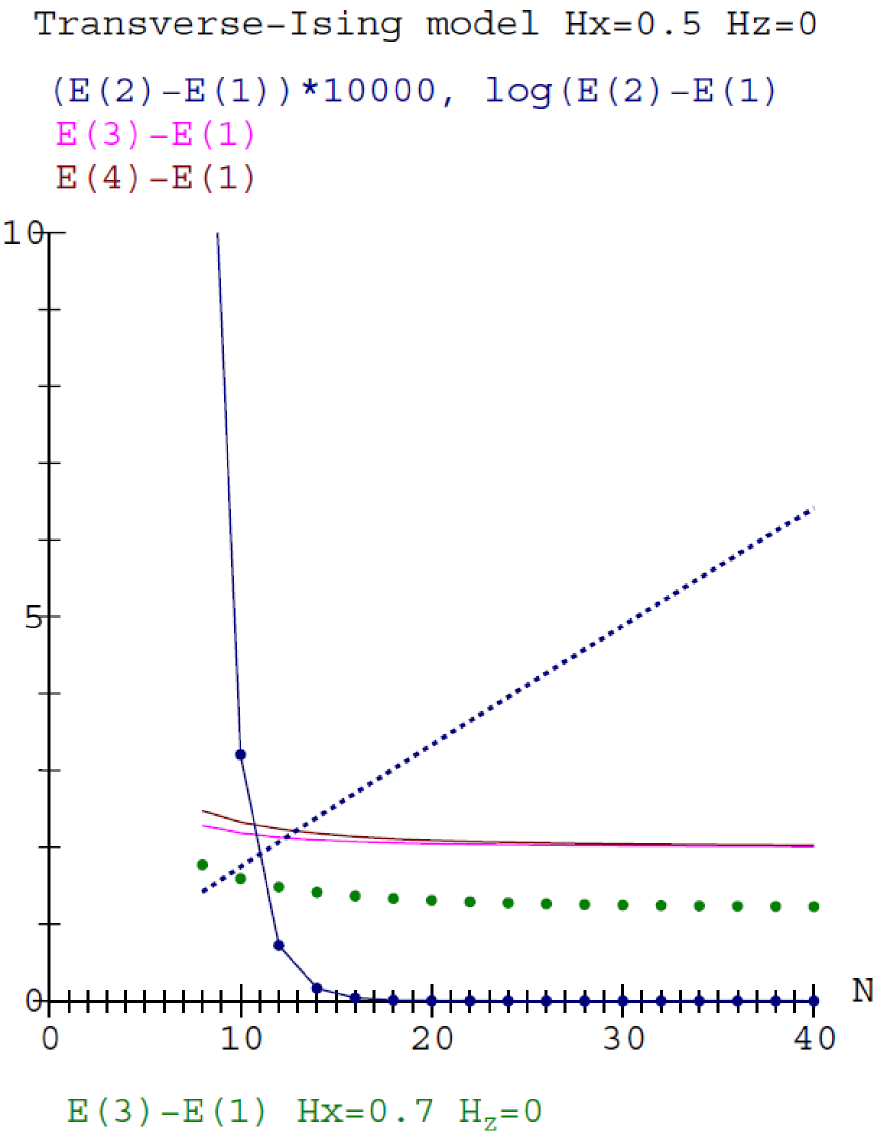




Hx=0.5 L=10,12,14,16

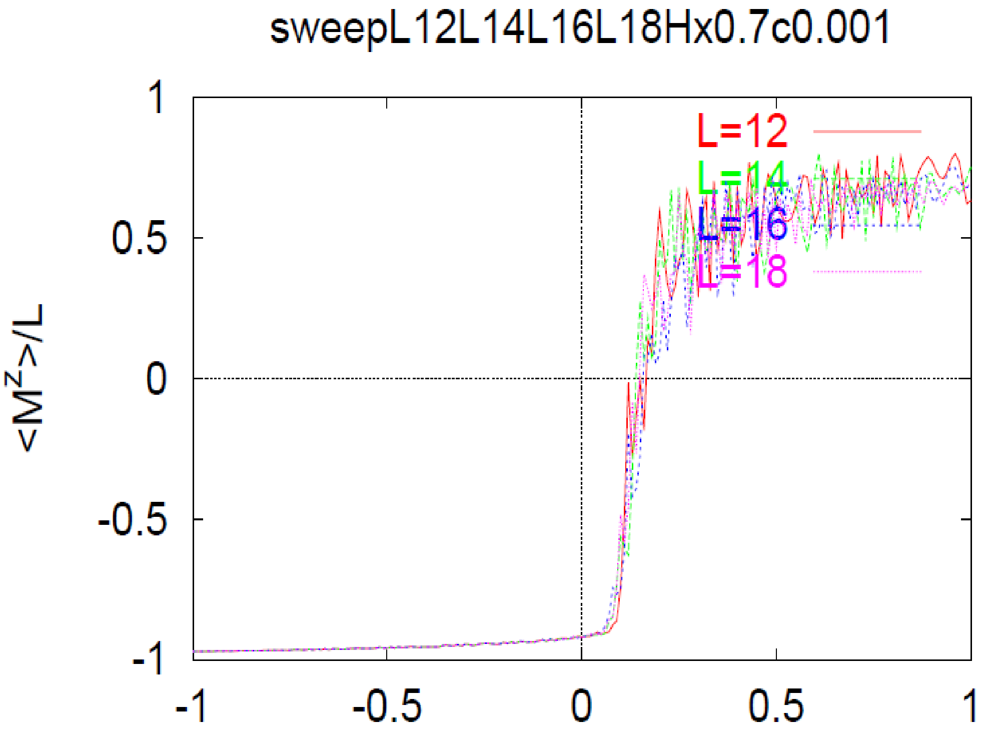
General structure

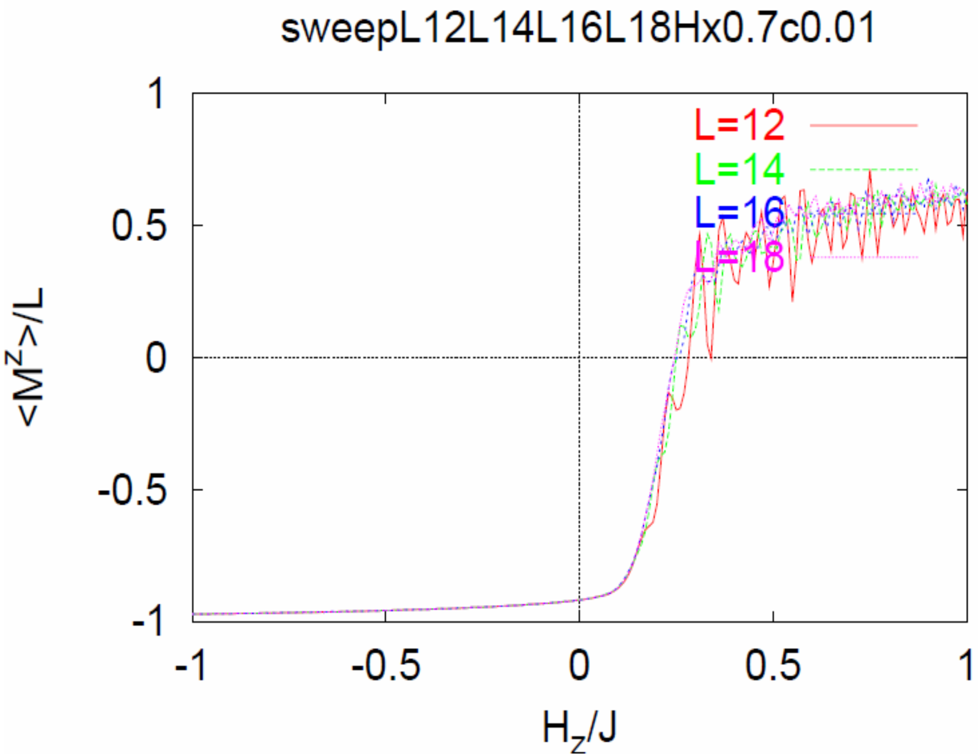


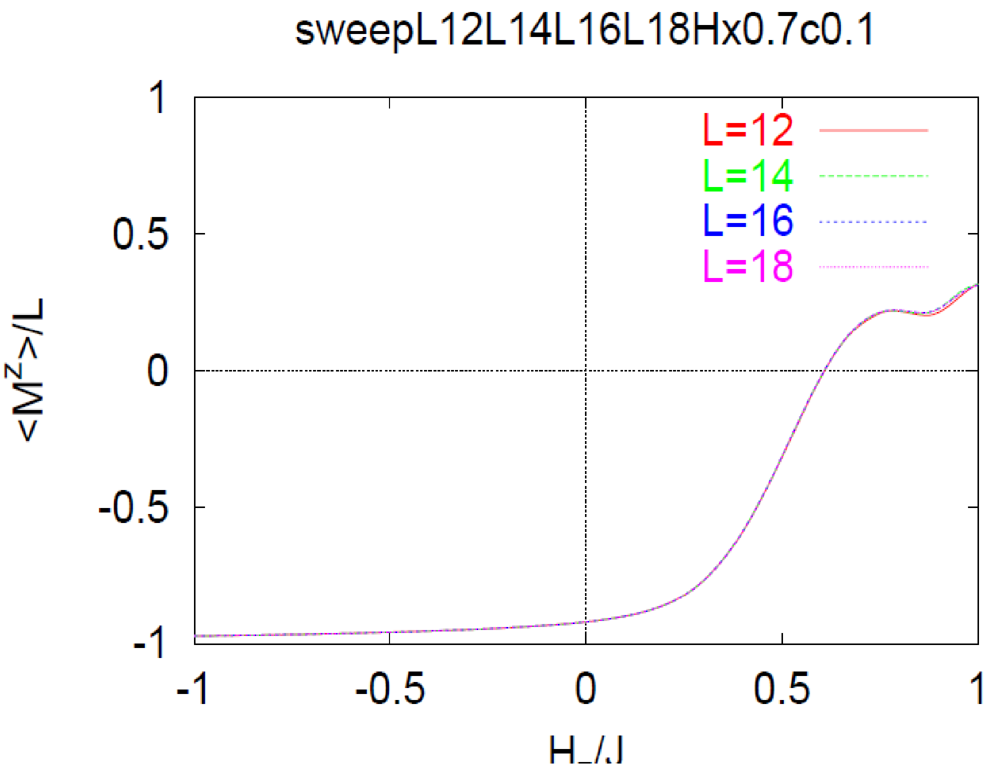


$$H_{ZC} = \Delta E_2 / L$$

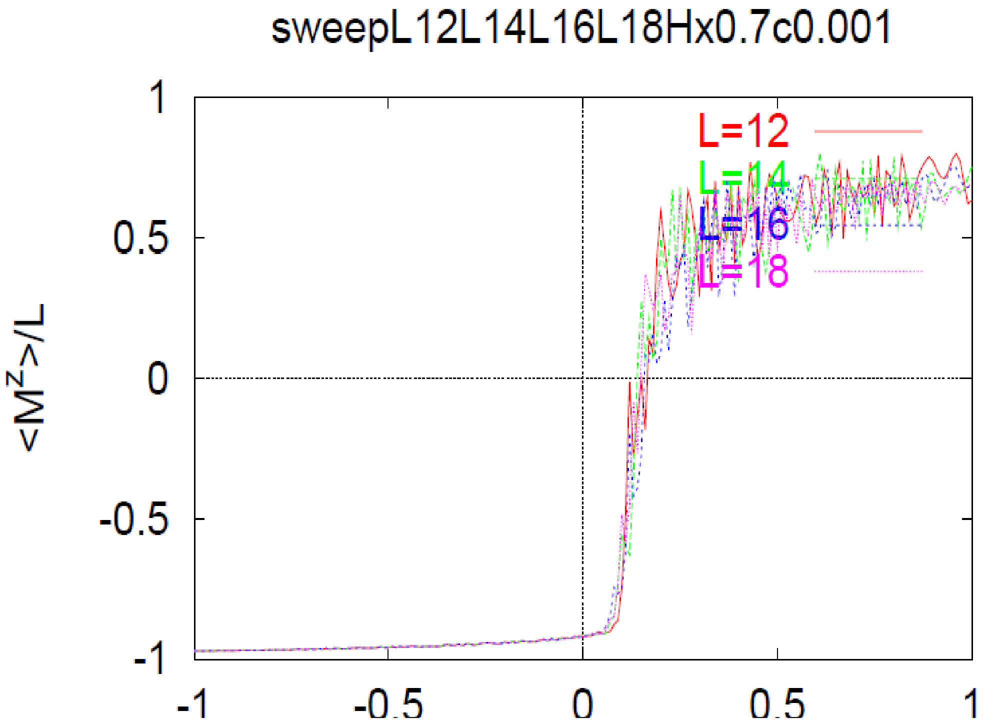
Sweep velocity dependence

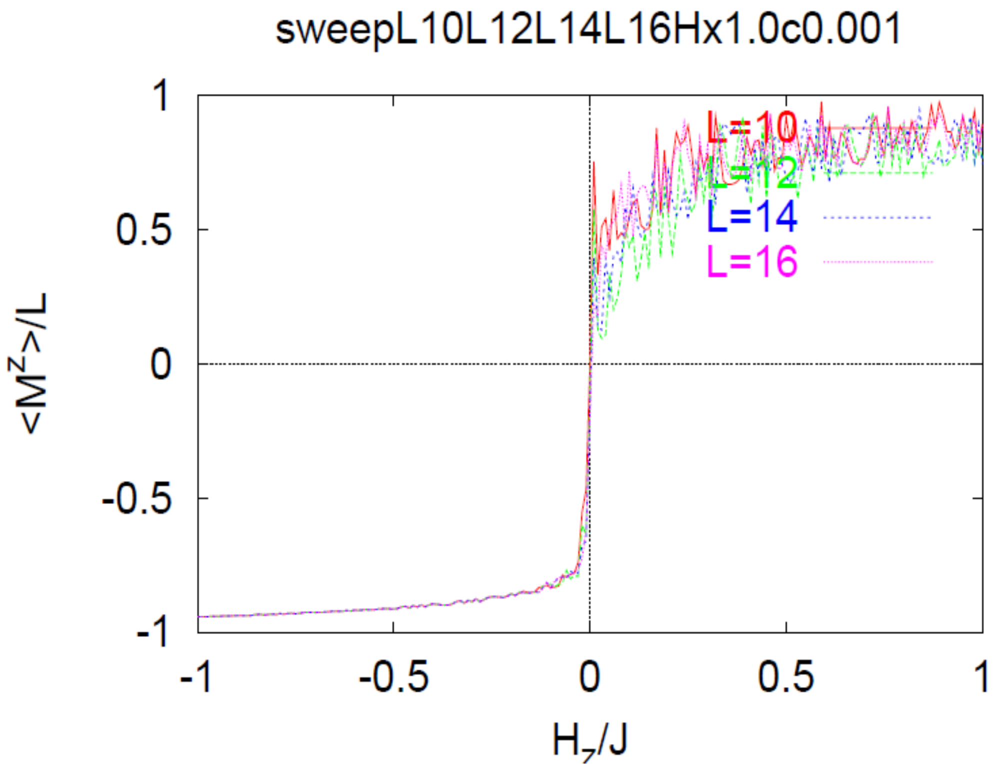


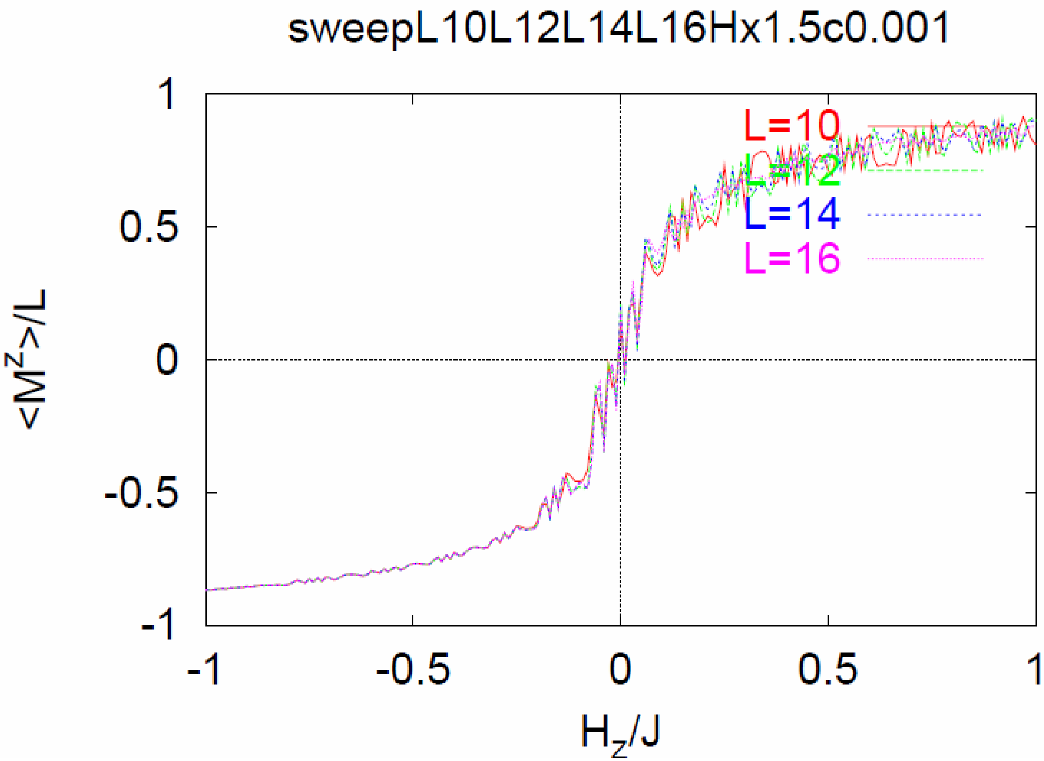




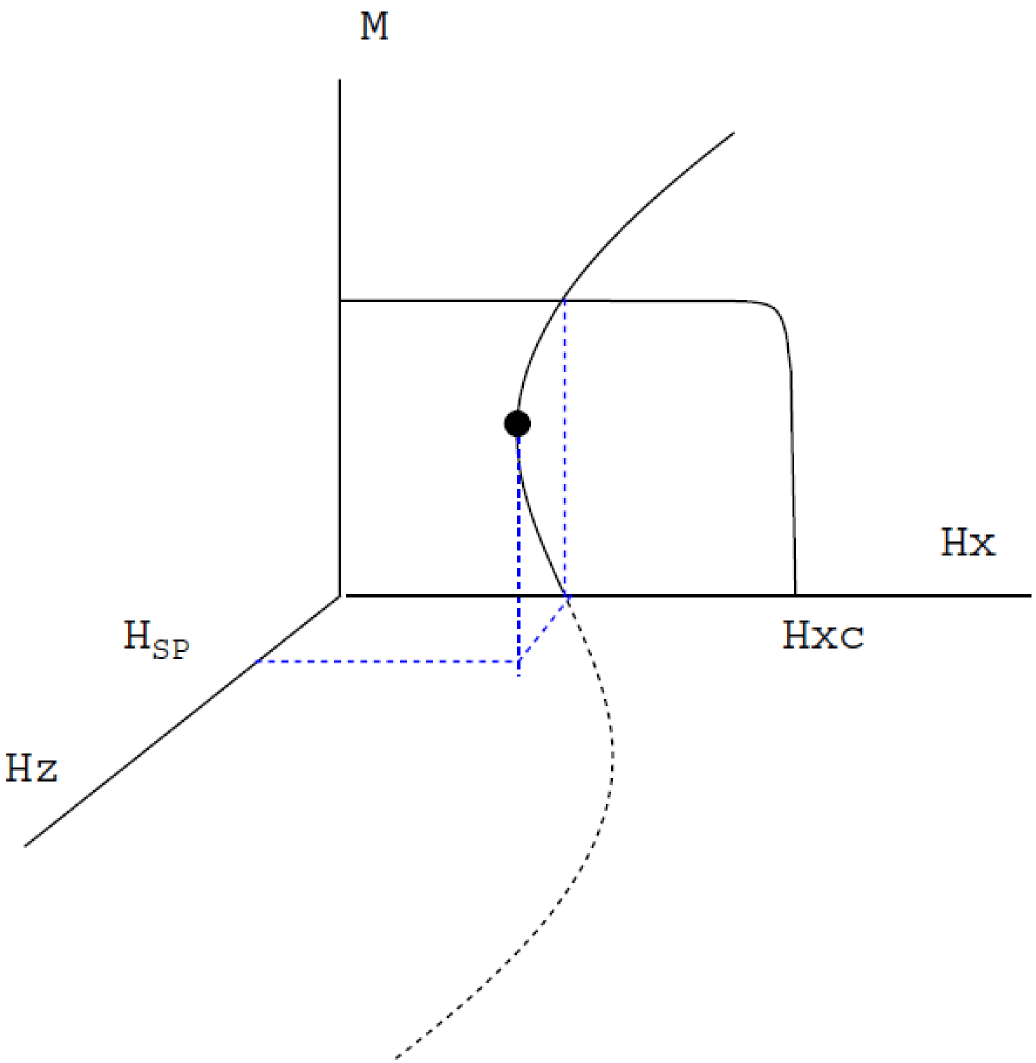
Dependence on Hx

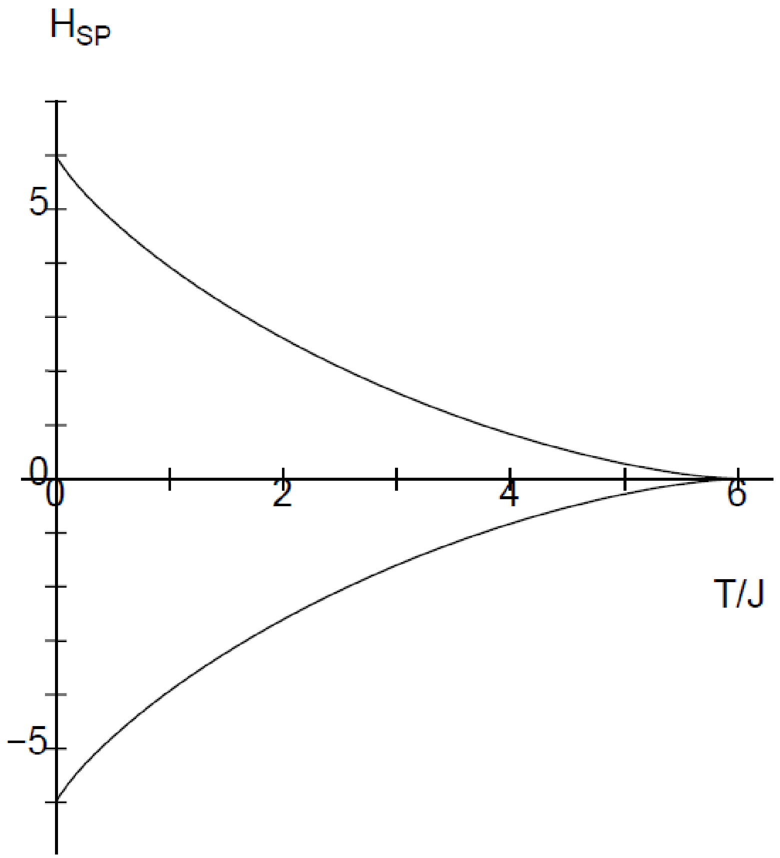






Metastability and Spinodal decomposition





Mean field theory : classical spin

Quantum spinodal decomposition

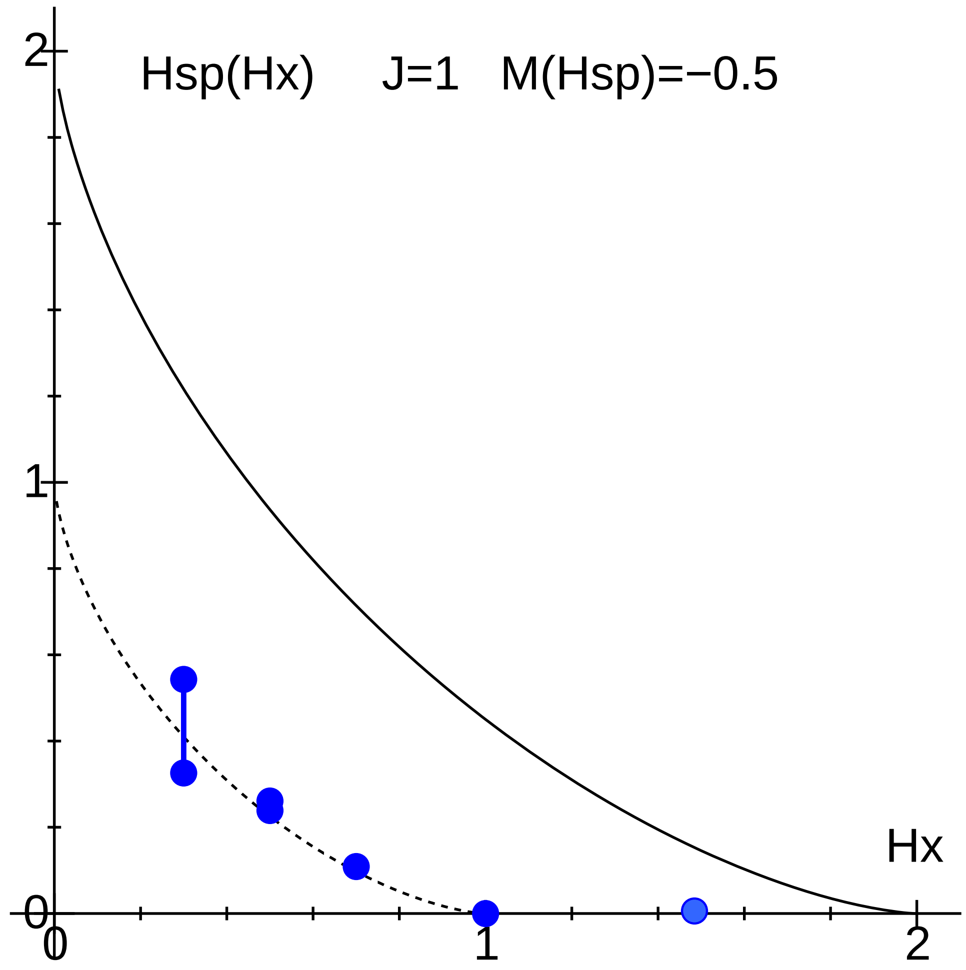
$$E = -J\sigma^2 - \Gamma\sqrt{1-\sigma^2} + H\sigma$$

$$\frac{dE}{d\sigma} = -J\sigma + \frac{\Gamma\sigma}{\sqrt{1-\sigma^2}} + H = 0$$

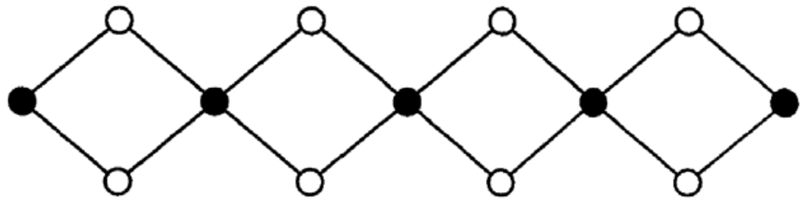
$$\frac{dH}{d\sigma} = 0 \quad \Rightarrow \quad \sigma = \left(1-\gamma^{2/3}\right)^{1/2},$$

$$\gamma = \frac{\Gamma}{2\mathrm{J}}$$

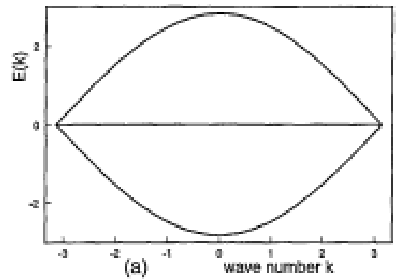
$$\frac{H_{\mathrm{SP}}}{2J} = \left(1-\gamma^{2/3}\right)^{3/2}$$

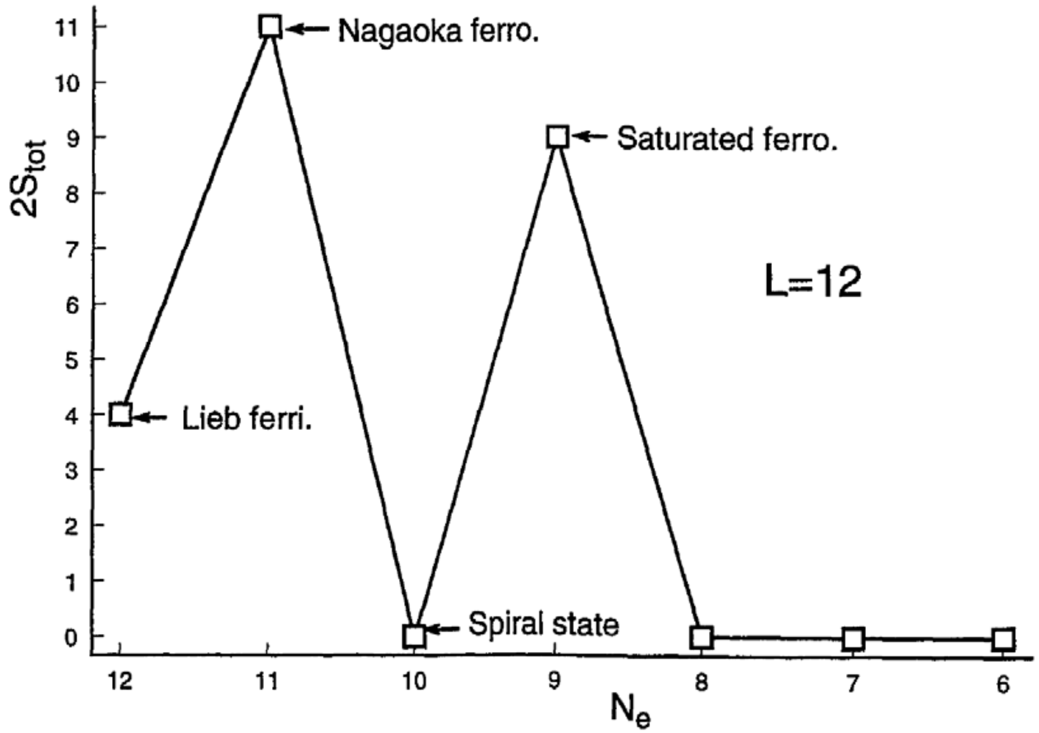


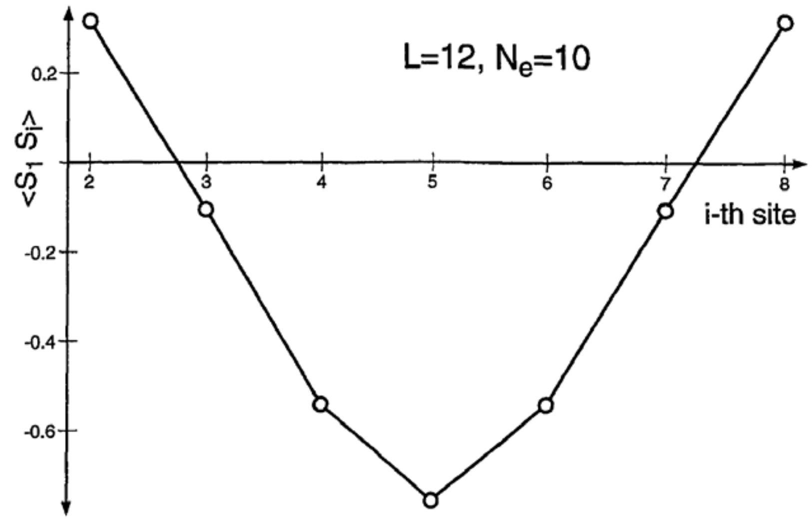
Itinerant ferromagnetism and its dynamics



$$H = H_{\text{hop}} + H_{\text{int}}$$
$$= -t \sum_{\langle i,j\rangle \in \Lambda} \sum_{\sigma=\uparrow,\downarrow} c^\dagger_{i,\sigma} c_{j,\sigma} + U \sum_{i\in\Lambda} n_{i,\uparrow} n_{i,\downarrow}$$

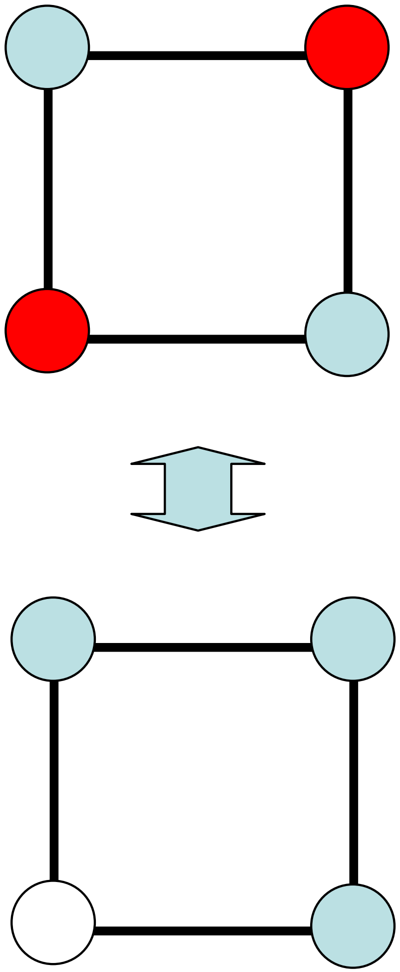


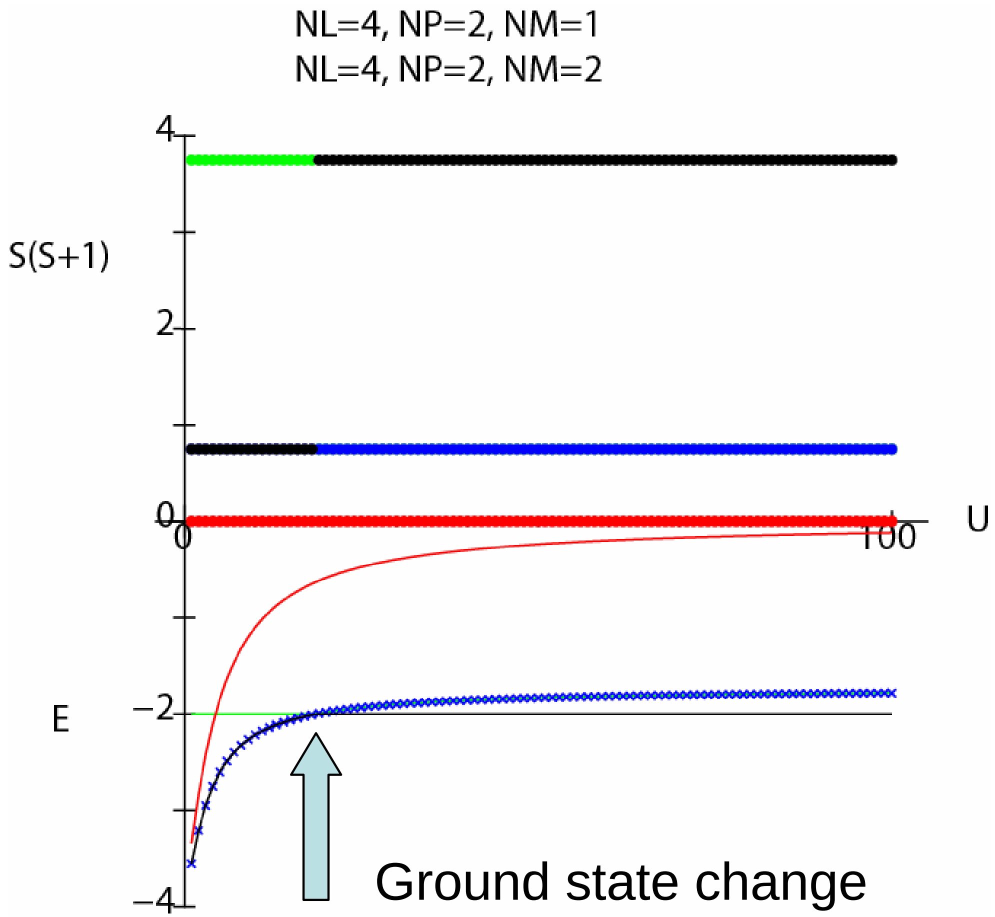




Y. Watanabe and SM: JPSJ 68 (1999) 3086.
66 (1997) 2123,

Transition between AF and Nagaoka-Ferromagnetic state





Dynamics after decimation

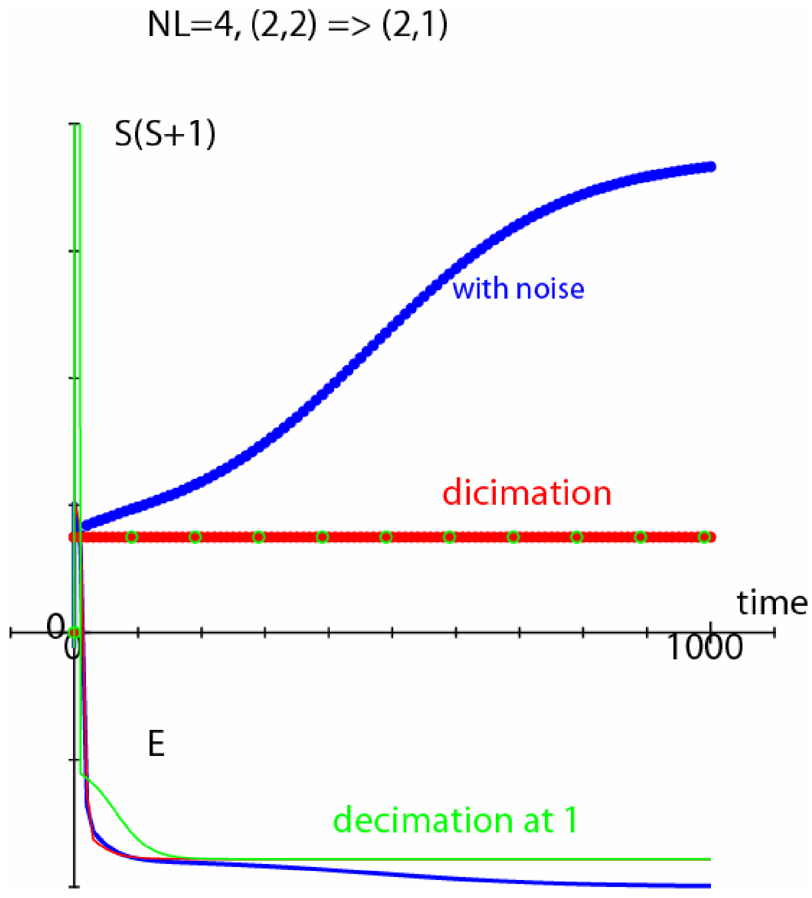
$$S^2 \left| G:(2+2) \right\rangle = 0$$

$$\Downarrow$$

$$\sum_i \left(c_{i\uparrow} + c_{i\downarrow} \right) \left| G:(2+2) \right\rangle = \left| initial \right\rangle$$

$$\left| t \right\rangle = e^{-iHt} \left| initial \right\rangle$$

$$S^2 \left| t \right\rangle = \frac{3}{2}$$



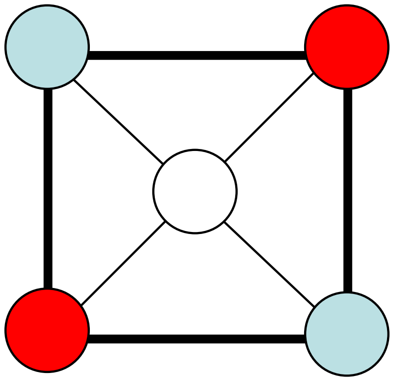
$$S^2 \left| G:(2+2) \right\rangle = 0$$

$$\Downarrow$$

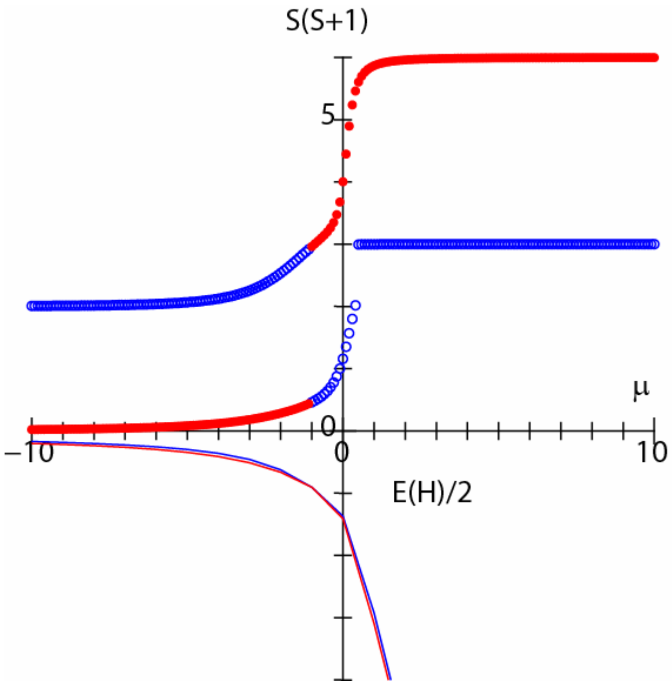
$$\sum_i \left((1+\delta_i) c_{i\uparrow} + (1+\delta_i') c_{i\downarrow} \right) \left| G:(2+2) \right\rangle = \left| initial ' \right\rangle$$

$$\left| t \right\rangle = e^{-iHt} \left| initial ' \right\rangle$$

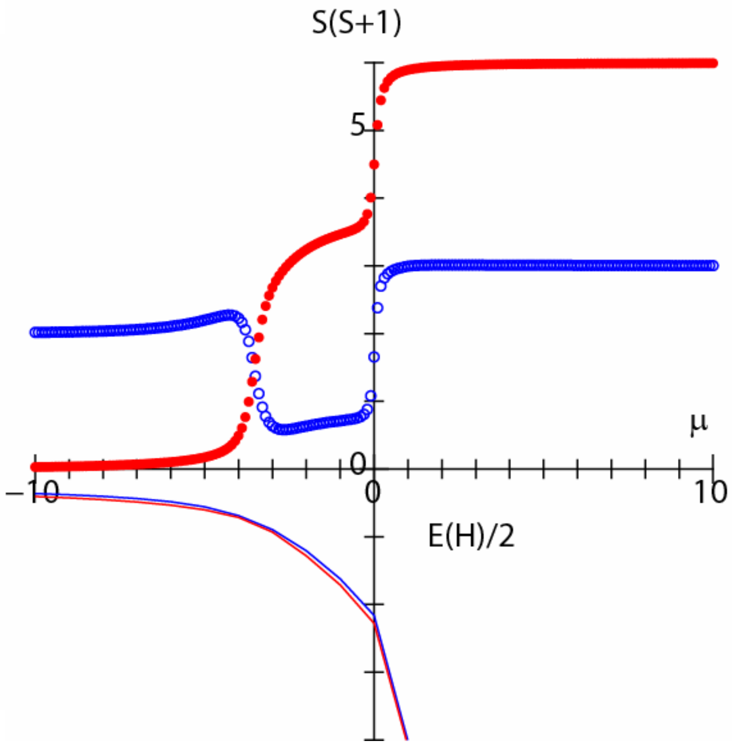
Adiabatic decimation



$$H = -t_{ij} \sum_{ij\sigma} \left(c^{+}_{i\sigma} c_{j\sigma} + c^{+}_{j\sigma} c_{i\sigma} \right) + U \sum_{i} n_{i\uparrow} n_{i\downarrow} - \mu \left(n_{5\uparrow} + n_{5\downarrow} \right)$$



Non−uniform lattice (t=2,3,1.5,1)

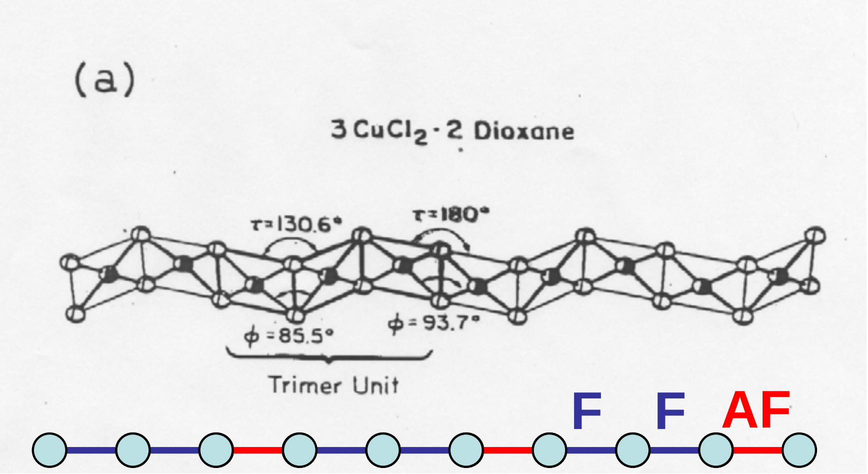


Quantum response in pure quantum and dissipative environments

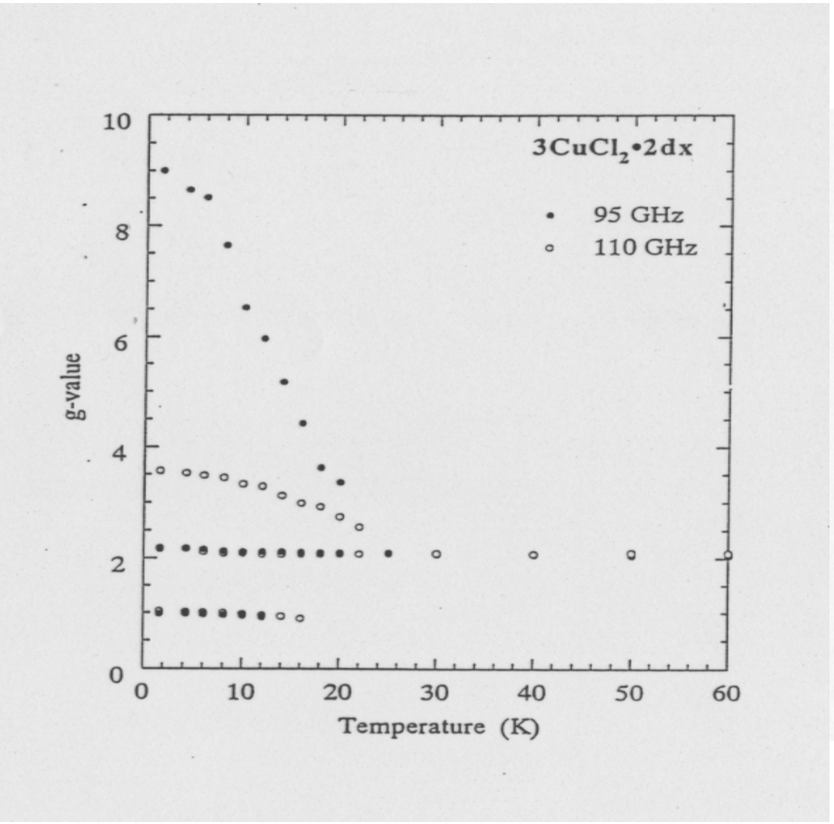
collaborators: Akira Ogasahara, Keiji Saito,
Chikako Uchiyama, and Mizuhiko Saeki

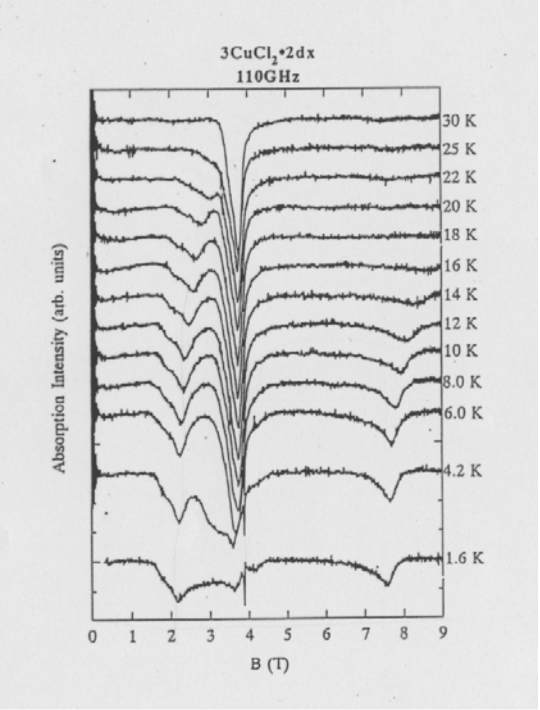
ESR line shape in strongly interacting spin systems

Temperature-dependence of the shift and width in low-dimensional quantum spin systems



Spin trimer: 3CuCl2 ･2Dioxane





Y. Ajiro, et al: JPSJ 63 (1994) 859.

Microscopic expression of the line shape from Hamiltonian

Kubo Formula

R. Kubo & K.Tomita JPSJ (1954) 888

R. Kubo: JPSJ 12 (1957) 570

$$\chi_{xx}''(\omega) = \frac{1}{2}(1 - \mathrm{e}^{-\beta\omega}) \int_{-\infty}^{\infty} \langle M^x(0) M^x(t) \rangle \, \mathrm{e}^{-i\omega t} dt$$

Pure quantum dynamics

$$M(t) = e^{iL(t)} M(0) \Rightarrow e^{iHt/\eta} M e^{-iHt/\eta}$$

$$H\,|m>= E_m\,|m>$$

$$\chi''(\omega) = \sum_{mn} D(\omega_{mn}) \delta(\omega - (E_n - E_m))$$

$$D(\omega_{mn}) = \pi \left(\mathrm{e}^{-\beta E_m} - \mathrm{e}^{-\beta E_n} \right) \frac{\left| \langle m | M^x | n \rangle \right|^2}{Z}, \quad (\omega = E_n - E_m)$$

Shift from the PMR

Isotropic models

$$H = -2\sum_{<ij>} J_{ij}\mathbf{S}_i \cdot \mathbf{S}_j - H_0\sum_i S_i^z - H_1\cos(\omega t)\sum_i S_i^x$$

Paramagnetic Resonance

$$\omega_R = \gamma H, \quad \gamma = \frac{1}{2\eta} g\mu_B$$

Perturbation

$$H_{\text{perturbati on}} = -2\sum_{<ij>}[J(S_i^x S_j^x + S_i^y S_j^y) + J_z S_i^z S_j^z]$$

$$+ D\sum_{<mn>}\left(\frac{\mathbf{S}_m \cdot \mathbf{S}_n}{r_{mn}^3} - \frac{3(\mathbf{S}_m \cdot \mathbf{r}_{mn})(\mathbf{S}_n \cdot \mathbf{r}_{mn})}{r_{mn}^5}\right) + \Lambda$$

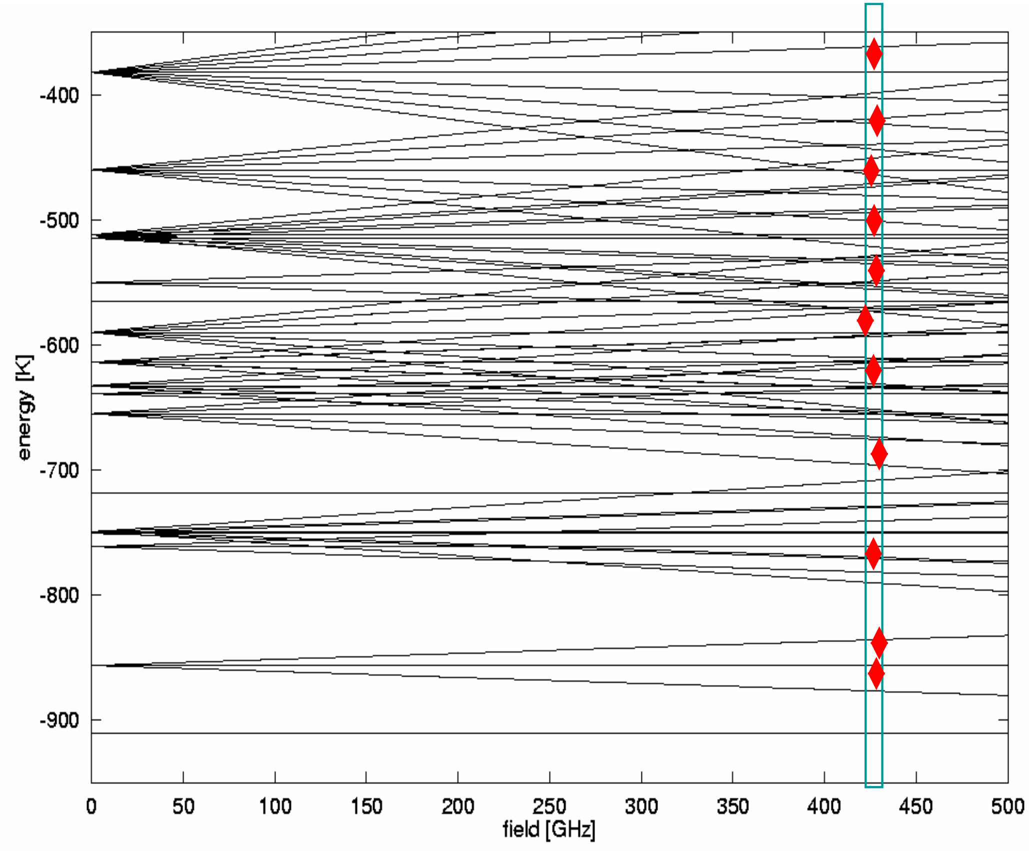
$$+ \mathbf{D} \cdot \sum_{<ij>} \mathbf{S}_i \times \mathbf{S}_j + \Lambda$$

Studies on the line shape

- F. Bloch: PR 70 (1946) 460. Nuclear Induction (Bloch equation)
- J. H. Van Vleck: PR 74 (1948) 1168.
  Dipolar broadening, and exchange narrowing
- N. Bloembergen, E. M. Purcell and R. V. Pound: PR 73 (1948) 679.
  Relaxation Effects in Nuclear Magnetic Resonance Absorption.
- I. Solomon: PR 99 (1955) 559.
  Relaxation processes in a system of two spins
- F. Bloch: PR 105 (1957) 1206. General theory of relaxation

- A. Abragam: The principles of Nuclear Magnetism,
  Oxford Univ. Press (1978)

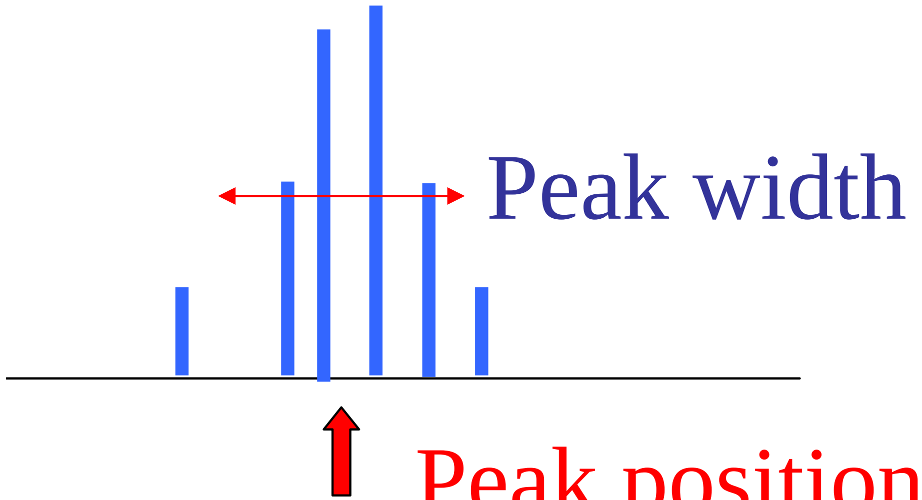
Shift & Width



$$\langle M^x(0)M^x(t)\rangle \cong m^2 e^{-i\omega_0 t - t/\tau}$$

$$\chi''(\omega) \propto \frac{\Gamma}{(\omega-\omega_0)^2+\Gamma^2}$$

$$\omega_0 = \omega_R + \delta\omega$$

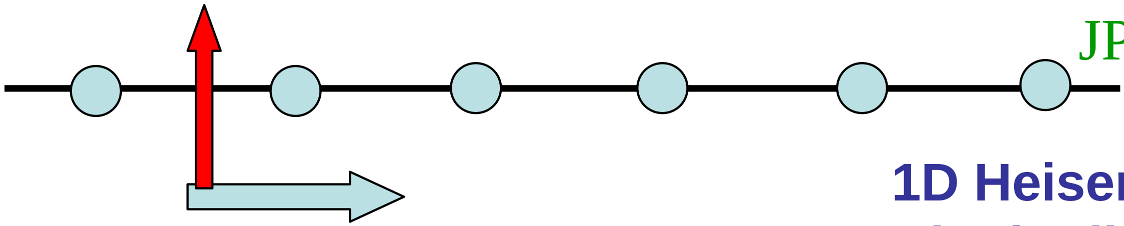


$$D(\omega_{mn}) = \pi\left(e^{-\beta E_m} - e^{-\beta E_n}\right)\frac{\left|\langle m|M^x|n\rangle\right|^2}{Z},$$

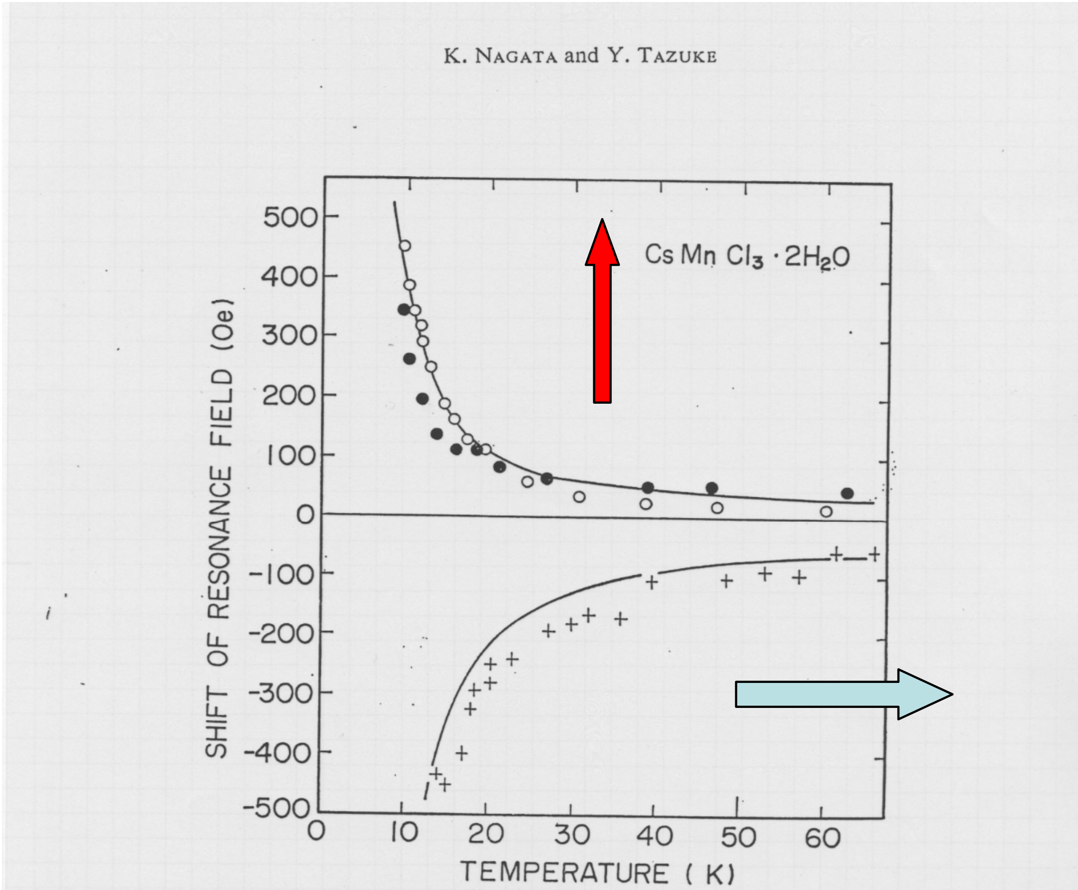
$$(\omega = E_n - E_m)$$

Nagata-Tazuke Dependence

K. Nagata and Y. Tazuke:
JPSJ 32 (1972) 337



1D Heisenberg model with Dipole-dipole interaction



K. NAGATA and Y. TAZUKE

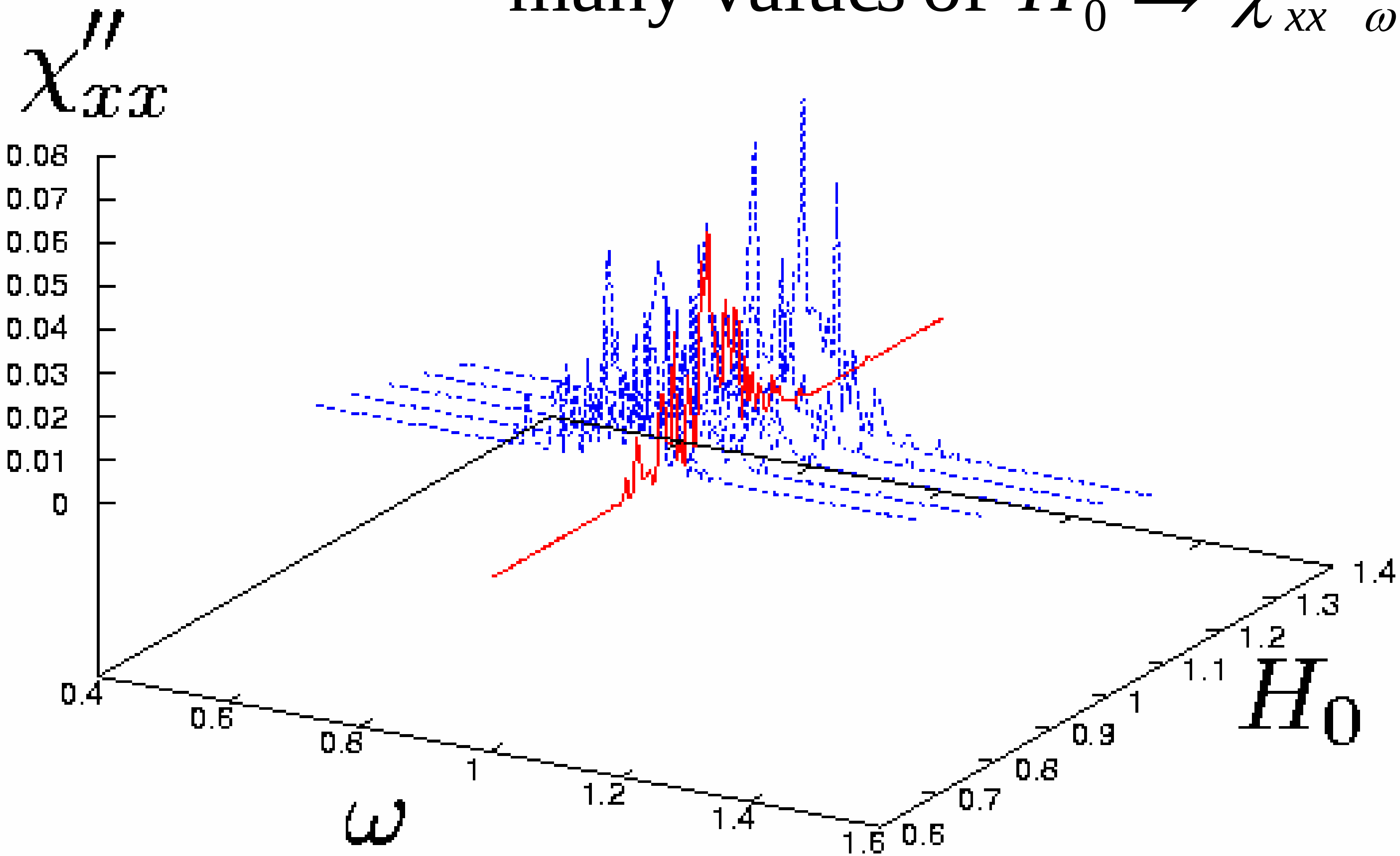
Fig. 3. Comparison of theory with experiment in the shift of resonance field in $CsMnCl_32H_2O$ at 34.4 GHz in the temperature range up to 70 K. Measured values of the shift are indicated by $+(H//a)$, $\bigcirc(H//b)$ and $\bullet(H//c)$. The solid curves are the result of the present calculation. The high temperature g-value is 2.000.

(J. Kanamori & M.Tachiki
JPSJ 48 (1962) 50)

Frequency sweep abd Field sweep

$$\chi_{xx}''(\omega, H_0) : H_0 \quad \text{given} \Rightarrow \chi_{xx}''_{H_0}(\omega)$$

$$\text{many values of } H_0 \Rightarrow \chi_{xx}''_{\omega}(H_0)$$

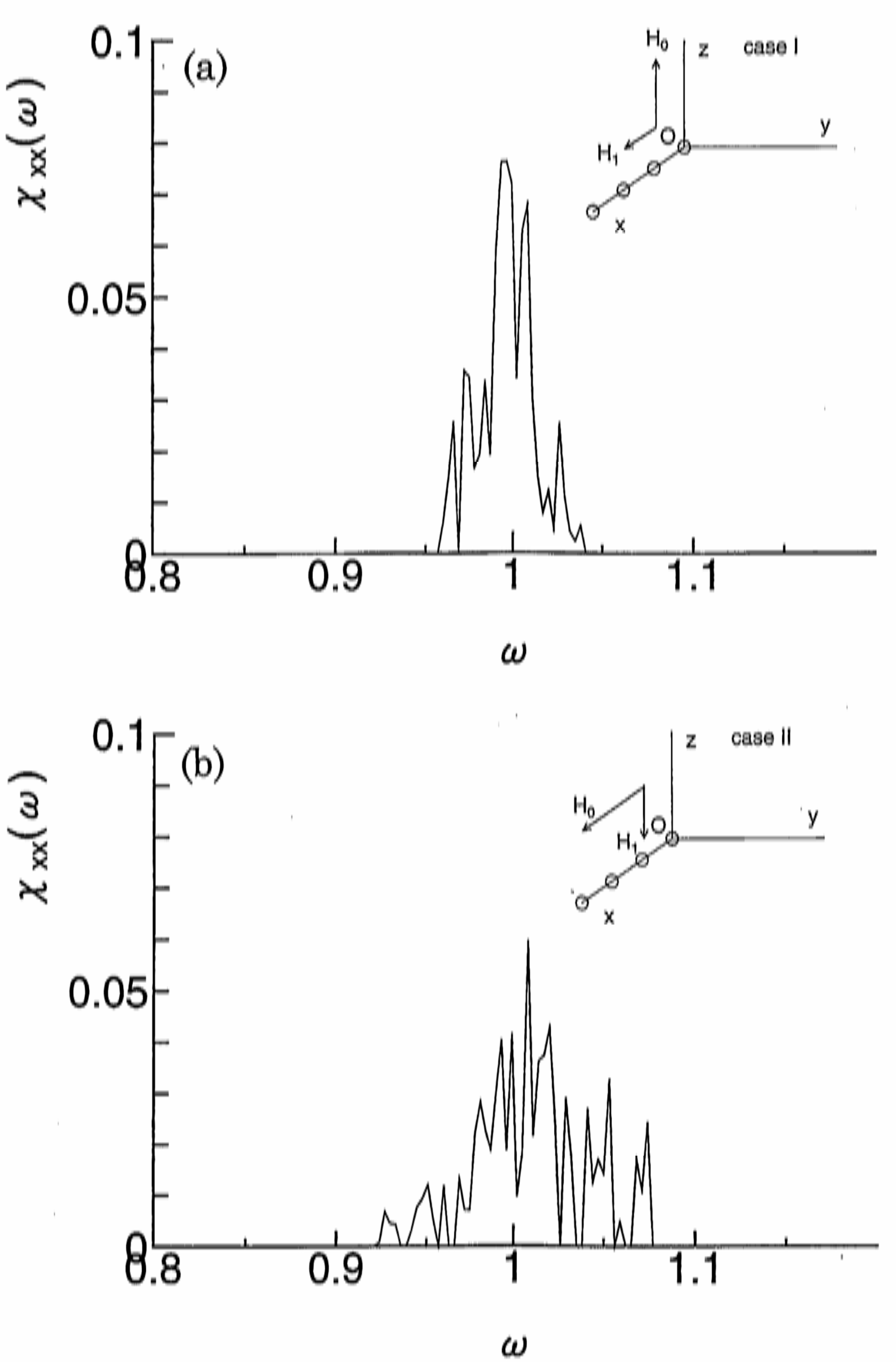


Line shape as an ensemble of delta-function

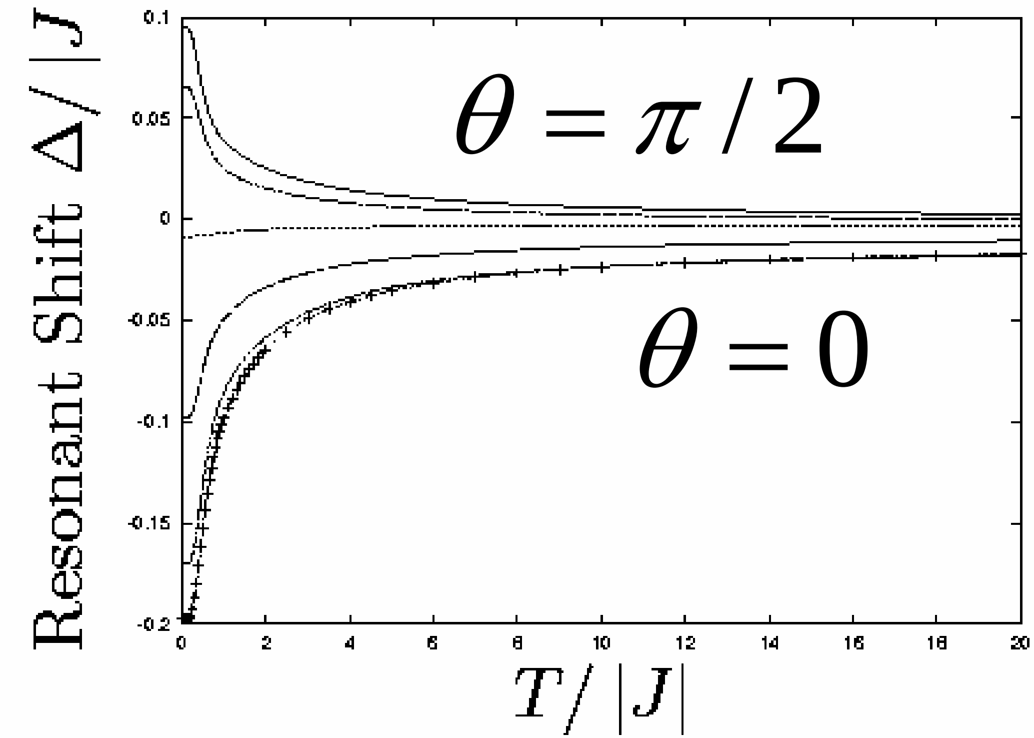
$$D(\omega_{mn}) = \pi\left(e^{-\beta E_m} - e^{-\beta E_n}\right)\frac{\left|\langle m|M^x|n\rangle\right|^2}{Z},$$

$$(\omega = E_n - E_m)$$

N=8



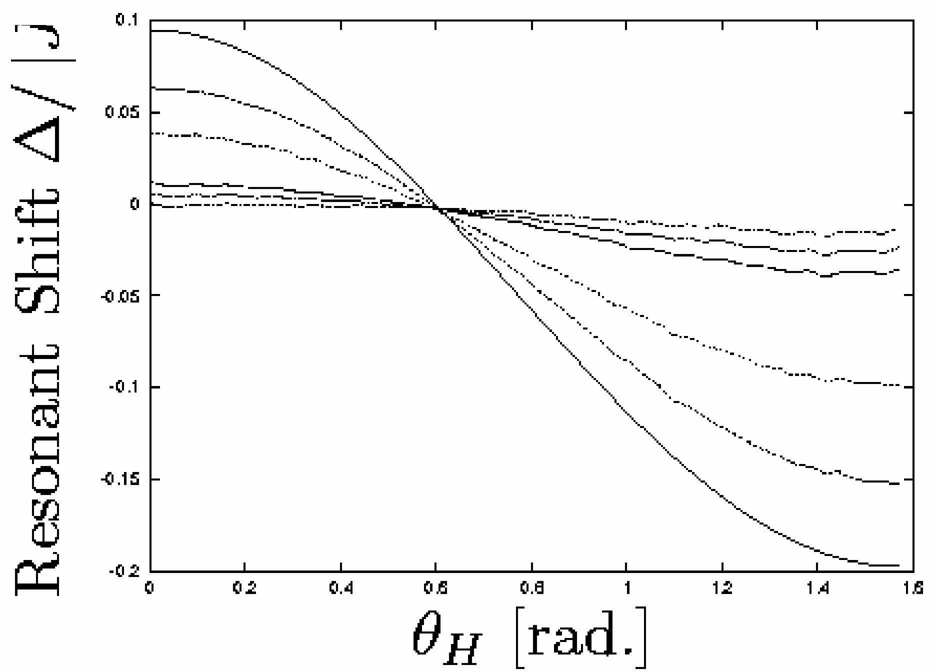
Temperature Dependence



Shift

1D Heisenberg AF

Angle Dependence

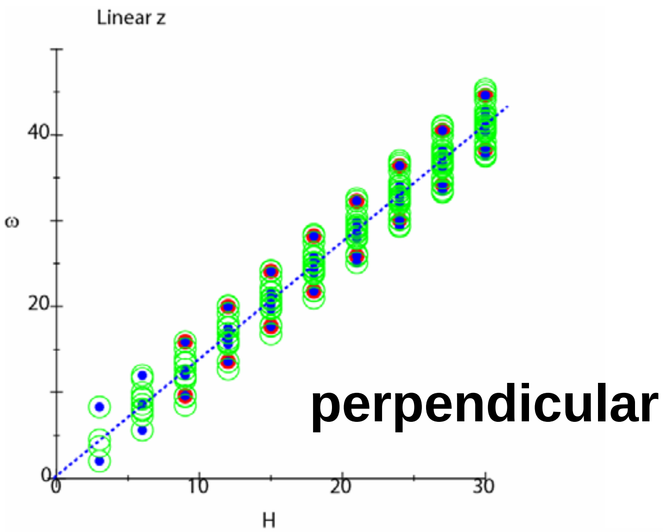


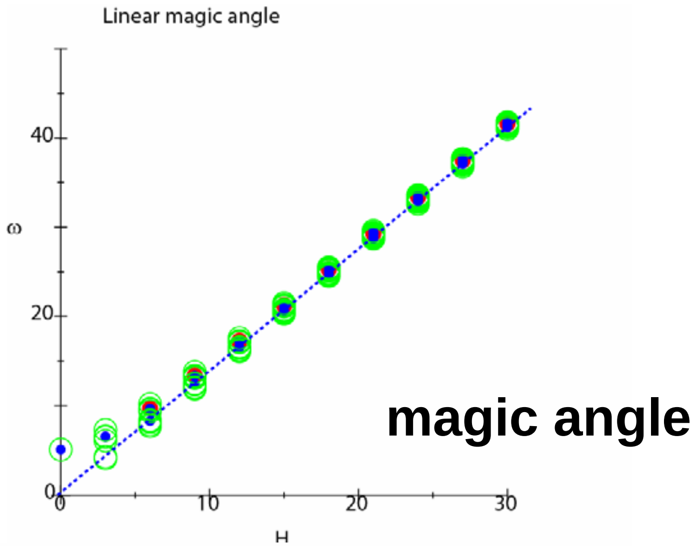
SM, T. Yoshino, A. Ogasahara
JPSJ 68 (1999) 655

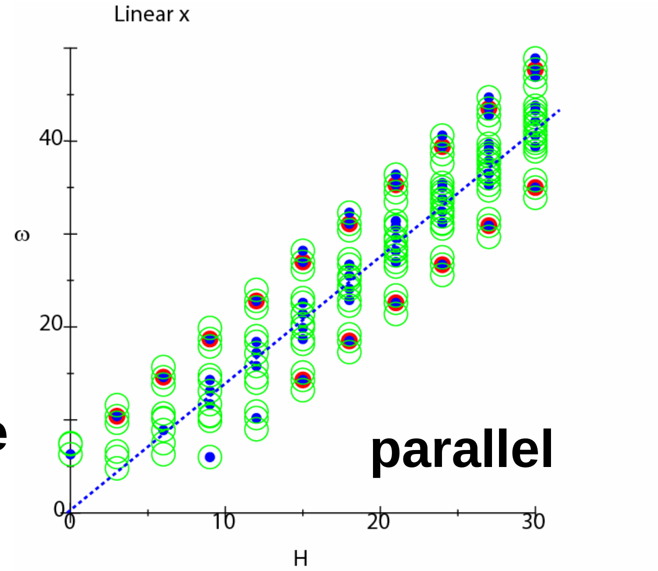
Width

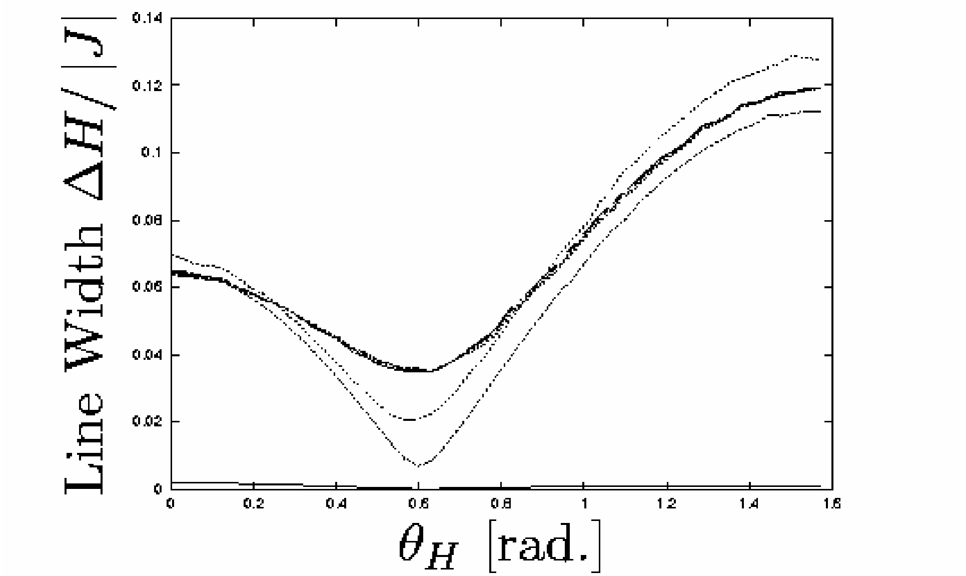
Magic Angle

R.E. Dietz, et al. PRL 26 (1971) 1186.
T.T. Cheung, et al. PRB 17 (1978) 1266



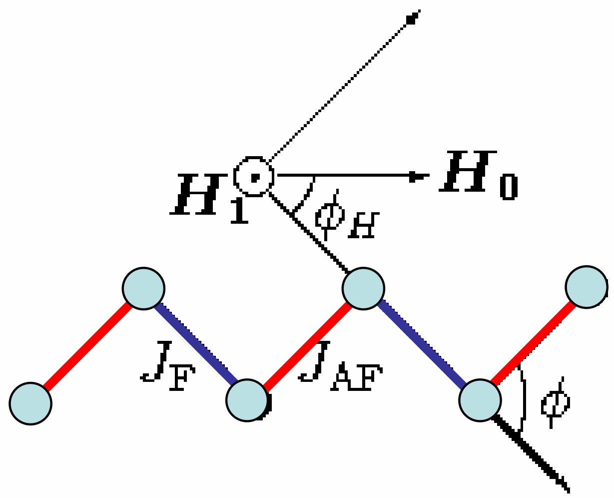




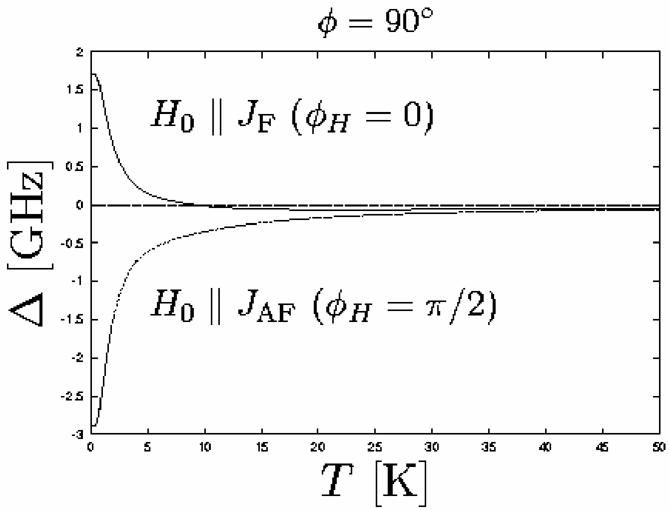


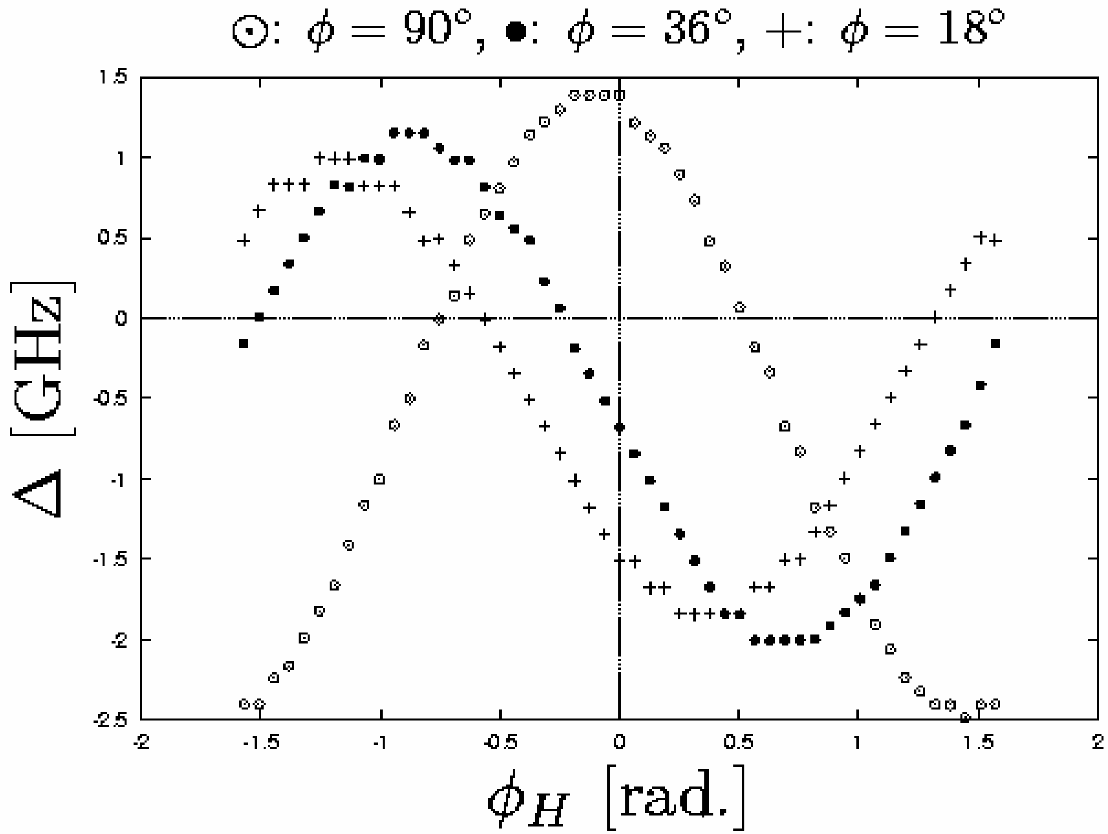
SM, T. Yoshino, A. Ogasahara
JPSJ 68 (1999) 655

Zigzag Chain



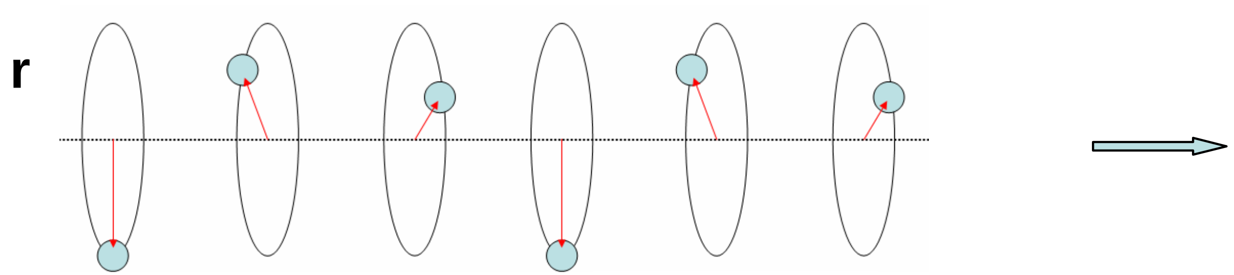
$Cu_{0.9}Zn_{0.1}Nb_2O_6$



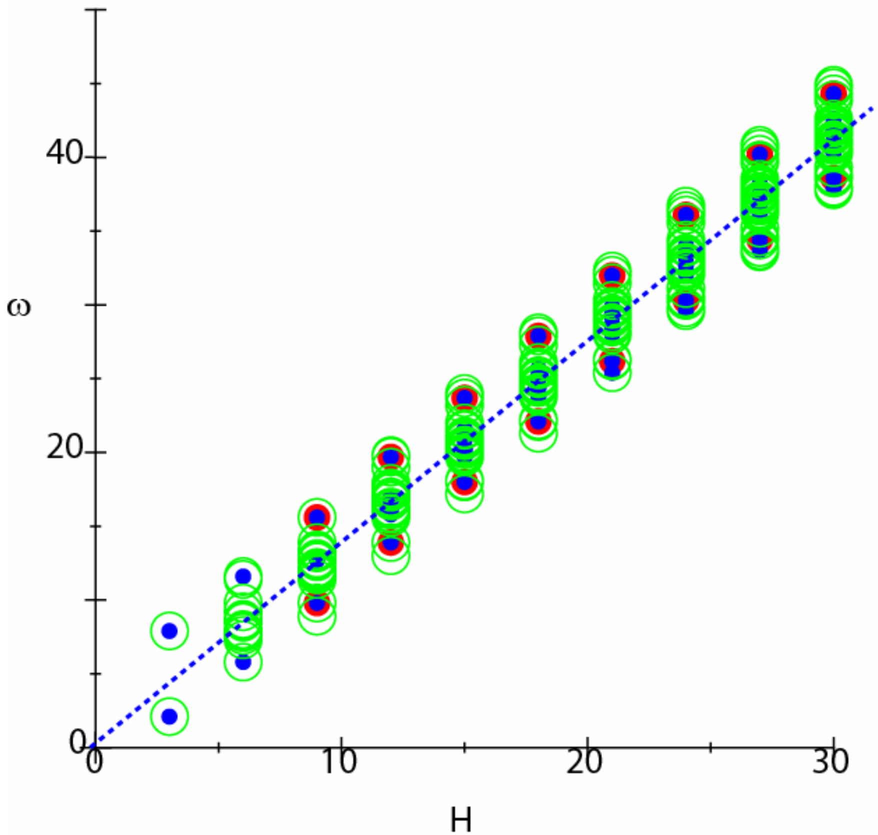


A. Ogasahara and S. Miyashita
J. Phys. Soc. Jpn. Suppl. B 72,44-52 (2003).

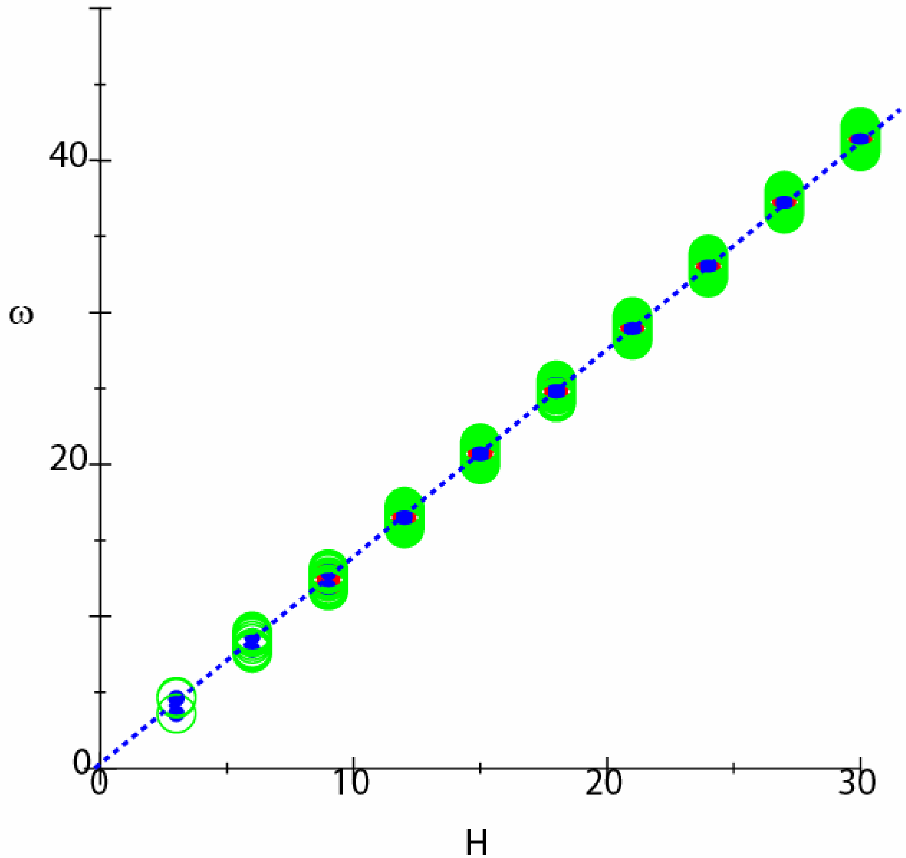
Spiral structure
Dipole-dipole interaction



r=0.1 parallel



r=0.2



Response in dissipative dynamics

$$\chi_{xx}''(\omega) = \frac{1}{2}(1 - \mathrm{e}^{-\beta\omega}) \int_{-\infty}^{\infty} \langle M^x(0) M^x(t) \rangle \, \mathrm{e}^{-i\omega t} dt$$

pure quantum dynamics

$$M^x(t) = e^{iHt/\eta} M^x e^{-iHt/\eta}$$

quantum dynamics with dissipation

Relaxation effects:

I. Solomon: PR 99 (1955) 559.

Relaxation processes in a system of two spins

F. Bloch: PR 105 (1957) 1206.

General theory of relaxation

Y. Hamano and F. Shibata: JPSJ 51 (1982) 1727,2721,2728.

M. Saeki: Prog. Theor. Phys. 67 (1982) 1313. : relaxation method

Prog. Theor. Phys. 115 (2006) 1. : TCLE method

Dissipative dynamics

Quantum Master equation method

$$\chi_{xx}''(\omega) = \frac{1}{2}\left(1 - e^{-\beta\omega}\right)\int_{-\infty}^{\infty}\left\langle M^x(0)M^x(t)\right\rangle e^{-i\omega t}dt$$

quantum dynamics with dissipation

$$M^x(t) = \mathrm{Tr}_B e^{i\left(H_S + H_I + H_B\right)t/\eta} M^x e^{i\left(H_S + H_I + H_B\right)t/\eta}$$

Quantum master equation

$$\frac{d\rho}{dt} = -\frac{i}{\eta}[H, \rho] - \frac{\pi\lambda^2}{\eta}\left([X, R\rho] + [X, R\rho]^+\right)$$

F. Bloch: PR 105 (1957) 1206.

S. Nakajima: PTP 20 (1958) 987, R. Zwanzig: J. Chem. Phys. 33 (1960) 1338.

A. G. Redfield: Adv. Magn. Reson. 1 (1965) 1.

H. Mori: PTP 33 (1965) 423. M. Tokuyama and H. Mori: PTP 55 (1976) 411.

N. Hashitsume, F. Shibata and M. Shingu: J. Stat. Phys. 17 (1977) 155 & 171.

T. Arimitsu and H. Umezawa: PTP 77 (1987) 32.

Formulation of line-shape with dissipative dynamics

$$\langle A(t)A\rangle = \mathrm{Tr}\, e^{iHt/\eta} A e^{-iHt/\eta} A\rho(t_0) = \mathrm{Tr} A e^{-iHt/\eta} A\rho(t_0) e^{iHt/\eta}$$

cf. $$\rho(t+t_0) = e^{-iHt/\eta}\rho(t_0)e^{iHt/\eta}$$

$$\frac{\partial}{\partial t}\rho = \frac{1}{i\eta}[H,\rho] - \gamma\left([X, R(t), \rho] + [X, R(t), \rho]^{+}\right) \equiv L\rho$$

K. Saito, S. Takesue and SM.
Phys. Rev. B61 (2000) 2397.

$$\frac{\partial}{\partial t}[A\rho(t_0)](t) = L\,[A\rho(t_0)]$$

$$[A\rho(t_0)](t) = \mathrm{e}^{Lt}[A\rho(t_0)](0)$$

Eigenmode of time-evolution operator

$$\frac{\partial}{\partial t}\rho = \frac{1}{i\eta}[H,\rho] - \gamma\left([X, R(t), \rho] + [X, R(t), \rho]^{+}\right)$$

matrix $\rho(i, j)$, $(i, j = 1, \Lambda\ N)$

vector $\vec{\rho}$, $(\rho(k), k = 1, \Lambda\ N^2)$

$$\frac{\partial}{\partial t}\vec{\rho}(t) = L\vec{\rho}(t) \qquad \vec{\rho}(t) = \mathrm{e}^{Lt}\vec{\rho}(0)$$

$$L\vec{\phi}_m = i\varepsilon_i\vec{\phi}_m$$

$$\vec{\phi}_m(t) = e^{i\varepsilon_i t}\vec{\phi}_m$$

$$\boxed{\vec{\rho}(t) = \sum_m c_m e^{i\varepsilon_i t}\vec{\phi}_m,} \qquad \left[\vec{\phi}_1, \vec{\phi}_2 \Lambda\ \vec{\phi}_M\right]\vec{c} = \vec{\rho}(0)$$

I. Knezevic and D. K. Ferry: Phys. Rev. E66(2003) 016131,
Phys. Rev.A 69 (2004) 012104.
S. Miyashita and K. Saito: Physica B 329-333 (2003) 1142.

Explicit form of the autocorrelation

$$[A\vec{\rho}(t_0)](t) = \sum_m c_m e^{i\varepsilon_i t}\vec{\phi}_m \qquad \left[\vec{\phi}_1, \vec{\phi}_2 \Lambda\ \vec{\phi}_M\right]\vec{c} = [A\vec{\rho}(t_0)]$$

$$\langle A(t)A\rangle = \sum_{ik}^{M} A_{ik}\left([A\vec{\rho}(t_0)](t)\right)_{ki} = \sum_{ik}^{M} A_{ik}\sum_m^{M^2} c_m\left(e^{i\varepsilon_i t}\vec{\phi}_m\right)_{M(k-1)+i}$$

$$\int_0^\infty \langle A(t)A\rangle e^{-i\omega t}dt = \sum_{ik}^{M}\ \sum_m^{M^2}\frac{1-e^{i(\varepsilon_i-\omega)\infty}}{i(\varepsilon_i-\omega)} A_{ik}c_m\left(\vec{\phi}_m\right)_{M(k-1)+i}$$

$$= -i\sum_{ik}^{M}\ \sum_m^{M^2}\frac{1}{(\varepsilon_i-\omega)} A_{ik}c_m\left(\vec{\phi}_m\right)_{M(k-1)+i}$$

Line shape

$$\chi_{AA} = \int_0^\infty \frac{i}{\eta}\left[\langle A(t)A\rangle - \langle AA(t)\rangle\right] e^{-i\omega t}dt$$

$$\int_0^\infty \langle AA(t)\rangle e^{-i\omega t}dt = -i\sum_{ik}^{M}\ \sum_m^{M^2}\frac{1}{(\varepsilon_i-\omega)} A_{ik}d_m\left(\vec{\phi}_m\right)_{M(k-1)+i}$$

$$\mathrm{Im}(\chi_{AA}) = \mathrm{Re}\sum_{ik}^{M}\ \sum_m^{M^2}\frac{1}{(\varepsilon_i-\omega)} A_{ik}(c_m-d_m)\left(\vec{\phi}_m\right)_{M(k-1)+i}$$

Paramagnetic Resonance

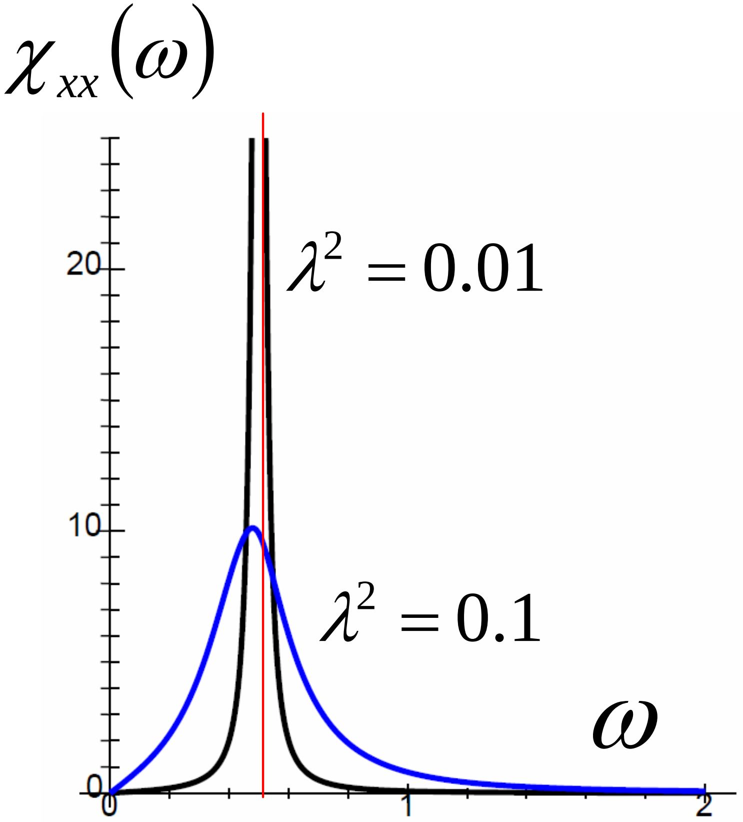
$$H = -H\sum_i S_i^z$$

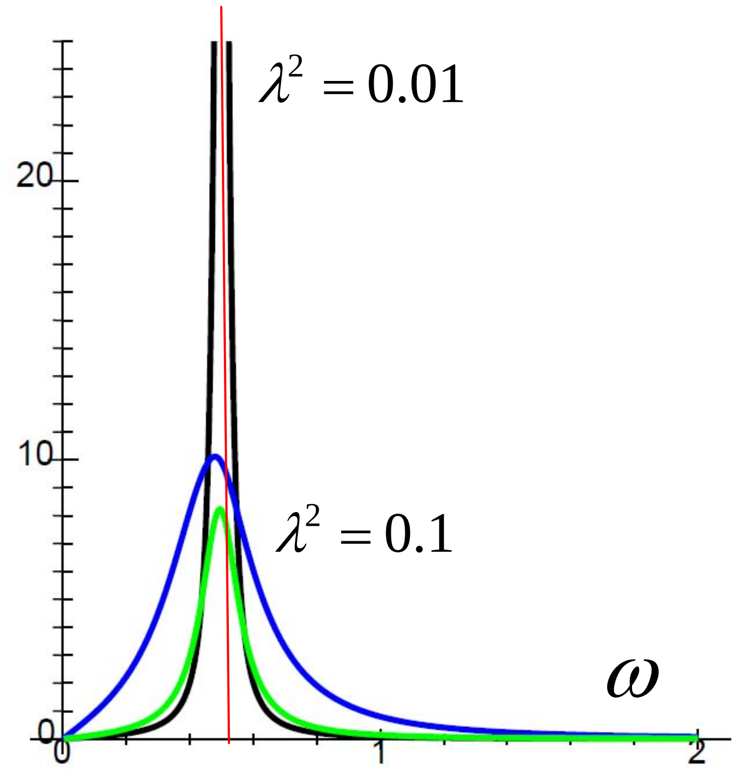
$$X = \sum_i \alpha_i S_i^x + \beta_i S_i^y + \gamma_i S_i^z$$

$$\Phi(\omega) = \frac{I_0\omega^2}{\left|e^{\beta\omega} - 1\right|} = e^{-\beta\omega}\Phi(-\omega)$$

Exchange narrowing

$$H = -H\sum_i S_i^z + J\sum_i \vec{S}_i \cdot \vec{S}_j$$

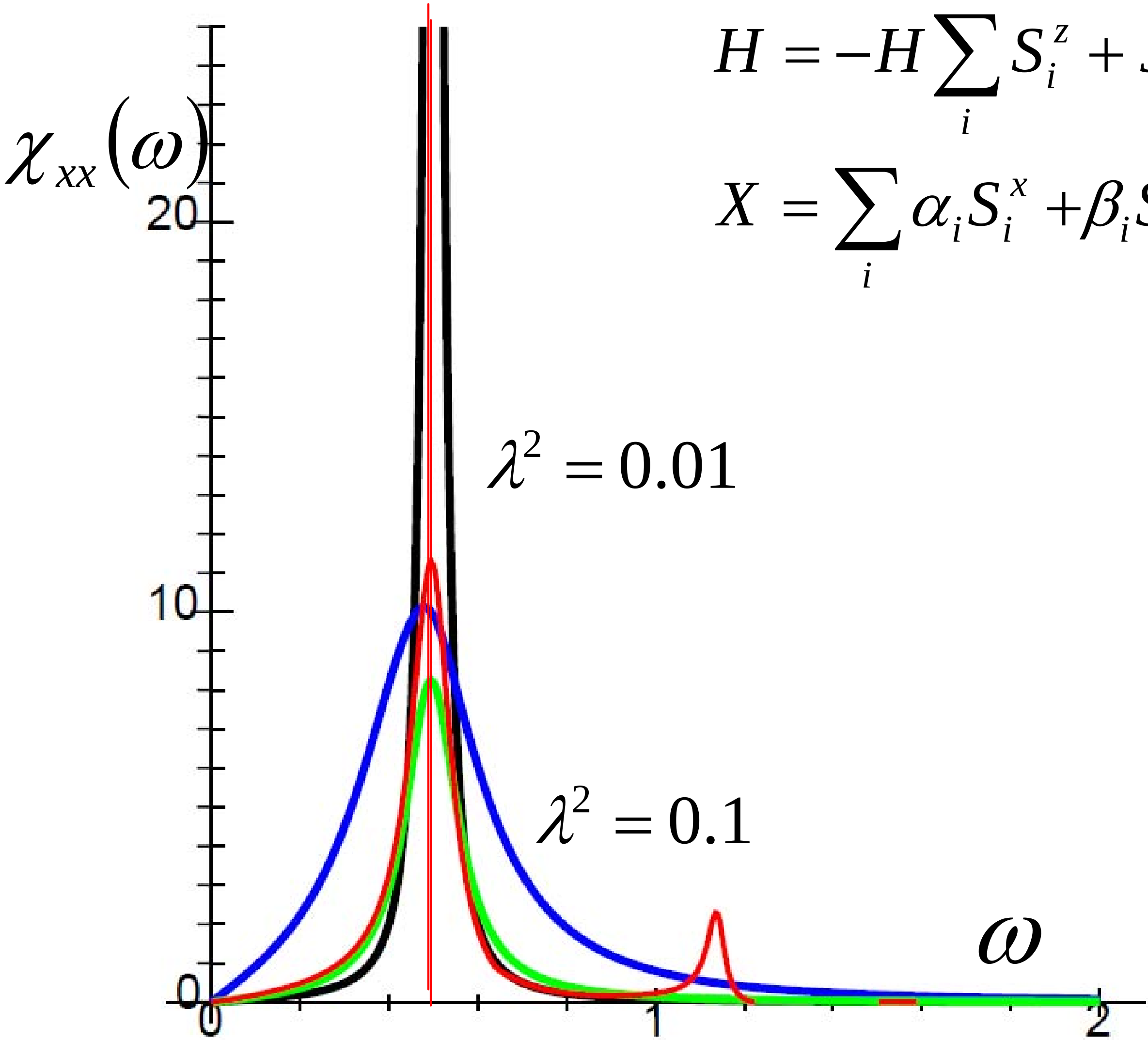




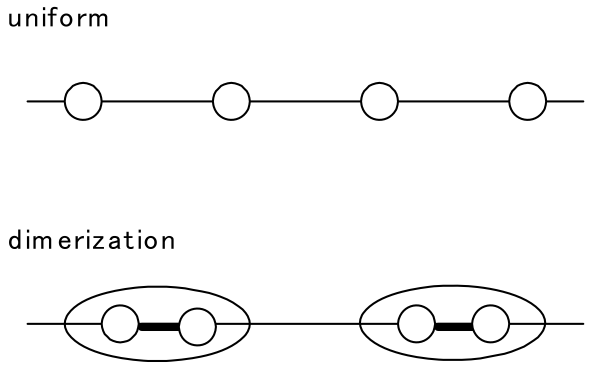
Dipole-dipole interaction

$$H = -H\sum_i S_i^z + J\sum_i \vec{S}_i \cdot \vec{S}_j + \mathrm{DD}$$

$$X = \sum_i \alpha_i S_i^x + \beta_i S_i^y + \gamma_i S_i^z$$

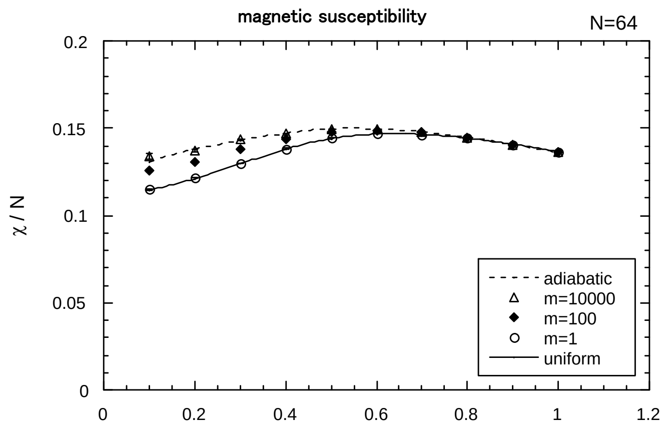


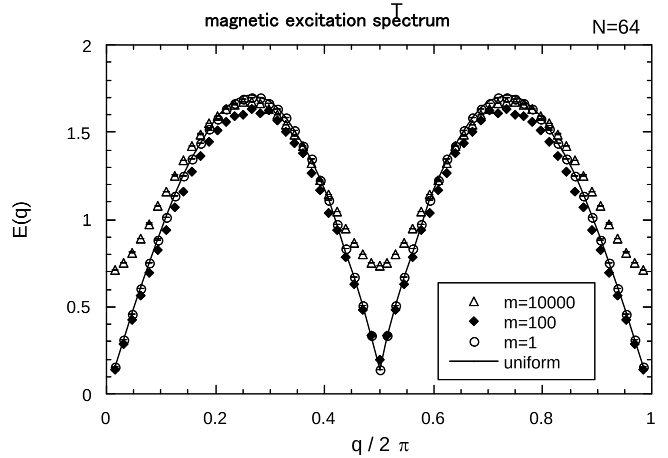
(Motional narrowing)
Quantum narrowing effect



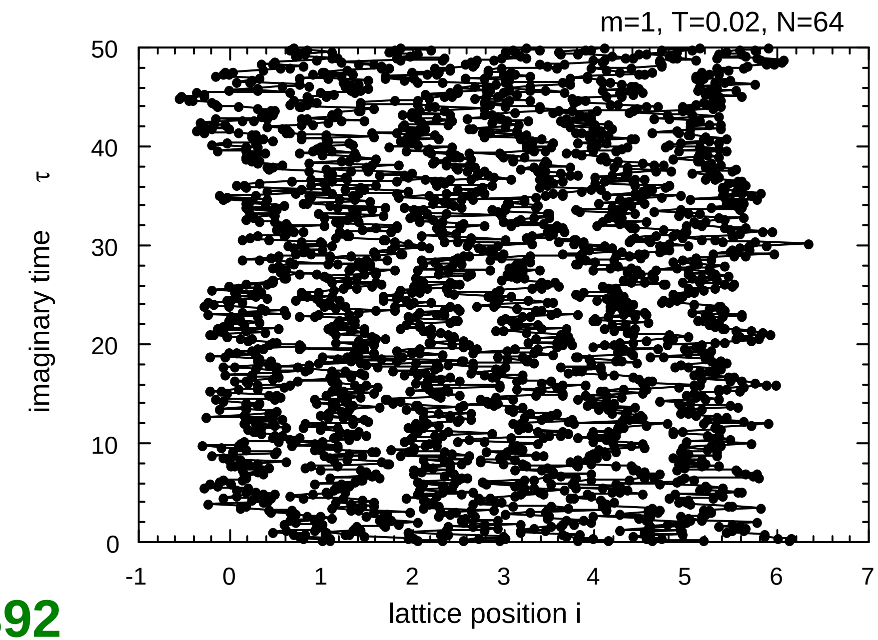
Spin-Peierls systems

$$H=\sum_{i=1}^{N} J[1+\alpha(u_{i+1}-u_i)]\mathbf{S}_i\cdot\mathbf{S}_{i+1}+\sum_{i=1}^{N}\left[\frac{1}{2m}p_i^2+\frac{k}{2}(u_{i+1}-u_i)^2\right]$$





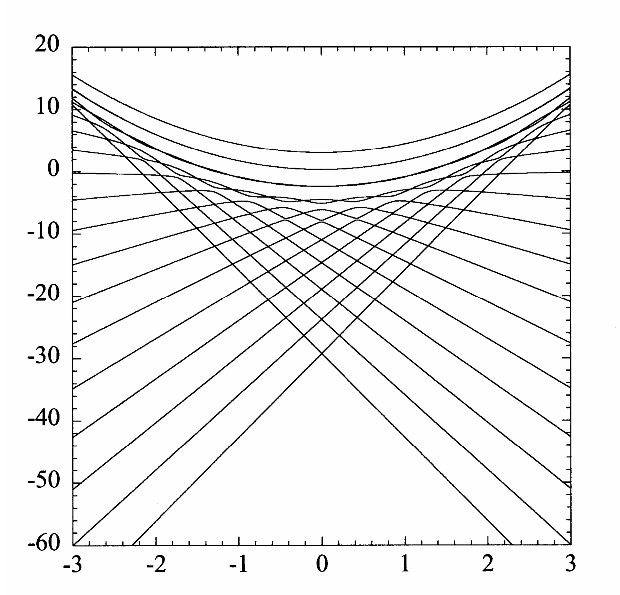
- effects of quantum lattice fluctuation becomes small when m small



H. Onishi and SM: JPSJ 72(2003) 392

Origin of the adiabatic change

S: even Large S (S=10) Mn12, Fe8

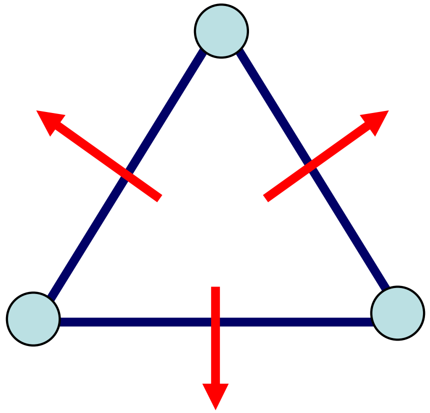


$$H = -D(S^z)^2 - hS^z + E((S^x)^2 - (S^y)^2) + C((S^+)^4 - (S^-)^4) + \text{etc.}$$

S: odd (S=1/2) V15 No anisotropy & Kramers doublet

Dzyloshinskii-Moriya interaction

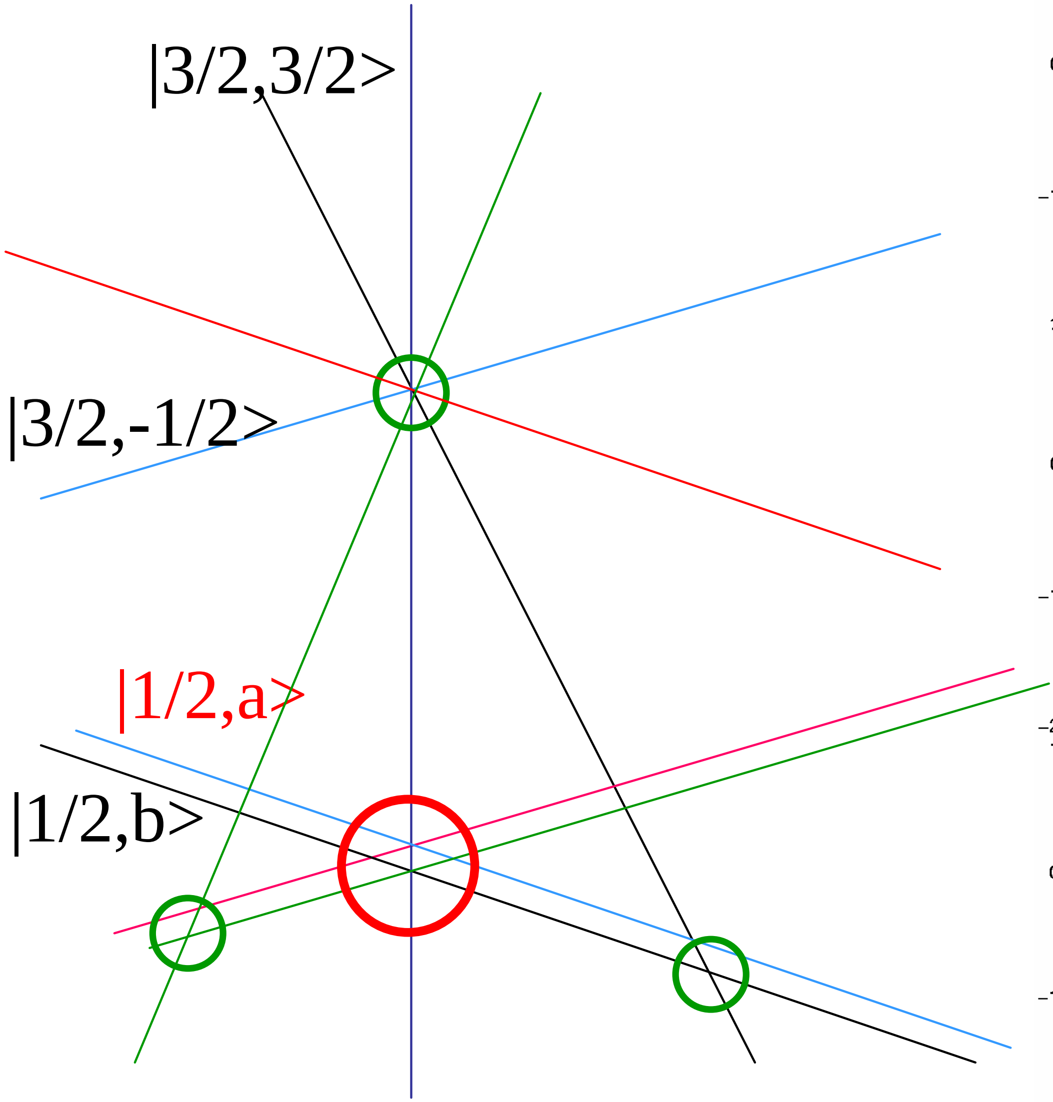
$$H_{\mathrm{D}} = \sum_{ij} \vec{D}_{ij} \left(\vec{S}_i \times \vec{S}_j \right)$$

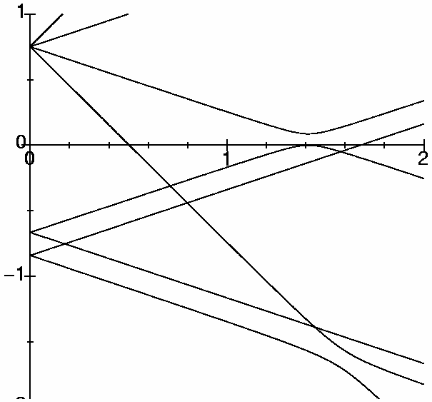


SM, &. N. Nagaosa, Prog. Theor. Phys. 106 (2001) 533

Energy structure with DM

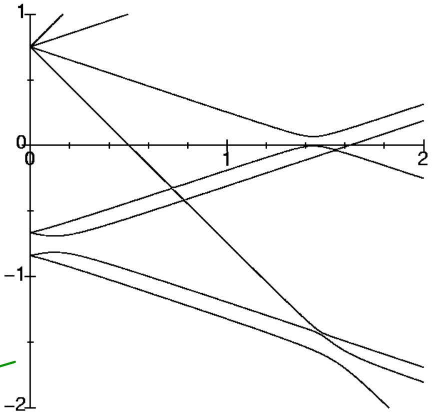
Anisotropy of DM interaction



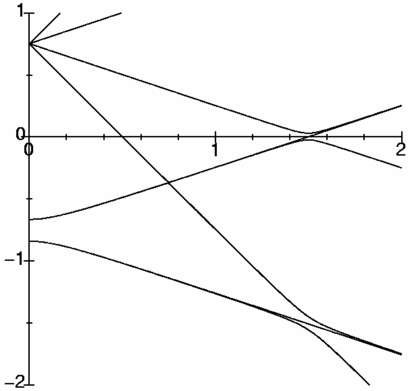


$\theta = 0^o$

No adiabatic change at H=0



$\theta = 45^o$

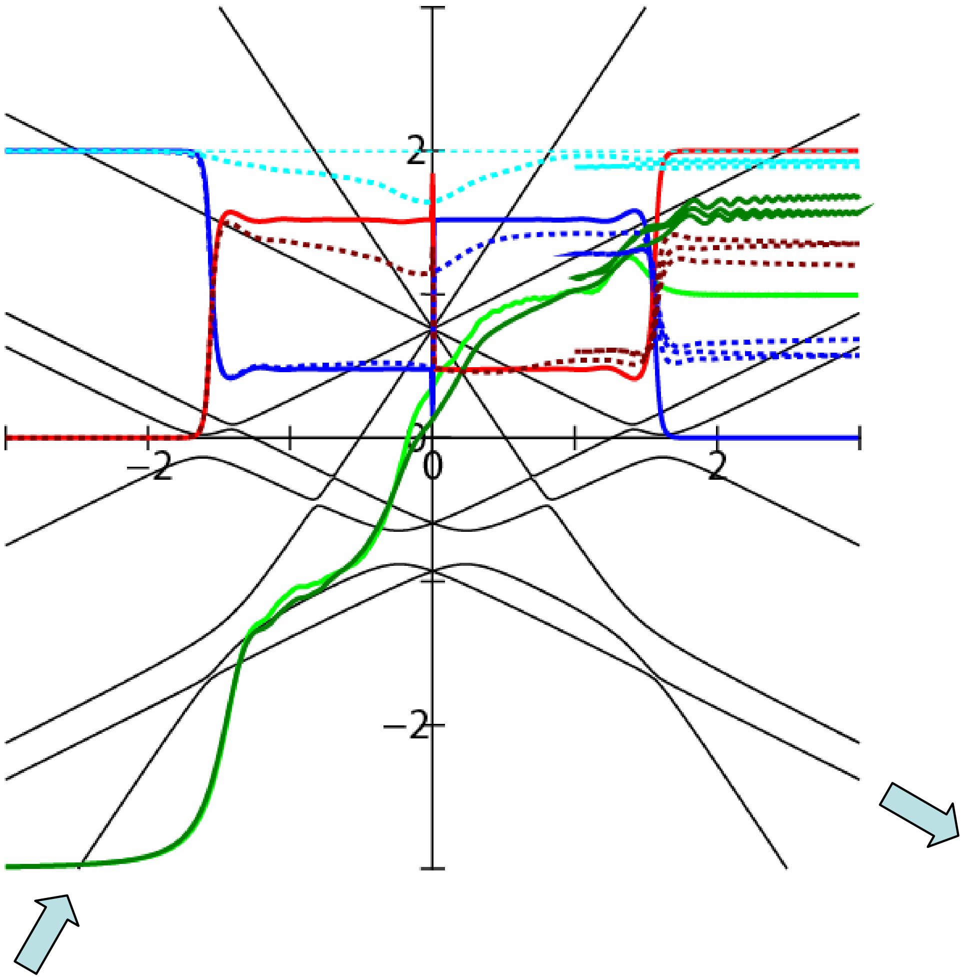


$\theta = 90^o$

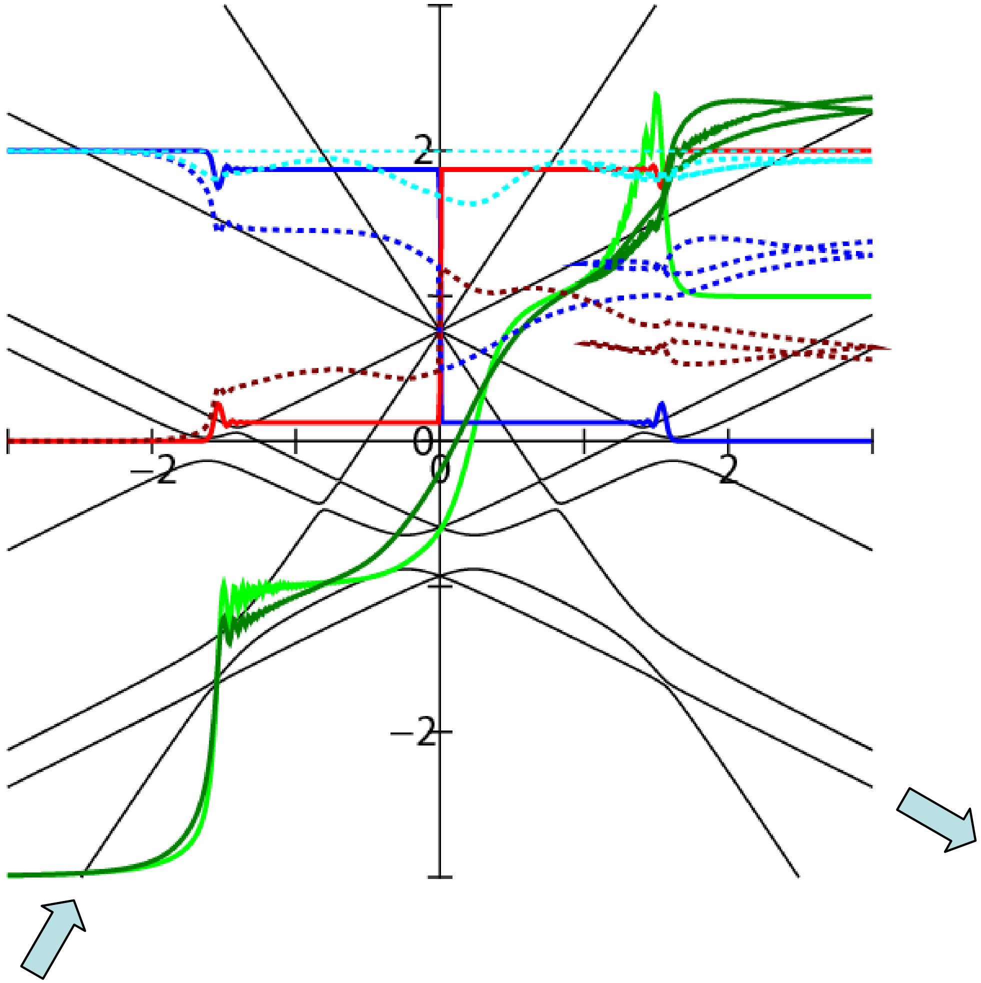
I.Chiorescu, W. Wernsdorfer, A. Mueller, SM, and B. Barbara: PRB 67 (2003) 020402

H. De Raedt, SM, K. Michielsen & M. Machida: PRB 70 (2004) 064401

Nontrivial coherence

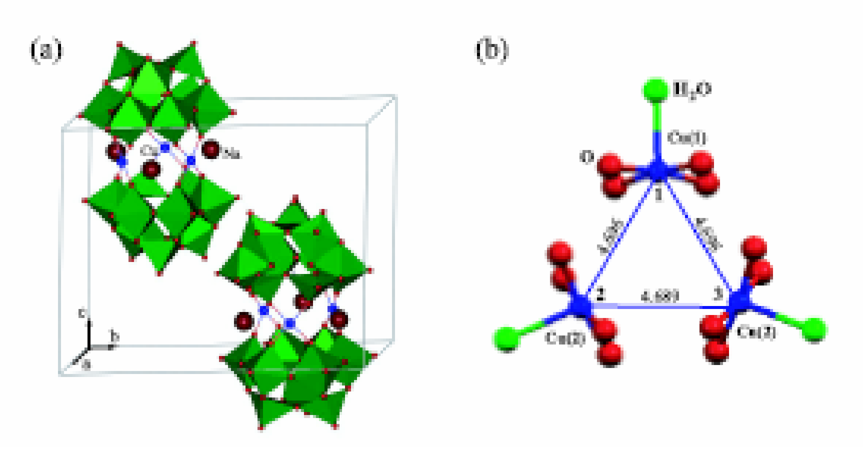


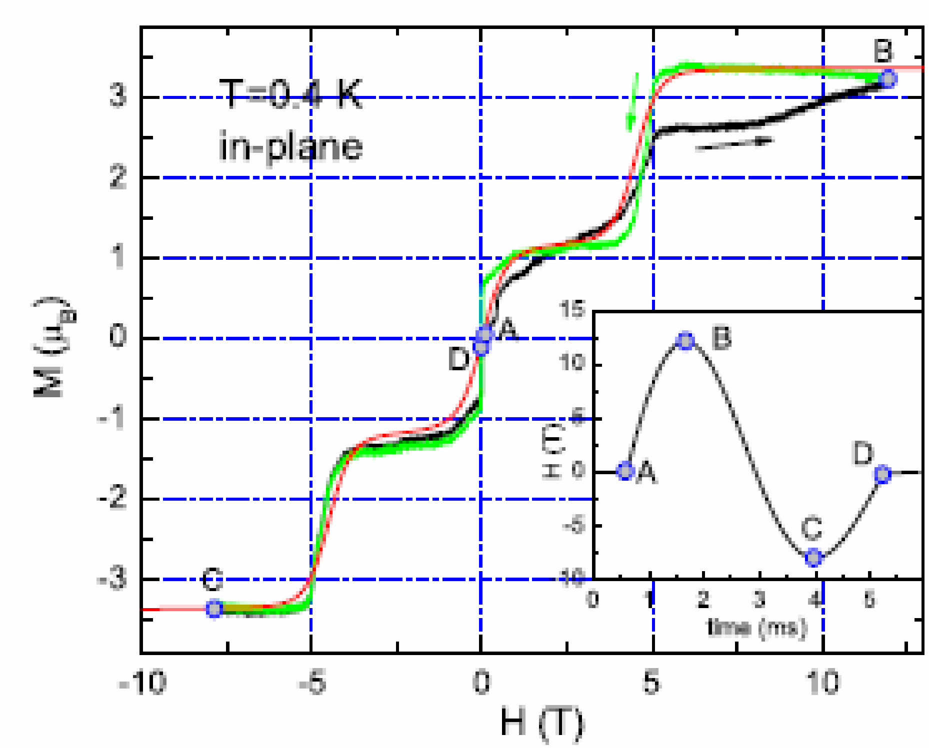
V=0.01

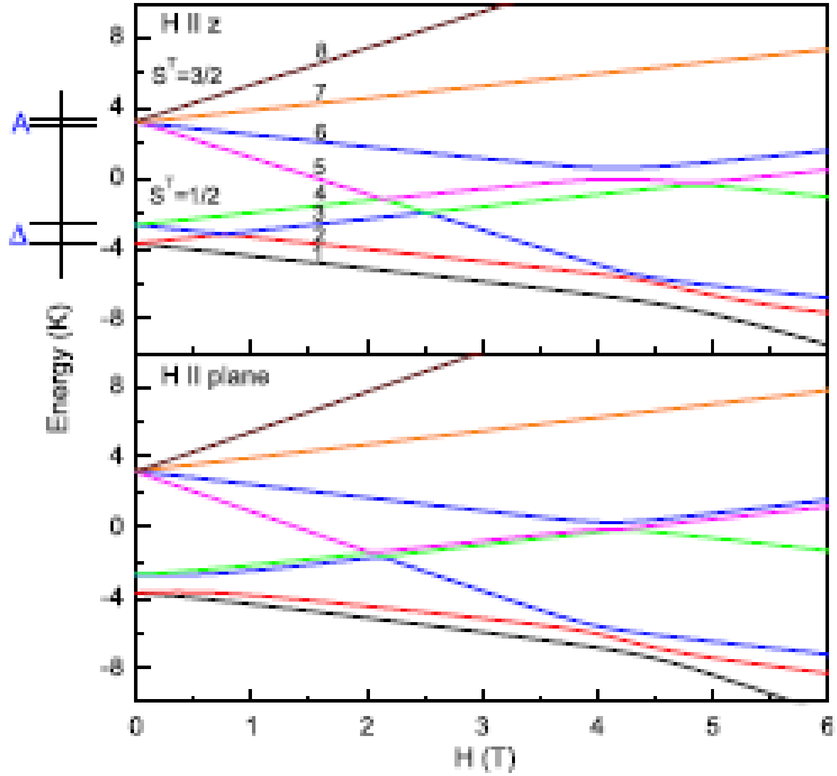


V=0.001

Cu3







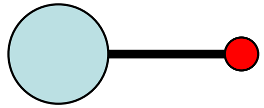
K.Y. Choi, et al. PRL 96 (2006) 107202

$$\mathcal{H} = \sum_{l=1}^{3} \sum_{\alpha=x,y,z} J_{ll+1}^{\alpha} \mathbf{S}_l \cdot \mathbf{S}_{l+1} + \sum_{l=1}^{3} \mathbf{D}_{ll+1} \cdot [\mathbf{S}_l \times \mathbf{S}_{l+1}] + \mu_B \sum_{l=1}^{3} \mathbf{S}_l \cdot \tilde{\mathbf{g}}_{ll} \cdot \mathbf{H}_l,$$

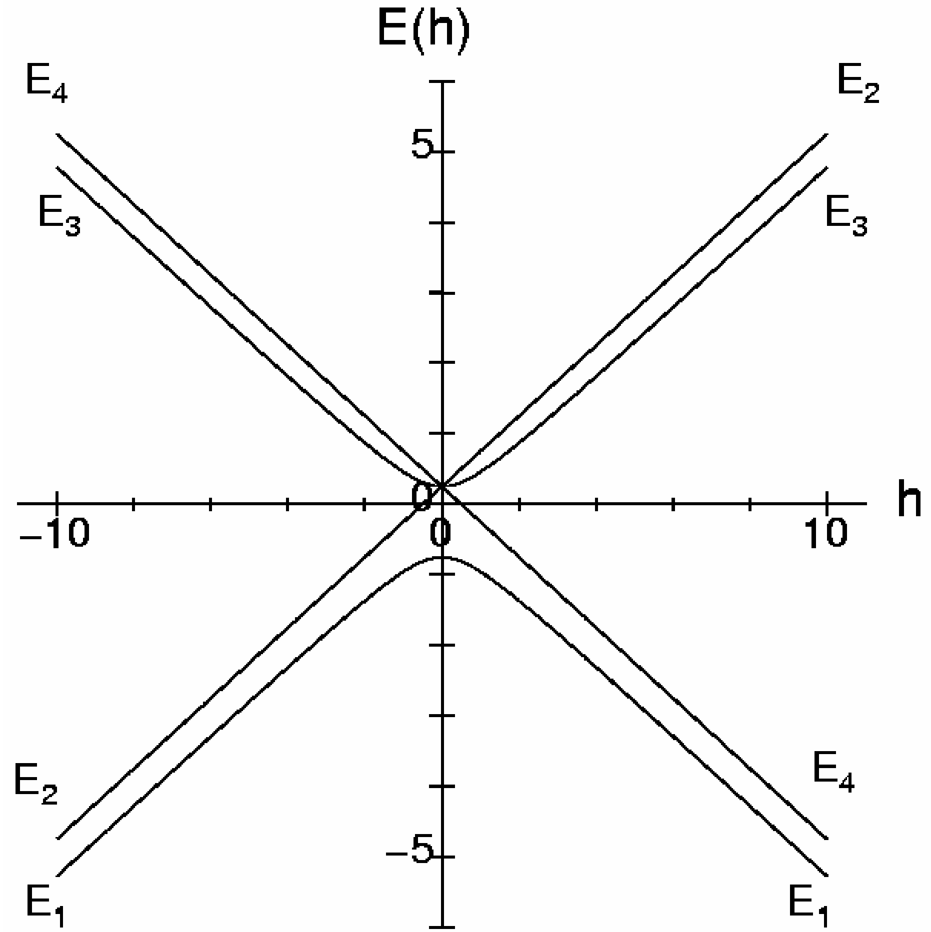
H. De Raedt, SM, K. Michielsen,
M. Machida: PRB 70 (2004) 064401

Directionally independent energy gap due to Hyperfine interaction

$$H = -A\vec{S}\cdot\vec{\sigma} - (g\mu_B S^z + g'\mu_{NB}\sigma^z)h$$



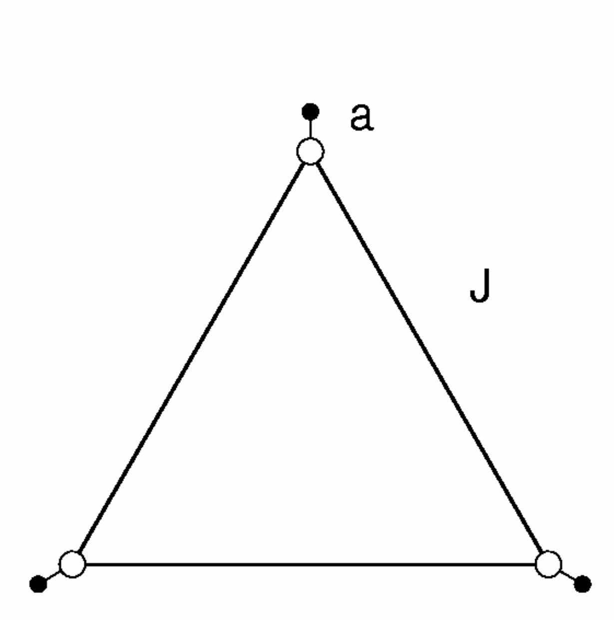
$$\begin{aligned}
E_1 &= -\tfrac{1}{4}a - \tfrac{1}{2}\sqrt{a^2 + h^2} \\
E_2 &= \tfrac{1}{4}a + \tfrac{1}{2}h \\
E_3 &= -\tfrac{1}{4}a + \tfrac{1}{2}\sqrt{a^2 + h^2} \\
E_4 &= \tfrac{1}{4}a - \tfrac{1}{2}h.
\end{aligned}$$

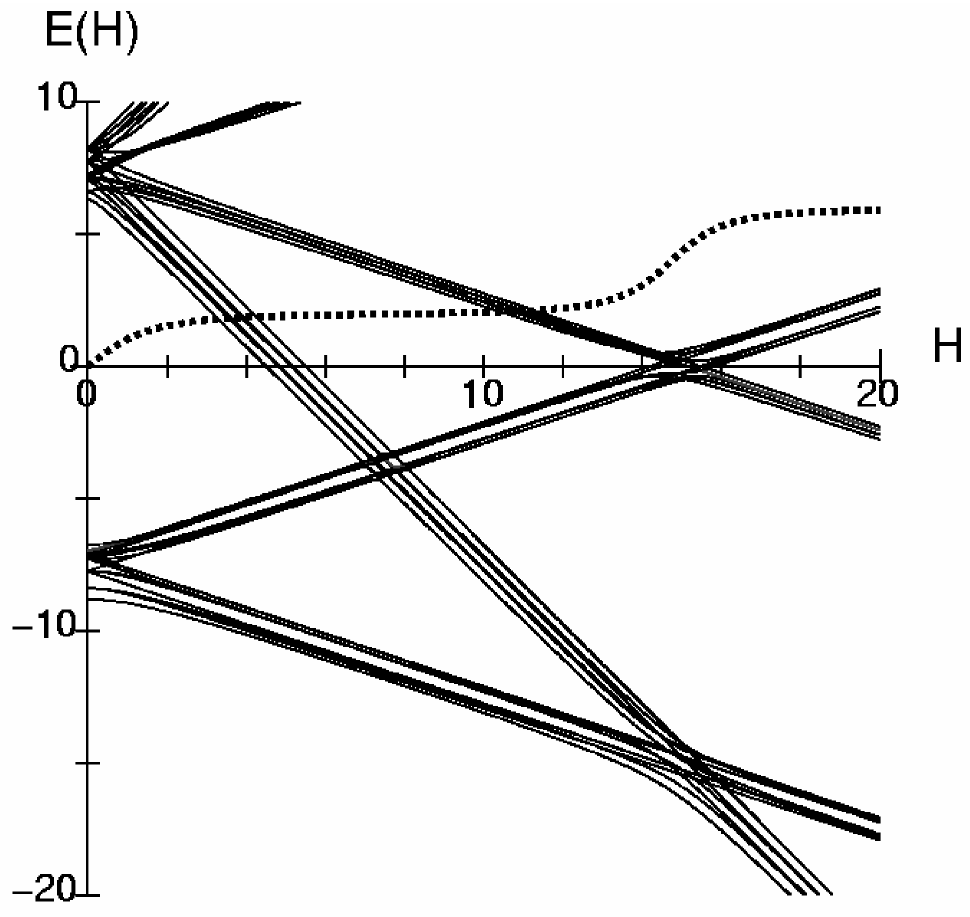


SM, H.de Raedt and K. Michielsen:
Prog. Thor. Phys.. 110 (2003) No.11

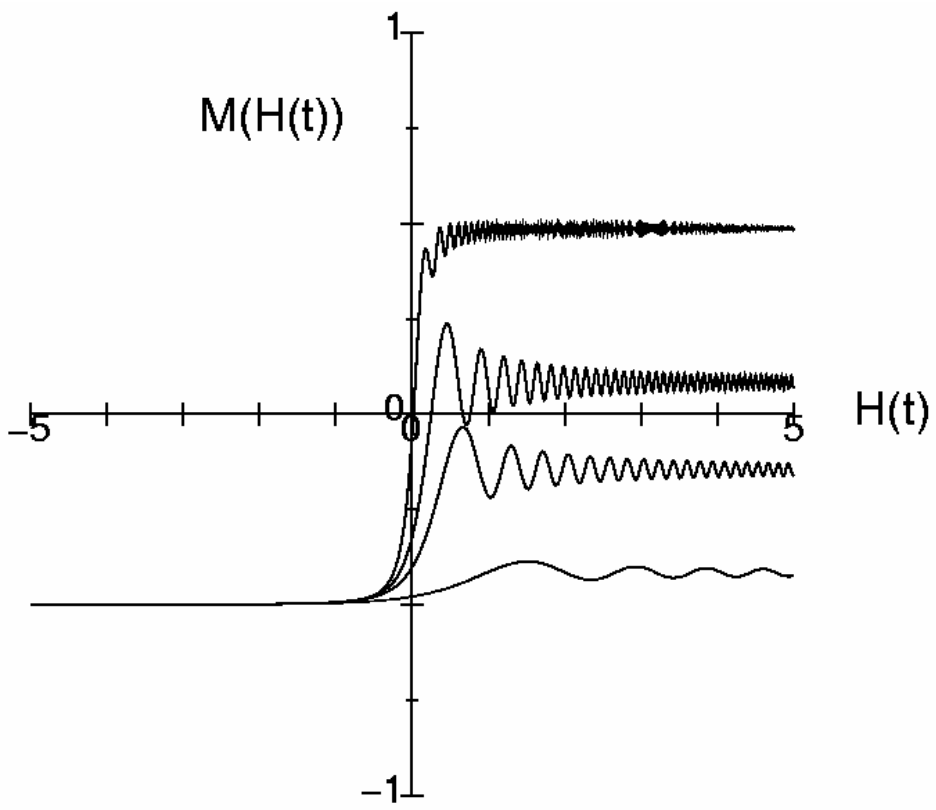
Triangle case

$$H = -A\vec{S}\cdot\vec{\sigma} - (g\mu_B S^z + g'\mu_{NB}\sigma^z)h$$





M(t) from the ground state



$$P = \left| \langle G(H_0) | \Psi(t_f) \rangle \right|^2$$

$$\Delta E = \sqrt{-2v \log(1-P)/\pi}$$

v	P	ΔE
0.500	0.08371	0.16681
0.250	0.16067	0.16697
0.100	0.35481	0.16702
0.050	0.58378	0.16704
0.025	0.82678	0.16704
0.010	0.98751	0.16704

Apparent LZS relation

Gap control using hidden symmetries

Transverse field

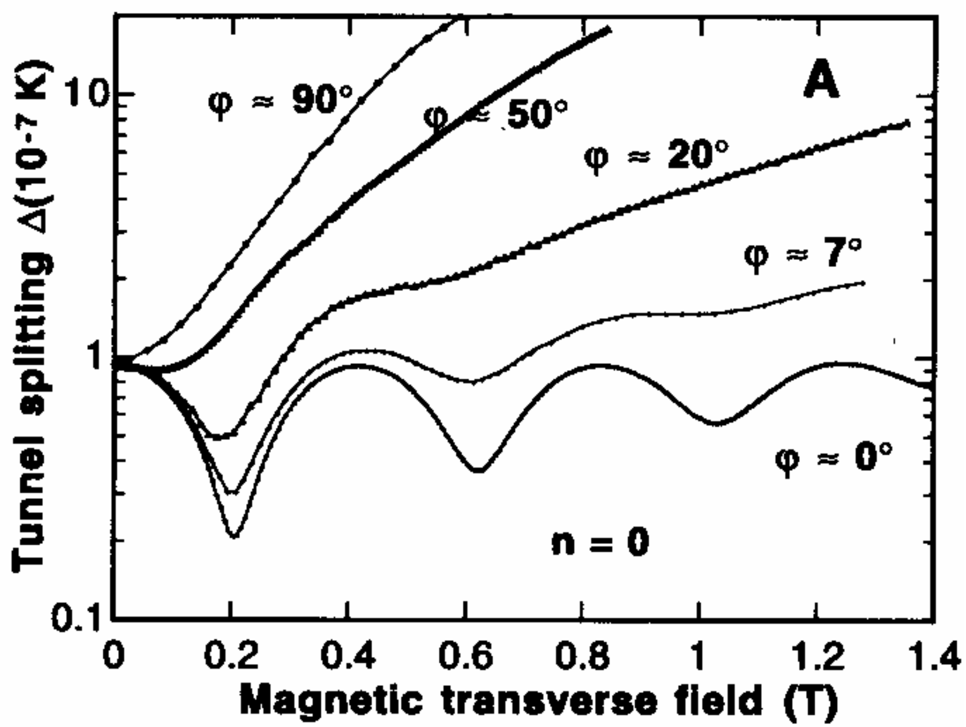
$$H = -DS_z^2 - h_x S_x \Rightarrow \Delta E \propto h_x^{|m-m'|}$$

Nontrivial control

$$H = -DS_z^2 + E(S_x^2 - S_y^2) + C\left((S^+)^4 + (S^-)^4\right) - h_x S_x$$

Quantum interference
Berry phase

W.Wernsdorfer & R. Sessoli:
Science 284 (1999) 133



Non-monotonic gap due to Hx

$$H = -DS_z^2 + 2E\left(S_x^2 - S_y^2\right) + C\left(S_+^4 + S_-^4\right) - \vec{H}(t)\cdot\vec{S}$$

$$E = 0.5D, \quad C = 0$$

$$H = -D\left(S_z^2 - S_x^2 + S_y^2\right) - H_x S_x$$

$$= 2DS_x^2 - H_x S_x - DS(S+1)$$

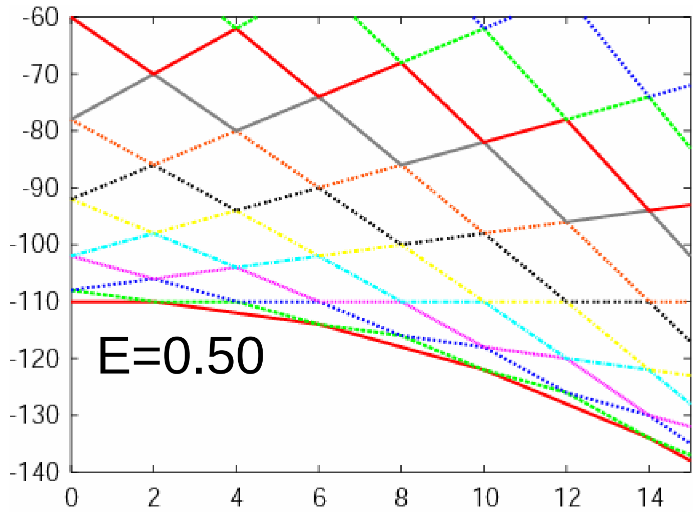
$$E = (0.5+\delta)D, \quad C = 0$$

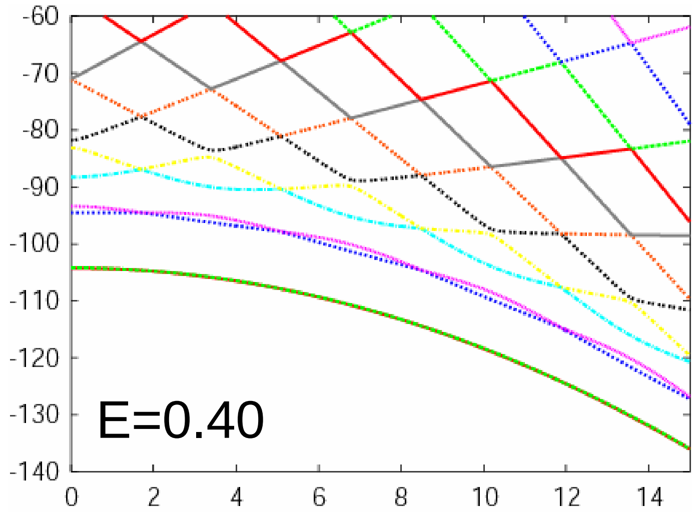
$$H = 2(D+\delta)S_x^2 - H_x S_x - 2\delta S_y^2$$

$$\Delta M_x = 0, \pm 2$$

Gaps open at

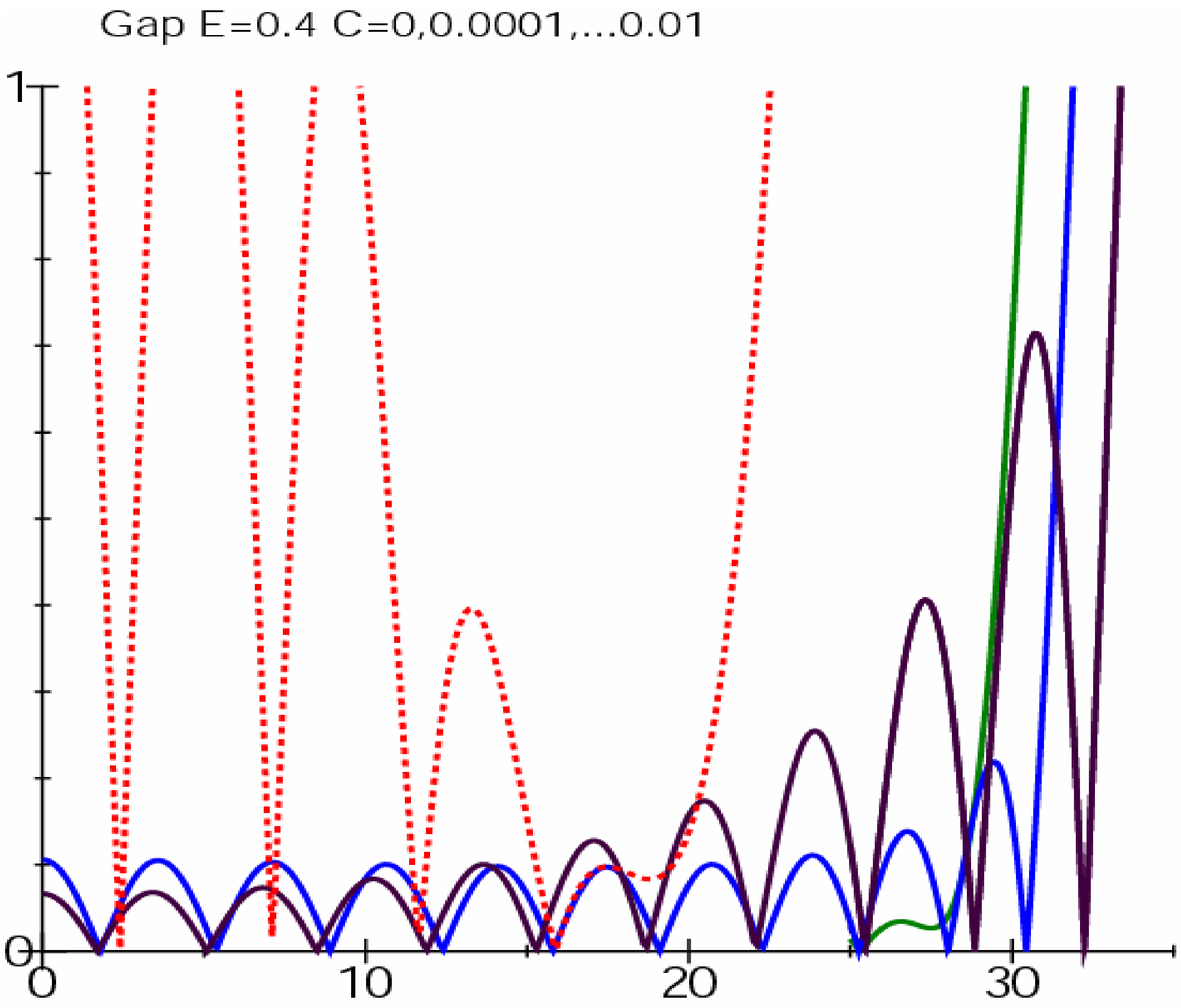
crossing remain at (M,M+1) etc. => 2S crossings



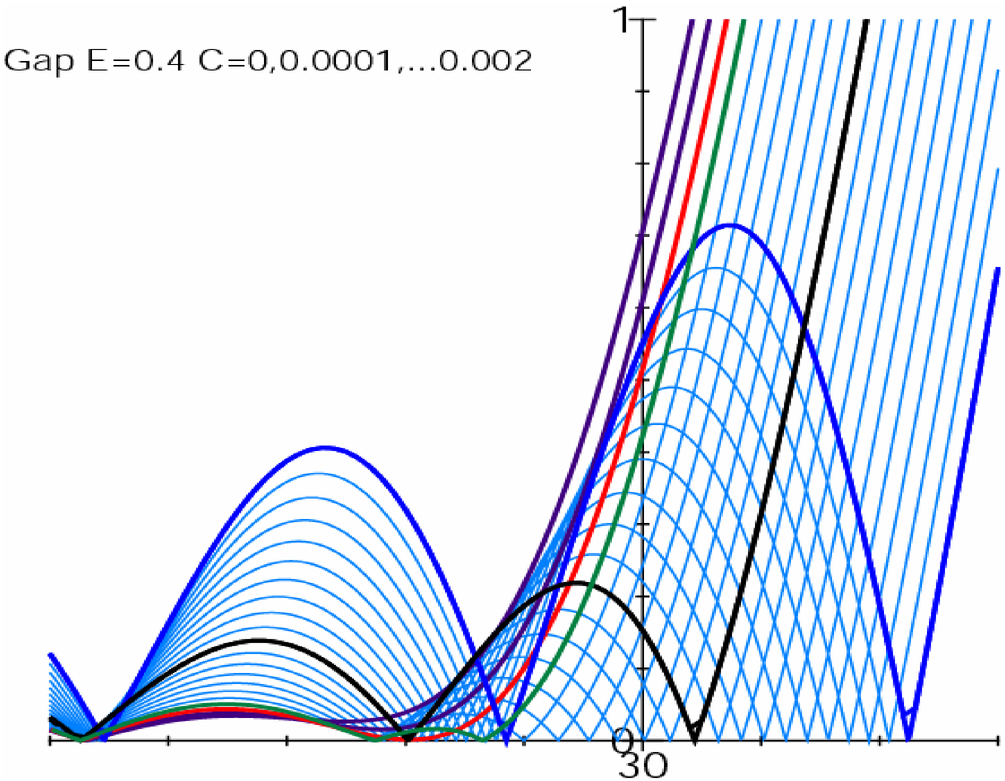


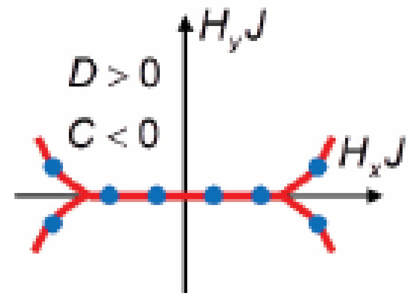
Gap with the C term

$$H = -DS_z^2 + 2E\left(S_x^2 - S_y^2\right) + C\left(S_+^4 + S_-^4\right) - \vec{H}(t)\cdot\vec{S}$$

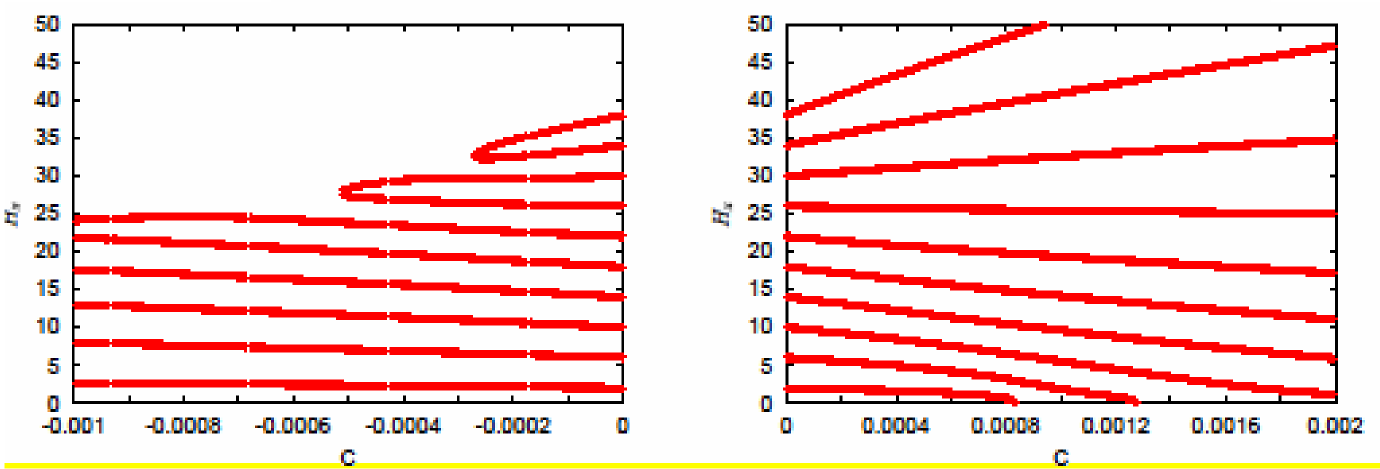


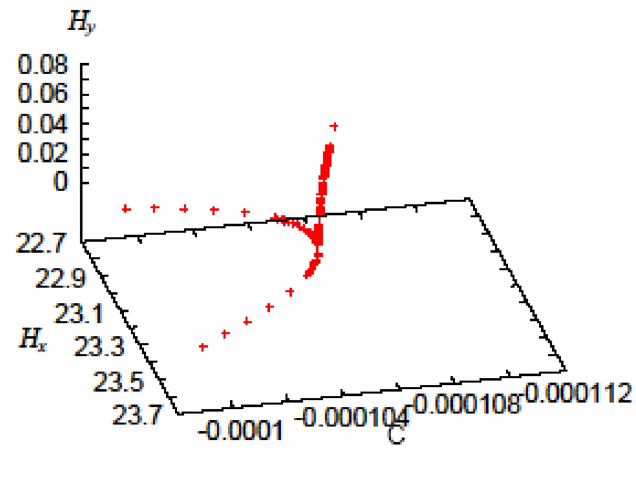
Collapse of degeneracy?





P. Bruno: PRL 96 (2006) 117208





Temporal symmetry-breaking induced DM interaction

NaV2O5 : charge fluctuation reduces the symmetry
=> virtual DM ESR

Nojiri, et al.: JPSJ 69 (2000) 2291

Fe12 : configuration fluctuation reduces the symmetry
=> virtual DM M(H)

H. Nakano and SM: JPSJ 71 (2002) 2580

SrCu2(BO3)2 : configuration fluctuation reduces the symmetry => Raman,ESR

Cepas and Zimann cond-mat 0401240
SM & Ogasahara: JPSJ 72 (2003) 2350

Charge transfer, Phonon,
Orbital degree of freedom, etc.

Fluctuating DM interaction model

$$H = J\vec{S}_1 \cdot \vec{S}_2 + \vec{d} \cdot \left(\vec{S}_1 \times \vec{S}_2\right) + H\left(S_1^z + S_1^z\right) + \frac{k}{2}x^2 + \frac{1}{2m}p^2$$

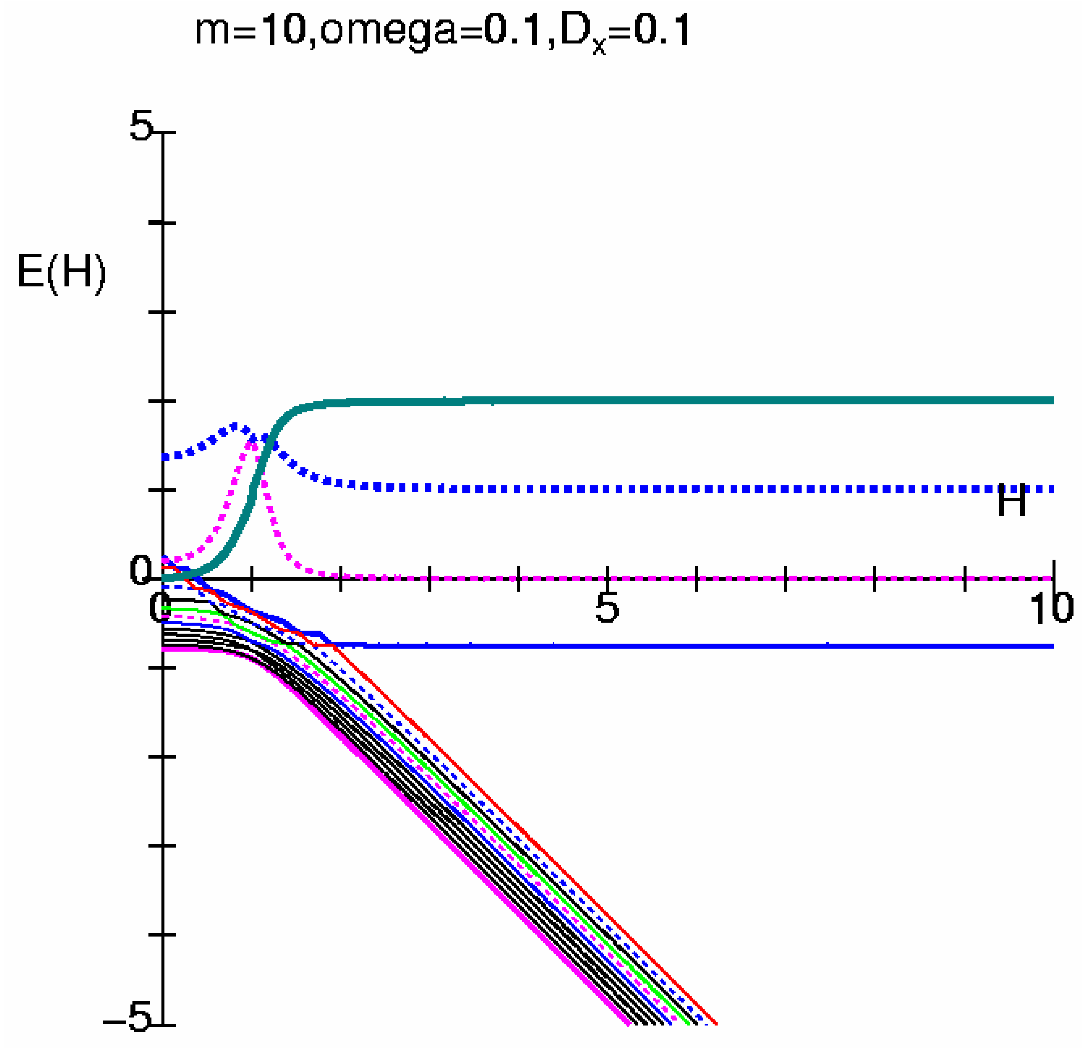
$$\vec{d} = \vec{d}_0 x$$

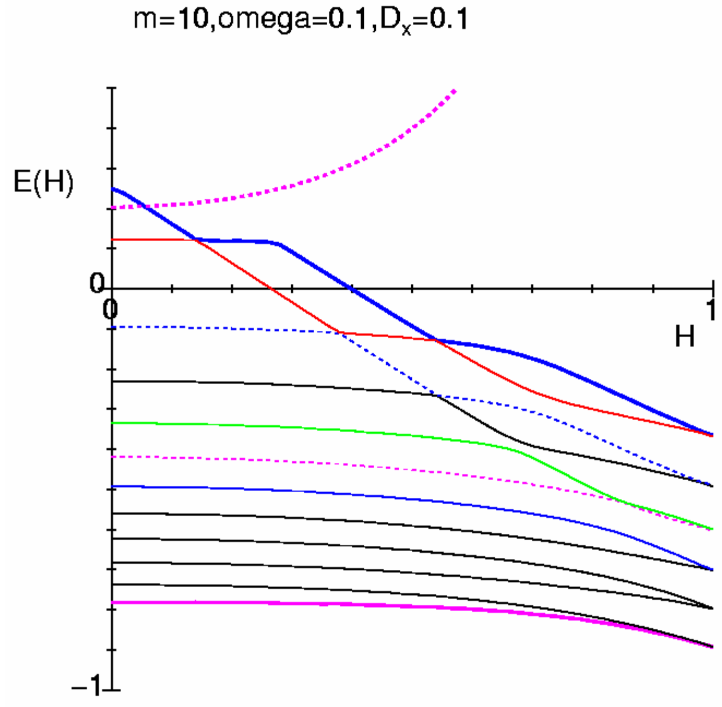
$$[x, p] = i\eta$$

$$\langle x \rangle = 0$$

$$\langle \text{singlet} | e^{iH} | \text{triplet} \rangle \neq 0 \quad ?$$

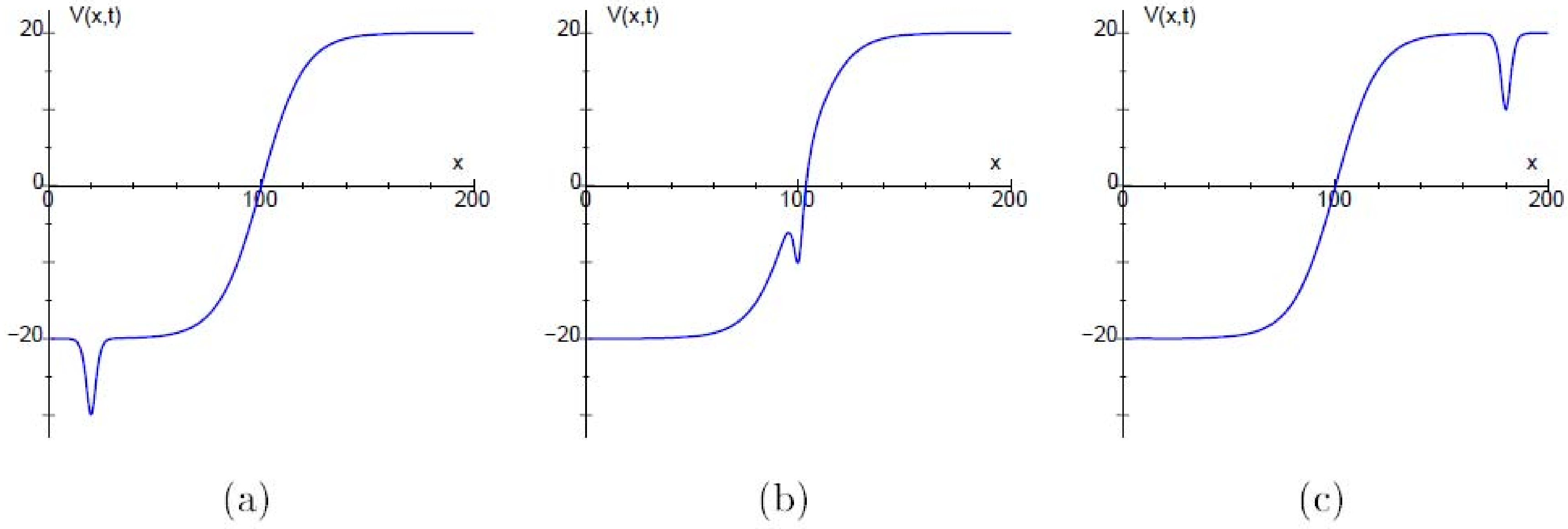
Smooth magnetization process





ポテンシャル移動による粒子運搬における量子効果

Particle trap by potential well --quantum dynamics for particle conveyance--



S. Miyashita,
Conveyance of quantum particles by a moving potential-well
J. Phys. Soc. Jpn. {¥bf 76} (2007) 104003.

Eigenstates in moving frame

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t) = \mathcal{H}(t)\Psi(x,t) \qquad \mathcal{H}(t) = \frac{p^2}{2m} + V(x-ct)$$

$$e^{ipct/\hbar}xe^{-ipct/\hbar} = x + ct$$

$$e^{ipct/\hbar}\mathcal{H}(t)e^{-ipct/\hbar} = \frac{p^2}{2m} + V(x) \equiv \mathcal{H}_0$$

$$\Phi(x,t) = e^{ipct/\hbar}\Psi(x,t)$$

$$i\hbar\frac{\partial}{\partial t}\Phi(x,t) = (\mathcal{H}_0 - cp)\,\Phi(x,t)$$

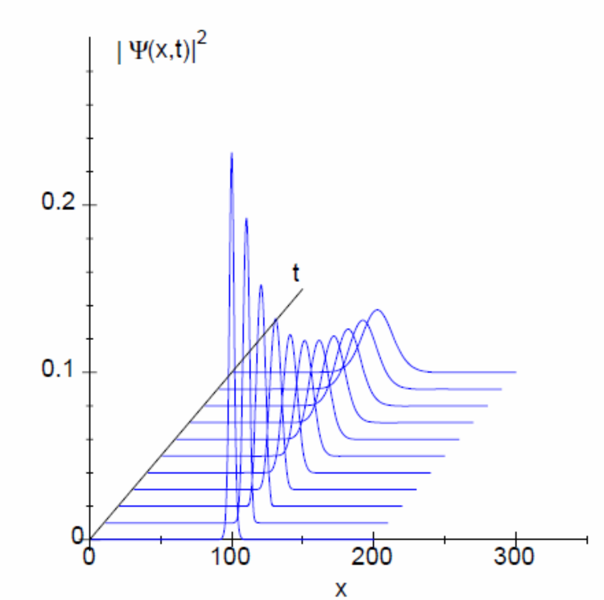
$$\mathcal{H}_0 - cp = \frac{1}{2m}(p-mc)^2 - \frac{1}{2}mc^2 + V(x)$$

$$e^{icmx/\hbar}pe^{-icmx/\hbar} = p - cm \qquad f(x,t) \equiv e^{-icmx/\hbar}\Phi(x,t)$$

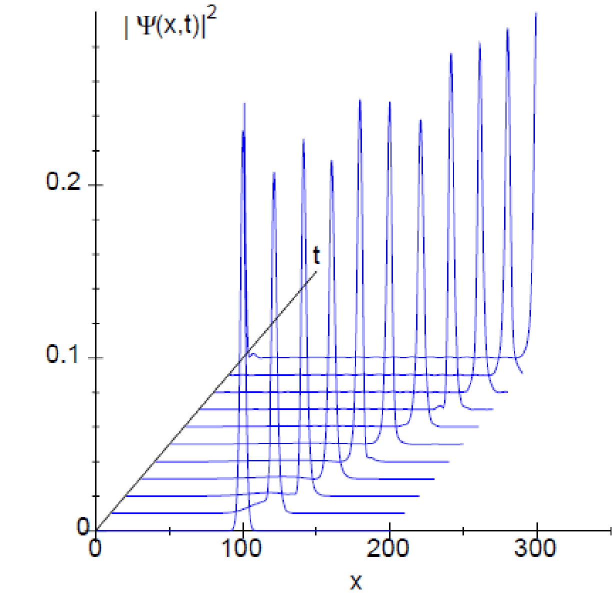
$$i\hbar\frac{\partial}{\partial t}f(x,t) = \left(\mathcal{H}_0 - \frac{1}{2}mc^2\right)f(x,t)$$

Sweep velocity dependence (flat)

fast



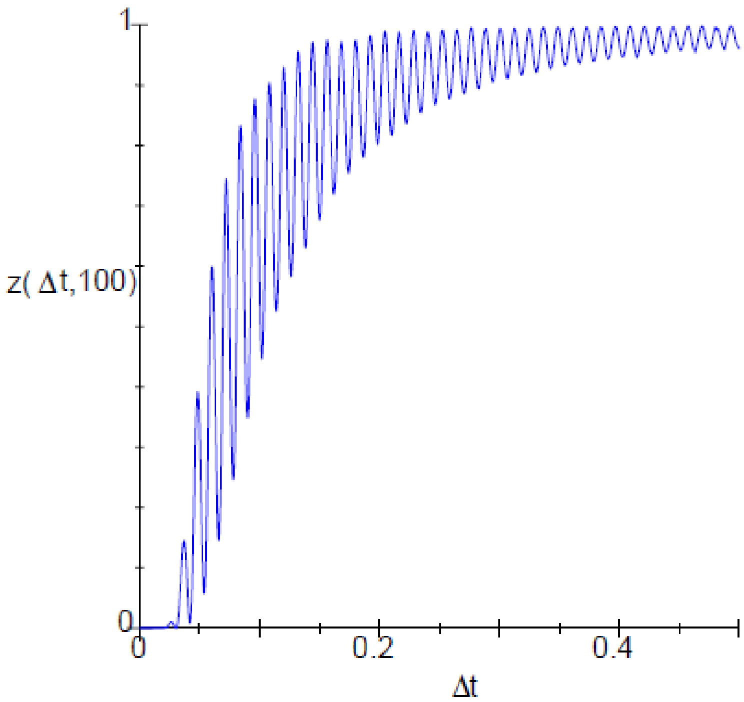
Slow



$$\Psi(x,t) = e^{-ictp/\hbar} e^{icmx/\hbar} e^{-i\mathcal{H}_0 t/\hbar} e^{-icmx/\hbar} |0\rangle$$

$$|\langle G(t)|\Psi(x,t)\rangle|^2 = \left| \langle 0| e^{icmx/\hbar} e^{-i\mathcal{H}_0 t/\hbar} e^{-icmx/\hbar} |0\rangle \right|^2$$

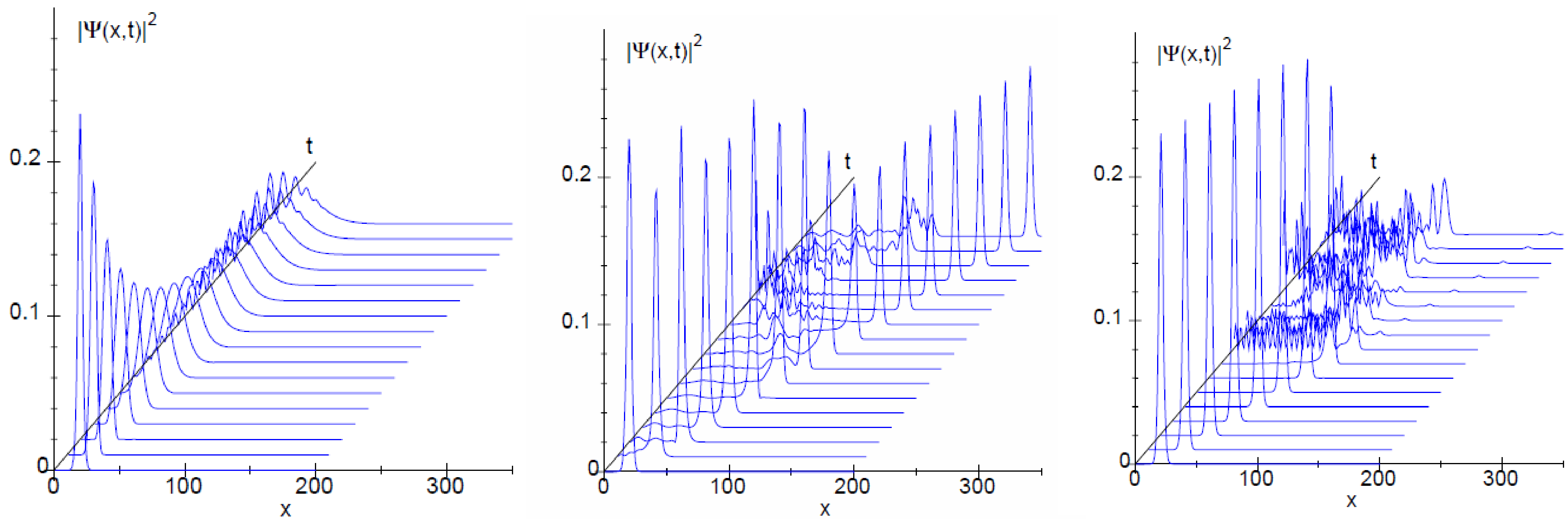
Trap probability

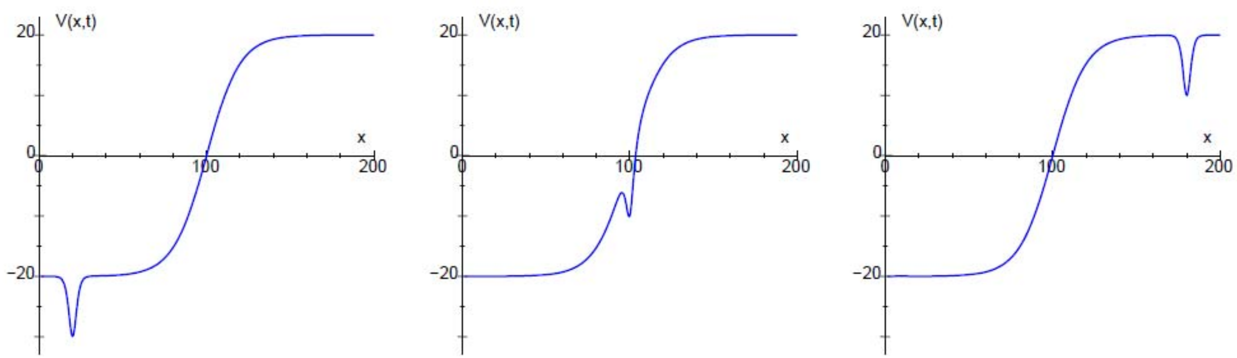


1/V

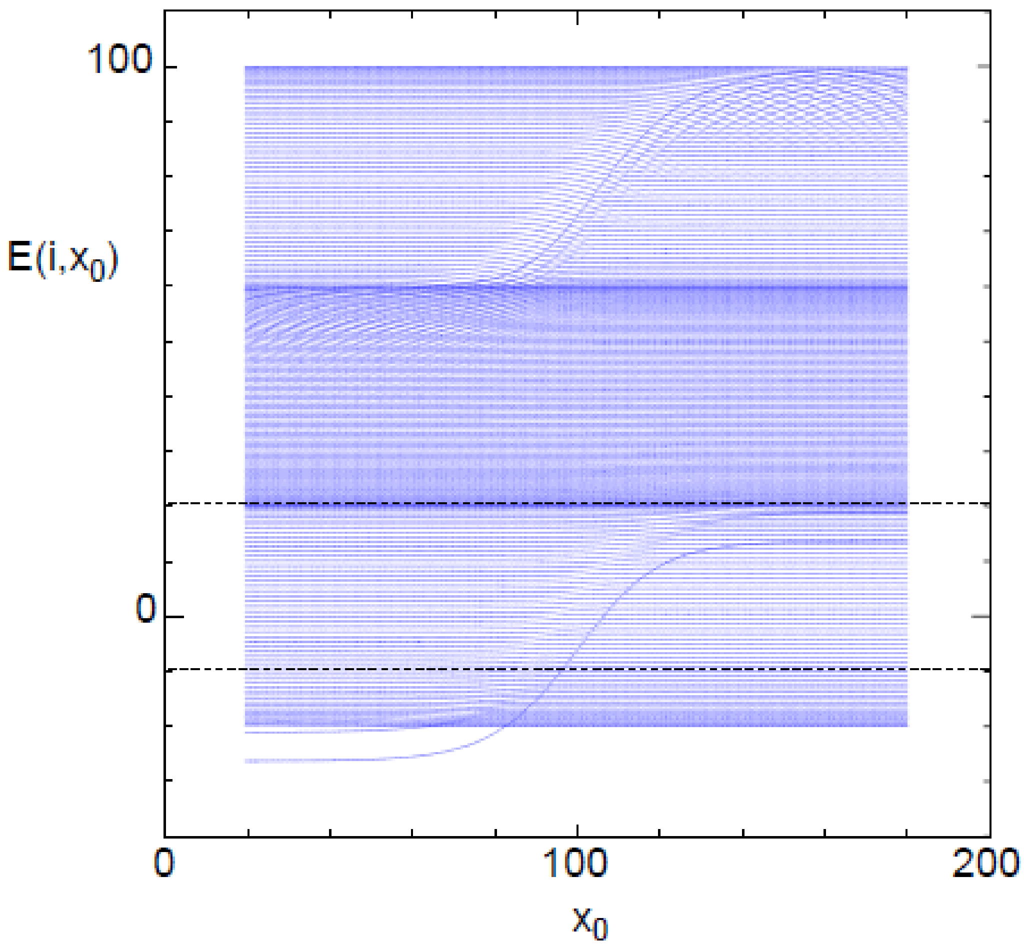
Sweep velocity dependence (carry-up)

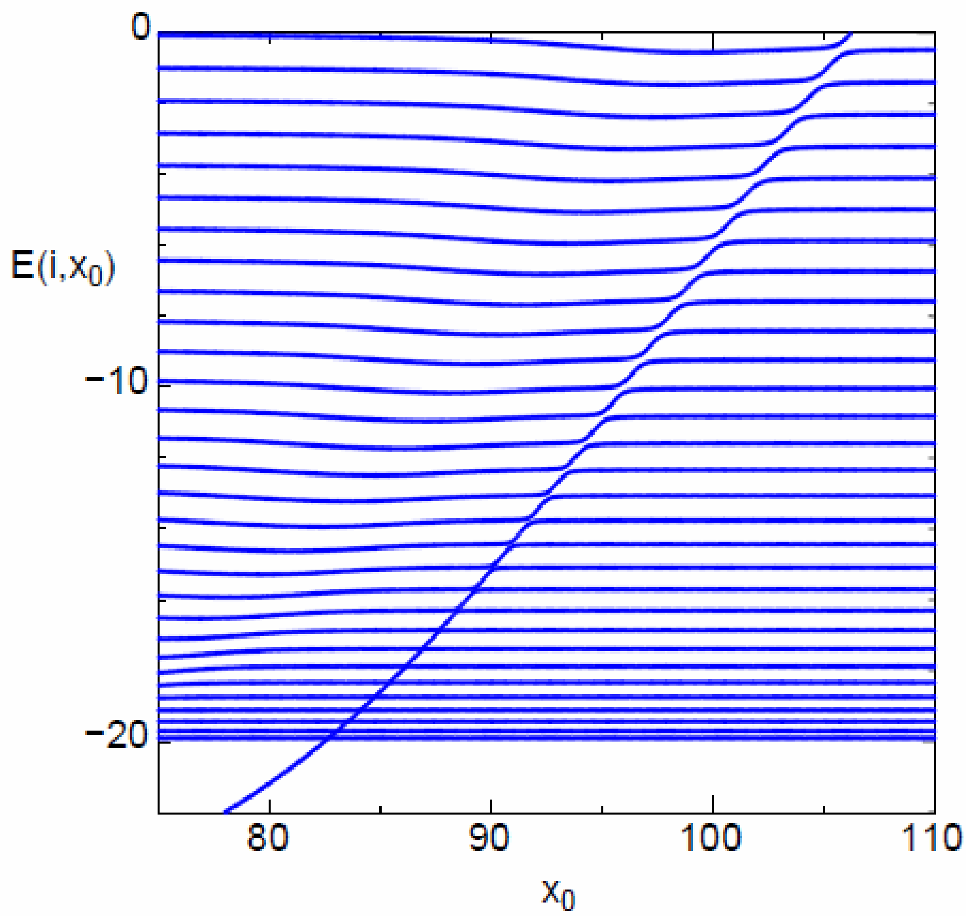
fast medium slow





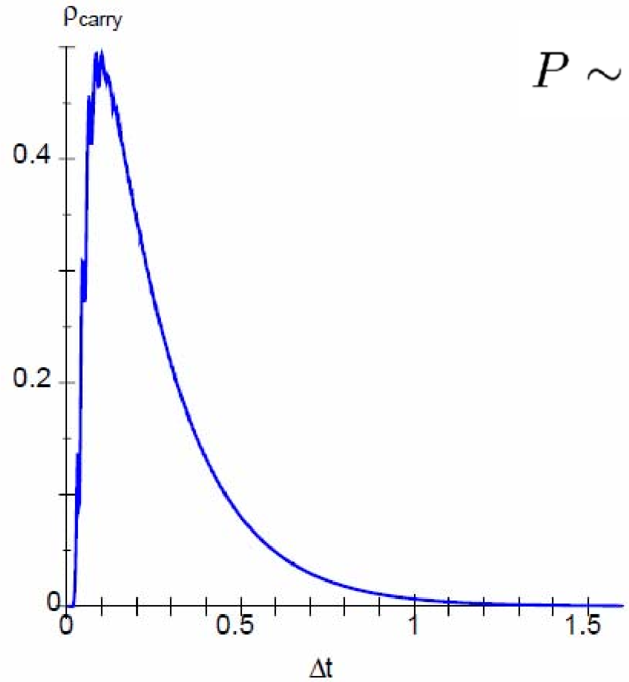
Adiabatic energy level as a function of the potential well



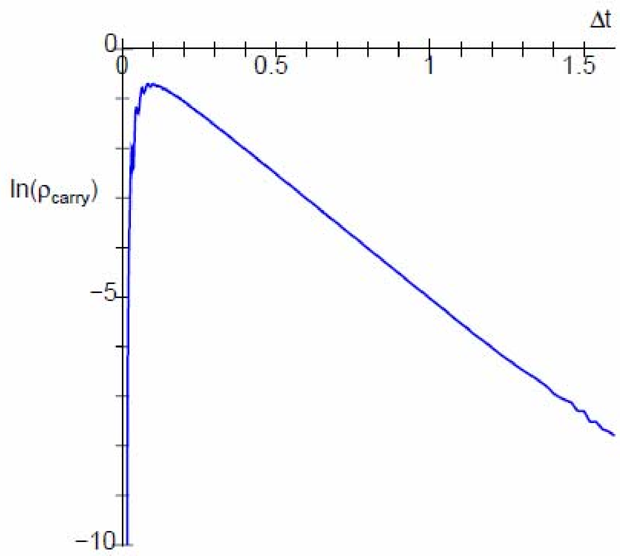


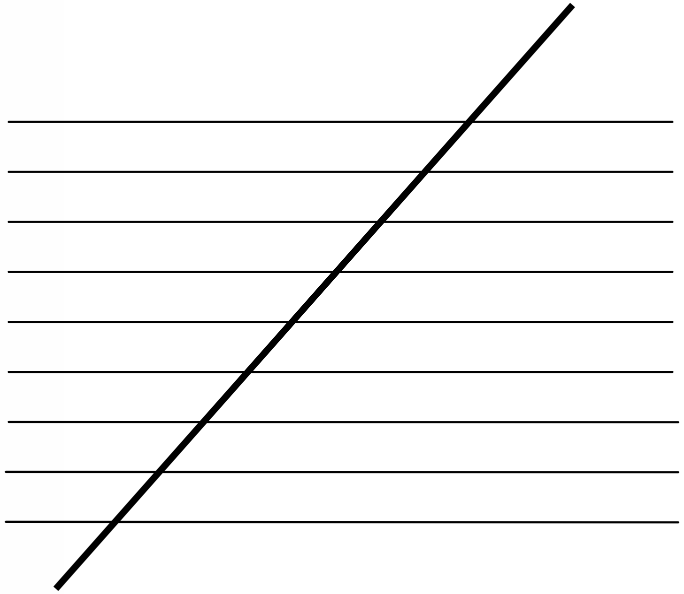
Successive Landau-Zener scattering

Adiabatic trap vs. tunneling



$$P \sim \exp\left(-\gamma/c\right) = \exp\left(-\gamma\Delta t\right)$$





$$\rho_{\mathrm{carry}} = \int_{x_0-2d_{\mathrm{pw}}}^{x_0+2d_{\mathrm{pw}}} \left|\Psi(x)\right|^2 dx$$

$$P = \exp\left(-\frac{2\pi}{\hbar}\sum_i J_i^2 |v|^{-1}\right)$$

Y. N. Demkov and V. I. Osherov, Sov. Phys.-JEPT 26 1211 (1968)

Y. Kayanuma and S. Fukuchi, JPSJ 53 (1985) 1869, J. Phys. B18 (1985) 4089.

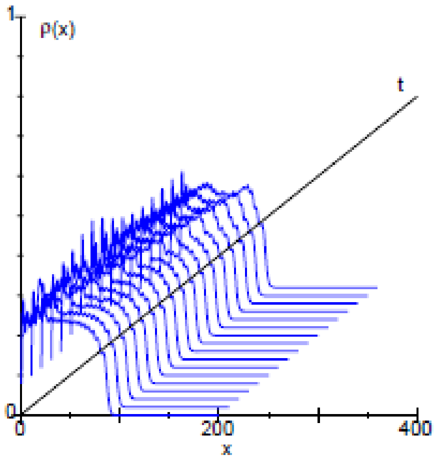
S. Tsuneyuki, et al. Surface Sci. 186 (1987) 26.

K. Kobayashi, et al. Physica A 265 (1999) 565.

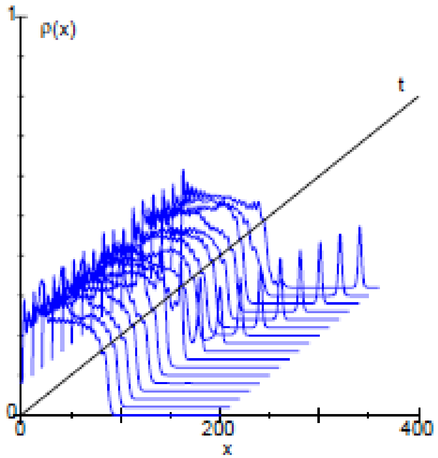
Keiji Saito, et al., Phys. Rev. B75 (2007) 75, 214308.

Multiple free particles (fermion)

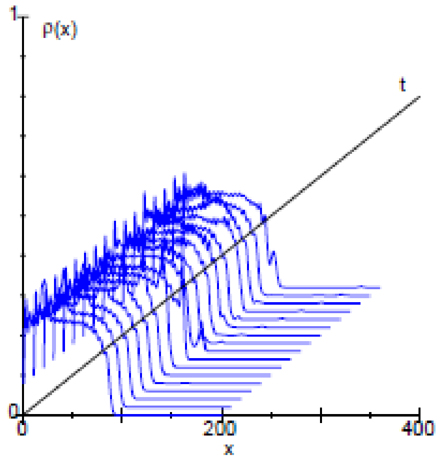
N=0.1L



(a)

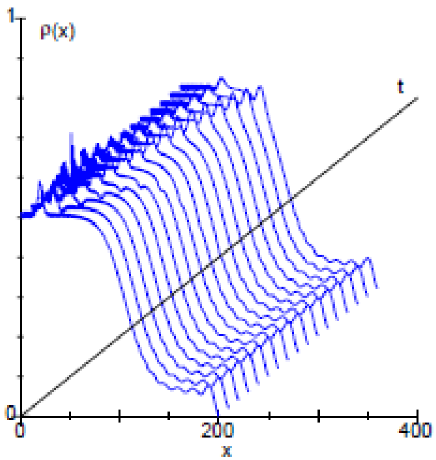


(b)

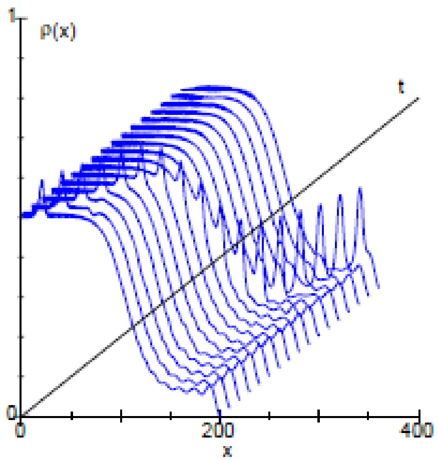


(c)

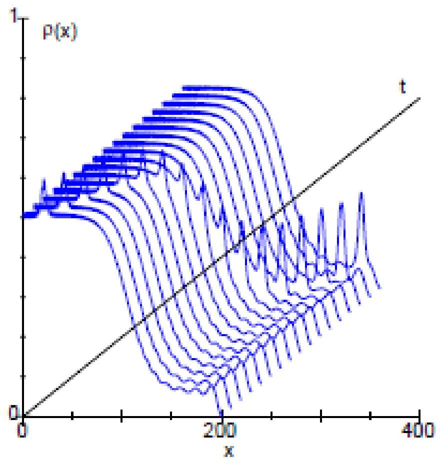
N=0.3L



(d)



(e)



(f)

Uniform acceleration

$$\mathcal{H}(t) = \frac{p^2}{2m} + V(x - \frac{1}{2}at^2) \qquad c = at$$

$$U_1 = e^{-i\frac{1}{2}at^2 p/\hbar} \qquad U_1^{-1}\mathcal{H}(t)U_1 = \mathcal{H}_0$$

$$\Phi(x,t) = U^{-1}\Psi(x,t)$$

$$i\hbar\frac{\partial}{\partial t}\Phi(x,t) = \left(\frac{1}{2m}(p - mat)^2 - \frac{1}{2}m(at)^2 + V(x)\right)\Phi(x,t) \equiv \mathcal{H}_1\Phi(x,t)$$

$$V = e^{-imatx/\hbar} \qquad V^{-1}pV = p - mat$$

$$i\hbar\frac{\partial}{\partial t}\Phi'(x,t) = \left(\mathcal{H}_0 + amx - \frac{1}{2}m(at)^2\right)\Phi'(x,t) \equiv \mathcal{H}_2\Phi(x,t)$$

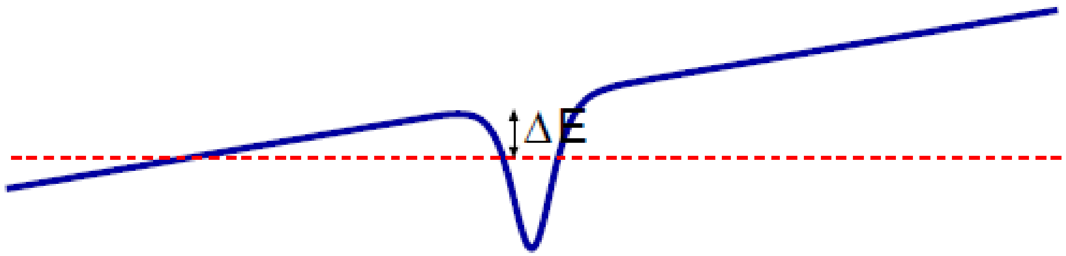
Adiabatic acceleration

$$c = at$$

$$t = c/a$$

$$a \to 0$$

$$V'(x) = V(x) + amx$$



$$x = \left|\langle G(0)|\Psi(x,t)\rangle\right|^2 = \left|\langle 0|e^{-i\mathcal{H}_2 t/\hbar}|0\rangle\right|^2$$

$$P = \exp\left(-\frac{2\sqrt{2mS}}{\hbar}\right) \qquad S \simeq \frac{\Delta E}{2am}$$

$$Pt = \frac{c}{a}\exp\left(-\frac{2\sqrt{\Delta E/a}}{\hbar}\right)$$

Thank you very much