Radboud Universiteit

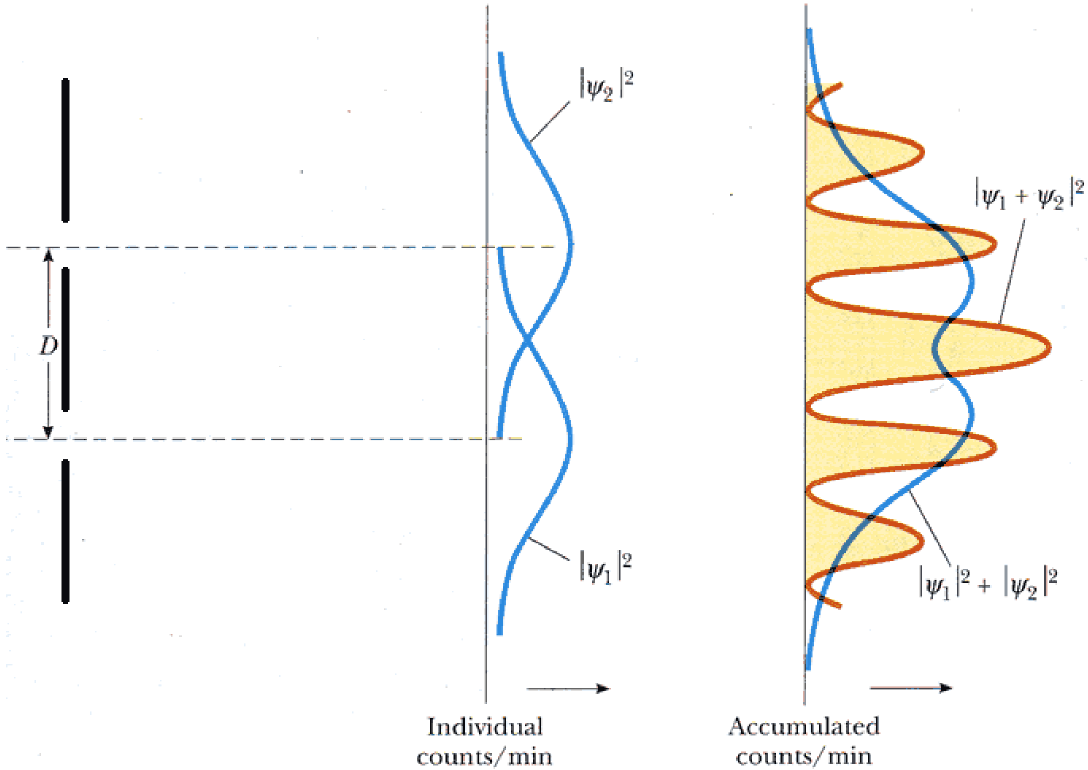
Origin of classicality in quantum spin systems

Mikhail Katsnelson

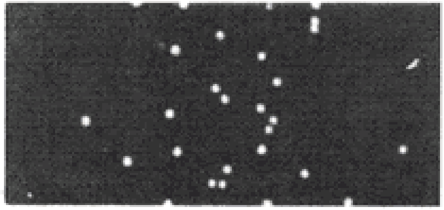
IMM
Institute for Molecules and Materials

Microworld: waves are corpuscles, corpuscles are waves

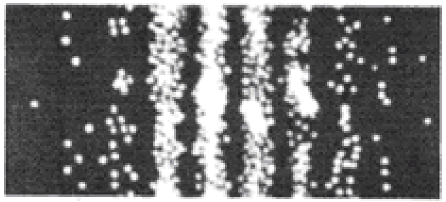
Einstein, 1905 – for light (photons)
L. de Broglie, 1924 – electrons and other microparticles



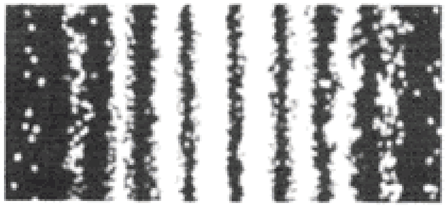
Electrons are particles (you cannot see half of electron) but moves along ***all*** possible directions (interference)



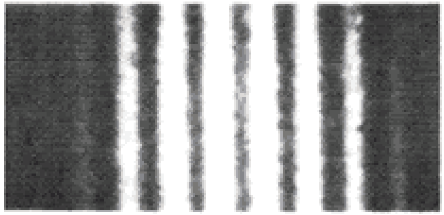
(a) After 28 electrons



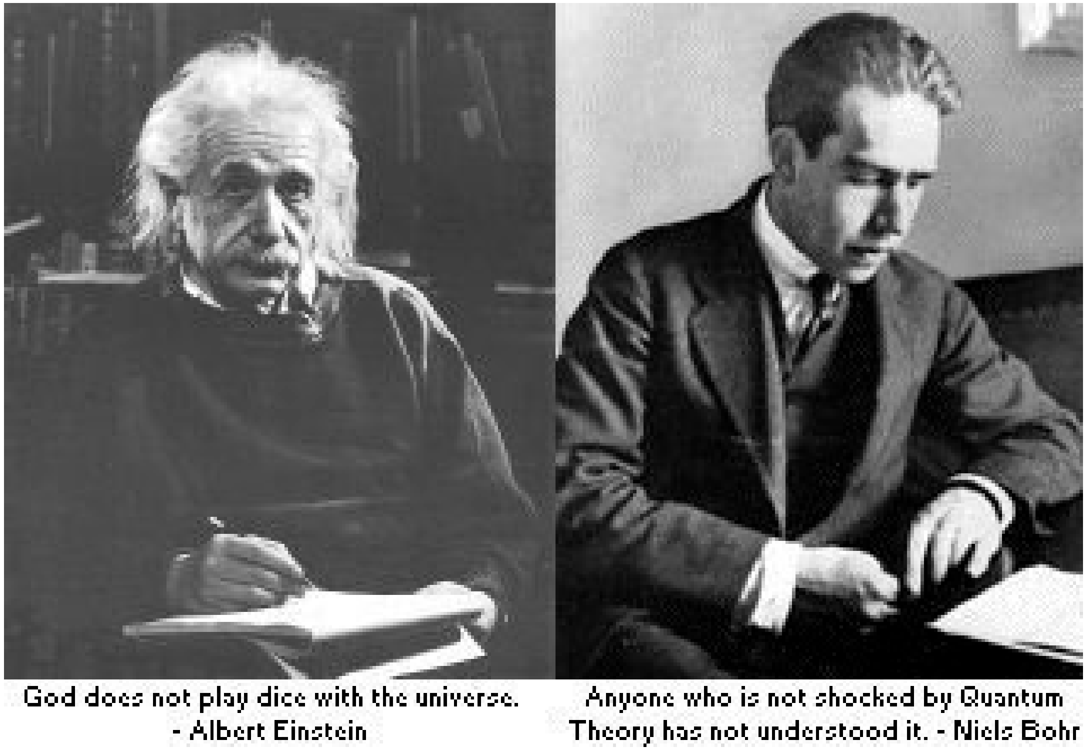
(b) After 1000 electrons



(c) After 10000 electrons



Interference phenomena: superposition principle
Does it work in the macroworld?! Seems to be - no



A. Einstein: Quantum mechanics is incomplete; superposition principle does not work in the macroworld

N. Bohr: Classical measurement devices is an important part of quantum reality

What is the origin of classical in the quantum world?

Complementary principle: we live in classical world, our language is classical, we know nothing on the electron itself, we deal only with the results of its interaction with classical measuring devices

Classical physics is not just a limit of quantum physics at $\hbar \to 0$: we need classical objects!

(cf relativity theory: $c \to \infty$)

Used to be mainstream but now: quantum cosmology (no classical objects in early Universe)... quantum informatics ("as you can buy wavefunction in a supermarket")... Many-world interpretation...

I will be talking on quantum description of world around us

Von Neumann theory of measurement (1932)

Density matrix for subsystem A of a total system A + B

$$\rho(\alpha,\alpha') = Tr_\beta \Psi^*(\alpha',\beta)\Psi(\alpha,\beta)$$

$$\rho = \sum_a W_a |a\rangle\langle a|$$

Pure state $\rho = |a\rangle\langle a|$

$$\rho^2 = \rho$$

Mixed state $Tr\rho^2 < Tr\rho$

Two ways of evolution

1. Unitary evolution

$$i\hbar\frac{\partial\rho}{\partial t} = [H,\rho]$$

$$\rho(t) = \exp(iHt/\hbar)\rho(0)\exp(-iHt/\hbar)$$

Entropy is conserved

$$S = -Tr\rho\ln\rho$$

2. Nonequilibrium evolution by the measurement

$$\rho_{after} = \sum_n P_n \rho_{before} P_n$$

$$P_n = |n\rangle\langle n|$$

$$S_{after} > S_{before}$$

Density matrix after the measurement is diagonal in *n*-representation

Application: decoherence wave

PHYSICAL REVIEW A, VOLUME 62, 022118

Propagation of local decohering action in distributed quantum systems

M. I. Katsnelson,* V. V. Dobrovitski, and B. N. Harmon

PHYSICAL REVIEW A **72**, 032316 (2005)

Quantum entanglement dynamics and decoherence wave in spin chains at finite temperatures

S. D. Hamieh and M. I. Katsnelson

Example: Bose-Einstein condensation in ideal and almost ideal gases

$$H=\sum_{\mu} E_{\mu}\alpha_{\mu}^{\dagger}\alpha_{\mu} \qquad |\Psi\rangle=\frac{1}{\sqrt{M!}}(\alpha_0^{\dagger})^M|0\rangle$$

0 is the state with minimal energy

We measure at $t = 0$ number of bosons at a given lattice site

Projection operator:

$$W_n=\delta_{n,N}=\int_0^{2\pi}\frac{d\phi}{2\pi}\exp[i\phi(n-N)]$$

Von Neumann prescription:

$$U(t)=\sum_{n=0}^{\infty}\exp(-iHt)W_nU_{\text{in}}W_n^{\dagger}\exp(iHt)$$

$U_{\text{in}}=|\Psi\rangle\langle\Psi|$ is the density matrix before measurement

Decoherence wave in BEC

Single-particle density matrix $\rho(\mathbf{r},\mathbf{r}',t)=\mathrm{Tr}[U(t)a^{\dagger}(\mathbf{r}')a(\mathbf{r})]$

Explicit calculations Poisson statistics for the measurement outcomes

$$p_n=e^{-n_0}n_0^n/(n!) \qquad n_0=n_B(0)$$

$$S=-\mathrm{Tr}[U(t)\ln U(t)]=-\sum_{n=0}^{\infty}p_n\ln p_n>0$$

$$\rho(\mathbf{r},\mathbf{r}',t)=\sqrt{n_B(\mathbf{r})n_B(\mathbf{r}')}-G^*(\mathbf{r}',t)\sqrt{n_B(\mathbf{r})n_0}-G(\mathbf{r},t)\sqrt{n_B(\mathbf{r}')n_0}+2n_0G^*(\mathbf{r}',t)G(\mathbf{r},t)$$

$$G(\mathbf{r},t)=V_0\left(\frac{m}{2\pi i\hbar t}\right)^{3/2}\exp\left(\frac{im\mathbf{r}^2}{2\pi\hbar t}\right)$$

$$\rho(\mathbf{r},\mathbf{r},t)=n_B+2n_BV_0^2\left(\frac{m}{2\pi\hbar t}\right)^3-2n_BV_0\left(\frac{m}{2\pi\hbar t}\right)^{3/2}\cos\left(\frac{m\mathbf{r}^2}{2\pi\hbar t}\right)$$

Decoherence wave in BEC II

Weakly nonideal gas: Bogoliubov transformation

$$H=\sum_{\mathbf{k}} E_{\mathbf{k}}\alpha_{\mathbf{k}}^{\dagger}\alpha_{\mathbf{k}}$$

$$+\frac{1}{2V}\sum_{\mathbf{k}_1+\mathbf{k}_2=\mathbf{k}_1'+\mathbf{k}_2'} v(\mathbf{k}_1-\mathbf{k}_1')\alpha_{\mathbf{k}_1'}^{\dagger}\alpha_{\mathbf{k}_2'}^{\dagger}\alpha_{\mathbf{k}_2}\alpha_{\mathbf{k}_1}$$

$$\alpha_{\mathbf{k}}=\xi_{\mathbf{k}}\cosh\chi_{\mathbf{k}}+\xi_{-\mathbf{k}}^{\dagger}\sinh\chi_{\mathbf{k}},$$

$$\alpha_{-\mathbf{k}}^{\dagger}=\xi_{\mathbf{k}}\sinh\chi_{\mathbf{k}}+\xi_{-\mathbf{k}}^{\dagger}\cosh\chi_{\mathbf{k}},$$

$$\tanh 2\chi_{\mathbf{k}}=-\frac{v(\mathbf{k})n_B}{E_{\mathbf{k}}+v(\mathbf{k})n_B}$$

Excitation spectrum $\omega_{\mathbf{k}}=\sqrt{E_{\mathbf{k}}^2+2E_{\mathbf{k}}v(\mathbf{k})n_B}.$

Acoustic for small *k*

$$\rho_n(\mathbf{r},\mathbf{r}',t)=\frac{n_B}{(n!)^2}\frac{\partial^{2n}}{\partial z^n\partial z'^n}\{[1+(z-1)G(\mathbf{r},t)]$$

$$\times[1+(z'-1)G^*(\mathbf{r}',t)]$$

$$\times\exp[n_B X(z,z')]\}_{z=z'=0},$$

$$X(z,z')=B(zz'-1)+(1-B)(z+z'-2)$$

$$+A[(z-1)^2+(z'-1)^2],$$

$$A=\frac{V_0}{2V}\sum_{\mathbf{k}}\frac{v(\mathbf{k})n_B}{\omega_{\mathbf{k}}},$$

$$B=\frac{V_0}{2V}\sum_{\mathbf{k}}\left[1+\frac{E_{\mathbf{k}}+v(\mathbf{k})n_B}{\omega_{\mathbf{k}}}\right],$$

$$G(\mathbf{r},t)=\sum_{\mathbf{k}}\exp(i\mathbf{k}\cdot\mathbf{r})\left\{\cos\omega_{\mathbf{k}}t-i\frac{E_{\mathbf{k}}+v(\mathbf{k})n_B}{\omega_{\mathbf{k}}}\sin\omega_{\mathbf{k}}t\right\}$$

Decoherence wave in BEC III

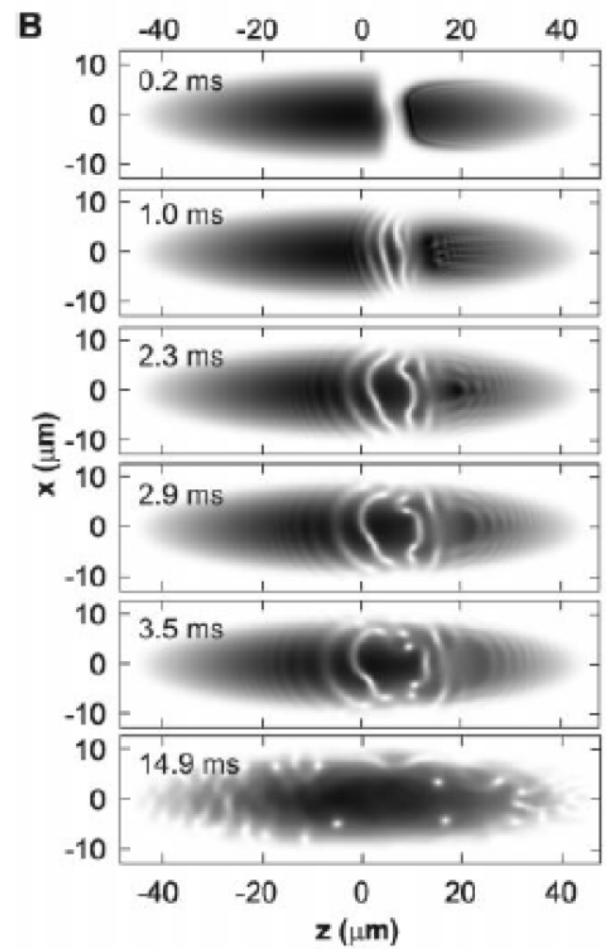
In this case, decoherent action propagates with sound velocity, nothing is "superluminal", etc – a smooth "wave function collapse"

Can be experimentally verified! But, in a sense...

Observation of Quantum Shock Waves Created with Ultra-Compressed Slow Light Pulses in a Bose-Einstein Condensate

Zachary Dutton,[1,2] Michael Budde,[1,3] Christopher Slowe,[1,2] Lene Vestergaard Hau[1,2,3]

SCIENCE VOL 293 27 JULY 2001 663



Interaction with light is a measurement!

Neel state of AFM: The role of entanglement

$$\mathcal{H}_0 = \sum_{\mathbf{q}} J_{\mathbf{q}} (S^+_{\mathbf{q}} S^-_{\mathbf{q}} + S^z_{\mathbf{q}} S^z_{\mathbf{q}})$$

Ground state is singlet, no sublattices!

$$\sum_{\mathbf{q}} J_{\mathbf{q}} = 0, \quad \min_{\mathbf{q}} J_{\mathbf{q}} = J_{\kappa}$$

Anomalous averages:

$$H \to H - hA$$

$$\lim_{h \to 0} \lim_{N \to \infty} \langle A \rangle \neq \lim_{N \to \infty} \lim_{h \to 0} \langle A \rangle$$

In the case of AFM (or superconductor) this field does not look physical!

On the Description of the Antiferromagnetism without Anomalous Averages

V.Yu. Irkhin and M.I. Katsnelson

Z. Phys. B – Condensed Matter 62, 201–205 (1986)

$$|\Phi_M\rangle \equiv |M\rangle = (S^-_{-\kappa})^M |F\rangle$$

$$|\Phi\rangle = \sum_{L=0}^{NS} \exp[\lambda(L)/2] |2L\rangle$$

$|F\rangle$ is the ferromagnetic state (all spins up)

In thermodynamic limit, this state (without anomalous averages!) gives the same results for observables as Neel state; can be used as starting point for local measurement and decoherence wave

ON THE GROUND-STATE WAVEFUNCTION OF A SUPERCONDUCTOR IN THE BCS MODEL

V.Yu. IRKHIN and M.I. KATSNELSON

Volume 104A, number 3 PHYSICS LETTERS 20 August 1984

Neel state of AFM: The role of entanglement II

PHYSICAL REVIEW B, VOLUME 63, 212404

Néel state of an antiferromagnet as a result of a local measurement in the distributed quantum system

M. I. Katsnelson,* V. V. Dobrovitski, and B. N. Harmon

Measuring local spin at site n = 0

Easy-axis anisotropy: in Ising limit, one single measurement leads to instans wave function collapse: all even spins up, all odd down (or vice versa)

Easy plane anisotropy (or isotropic case) – broken continuous symmetry; Decoherence wave and of the order of *N* measurements to create Neel state

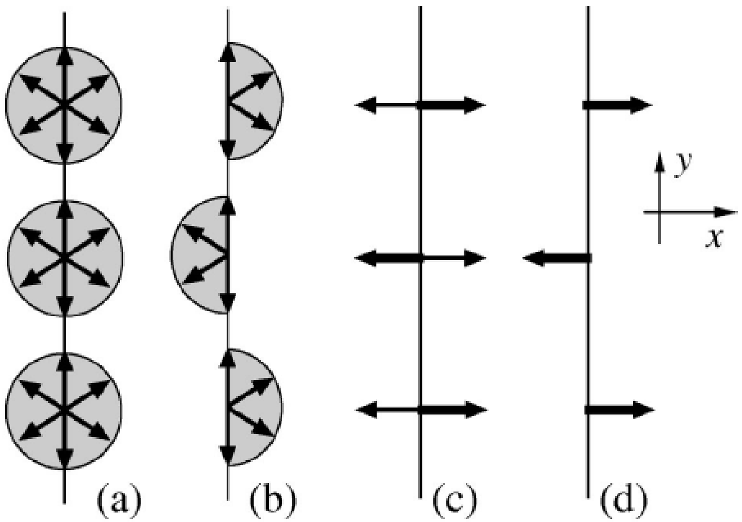


FIG. 1. Sketch of the spin arrangement. Easy plane case: (a) before measurement, sublattices are absent and the total AFM axis is not fixed; (b) after measurement, the "fan" sublattices emerge but an AFM axis is not fixed. Easy axis case: (c) before measurement, sublattices are absent; (d) after measurement, the Néel state appears.

However... This is for classical spins!

In AFM, there are zero-point oscillations: nominal spin is less than in classical Neel picture. E.g., square lattice Heisenberg AFM, NN interactions only:

$$\overline{S_0} = S - 0.1971$$

It means that for S=1/2 if a spin belongs to (nominally) spin-up sublattice in reality it is up with 80% probability and down with 20% probability (average spin is roughly 0.3)

Than, even in easy-axis case one single local measurement is not enough to establish sublattices – may be by accident it is done in a "wrong" instant

Decoherence waves in AFM for quantum spins

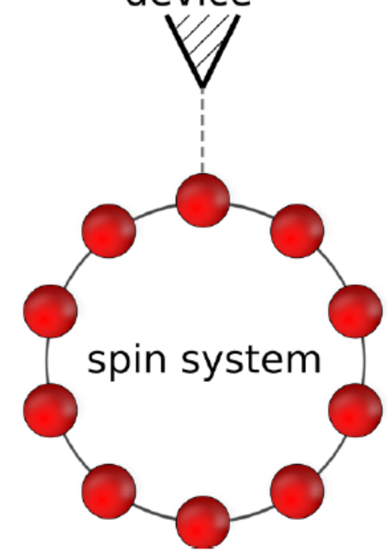
PHYSICAL REVIEW B **93**, 184426 (2016)

Decoherence wave in magnetic systems and creation of Néel antiferromagnetic state by measurement

Hylke C. Donker*
Radboud University, Institute for Molecules and Materials, Heyendaalseweg 135, NL-6525AJ Nijmegen, The Netherlands

Hans De Raedt
Zernike Institute for Advanced Materials, University of Groningen, Nijenborgh 4, NL-9747AG Groningen, The Netherlands

Mikhail I. Katsnelson
Radboud University, Institute for Molecules and Materials, Heyendaalseweg 135, NL-6525AJ Nijmegen, The Netherlands
(Received 15 February 2016; published 20 May 2016)



Simulations by numerically exact solution of time-dependent Schrödinger equation

$$\rho \to \rho' = \sum_i P_i \rho P_i \qquad P_m^{\pm\alpha} = \frac{1 \pm 2S_m^\alpha}{2} \qquad \langle S_l^\beta(t)\rangle = \mathrm{Tr}\left[S_l^\beta(t)\frac{P_m^{\pm\alpha}\rho_0 P_m^{\pm\alpha}}{N_0}\right]$$

Hamiltonian is the sum of Heisenberg and Ising parts:

$$H_0 = J\sum_{\langle i,j\rangle} \mathbf{S}_i \cdot \mathbf{S}_j \qquad H' = J\Delta \sum_{\langle i,j\rangle} S_i^z S_j^z$$

The larger Δ, the weaker are quantum zero-point oscillations

Chebyshev Polynomial Algorithm

Chebyshev Polynomial Algorithm: based on the numerically exact polynomial decomposition of the time evolution operator Ũ. It is very efficient if *H* is a sparse matrix.

$$\left|\varphi(t)\right\rangle = \widetilde{U}\left|\varphi(0)\right\rangle = e^{-itH}\left|\varphi(0)\right\rangle$$

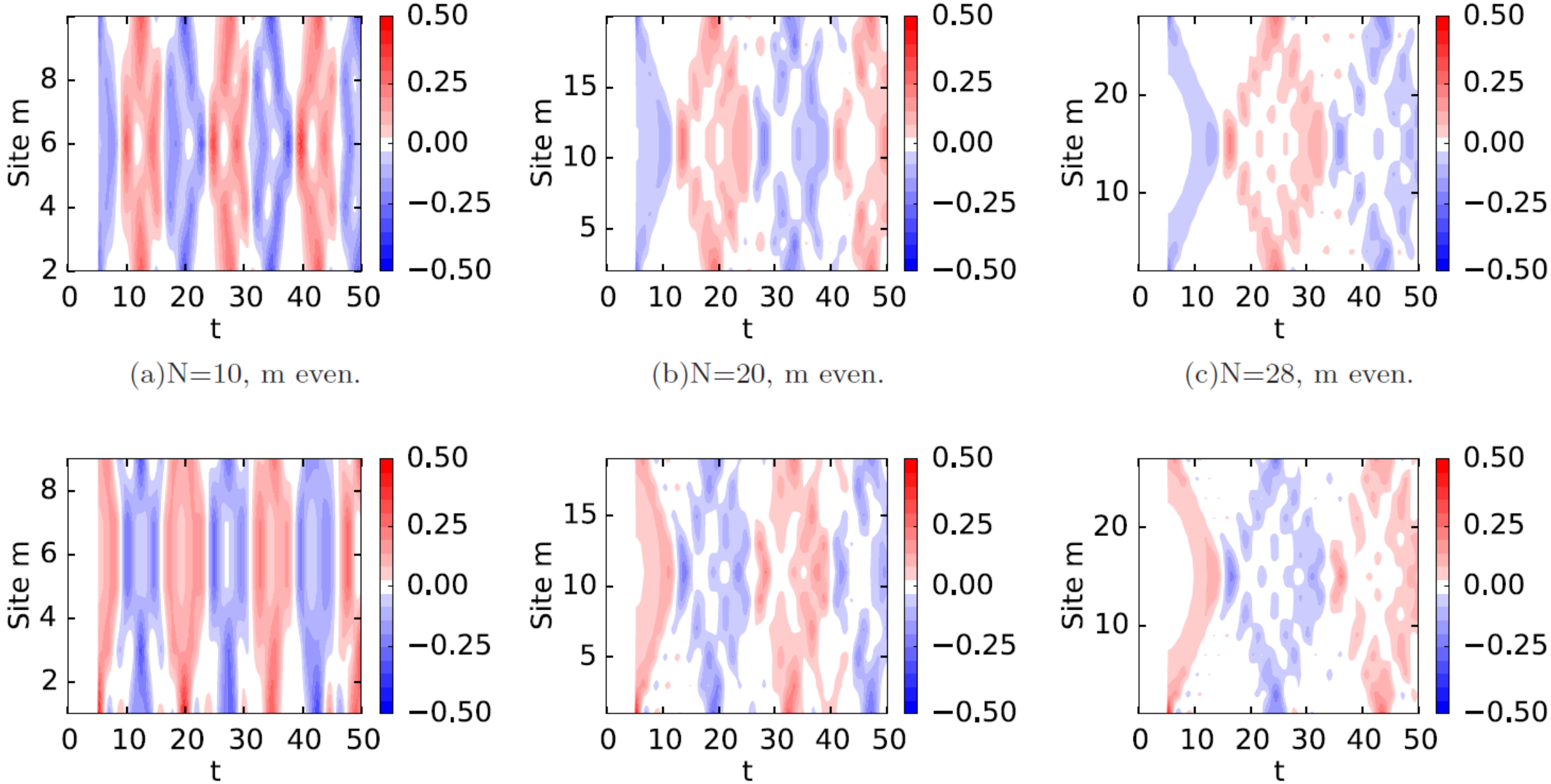
$$e^{-izx} = J_0(z) + 2\sum_{m=1}^{\infty}(-i)^m J_m(z) T_m(x)$$

$$T_m(x) = \cos[m \arccos(x)], x \in [-1,1]$$

$$T_{m+1}(x) + T_{m-1}(x) = 2xT_m(x)$$

Decoherence waves in AFM for quantum spins II

Single measurement



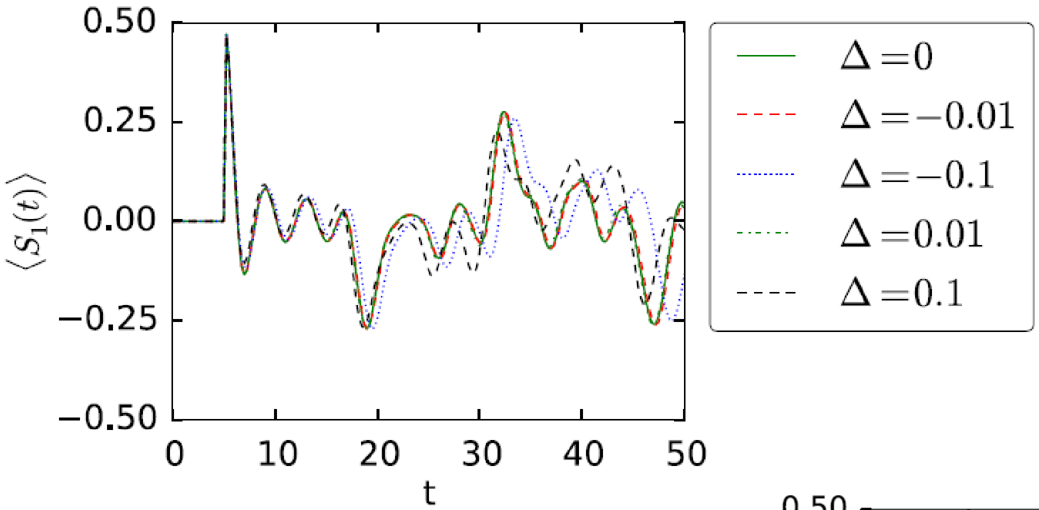
(a)N=10, m even. (b)N=20, m even. (c)N=28, m even.

(d)N=10, m odd. (e)N=20, m odd. (f)N=28, m odd.

FIG. 3. Time evolution of the magnetization $\langle S_m^z(t)\rangle$ for the isotropic (i.e., XXX) AFM Heisenberg spin chain of length N. The system at $t = 0$ is prepared in the ground state after which at $t = 5$ spin 1 is projected on the $+z$ axis.

Decoherence waves in AFM for quantum spins III

The sign of anisotropy is not important if it is small



Also, multiple measurements were studied

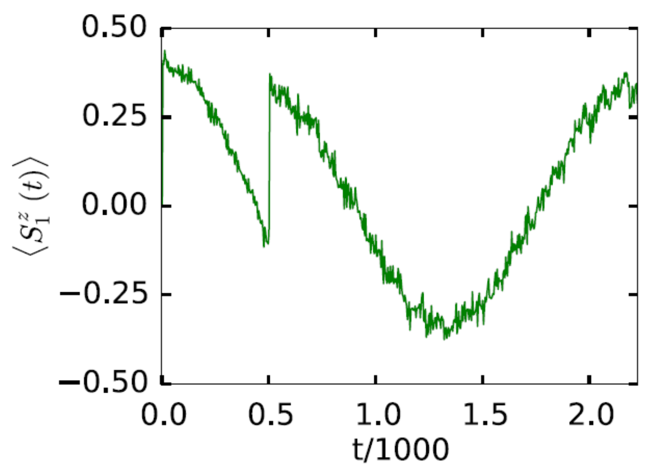


FIG. 7. Magnetization $\langle S_1^z \rangle$ for $N = 20$ and $\Delta = 2$, projections P_1^z are performed at $t = 1$ and $t = 500$. The subsequent measurement (at $t = 500$) restores the sublattice order (close) to the state after the first measurement.

Decoherence waves in AFM for quantum spins IV

Oscillations of total magnetization after single local measurement

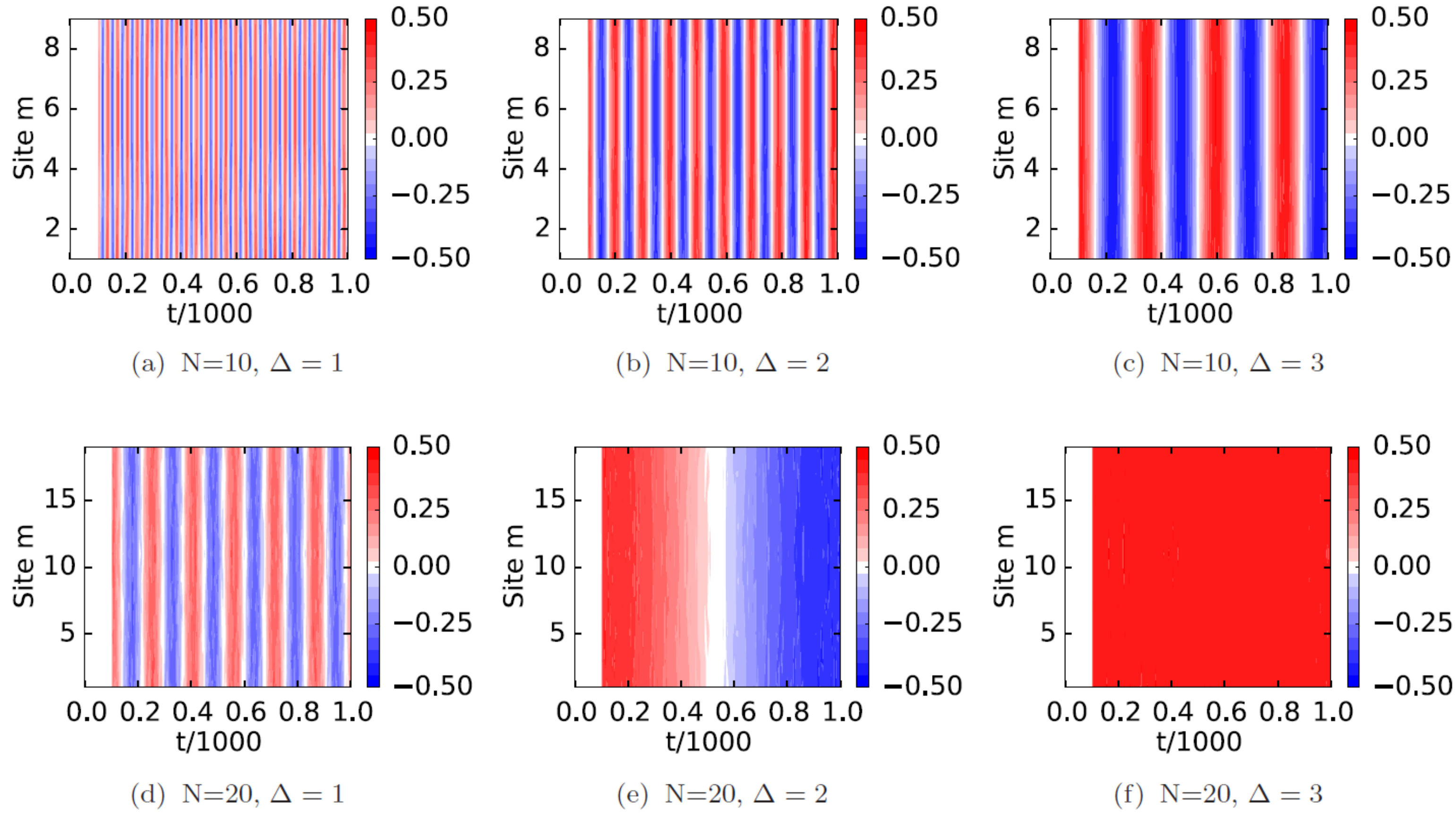


FIG. 9. Magnetization $\langle S_m^z \rangle$ for odd values of m for different values of the anisotropy Δ and chain length N. At $t = 0$, the system is prepared in the ground state, and at $t = 100$ a single measurement is performed on spin 1 along the z direction.

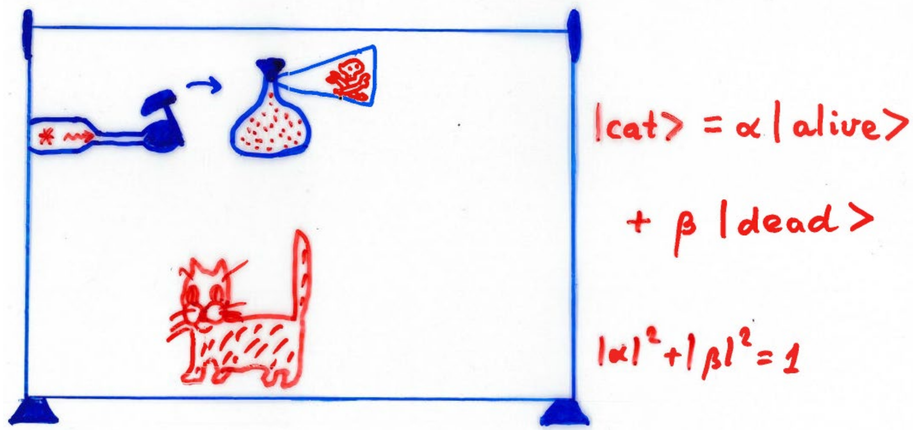
"Decoherence program"

Measurement eliminates off-diagonal elements of the density matrix, creates preferable basis (eigenstates of the operator corresponding to the measured Quantity) and therefore kills superposition principle. But why and how?

(Von Neumann theory is pure phenomenology)

"Big" is not necessarily means "classical"

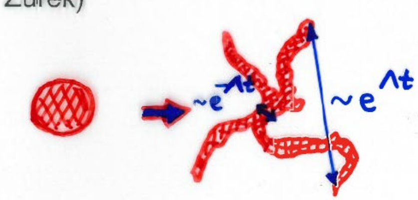
1. Schroedinger cat paradox



2. Unstable systems (W. Zurek)

$$\delta q \propto \exp(\Lambda t)$$

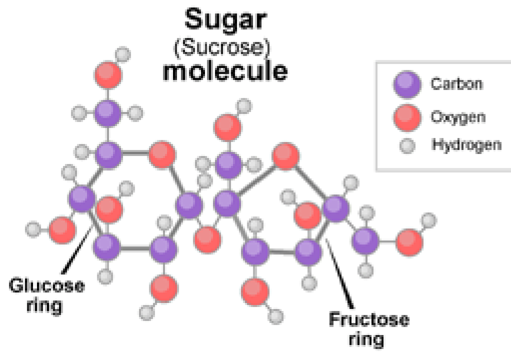
$$\delta p \propto \exp(\Lambda t)$$



Λ is the Kolmogorov entropy

“Decoherence program” II

Optical activity of biological substances



It is not equivalent to its mirror reflection → optical activity

Why it is not a superposition $1/\sqrt{2}(|\text{left}\rangle + |\text{right}\rangle)$?

The “Schrödinger cat” problem!

Superposition principle does not work

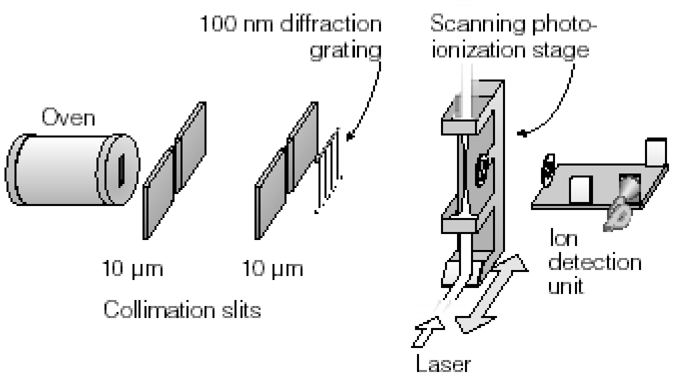
On the other hand: inverse splitting in NH_3 (ammonia maser)

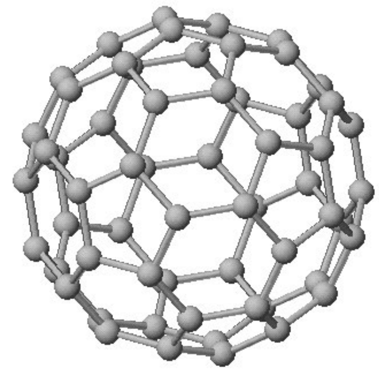
“Decoherence program” III

Wave–particle duality of C_{60} molecules

Markus Arndt, Olaf Nairz, Julian Vos-Andreae, Claudia Keller, Gerbrand van der Zouw & Anton Zeilinger

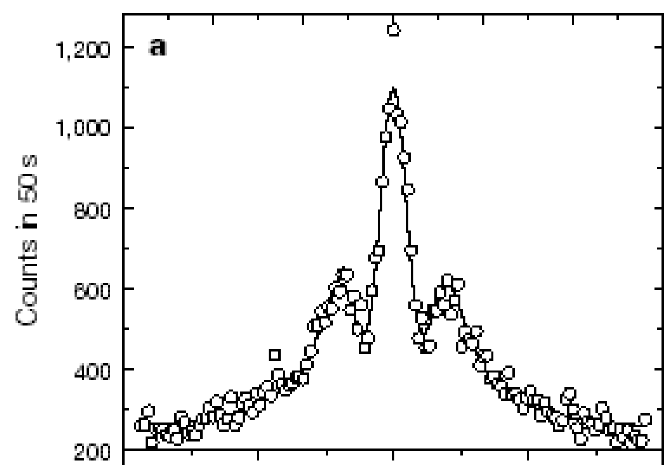
NATURE | VOL 401 | 14 OCTOBER 1999 |





C_{60}

Matter waves for C_{60} molecules



"Solution": decoherence by an environment

Physics of decoherence = physics of *open* quantum systems

E. Wigner, R. Feynman, A. Leggett, W. Zurek, E. Joos, H. Zeh...

Formal solution of the Schrödinger cat paradox: Zurek 1982, Joos & Zeh 1985

Suppression of off-diagonal matrix elements of the density matrix due to scattering of air molecules, photons…

Very small decoherence time $t_{decoh}^{-1} \propto N\left(\frac{\delta f}{\lambda}\right)^2$

N is the number of scattering acts, δf is the difference of scattering lengths for "dead" and "alive" cat, λ is de Broglie wave-length.

Even in intergalactic space: scattering of background microwave radiation

Still controversial...

Key words

1. Superselection rules

Suppression of some quantum transitions due to environment rather than to symmetry (e.g., dead cat – alive cat, right molecule – left molecule).

2. Pointer states

"Robust" states with respect to the interaction with an environment. Only pointer states survive in the macroworld. Superposition of the pointer states is not, in general, a pointer state!

Mathematical status of this concept is still not clear: something like "attractors", but… the Schrödinger equation is linear…

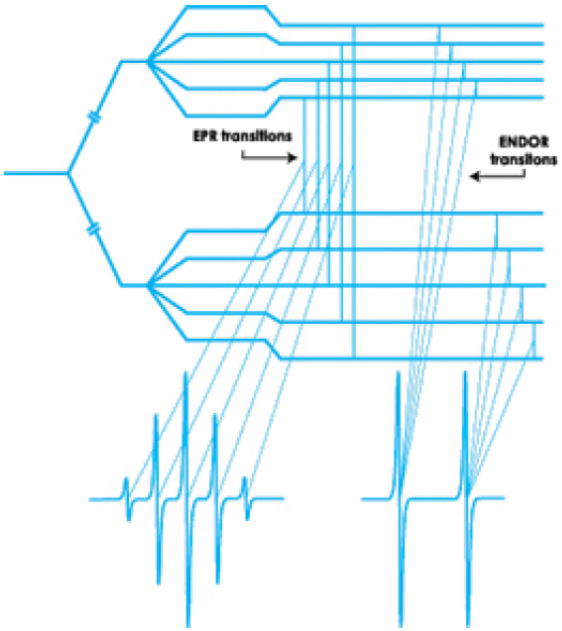
3. Difference between dissipation and dephasing

In terms of NMR: difference between T_1 and T_2.

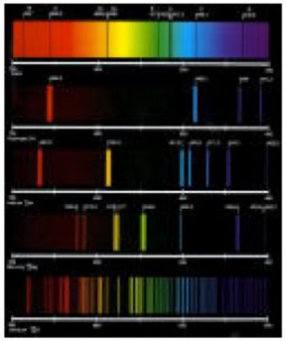
An isolated system is always quantum

Electron spin resonance:
(1) Initial electron state is known
(2) Final electron state is known
(3) Nuclear spin states are arbitrary
Nuclear spins is a thermal bath

ENDOR: both electron and nuclear initial and final states are known
Nuclear spins is a part of the system



Bohr transitions in atoms



Quantum: energy spectrum is not equidistant so for a given frequency $\hbar\omega_{mn} = E_m - E_n$ we know both initial and final state

Classical resonance: the spectrum is equidistant $E_n = \hbar\omega_0(n+1/2)$ + selection rules for the coordinate operator $|n\rangle \to |n \pm 1\rangle$: $\omega=\omega_0$ means nothing

Oscillations in this system are not quantum!

What are pointer states?

$$H = H_S + H_E + H_{SE}$$

S system E environment

Hypotheses (Zurek et al): if $H_{\mathrm{SE}} >> \Delta E_{\mathrm{S}}$ pointer states are eigenstates of H_{SE}

If $H_{\mathrm{SE}} << \Delta E_{\mathrm{S}}$ pointer states are eigenstates of H_{S}

ΔE_{S} difference of energy levels of central system (vanishes in thermodynamic limit)

Second: assumes evolution to Gibbs distribution (in particular)

S. Yuan, M. I. Katsnelson and H. De Raedt, JETP Lett. 84, 99 (2006); Phys. Rev. A 75, 052109 (2007); Phys. Rev. B 77, 184301 (2008); J. Phys. Soc. Japan 78, 094003 (2009)

$$H_S = -\sum_{i=1}^{n_S-1} \sum_{j=i+1}^{n_S} \sum_{\alpha=x,y,z} J_{i,j}^{(\alpha)} S_i^\alpha S_j^\alpha$$

$$H_E = -\sum_{i=1}^{n_E-1} \sum_{j=i+1}^{n_E} \sum_{\alpha=x,y,z} \Omega_{i,j}^{(\alpha)} I_i^\alpha I_j^\alpha$$

$$H_{SE} = -\sum_{i=1}^{n_S} \sum_{j=1}^{n_E} \sum_{\alpha=x,y,z} \Delta_{i,j}^{(\alpha)} S_i^\alpha I_j^\alpha$$

Seems to be confirmed by all simulations!

Dynamical Evolution to Canonical Ensemble

- Quantities to measure the difference between the state and the canonical distribution

Digonal Terms (Measurement of Energy Distribution)

$$\delta(t) = \sqrt{\sum_{i=1}^{N}\left(\rho_{ii}(t) - e^{-b(t)E_i} / \sum_{i=1}^{N} e^{-b(t)E_i}\right)^2}$$

Off - Digonal Terms (Measurement of Decoherence)

$$\sigma(t) = \sqrt{\sum_{i=1}^{N-1}\sum_{j=i+1}^{N} |\rho_{ij}(t)|^2}$$

Effective Temperature

$$b(t) = \frac{\sum_{i<j, E_i \neq E_j} [\ln \rho_{ii}(t) - \ln \rho_{jj}(t)] / (E_j - E_i)}{\sum_{i<j, E_i \neq E_j} 1}$$

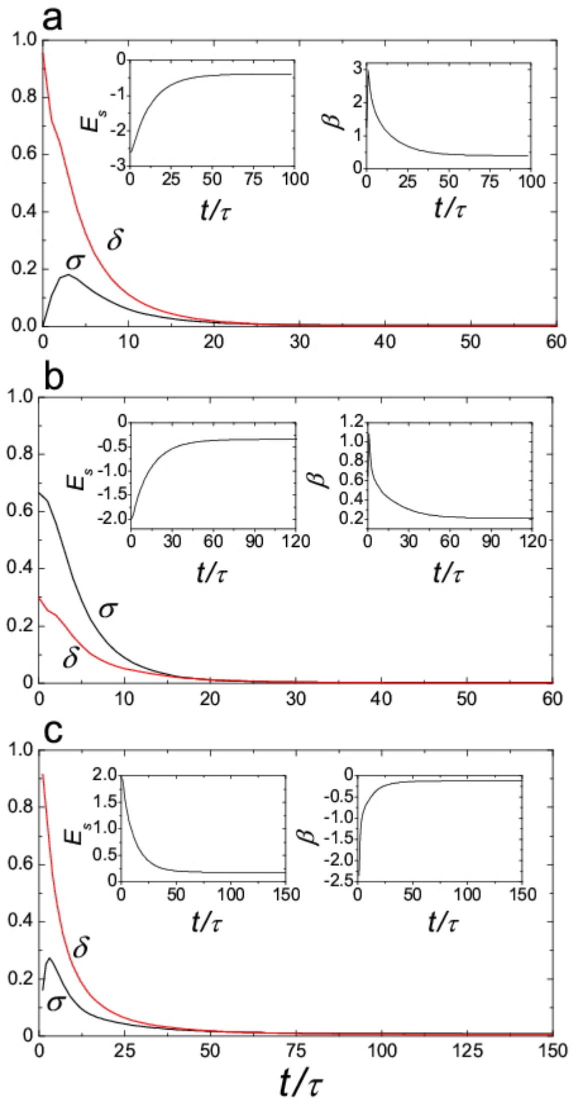
Canonical Ensemble

$$\delta(t) \to 0$$

$$\sigma(t) \to 0$$

$$b(t) \to \beta$$

Dynamical Evolution to Canonical Ensemble II



H_S : ***(a) XY - ring***

(b) Heisenberg - ring

(c) Ising - ring

H_E : ***Heisenberg - type - spin - glass***

H_{SE} : ***Heisenberg - type***

$n_S = 8, n_E = 16$

$J = -1, \Omega = 1, \Delta = 0.3$

$(a)\ |\phi(0)\rangle = |GROUND\rangle_S \otimes |RANDOM\rangle_E$

$(b)\ |\phi(0)\rangle = |UDUD\rangle_S \otimes |RANDOM\rangle_E$

$(c)\ |\phi(0)\rangle = |UUUU\rangle_S \otimes |RRRR\rangle_E$

Pointer states for strong interaction with environment

The situation is not so clear

Important to clarify (e.g. to derive von Neumann prescription for measurement)

SciPost SciPost Phys. 2, 010 (2017)

Decoherence and pointer states in small antiferromagnets: A benchmark test

Hylke C. Donker[1*], Hans De Raedt[2] and Mikhail I. Katsnelson[1]

Suppose it is correct; why macroobjects have definite coordinates rather than momenta (do not form standing waves etc.)? Because interatomic interactions are dependent mostly on coordinates and not on momenta!

Can we invent the situation when it will be dependent on momenta?

Yes!!! Edge states in topological insulators where momentum is entangled with spin, and the Hamiltonian can be spin-dependent!

PHYSICAL REVIEW B **100**, 195426 (2019)

Suppressing backscattering of helical edge modes with a spin bath

Andrey A. Bagrov,[1,2,*] Francisco Guinea,[3,4,†] and Mikhail I. Katsnelson[1,‡]

Protection of propagation direction by environment

Two electron modes (one is edge mode), zero Hamiltonian

$$\mathcal{H} = \sum_k c^\dagger(k) H^c(k) c(k) + \sum_{k;i=1,2} d_i^\dagger(k) H_i^d(k) d_i(k)$$

$$H^c(k) = \begin{pmatrix} \hbar v_F k & h_0 \\ h_0 & -\hbar v_F k \end{pmatrix}$$

$$H_{1,2}^d(k) = \begin{pmatrix} \pm\hbar c k & 0 \\ 0 & \pm\hbar c k \end{pmatrix}$$

c edge mode, h_0 back scattering, d fermionic thermal bath.

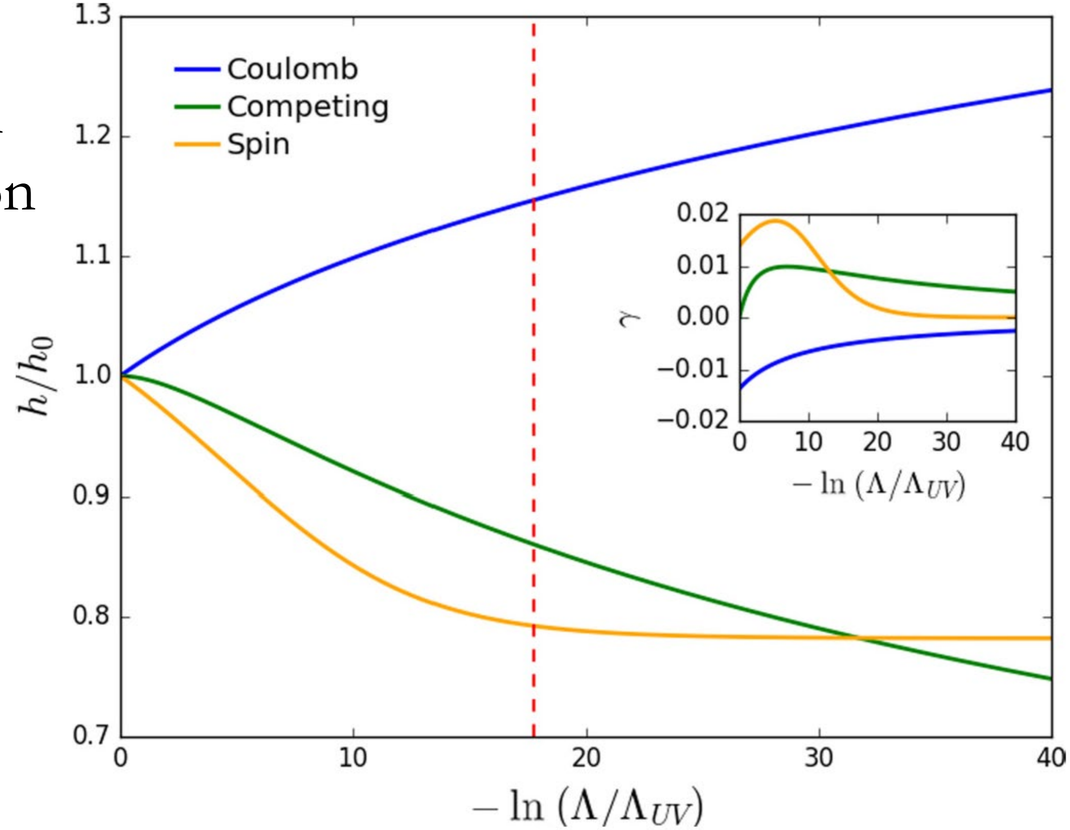
Interaction:

$$\mathcal{H}_{\text{int}} = \Gamma^{(i)}_{\alpha\beta\gamma\delta} \sum_{q,p,k} c^\dagger_\alpha(k) c_\beta(k+q) d^\dagger_{i,\gamma}(p) d_{i,\delta}(p-q),$$

$$\begin{aligned}\Gamma^{(i)}_{\alpha\beta\gamma\delta} &= J^{(i)}_{00} \mathbb{I}_{\alpha\beta} \otimes \mathbb{I}_{\gamma\delta} + J^{(i)}_{zz} \sigma^z_{\alpha\beta} \otimes \sigma^z_{\gamma\delta} \\ &+ J^{(i)} \left(\sigma^x_{\alpha\beta} \otimes \sigma^x_{\gamma\delta} + \sigma^y_{\alpha\beta} \otimes \sigma^y_{\gamma\delta}\right) \\ &+ J^{(i)}_{0z} \mathbb{I}_{\alpha\beta} \otimes \sigma^z_{\gamma\delta} + J^{(i)}_{z0} \sigma^z_{\alpha\beta} \otimes \mathbb{I}_{\gamma\delta},\end{aligned}$$

Pointer states for strong interaction with environment II

RG analysis: renormalization of back scattering as a function of cutoff parameter

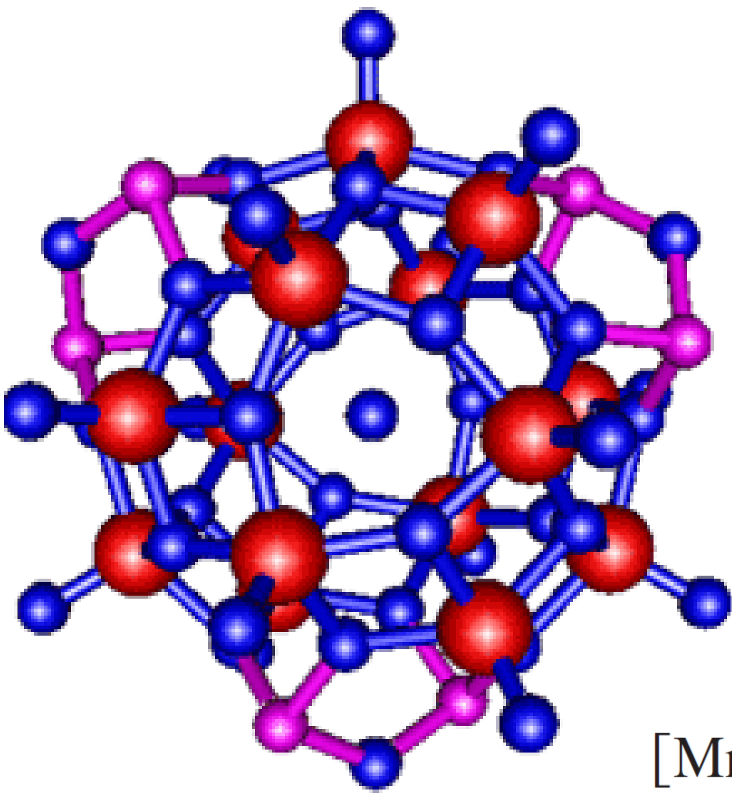


When interaction Hamiltonian depends mostly on spins back-scattering is suppressed (direction of momentum is protected), when mostly on coordinates – the effect is opposite

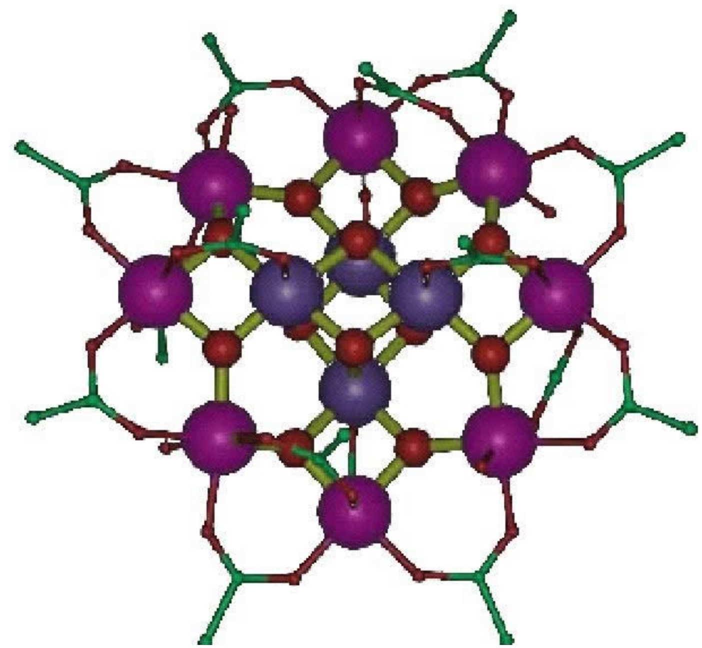
Decoherence in quantum spin systems: Motivation

Molecular magnets

V_{15}



Mn_{12}



$[Mn_{12}O_{12}(CH_3COO)_{16}(H_2O)_4]\cdot 2CH_3COOH\cdot 4H_2O$

$V_{15}(K_6[V_{15}As_6O_{42}(H_2O)]\cdot 8H_2O)$

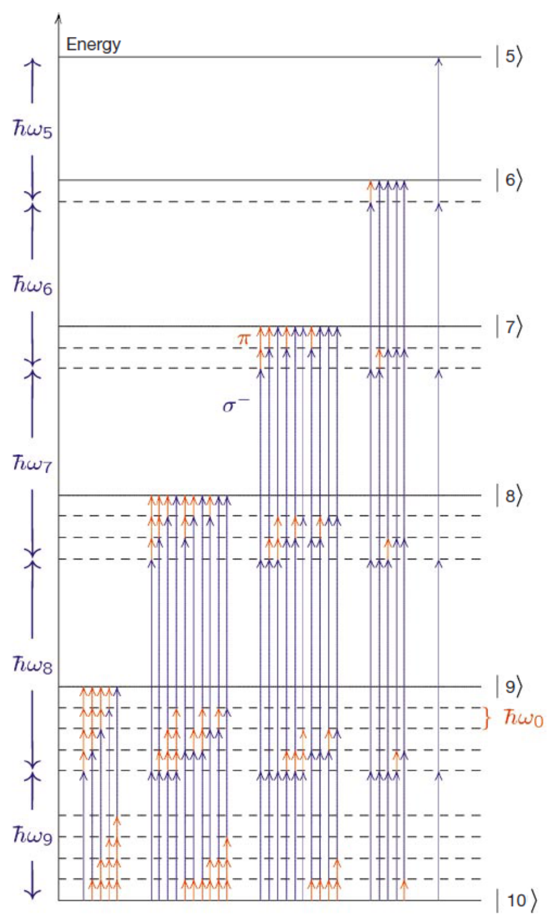
Molecular magnets II

Quantum computing in molecular magnets

Michael N. Leuenberger & Daniel Loss

NATURE | VOL 410 | 12 APRIL 2001 |

Very attractive but...
Decoherence by nuclear spins
(chaotic thermal bath at any reasonable temperature)



VOLUME 90, NUMBER 21 PHYSICAL REVIEW LETTERS week ending 30 MAY 2003

Quantum Oscillations without Quantum Coherence

V.V. Dobrovitski,[1] H. A. De Raedt,[2] M. I. Katsnelson,[3] and B. N. Harmon[1]

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{V} = \mathcal{H}_S + \mathcal{H}_B + \mathcal{V}$$

$$\mathcal{H}_S = 2J\mathbf{s}_1\mathbf{s}_2 \qquad \mathcal{V} = \sum_k A_k^{(1)}\mathbf{s}_1\mathbf{I}_k + A_k^{(2)}\mathbf{s}_2\mathbf{I}_k \qquad \mathcal{H}_B = 0$$

One can have "Rabi oscillations" but entropy is high (a very small part of Hilbert space is available for manipulations)

STM probe of magnetic clusters

Revealing Magnetic Interactions from Single-Atom Magnetization Curves

Focko Meier,* Lihui Zhou, Jens Wiebe,† Roland Wiesendanger

4 APRIL 2008 VOL 320 SCIENCE

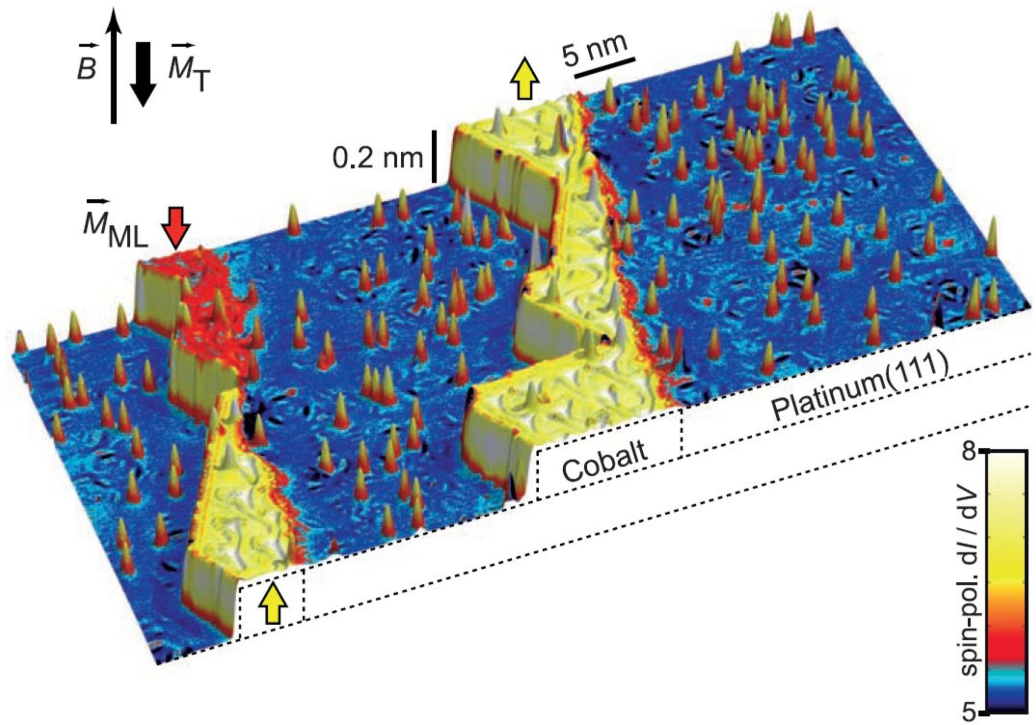
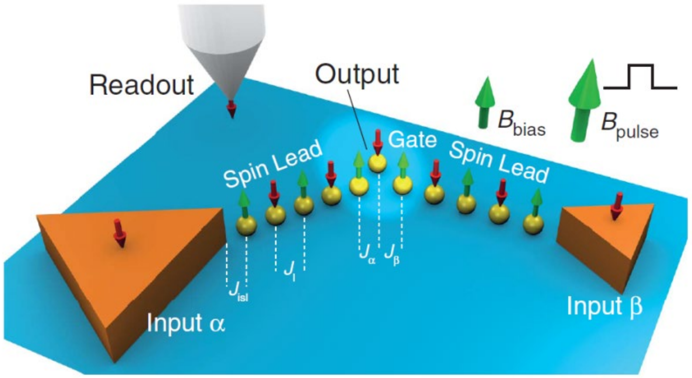


Fig. 1. Overview of the sample of individual Co adatoms on the Pt(111) surface (blue) and Co ML stripes (red and yellow) attached to the step edges (STM topograph colorized with the simultaneously recorded spin-polarized d*I*/d*V* map measured with an STM tip magnetized antiparallel to the surface normal). An external $\vec{B}$ can be applied perpendicular to the sample surface in order to change the magnetization of adatoms $\vec{M}_A$, ML stripes $\vec{M}_{ML}$, or tip $\vec{M}_T$. The ML appears red when $\vec{M}_{ML}$ is parallel to $\vec{M}_T$ and yellow when $\vec{M}_{ML}$ is antiparallel to $\vec{M}_T$. (Tunneling parameters are as follows: $I = 0.8$ nA, $V = 0.3$ V, modulation voltage $V_{mod} = 20$ mV, $T = 0.3$ K.)

Realizing All-Spin–Based Logic Operations Atom by Atom

Alexander Ako Khajetoorians, Jens Wiebe,* Bruno Chilian, Roland Wiesendanger

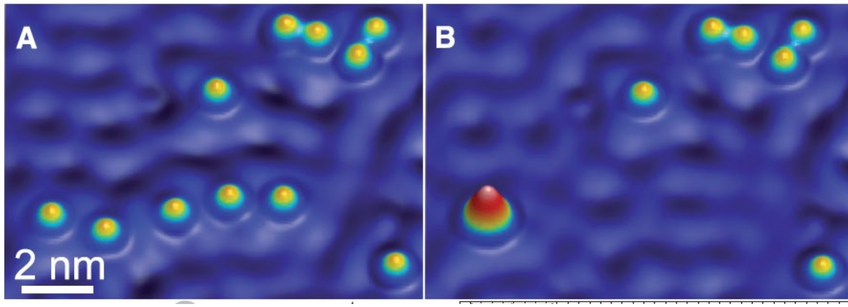
27 MAY 2011 VOL 332 SCIENCE



Current-Driven Spin Dynamics of Artificially Constructed Quantum Magnets

Alexander Ako Khajetoorians,[1*] Benjamin Baxevanis,[2] Christoph Hübner,[2] Tobias Schlenk,[1] Stefan Krause,[1] Tim Oliver Wehling,[3,4] Samir Lounis,[5] Alexander Lichtenstein,[2] Daniela Pfannkuche,[2] Jens Wiebe,[1*] Roland Wiesendanger[1]

SCIENCE VOL 339 4 JANUARY 2013



Constant-current STM images of single Fe atoms on the surface of Cu(111)

STM probe of magnetic clusters II

PRL 107, 106804 (2011) PHYSICAL REVIEW LETTERS week ending 2 SEPTEMBER 2011

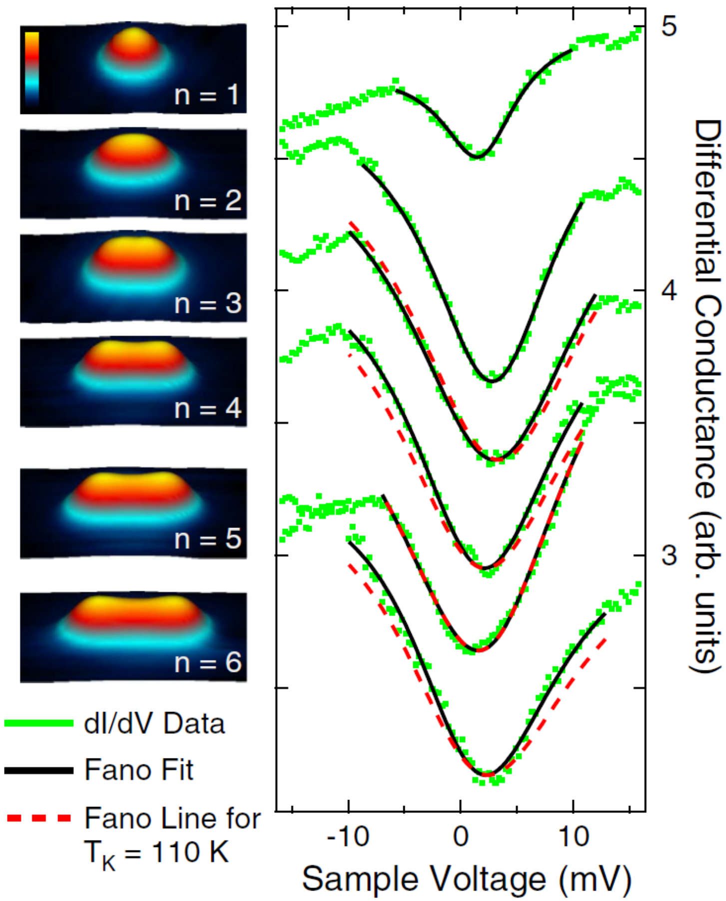
Two-Site Kondo Effect in Atomic Chains

N. Néel and R. Berndt
Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany

J. Kröger
Institut für Physik, Technische Universität Ilmenau, D-98693 Ilmenau, Germany

T. O. Wehling and A. I. Lichtenstein
Institut für Theoretische Physik, Universität Hamburg, D-20355 Hamburg, Germany

M. I. Katsnelson
Institute for Molecules and Materials, Radboud University Nijmegen, NL-6525 AJ Nijmegen, The Netherlands
(Received 10 August 2010; published 1 September 2011)

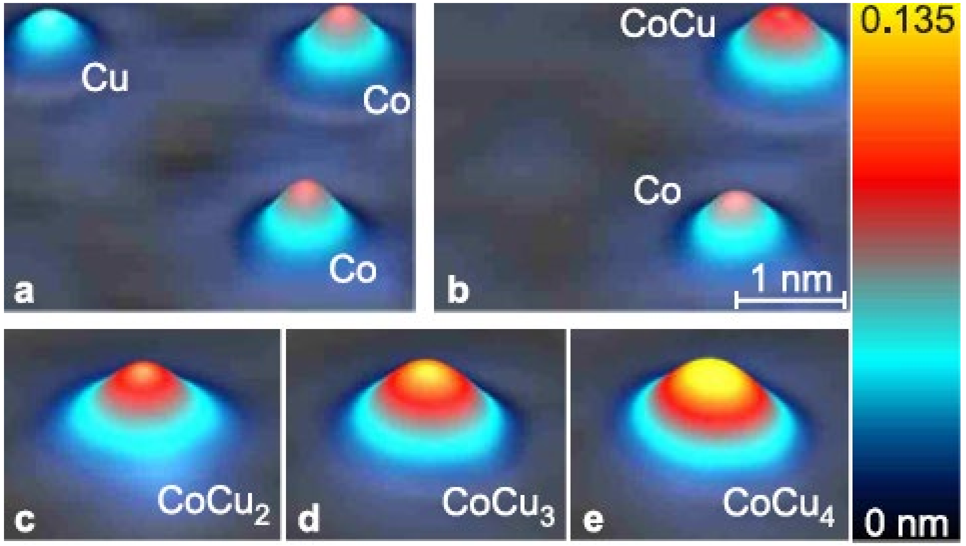


PRL 101, 266803 (2008) PHYSICAL REVIEW LETTERS week ending 31 DECEMBER 2008

Controlling the Kondo Effect in $CoCu_n$ Clusters Atom by Atom

N. Néel,[1] J. Kröger,[1,*] R. Berndt,[1] T. O. Wehling,[2] A. I. Lichtenstein,[2] and M. I. Katsnelson[3]
[1]*Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany*
[2]*Institut für Theoretische Physik I, Universität Hamburg, D-20355 Hamburg, Germany*
[3]*Institute for Molecules and Materials, Radboud University Nijmegen, NL-6525 AJ Nijmegen, The Netherlands*
(Received 1 October 2008; published 30 December 2008)

Clusters containing a single magnetic impurity were investigated by scanning tunneling microscopy, spectroscopy, and *ab initio* electronic structure calculations. The Kondo temperature of a Co atom embedded in Cu clusters on Cu(111) exhibits a nonmonotonic variation with the cluster size. Calculations model the experimental observations and demonstrate the importance of the local and anisotropic electronic structure for correlation effects in small clusters.



Decoherence by conduction electrons in substrate

Model consideration

Metal-insulator transition by suppression of spin fluctuations

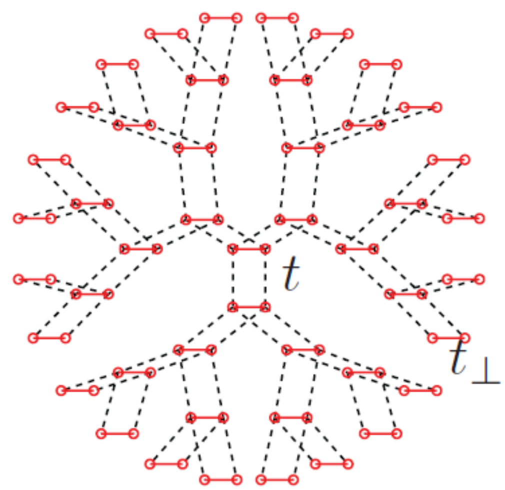
H. Hafermann, M. I. Katsnelson and A. I. Lichtenstein

EPL, **85** (2009) 37006

Two atoms, each connects with a thermal bath (double Bethe model)

Fig. 1: (Color online) The two-plane Hubbard model on the Bethe lattice visualized for coordination number $z = 3$. It can be viewed as a lattice of dimers, or equivalently as two planes with opposing sites coupled by a perpendicular hopping $t_\perp$.

$$H = -t \sum_{\langle ij \rangle, \sigma} (a^\dagger_{i\sigma} a_{j\sigma} + b^\dagger_{i\sigma} b_{j\sigma}) - t_\perp \sum_{i\sigma} (a^\dagger_{i\sigma} b_{i\sigma} + b^\dagger_{i\sigma} a_{i\sigma}) + U \sum_{i\sigma} (n_{ai\uparrow} n_{ai\downarrow} + n_{bi\uparrow} n_{bi\downarrow}), \quad (1)$$



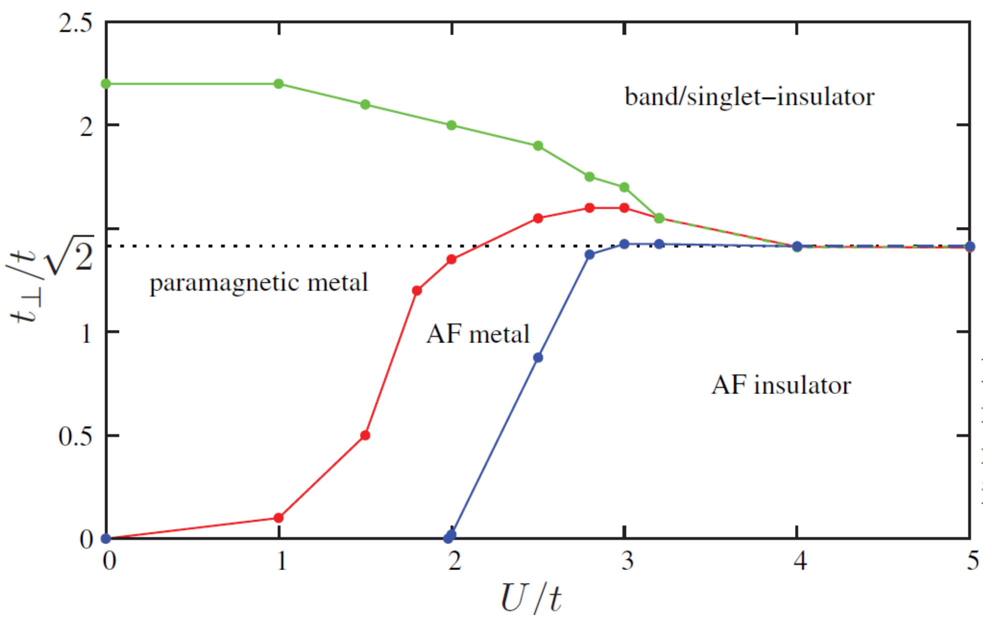


Fig. 2: (Color online) Phase diagram of the two-plane Hubbard model on the Bethe lattice at temperature $T/t = 0.1$. The mean-field value of $t_\perp$ for the AF to singlet insulating transition is marked by a dashed line.

Model consideration II

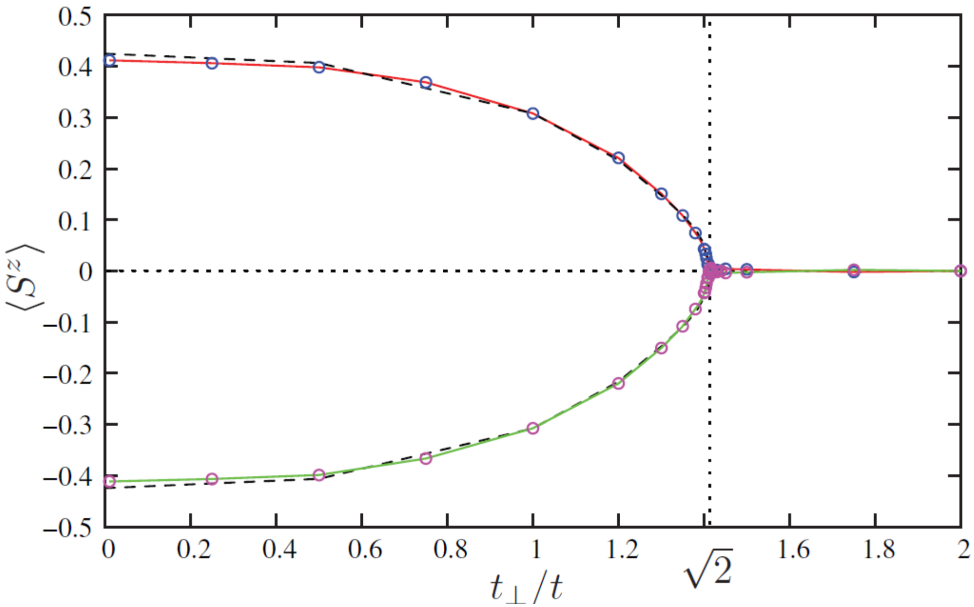


Fig. 4: (Color online) Magnetization $\langle S_i^z \rangle$ on opposite sites of the two Bethe lattices for $U/t = 4$ and temperature $T/t = 0.1$. The dashed lines show the correspondig result for $T/t = 0.04$.

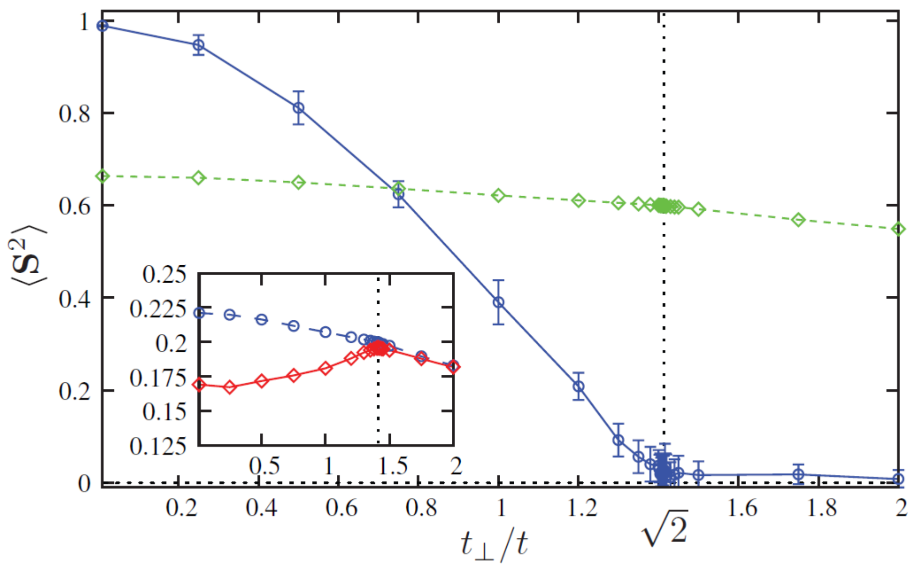


Fig. 5: (Color online) Spin-correlations $\langle \mathbf{S}_i^2 \rangle$ on opposite sites of the two Bethe lattices (dashed line) and total spin $\langle \mathbf{S}^2 \rangle$ (solid line) for the dimer for $U/t = 4$ and temperature $T/t = 0.1$. The inset compares the correlations $\langle S_i^z S_i^z \rangle$ (upper dashed line) and $-\langle S_i^z S_j^z \rangle$ for $i \neq j$ (solid line). The transition point is marked by the vertical dashed line.

Possible experiment with spin-polarized STM:

- changing distance between magnetic adatoms;
- changing hybridization with substrate

Transition from Neel state to singlet state (e.g. for dimer) when the coupling to substrate is weaker than the coupling between adatoms

Anderson tower and origin of classicality for Heisenberg AFM

PHYSICAL REVIEW X **13,** 041027 (2023)

Emergence of Classical Magnetic Order from Anderson Towers: Quantum Darwinism in Action

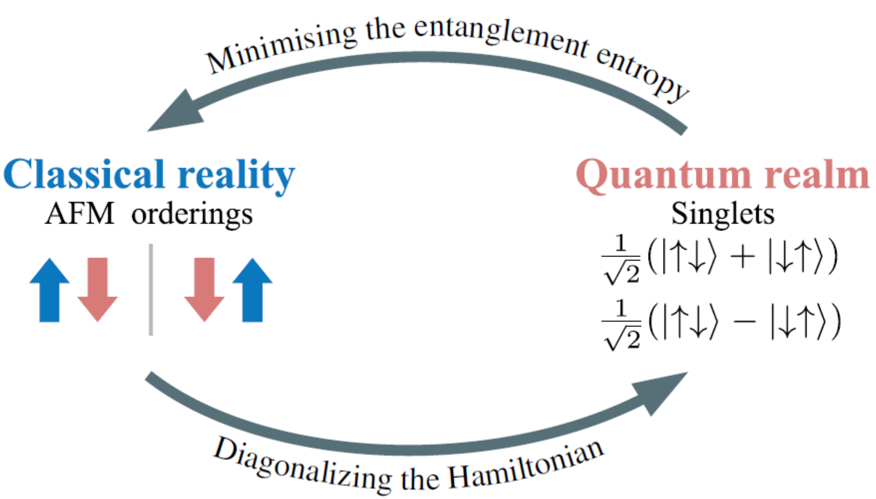
O. M. Sotnikov,[1,2] E. A. Stepanov,[3] M. I. Katsnelson,[4] F. Mila,[5] and V. V. Mazurenko[1,2,*]

P. W. Anderson (1952) noticed that despite singlet ground state is very different from Neel state their energies are close: $E_N\,(1+1/zS) < E_0 < E_N$

(bipartite lattice, nearest-neighbors, z coordination number)

Neel state can be build as a superposition of low-excited state (Anderson tower), supposed to be stable in thermodynamic limit

The idea: to prove robustness of classical Neel state with respect to (arbitrary) interaction with environment, within the concept of "quantum Darwinism" (W. Zurek)



Anderson tower and origin of classicality for Heisenberg AFM II

"Classical" states: product of spin coherent states (product state, no entanglement)

$$|\Psi_T\rangle = \prod_i \left[\cos\frac{\theta_i}{2} e^{i(\phi_i/2)}|\uparrow\rangle + \sin\frac{\theta_i}{2} e^{-i(\phi_i/2)}|\downarrow\rangle\right]$$

Tower states

magnetic moment $\mathbf{m}_i$

$$\langle m_i^x \rangle = \sin\theta_i \cos\phi_i \quad \langle m_i^y \rangle = \sin\theta_i \sin\phi_i \quad \langle m_i^z \rangle = \cos\theta_i$$

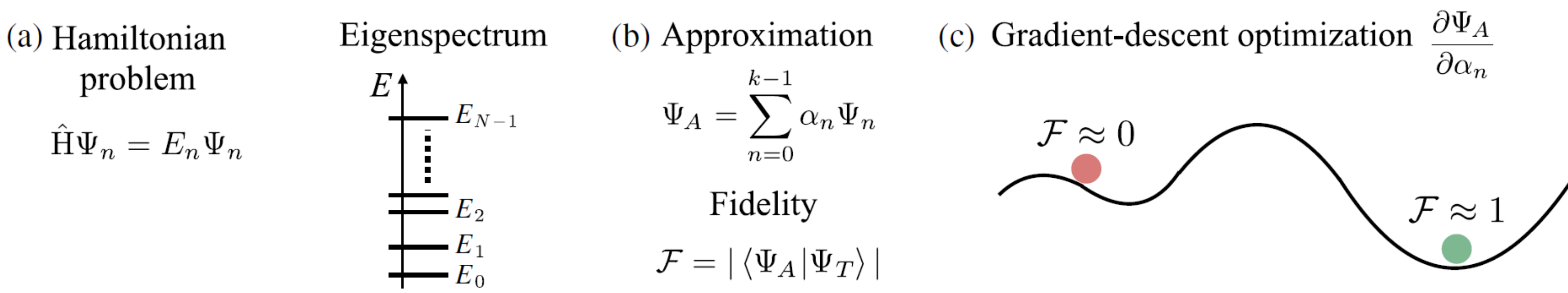
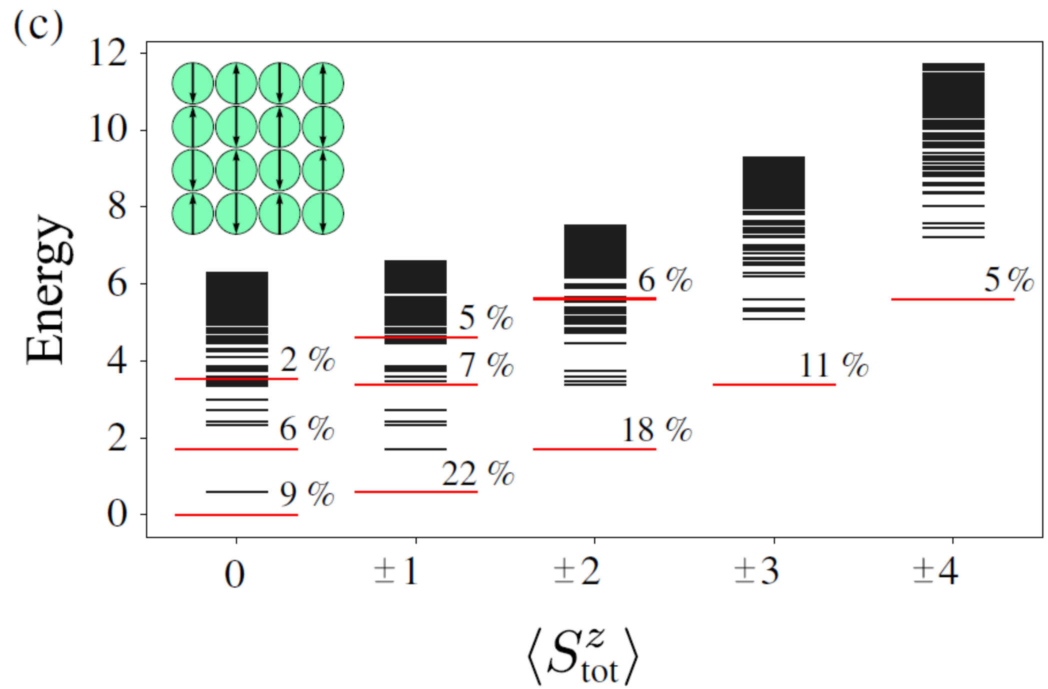


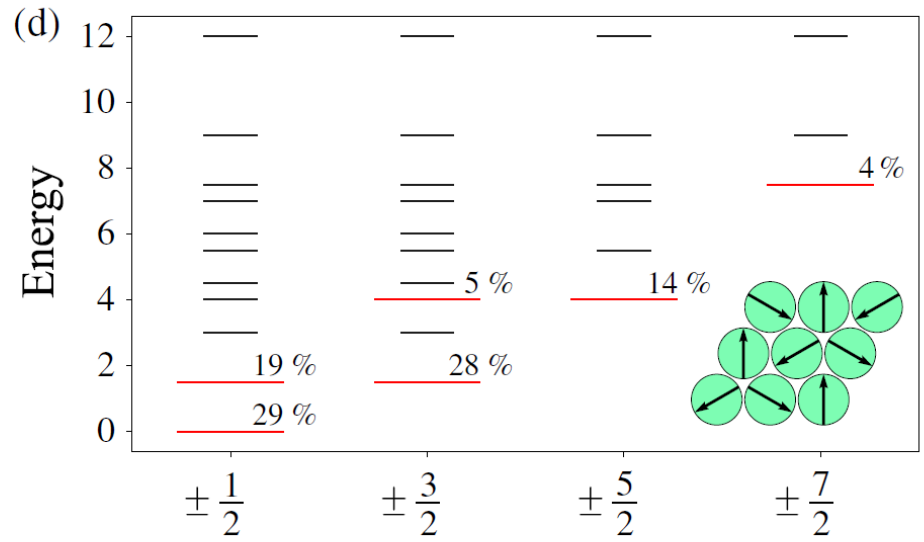
FIG. 2. Protocol for constructing Anderson's towers of states. (a) For the given Hamiltonian, one calculates a set of low-lying eigenstates. (b) On the basis of the calculated eigenstates, an initial approximation of the target state is prepared. The complex coefficients α_n are chosen to be random. (c) The coefficients are optimized within a gradient-descent approach aiming to maximize the fidelity between approximation and target wave functions. N is the corresponding number of energy levels.

Anderson tower and origin of classicality for Heisenberg AFM III

Composition of some slassical AFM states for small quantum systems



TOS states: eigenstates with maximal contribution to classical states (shown in red)



Anderson tower and origin of classicality for Heiseneberg AFM IV

Selection of pointer states via "quantum Darwinism" (optimization of robustness)

$$\Psi_R(\boldsymbol{\alpha}) = \sum_{n=0}^{k-1} \alpha_n \Psi_n^{\mathrm{TOS}}$$

Trial combinations of TOS states

Selected states (red) forms subsystem A, other states subsystem B; B plays the role of environment for TOS

Entanglement entropy

$$\mathbb{E}_A(\boldsymbol{\alpha}) = -\mathrm{Tr}\rho_A(\boldsymbol{\alpha})\log_2\rho_A(\boldsymbol{\alpha})$$

$$\rho_A(\boldsymbol{\alpha}) = \mathrm{Tr}_B\rho_{AB}(\boldsymbol{\alpha})$$

If necessary symmetrize – e.g. for triangular lattice with three sublattices A,B,C

$$\mathbb{E}_\Delta(\boldsymbol{\alpha}) = \frac{1}{3}[\mathbb{E}_A(\boldsymbol{\alpha}) + \mathbb{E}_B(\boldsymbol{\alpha}) + \mathbb{E}_C(\boldsymbol{\alpha})]$$

Anderson tower and origin of classicality for Heisenberg AFM V

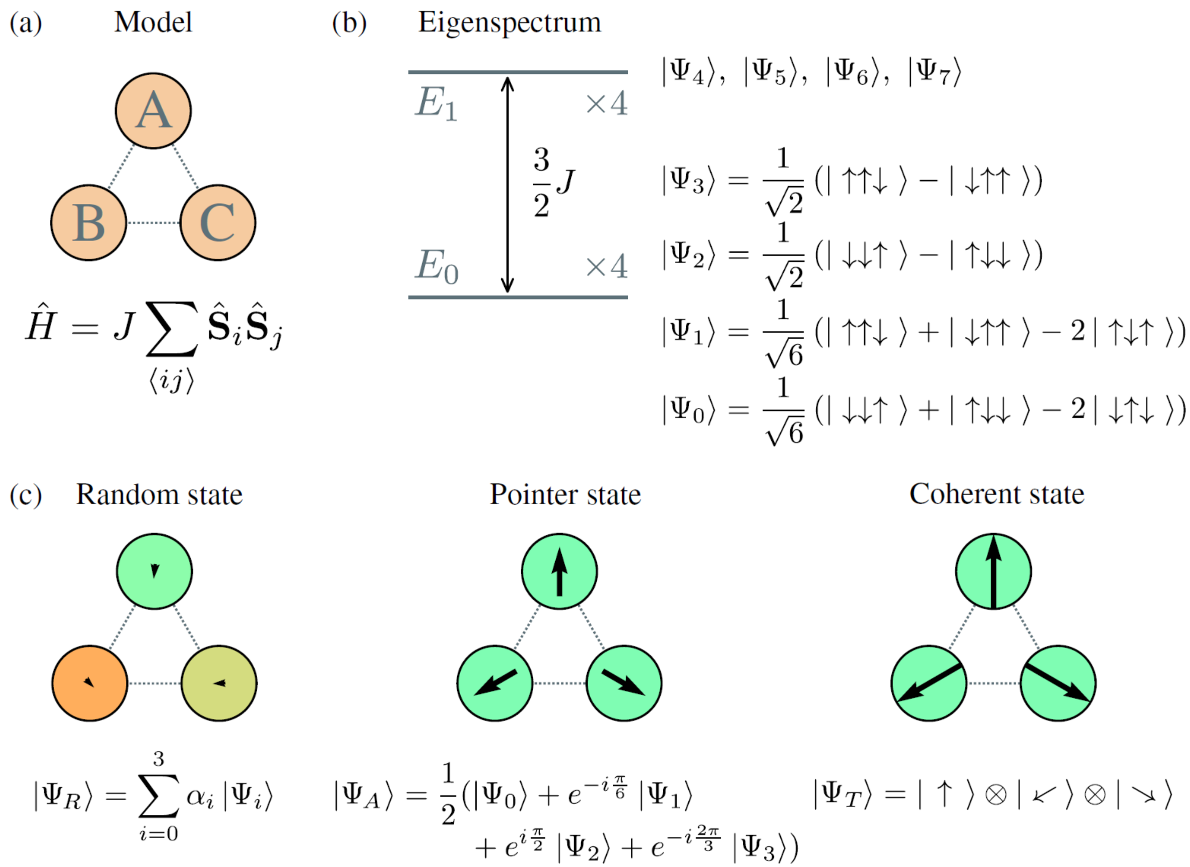
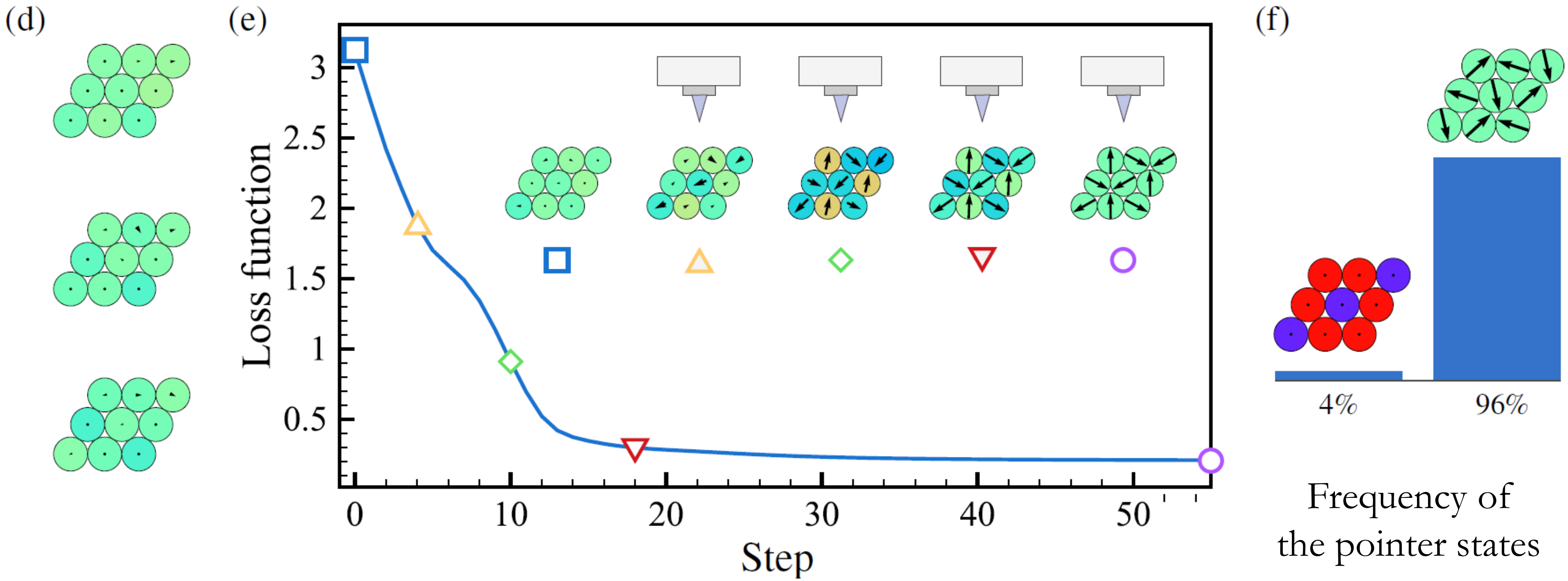


FIG. 5. Candidate for demonstrating the quantum Darwinism of degenerate quantum systems in real experiments. (a) Antiferromagnetic Heisenberg model defined on the triangular plaquette. (b) Eigenspectrum of the Heisenberg model characterized by fourfold degenerate ground and excited states. (c) Example of a magnetic structure corresponding to a random superposition Ψ_R of ground eigenstates, pointer state Ψ_A optimized with respect to von Neumann entropy showing reduced local magnetization, and classical model solution Ψ_T.

Optimized state: ent. entropy 0.65, sublattice spin 0.33 (instead of 0.5)

Anderson tower and origin of classicality for Heisenberg AFM VI

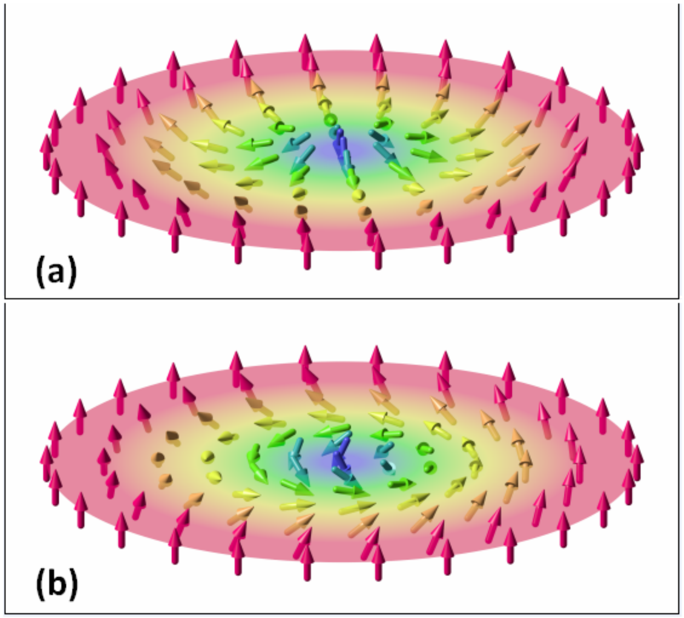
Optimization for larger system



Conclusion: classical states correspond to linear combination of low-excited states (or the states belonging to degenerate ground states) which are robust if the rest of quantum Hilbert state is considered as environment

Quantum skyrmion

Classical skyrmion: magnetic topological defect of great fundamental interest and perspectives of important applications



Wikipedia

Characterized by topological charge, conserving integer quantity

$$Q = \frac{1}{4\pi} \int \mathbf{m} \cdot [\partial_x \mathbf{m} \times \partial_y \mathbf{m}] dx\, dy$$

Can we have quantum analog?

Several works, I will follow this one:

PHYSICAL REVIEW B **103**, L060404 (2021)

Letter | Editors' Suggestion

Probing the topology of the quantum analog of a classical skyrmion

O. M. Sotnikov,[1] V. V. Mazurenko,[1,*] J. Colbois,[2] F. Mila,[2] M. I. Katsnelson,[3,1] and E. A. Stepanov[4,1]

Quantum skyrmion II

Exchange + DMI +
External magnetic field

$$\hat{H} = \sum_{ij} J_{ij} \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j + \sum_{ij} \mathbf{D}_{ij} [\hat{\mathbf{S}}_i \times \hat{\mathbf{S}}_j] + \sum_i B^z \hat{S}_i^z$$

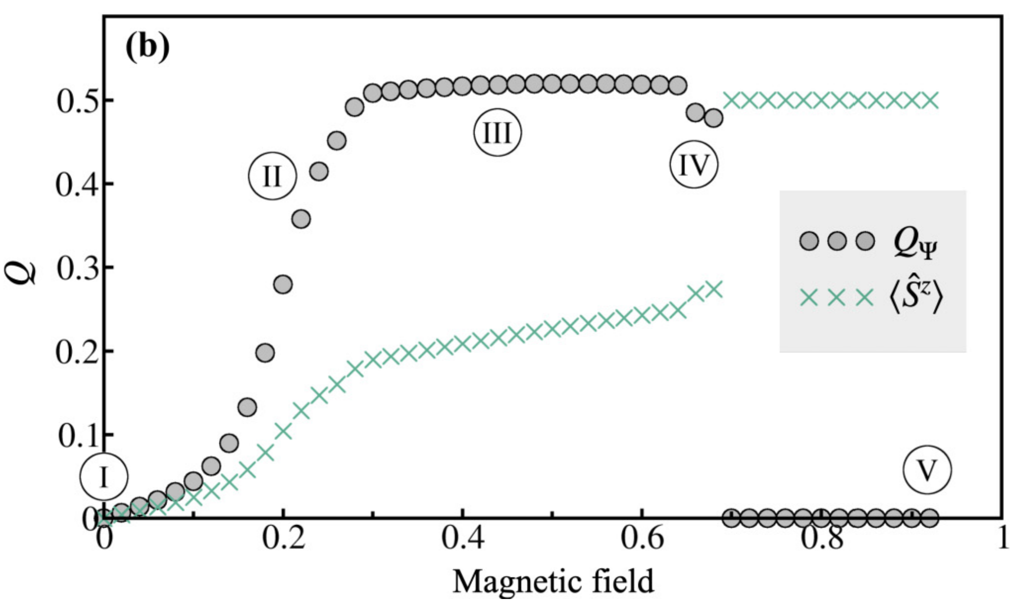
Important: strictly speaking, no topological protection in quantum case (informally: unstable with respect to tunneling)

quantum scalar chirality

$$Q_\Psi = \frac{N}{\pi} \langle \hat{\mathbf{S}}_1 \cdot [\hat{\mathbf{S}}_2 \times \hat{\mathbf{S}}_3] \rangle$$

where N is the number of nonoverlapping elementary triangular plaquettes that cover the lattice. Labels 1, 2, and 3 depict three different spins that form an elementary plaquette. Here

quantum problem



$$J = -0.5D$$

Plateau region corresponding to skyrmion state?!

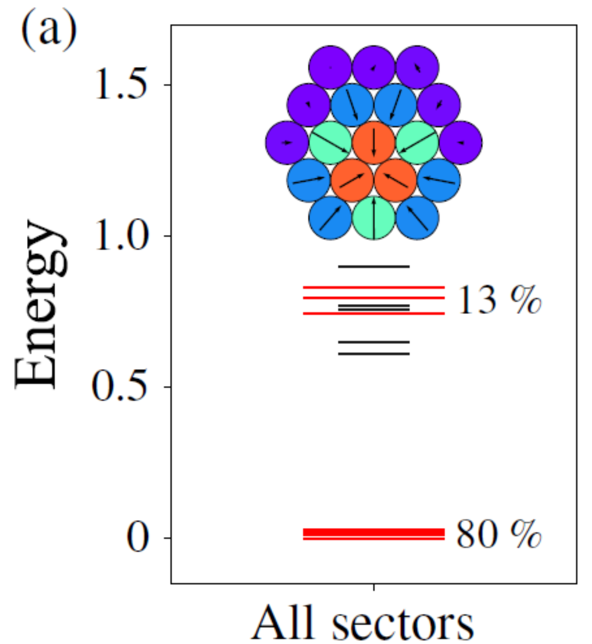
Quantum skyrmion III

PHYSICAL REVIEW X **13**, 041027 (2023)

Emergence of Classical Magnetic Order from Anderson Towers: Quantum Darwinism in Action

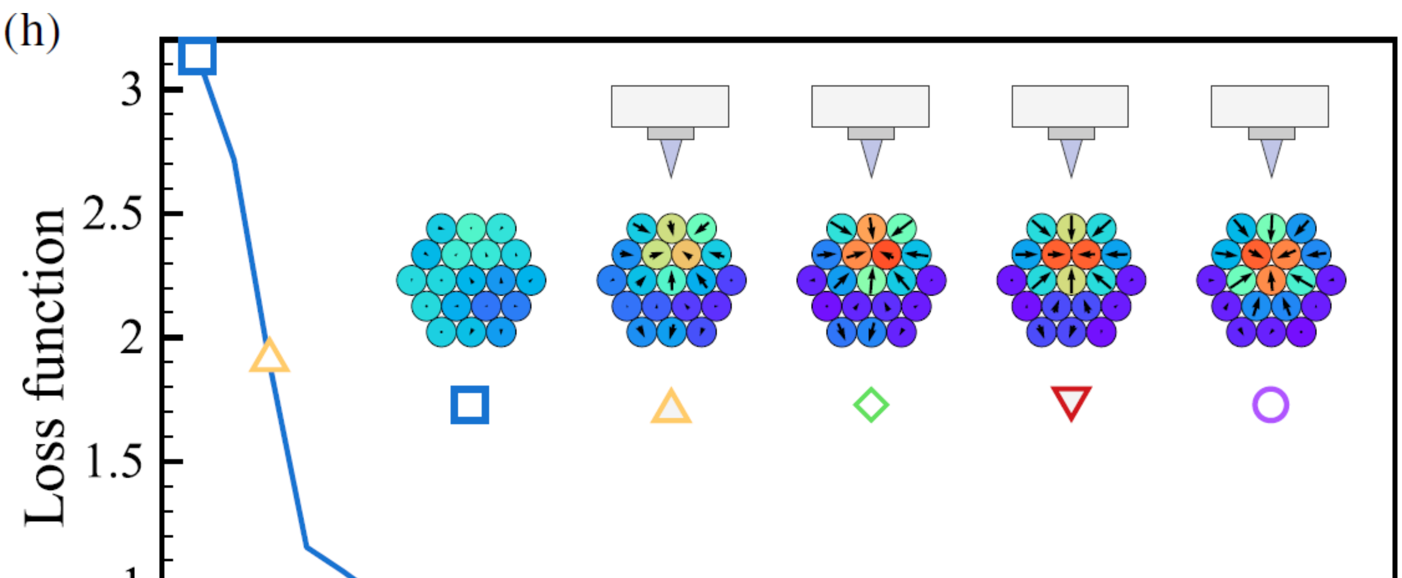
O. M. Sotnikov,[1,2] E. A. Stepanov,[3] M. I. Katsnelson,[4] F. Mila,[5] and V. V. Mazurenko[1,2,*]

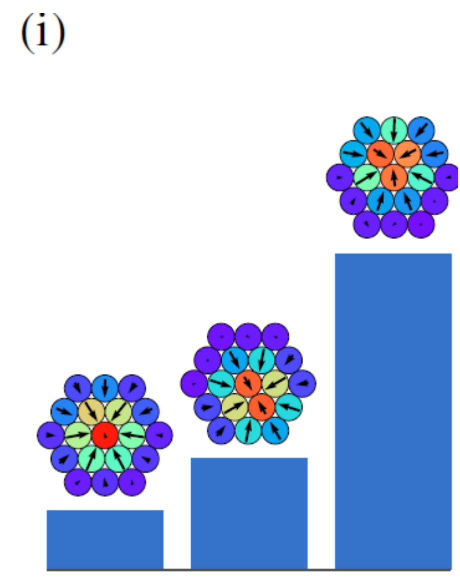
Tower of states



The same problem of classical-quantum correspondence as for AFM

Optimization to pointer states





Quantum skyrmion IV

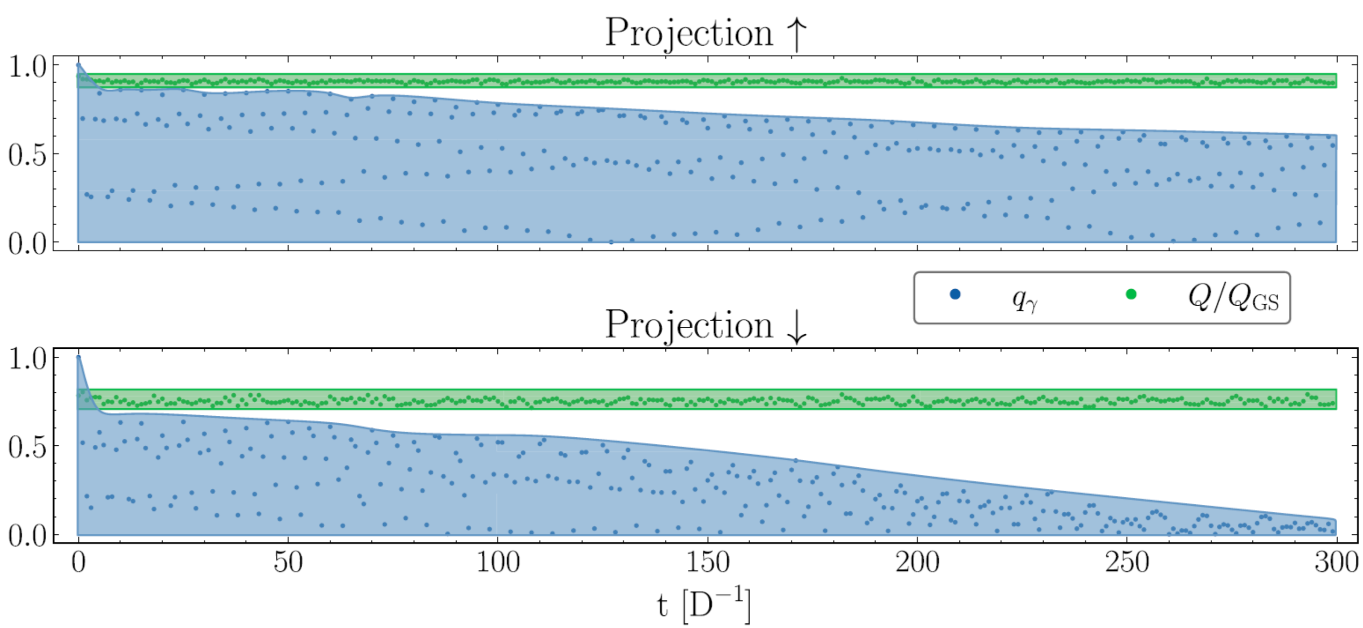
PHYSICAL REVIEW B **109**, 064409 (2024)

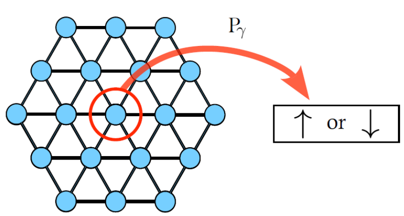
Stability of a quantum skyrmion: Projective measurements and the quantum Zeno effect

Fabio Salvati,* Mikhail I. Katsnelson, Andrey A. Bagrov, and Tom Westerhout

Despite the absence of exact topological protection quantum skyrmion state is reasonably robust with respect to the local measurements

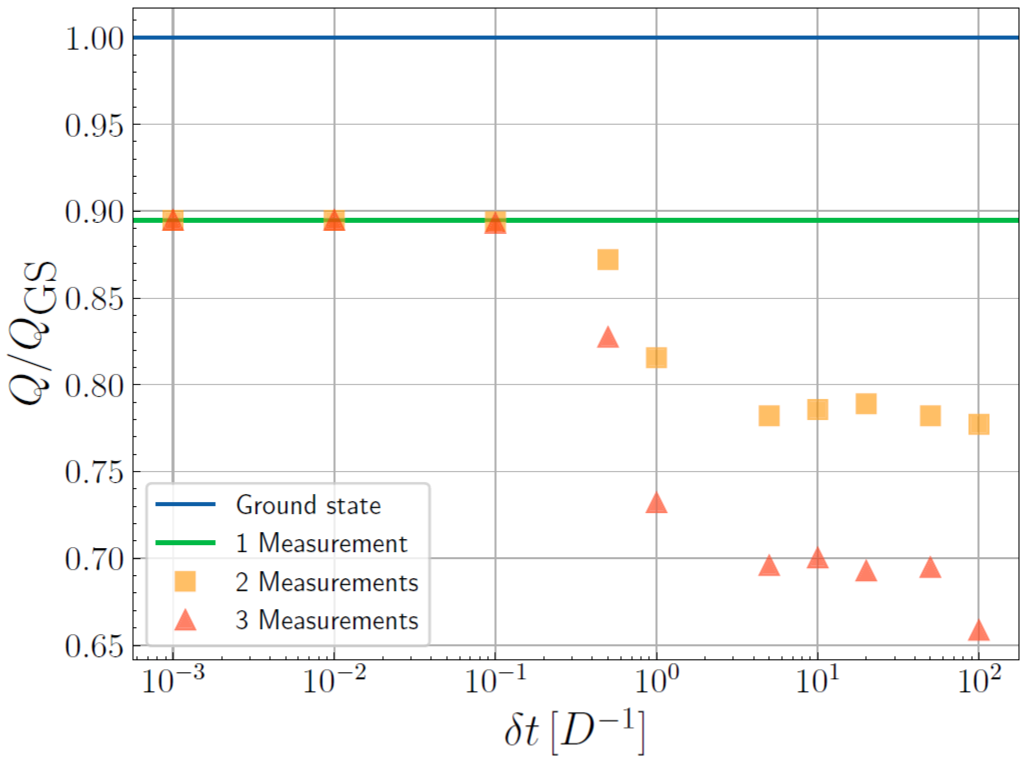
Evolution of quantum chirality after projective local measurement





Anderson tower and origin of classicality for Heisenberg AFM VI

Repeated measurement and "quantum Zeno" effect (stabilization of quantum state by repeated measurements, initially introduced for two-level problem)



Like for AFM repeated local measurements make system more classical

Emergent topological protection!

FIG. 4. Averaged normalized chirality for one and repetitive measurements as a function of time interval δt between measurements. Quantum Zeno effect stabilizes the quantum skyrmion when projective measurements are performed for time intervals below $\delta t \leqslant 0.1D^{-1}$

Main collaborators

H. Donker, A. Bagrov, F. Salvati, T. Westerhout (Radboud Univ., Nijmegen)

H. De Raedt (Groningen Univ.)

O. Sotnikov and V. Mazurenko (Ural Federal Univ., Ekaterinburg)

F. Mila (EPFL, Lausanne)

E. Stepanov (Ecole Polytechnique, Paris)

MANY THANKS
FOR YOUR ATTENTION