# Teoria della Materia Condensata

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# Temi di Ricerca

1. Low dimensional magnets
   - (quasi) 2-d: Layered materials and films
   - (quasi) 1-d: Weakly coupled chains
2. From magnetic systems to entanglement and back
   - Entanglement, QPT and factorization in 1D & 2D AFM
   - Qbit-environment coupling: entanglement preservation and control
3. Open Quantum Systems
   - Josephson Junction Arrays
   - Spin-Environment coupling
4. Idrogeno solido $\longrightarrow$ Moraldi

# Low dimensional magnets

Different systems were investigated in last 10 years ...

- $0-d$ Molecular magnets
- $1-d$ Spin-chains and quasi-1d materials
- $2-d$ Layered materials and films

... focusing attention on different aspects as ...

- Dynamical processes (e.g. slow magnetizaton relaxation)
- Classical and quantum correlations and phase-transitions

... developing and applying different methods ...

- Analytical (Transfer-matrix, spin-wave theory, PQSCHA ...)
- Numerical (Classical and Quantum Monte Carlo simulations ...)

# Classical Monte Carlo simulation of Ho films

$$\mathcal{H} = -\sum_{i,j}^{N} J_{ij}\vec{\sigma}_i \cdot \vec{\sigma}_j + D_z \sum_{i=1}^{N} \left(\sigma_i^z\right)^2$$

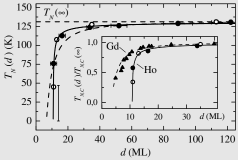
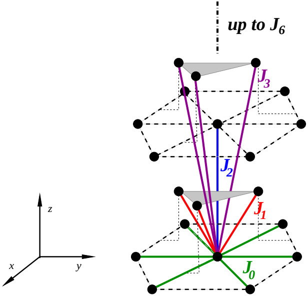



FIG. 3. $T_N$ as a function of Ho film thickness $d$, including data from MBE films (solid circles) and films grown *in situ* on W(110) (open circles). The MBE films with $d \geq 16$ ML were also studied by neutron diffraction, with identical results for $T_N$ within the error bars. For $T_N$ of the 11 ML *in situ* -grown film, see [24]. Inset: Comparison to thin-film data for Gd (solid triangles; from Ref. [9]).

From Wescke et al., Phys. Rev. Lett. **93**, 157204 (2004).

- Helimagnetic order up to $\simeq$ 10 ML
- Deacreasing $T_N$

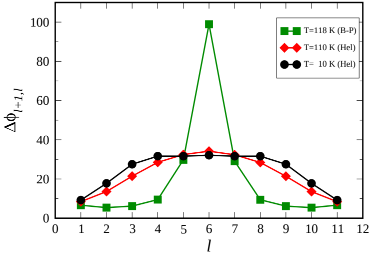
- $D_z = 16$ K
- Six-interlayers exchange model




- MC agrees with exp. picture, but ....

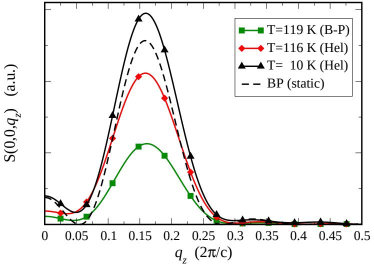
# Ho films: Blocked phase

- $n = 12$ - Magnetization rotation angle between neighboring layers




⇒ Block-Phase ( ↑↑↑↑↑ ∘∘ ↓↓↓↓↓ ) in the intermediate temperature region $T_{\rm hel} \lesssim T \lesssim T_C(l)_{\rm max}$: alternating disordered and collinear, antialigned blocks.

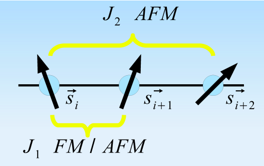
- $n = 16$ - Static structure factor at $T = 10$, $T = 116$, $T = 119$ K, and for *static* BP configuration ( ↑↑↑↑ ∘∘ ↓↓↓↓ ∘∘ ↑↑↑↑ )




⇒ Static structure factors of helical and BP spin arrangements are almost identical.

F. Cinti et al. PRB (2009)

# Competitive interactions, helical order and chirality

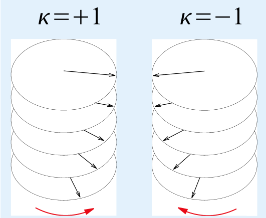



$$\frac{|J_2|}{J_1} \geq \frac{1}{4}$$
$$\Downarrow$$

Helical order at $T = 0$

$$Q = \arccos\left(\frac{J_1}{4|J_2|}\right)$$

$Z_2 \times SO(2)$ symmetry may separately break




Chiral order may be relevant

$$\kappa = \frac{[\vec{s}_i \times \vec{s}_{i+1}]^z}{|\sin(Q)|}$$

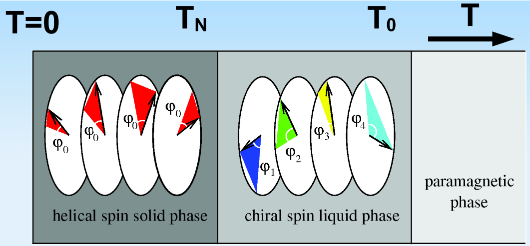
# Villain Conjecture (VC)

- Chiral order
  four-spin correlation function

$$\langle \kappa_i \kappa_{n+i} \rangle \sim e^{-\frac{na}{\xi_\kappa}} \qquad \xi_\kappa \sim e^{\frac{J}{T}}$$

- Helical (spin) order
  two-spin correlation function

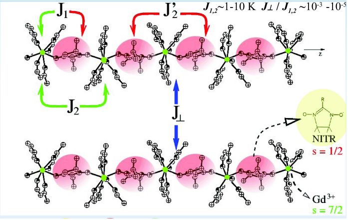
$$\langle \vec{s}_i \vec{s}_{n+i} \rangle \sim e^{-\frac{na}{\xi_s}} \qquad \xi_s \sim \frac{J}{T}$$

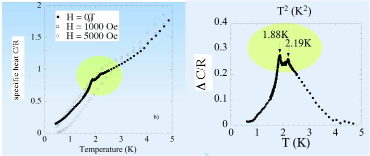


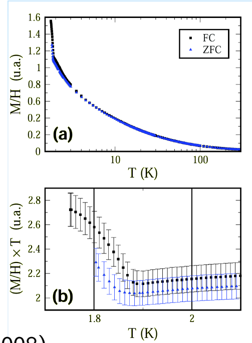

J. Villain, Ann. Isr. Phys. Soc. **2**, 565 (1978).

- 3d systems made up by weakly coupled chains could display two different critical points

# Experimental validation of VC on $GD(hfac)_3NITR$



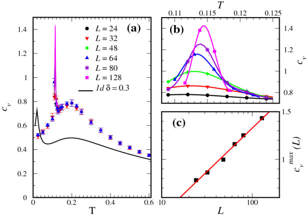




- Two $\lambda$ anomalies in specific heat
- No anomaly in susceptibility at highest $T$

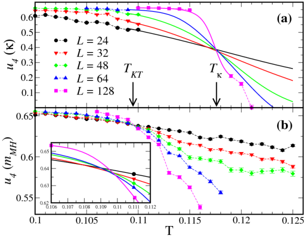
Cinti et al. PRL 100, (2008)

# Numerical validation of VC on 2d anisotropic magnet

$$\mathcal{H} = -\sum_{i=1}^{L}\sum_{j=1}^{L}\left\{J_1\vec{S}_{i,j}\cdot\vec{S}_{i,j+1} + J_2\vec{S}_{i,j}\cdot\vec{S}_{i,j+2} + J'\vec{S}_{i,j}\cdot\vec{S}_{i+1,j}\right\}$$




- Tipical $BKT$ broad maximum
  and
  Ising-like peak
  in specific heat




- Critical temperatures location
  by Binder's cumulants

Cinti et al., in preparation

# Spins systems and Quantum Information (QI)

Investigating and understanding spin models helps QI ...

- Q-bit $\leftrightarrow$ Quantum two-state system $\Longrightarrow S = 1/2$ spin

$\Rightarrow$ Spin models: natural, reference system to investigate properties of (interacting) Q-bit systems

- Almost all relevant physical realizations of QI devices can be easily mapped to spin models

$\Rightarrow$ Spin systems: universal model to investigate Entanglement in quantum information devices

- Few parameters, large variety of behaviours

# Spins systems and Quantum Information

The way back ... QI helps investigating spin models

- QI and QC call our attention on Entanglement, the essential resource for Quantum Computation (QC)
- Entanglement: sort of correlation between quantum systems of purely quantum origin

$\Rightarrow$ Investigating entanglement properties may shed new light on peculiar behaviours of spin systems of genuine quantum origin

# AFM Spin chain models

- XYZ model Hamiltonian

$$\hat{\mathcal{H}} = J \sum_i \Big( (1+\gamma) \hat{S}_i^x \hat{S}_{i+1}^x + (1-\gamma) \hat{S}_i^y \hat{S}_{i+1}^y + \lambda \hat{S}_i^z \hat{S}_{i+1}^z - h \hat{S}_i^z \Big)$$

- Exchange coupling: $J > 0 \implies$ antiferromagnetic coupling (AFM)
- Anisotropy constants:
  - $0 \leq \lambda \leq 1$: easy-plane anisotropy $\implies$ $z$-components quenched
  - $0 \leq \gamma \leq 1$: in-plane, easy-axis anisotropy

# AFM chain phenomenology at $T = 0$

- Factorization : $\exists \; h_{\rm f} = \sqrt{(1-\gamma+\lambda)(1+\gamma+\lambda)}$ such that:

  $h = h_{\rm f} \quad \Longrightarrow \quad |GS\rangle = \prod_i |\phi_i>$ (Néel, *classical-like* ground state)

- Quantum Phase Transition (QPT) : $\exists \; h_{\rm c}$ such that:

  $h > h_{\rm c} \quad \Longrightarrow$ disordered GS: $\langle S^x \rangle = 0$, $\quad \langle S^x_i S^x_{i+r} \rangle \simeq e^{-r/\xi}$

  $h < h_{\rm c} \quad \Longrightarrow$ long-range correlations on $XY$ plane ($\xi = \infty$)

  - $XY(Z)$ model: $\quad 0 < \gamma \leq 1 \quad 0 \leq \lambda < 1$

    $\Longrightarrow$ Ising transition $\Longrightarrow$ LRO $\quad \langle S^x_i S^x_{i+r} \rangle \underset{r\to\infty}{\longrightarrow} \mathrm{const} \neq 0$

  - $XX(Z)$ model: $\quad \gamma = 0 \quad 0 \leq \lambda < 1$

    $\Longrightarrow$ BKT transition $\Longrightarrow$ QLRO $\quad \langle S^x_i S^x_{i+r} \rangle \underset{r\to\infty}{\longrightarrow} \dfrac{1}{r^\eta}$

- $h_{\rm f} \leq h_{\rm c} \leq h_{\rm s}$ $\quad$ ( $h_{\rm s}$: saturation field )

# Entanglement in spin chains

Estimators of entaglement of formation of $S = 1/2$ systems:

- One-tangle:

$$\tau_1 = 1 - 4\sum_\alpha (m^\alpha)^2$$

quantifies entanglement between $i$-th spin and the rest of the system

- Concurrence:

$$C_{ij} = 2\ \max\left\{0, C_{ij}^{(1)}, C_{ij}^{(2)}\right\}$$

$$C_{ij}^{(1)} = g_{ij}^{zz} - \frac{1}{4} + |g_{ij}^{xx} - g_{ij}^{yy}|$$

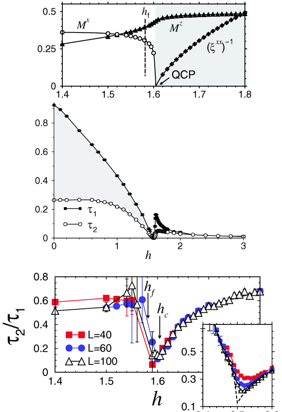
$$C_{ij}^{(2)} = |g_{ij}^{xx} + g_{ij}^{yy}| - \sqrt{\left(\frac{1}{4} + g_{ij}^{zz}\right)^2 - (m^z)^2}$$

quantifies pair-wise entanglement between spins at sites $i$ and $j$

$$g_{ij}^{\alpha\alpha} = \langle \hat{S}_i^\alpha \hat{S}_j^\alpha \rangle \qquad m^\alpha = \langle S^\alpha \rangle$$

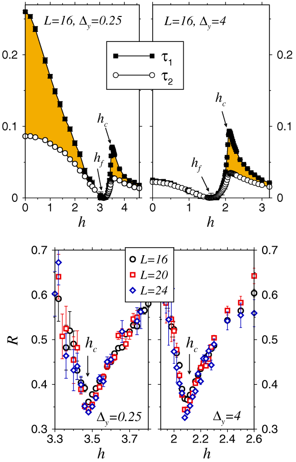
# Entanglement, QPT and factorization in 1D & 2D AFM

- AFM XYZ Chain in field



(Roscilde et. al., PRL (2004))

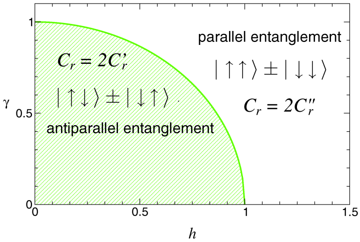
- 2D AFM in field



(Roscilde et. al., PRL (2005))

# Entanglement range in AFM XY chain in field

- Parallel and antiparallel entanglement

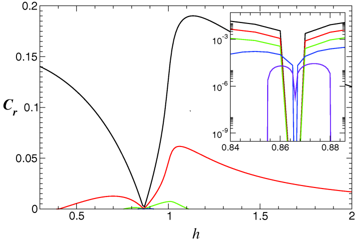


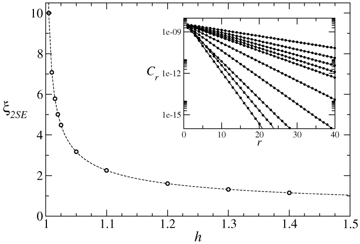

Bell states

$$|\phi_\pm\rangle = \frac{1}{\sqrt{2}}\left(|00\rangle \pm |11\rangle\right)$$

$$|\psi_\pm\rangle = \frac{1}{\sqrt{2}}\left(|01\rangle \pm |10\rangle\right)$$

- Range of entanglement




(Verrucchi et al. PRA (2006) & EPJD (2007))

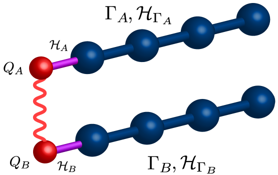
# Qbits with transverse coupling to $XY$ spin chain

- Model: two (entangled) Qbits ($Q_A$ and $Q_B$) locally coupled to two independent $XY$ spin environments $\Gamma_A$ and $\Gamma_B$

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_{\Gamma_A} + \hat{\mathcal{H}}_{0_A} + \hat{\mathcal{H}}_{\Gamma_B} + \hat{\mathcal{H}}_{0_B}$$

$$\hat{\mathcal{H}}_{\Gamma_\kappa} = -2\sum_{n_\kappa=1}^{N_\kappa-1}\left(J^x_{n_\kappa}\hat{s}^x_{n_\kappa}\hat{s}^x_{n_\kappa+1} + J^y_{n_\kappa}\hat{s}^y_{n_\kappa}\hat{s}^y_{n_\kappa+1}\right) - 2\sum_{n_\kappa=1}^{N_\kappa} h_{n_\kappa}\hat{s}^z_{n_\kappa}$$

$$\hat{\mathcal{H}}_{0_\kappa} = -2h_{0_\kappa}\hat{s}^z_{0_\kappa} - 2\left(J^x_{0_\kappa}\hat{s}^x_{0_\kappa}\hat{s}^x_{1_\kappa} + J^y_{0_\kappa}\hat{s}^y_{0_\kappa}\hat{s}^y_{1_\kappa}\right)$$

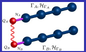



- Subsystems $A$ and $B$ do not interact

$$\hat{\mathcal{U}}_{A\cup B}(t) = \hat{\mathcal{U}}_A(t) \otimes \hat{\mathcal{U}}_B(t)$$

- Dynamics can be solved separately for subsystems $A$ and $B$
- Joined non-trivial dynamics only follows from quantum correlations embodied in initial preparation of $Q_A$ and $Q_B$ in a proper entangled state

# Qbits with transverse coupling to $XY$ spin chain



- Identical environments, $XX$ in transverse field, $N >> 1$ and even

$$J^x_{n_\kappa} = J^y_{n_\kappa} = J \qquad h_{n_\kappa} = h \; (n_\kappa > 0)$$

- Uncorrelated initial state of Qbits and environments

$$\hat{\rho}(0) = \hat{\rho}^{Q_A Q_B}(0) \otimes \hat{\rho}^{\Gamma_A}(0) \otimes \hat{\rho}^{\Gamma_B}(0)$$

- Initial state of environment: ground state
- Initial state of Qbits: one of (maximally entangled) Bell states

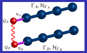
$$|\phi_\pm\rangle = \frac{1}{\sqrt{2}}(|00\rangle \pm |11\rangle) \qquad |\psi_\pm\rangle = \frac{1}{\sqrt{2}}(|01\rangle \pm |10\rangle)$$

- Entanglement evolution quantified by concurrence:

$$C(t) = 2\max\{0, C_{\uparrow\uparrow}(t), C_{\uparrow\downarrow}(t)\}$$

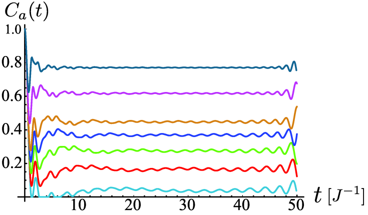
$$\begin{aligned} C_{\uparrow\downarrow}(t) &= |\tilde{\rho}_{23}| - \sqrt{\tilde{\rho}_{11}\tilde{\rho}_{44}} \\ C_{\uparrow\uparrow}(t) &= |\tilde{\rho}_{14}| - \sqrt{\tilde{\rho}_{22}\tilde{\rho}_{33}} \end{aligned}$$

# Isotropic coupling - $J_0 = J \quad h_0 \neq 0 \; h = 0$

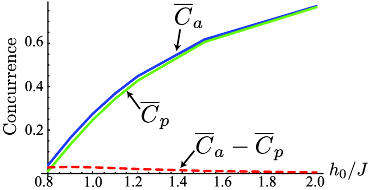


Field applied on Qbits only - $h_{0_A} = h_{0_B} = h_0$

- Antiparallel concurrence
  $\frac{h_0}{J} = 0.8, 0.9, 1, 1.1, 1.2, 1.5, 2$



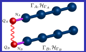

- Average antiparallel & parallel concurrence $\overline{C}_a$, $\overline{C}_p$




- Effective dynamic decoupling of each Qbit from its environment
- $h_{0_A} = h_{0_B} \Longrightarrow$ correlated dynamics of Qbits
  $\Longrightarrow$ entanglement preservation

Apollaro et al., submitted (2010)

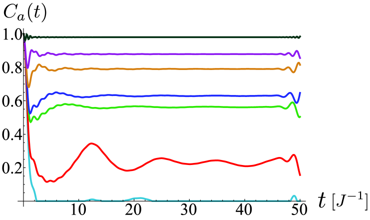
# Isotropic coupling - $J_0 = J \quad h_0 = 0 \ h \neq 0$



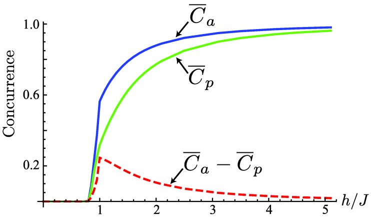
Field applied on environment only

- Antiparallel concurrence

  $\frac{h}{J}$ = 0.8, 0.9, 1, 1.1, 1.5, 2, 5




- Average antiparallel & parallel concurrence $\overline{C}_a$, $\overline{C}_p$



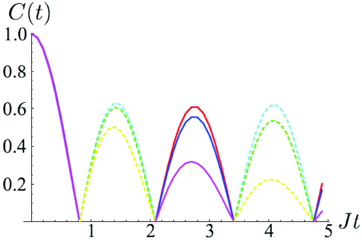

- Abrupt entanglement dynamics freezing as $h \geq J$
- Long time entanglement memory for $h \geq J$
- $\overline{C}_a - \overline{C}_p$ peak at $h = J$: drastic change of entanglement behaviour at environment QPT

Apollaro et al., submitted (2010)

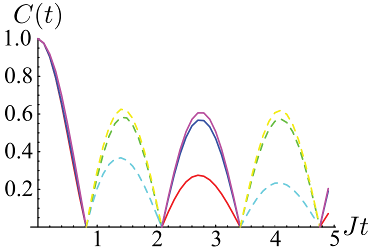
# Anisotropic coupling

$$J^y_{0_A} = J^y_{0_B} = 0; \quad h_{0_A} = h_{0_B} = h_B = 0$$

- Concurrence
  $J^x_{0_B} = 2J$; $J^x_{0_A} = 0.5, 0.2, 0.0\ J$
  $h_A = 0$




- Concurrence
  $J^x_{0_B} = J^x_{0_A} = J$
  $\frac{h_A}{J} = 1, 2, 10$




- $A$ and $B$ differential dynamics leads to entanglement type switching
- Setting $h_A > J_A$ freezes entanglement relaxation, increasing switching efficiency

Apollaro et al., submitted (2010)

# Open Quantum Systems

- Quantization $\Leftrightarrow$ Hamiltonian formulation
- Modeling Environment (Caldeira-Leggett):
  - Harmonic Oscillators set

$$\hat{\mathcal{H}}_{\mathrm{S}} = \frac{\hat{p}^2}{2m} + V(\hat{q}) \; ; \qquad \hat{\mathcal{H}}_{\mathrm{I}} = \frac{1}{2}\sum_\alpha \left[a_\alpha^2 \hat{p}_\alpha^2 + b_\alpha^2(\hat{q}_\alpha - \hat{q})^2\right]$$

  - Path-Integral formulation of QM
  - Tracing out environment variables $\Rightarrow$ system's effective action

$$\mathcal{S}_{\mathrm{I}}[q] = -\frac{1}{2}\int_0^\beta du\, du' \; k(u-u') \; q(u)q(u') = -\frac{\beta}{2}\sum_n k_n \; q_n q_{-n}$$

- Non-local effective action in imaginary-time
- Dissipation $\Rightarrow$ Langevin's Equation

$$m\ddot{\hat{q}} + \int_{-\infty}^t dt' \; \gamma(t-t') \; \dot{\hat{q}}(t') + V'(\hat{q}) = \hat{\xi}(t)$$

- Microscopic or phenomenological Kernel choice

$$k_n = \nu_n^2 \sum_\alpha \frac{b_\alpha^2}{\nu_n^2 + \omega_\alpha^2} \; ; \quad \gamma(z) = z\sum_\alpha \frac{b_\alpha^2}{z^2+\omega_\alpha^2} \quad \Longrightarrow \quad k_n = |\nu_n|\,\gamma(z{=}|\nu_n|)$$

# Methods

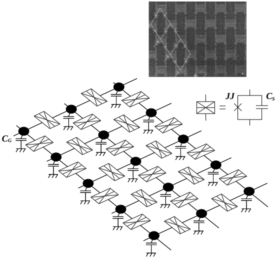
Standard: $q$-coupling and linear coupling with environment

- FPIMC pimc in (Matsubara) Fourier space - numerical, *exact* :
  - $\Rightarrow$ diagonal dissipative Kernel in Fourier space makes it efficient
- PQSCHA - Analytic, but approximate :
  - $\Rightarrow$ Quantum effects treated exactly at the Harmonic level
  - $\Rightarrow$ Approximation of Non-linear quantum effects only
  - Linear dissipative Kernel $\Rightarrow$ quantum dissipative effects correctly accounted for

Non-standard: $q-p$-coupling, and/or non-linear coupling

- Needed for magnetic system investigation
- Developement of formalism and approximation schemes

# Phase diagram of Josephson's Junctions Arrays (FPIMC)



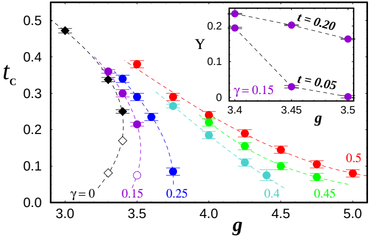

$$\hat{\mathcal{H}} = \frac{(2e)^2}{2} \sum_{ij} C^{-1}_{ij}\, \hat{n}_i \hat{n}_j - \frac{E_J}{2} \sum_{id} \cos(\hat{\varphi}_i - \hat{\varphi}_{i+d})$$

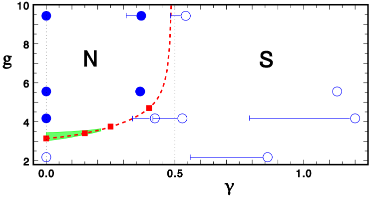
quantum coupling $g = \sqrt{E_C / E_J}$

dissipative coupling strength $\gamma = R_Q / R_S$

$E_C = (2e)^2 / 2C$

$R_S$ = Ohmic shunt resistors, $R_Q = h/(2e)^2$




(Exp. data: Takahide et al., PRL 85 (2000))

reentrance - role of dissipation

(Cuccoli et al., PRL 94, 157001(2005))

# Spin systems in phonon's environment

$$\hat{\mathcal{H}} = -\sum_{\langle ij \rangle} J \left[ \mu \left( \hat{S}^x_{\mathbf{i}} \hat{S}^x_{\mathbf{j}} + \hat{S}^y_{\mathbf{i}} \hat{S}^y_{\mathbf{j}} \right) + \hat{S}^z_{\mathbf{i}} \hat{S}^z_{\mathbf{j}} \right]$$

- Phonons $\Leftrightarrow$ Exchange constant modulation

$$J \longrightarrow J\left(\hat{r}_{\mathbf{ij}}\right) \simeq J + \delta J_{\mathbf{ij}} = J + J' \boldsymbol{d} \cdot \delta \hat{\boldsymbol{r}}_{\mathbf{ij}}$$

$\Rightarrow$ Spin are naturally coupled with environment

$\Rightarrow$ Spin-Environment coupling possibly non-linear

- Spin systems + spin-boson transformations:

$$S^z_{\mathbf{i}} = \widetilde{S}\left(1 - \frac{q_{\mathbf{i}}^2 + p_{\mathbf{i}}^2}{2}\right) , \qquad S^{\pm}_{\mathbf{i}} = \widetilde{S} \sqrt{1 - \frac{p_{\mathbf{i}}^2 + q_{\mathbf{i}}^2}{4}} \, (q_{\mathbf{i}} \pm i p_{\mathbf{i}}) + O(\widetilde{S}^{-1})$$

$\Rightarrow$ Symmetric role played by $q$ e $p$

# Non-standard couplings (PQSCHA)

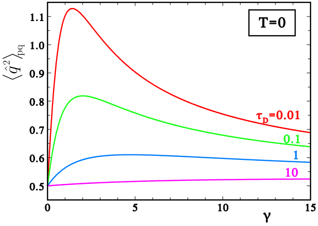
- Reference model (HO)

  exact calculation

  $q$–$p$ coupling

  Drude memory function

  independent $q$, $p$ baths




Quantum fluctuations are enhanced and reentrant

⇒ QPT ?

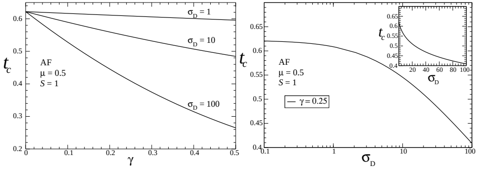
(Cuccoli et. al., PRE in stampa (2010))

- Spin-Environment linear coupling

$$\hat{\mathcal{H}}_{\mathrm{E}}^{(\mathbf{i}\sigma)} = \frac{1}{2}\sum_\alpha \left[ a_{\sigma\alpha}^2\,\hat{p}_\alpha^2 + b_{\sigma\alpha}^2\,(\hat{q}_\alpha - \hat{S}_{\mathbf{i}}^{\sigma})^2 \right]$$

Drude memory function:

$$\kappa_n = \gamma\,\frac{\sigma_{\mathrm{D}}\,\tilde{\nu}_n}{\sigma_{\mathrm{D}}+\tilde{\nu}_n}\;;\quad \sigma_{\mathrm{D}} \equiv \omega_{\mathrm{D}}/J\widetilde{S}^2$$




Phase diagram

- Non-linear spin-environment coupling ...

  ... work in progress ...

# Progetti e collaborazioni

- PRIN 2005 (Concluso gennaio 2008) -
  UniFi+UniCT+UniSA+UniTO
  Fenomeni collettivi e loro controllo in sistemi di spin su reticolo: proprieta' statiche e dinamiche al variare dei parametri dell'interazione.
- PRIN 2008 (marzo 2010 - marzo 2012)
  UniFI+UniMO+UniPR+UniPV
  Teoria degli effetti topologici in clusters e catene di spin molecolari
  - 1 Assegno di Ricerca annuale da bandire

Idrogeno solido $\longrightarrow$ Moraldi