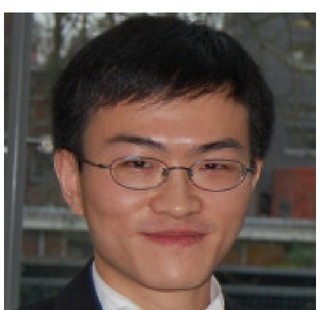
Radboud Universiteit

Decoherence in quantum spin systems

Mikhail Katsnelson

Main collaborators:

Shengjun Yuan, Nijmegen (now Wuhan)



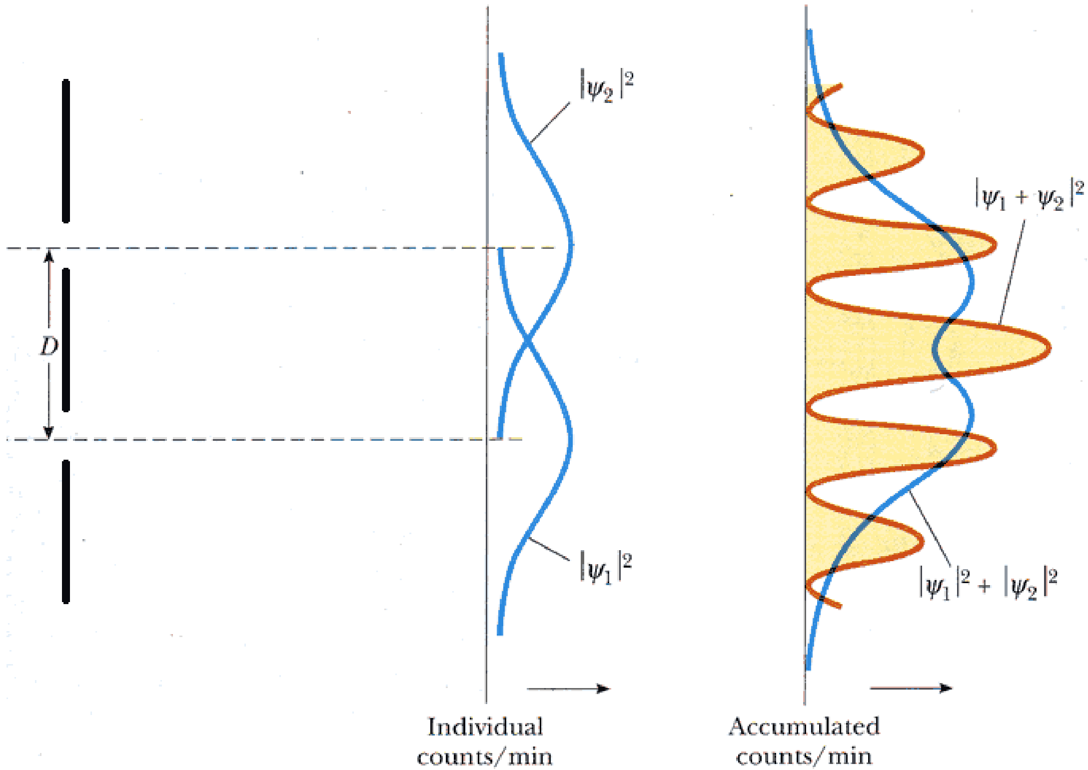
Hans de Raedt, Groningen

Hylke Donker, Nijmegen

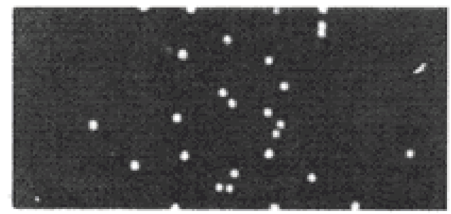
Slava Dobrovitski, Ames Iowa (now Delft)

Microworld: waves are corpuscles, corpuscles are waves

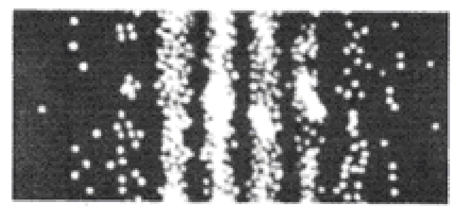
Einstein, 1905 – for light (photons)
L. de Broglie, 1924 – electrons and other microparticles



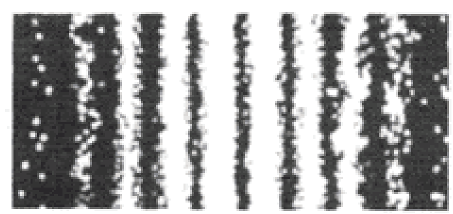
Electrons are particles (you cannot see half of electron) but moves along ***all*** possible directions (interference)



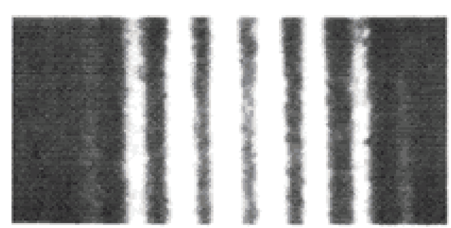
(a) After 28 electrons



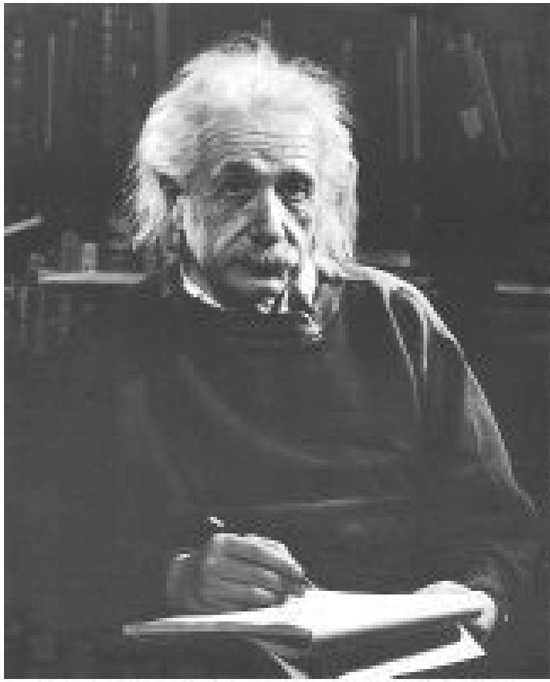
(b) After 1000 electrons



(c) After 10000 electrons



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



God does not play dice with the universe.
- Albert Einstein

Anyone who is not shocked by Quantum Theory has not understood it. - Niels Bohr

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 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

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

$$H=\sum_{\mu} E_{\mu}\alpha_{\mu}^{\dagger}\alpha_{\mu}$$

$$|\Psi\rangle=\frac{1}{\sqrt{M!}}(\alpha_0^{\dagger})^M|0\rangle$$

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

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

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

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

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

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

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

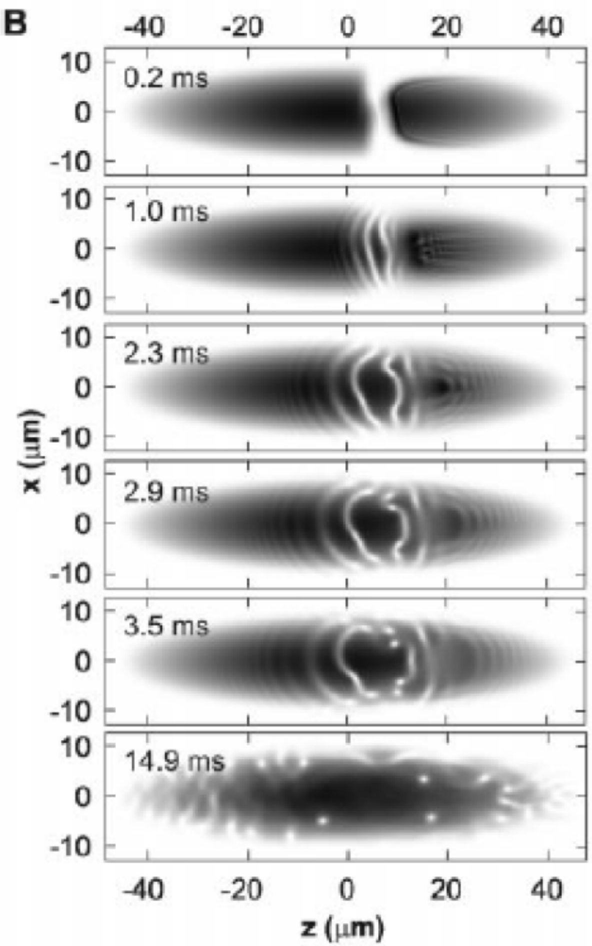
In this case, decoherent action propagates with sound velocity, nothing is “superluminal”, etc – a smooth “wave function collapse”

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

$$\mathcal{H}_0 = \sum_{\mathbf{q}} J_{\mathbf{q}} (S_{\mathbf{q}}^{+} S_{\mathbf{q}}^{-} + S_{\mathbf{q}}^{z} S_{\mathbf{q}}^{z})$$

Ground state is singlet, no sublattices!

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

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

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

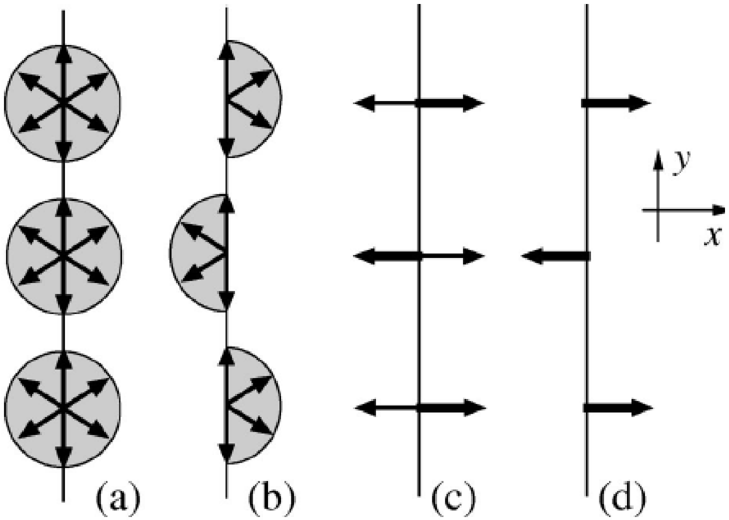


FIG. 1. Sketch of the spin arrangement. Easy plane case: (a) before measurement, sublattices are absent and the total AFM axis is not fixed; (b) after measurement, the ‘‘fan’’ sublattices emerge but an AFM axis is not fixed. Easy axis case: (c) before measurement, sublattices are absent; (d) after measurement,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

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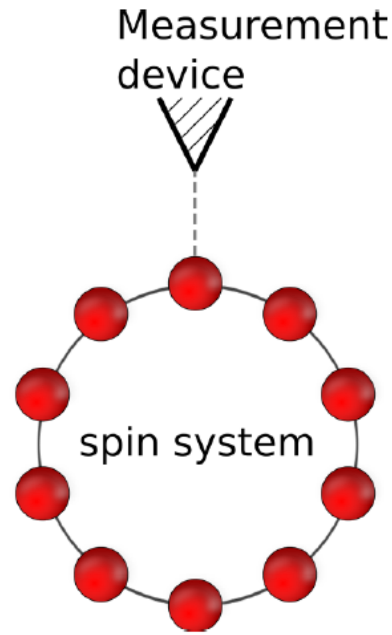


Simulations by numerically exact solution of time-dependent Schrödinger equation

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

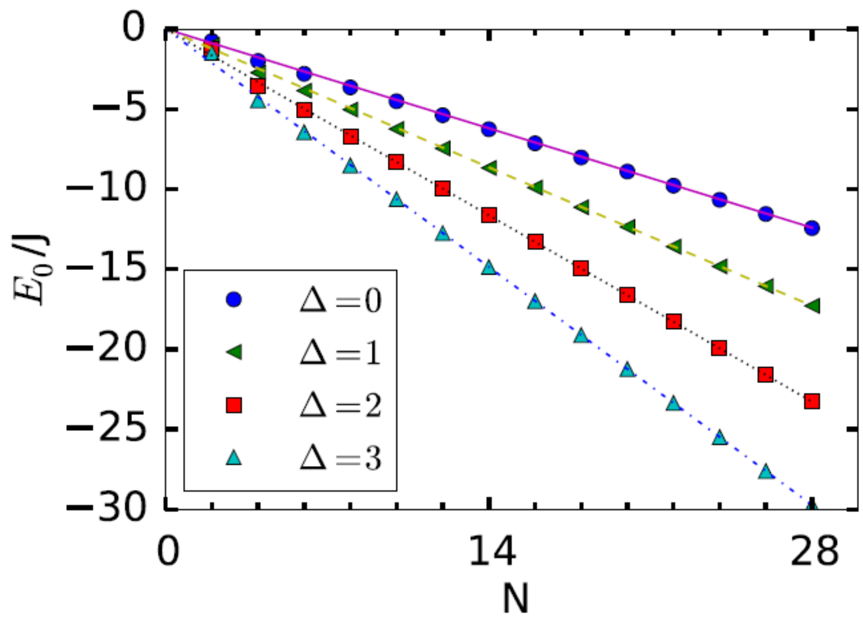
Hamiltonian is the sum of Heisenberg and Ising parts:

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

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

Decoherence waves in AFM for quantum spins II

To find ground state: Lanczos algorithm $\rho = |\Psi\rangle\langle\Psi|$



Agrees very well with Bethe Ansatz Solution (funny – straight line already for small N)

Time evolution – Chebyshev polynom expansion algorithm

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.

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

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

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

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

Chebyshev Polynomial Algorithm II

- Introduce modified time and energy

$$\left|\phi(t)\right\rangle = \sum_{n=1}^{N} e^{-i\hat{t}\hat{E}_n} \left|E_n\right\rangle\left\langle E_n\right|\phi(0)\rangle, \quad \hat{E}_n = E/\left|E\right|_{\max}, \hat{t} = t\left|E\right|_{\max}$$

$$\left|\phi(t)\right\rangle = \sum_{n=1}^{N}\left[J_0(\hat{t}) + 2\sum_{m=1}^{\infty}(-i)^m J_m(\hat{t})T_m(\hat{E}_n)\right]\left|E_n\right\rangle\left\langle E_n\right|\phi(0)\rangle$$

- Cut off of the Bessel function

$$\left|J_m(\hat{t})\right| < \varepsilon, \quad for\ m \geq M = \hat{t}\exp[1-(\ln\varepsilon)/\hat{t}]/2$$

$$\left|\phi(t)\right\rangle \cong \left[J_0(\hat{t})\hat{T}_0(\hat{H}) + 2\sum_{m=1}^{M} J_m(\hat{t})\hat{T}_m(\hat{H})\right]\left|\phi(0)\right\rangle$$

Chebyshev Polynomial Algorithm III

- Definition of the modified Chebyshev Polynomial

$$\hat{T}_m(\hat{H}) = (-i)^m T_m(\hat{H}) = (-i)^m \sum_{n=1}^{N} T_m(\hat{E}_n) \left| E_n \right\rangle \left\langle E_n \right|$$

- Recurrence relations of the modified Chebyshev Polynomial

$$\hat{T}_0(\hat{H}) \left| \phi \right\rangle = \left| \phi \right\rangle$$

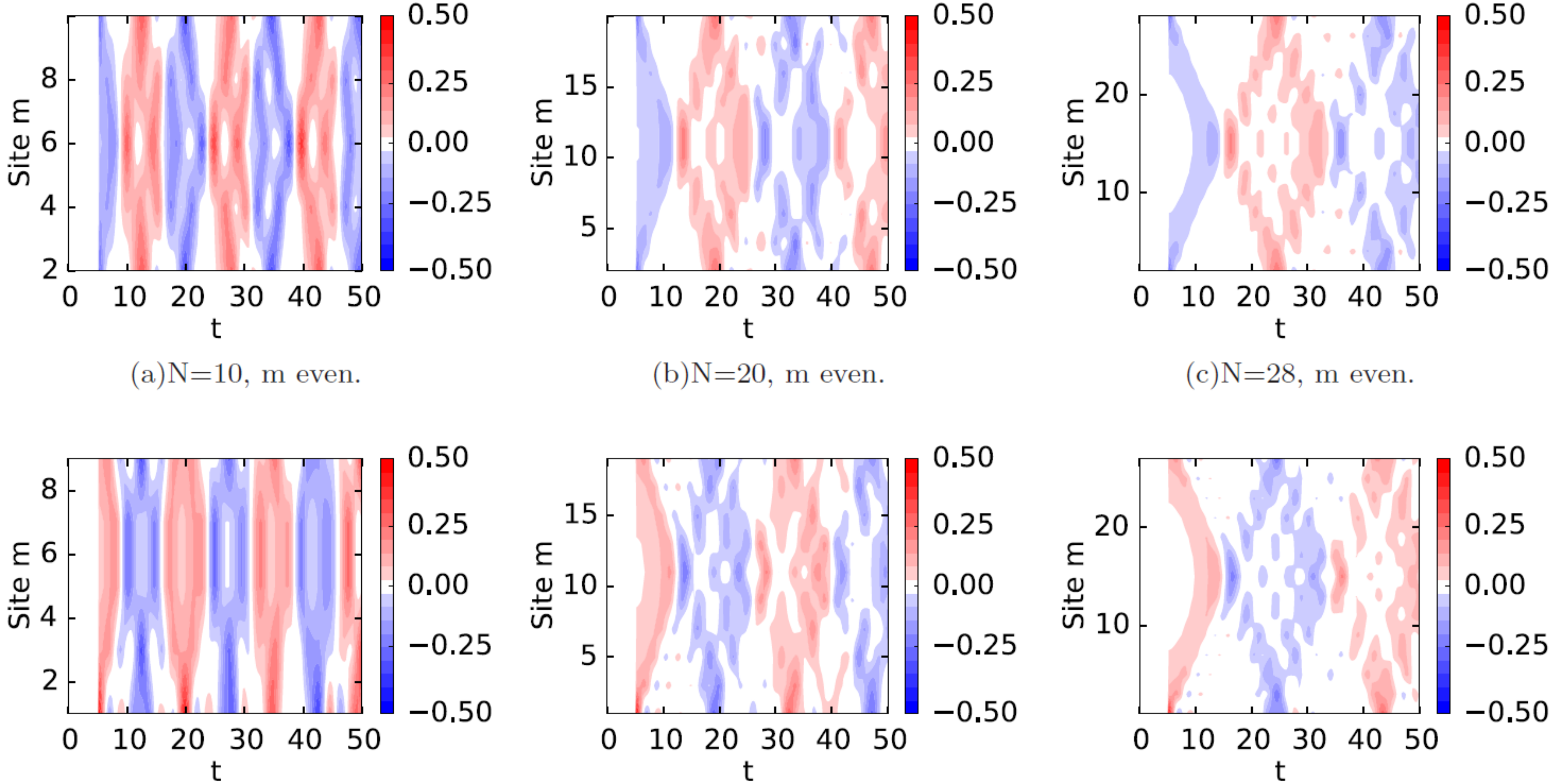
$$\hat{T}_1(\hat{H}) \left| \phi \right\rangle = -i\hat{H} \left| \phi \right\rangle$$

$$\hat{T}_{m+1}(\hat{H}) \left| \phi \right\rangle = -2i\hat{H}\hat{T}_m(\hat{H}) \left| \phi \right\rangle + \hat{T}_{m-1}(\hat{H}) \left| \phi \right\rangle$$

$$\left| \phi(t) \right\rangle \cong \left[J_0(\hat{t})\hat{T}_0(\hat{H}) + 2\sum_{m=1}^{M} J_m(\hat{t})\hat{T}_m(\hat{H}) \right] \left| \phi(0) \right\rangle$$

Decoherence waves in AFM for quantum spins III

Single measurement



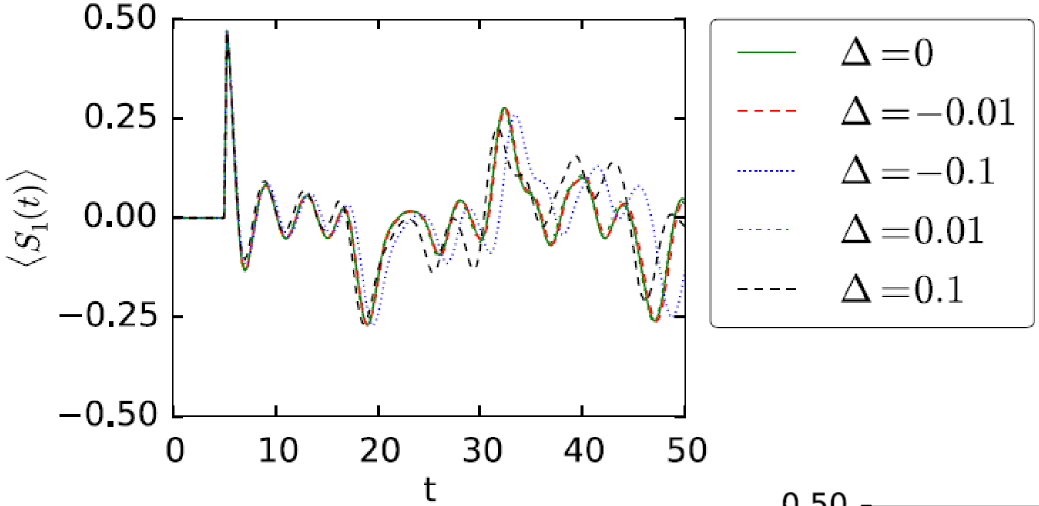
(a)N=10, m even. (b)N=20, m even. (c)N=28, m even.

(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 IV

The sign of anisotropy is not important if it is small



Also, multiple measurements were studied

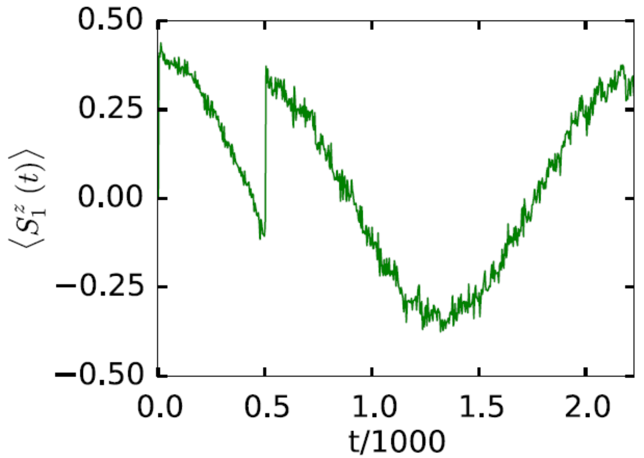
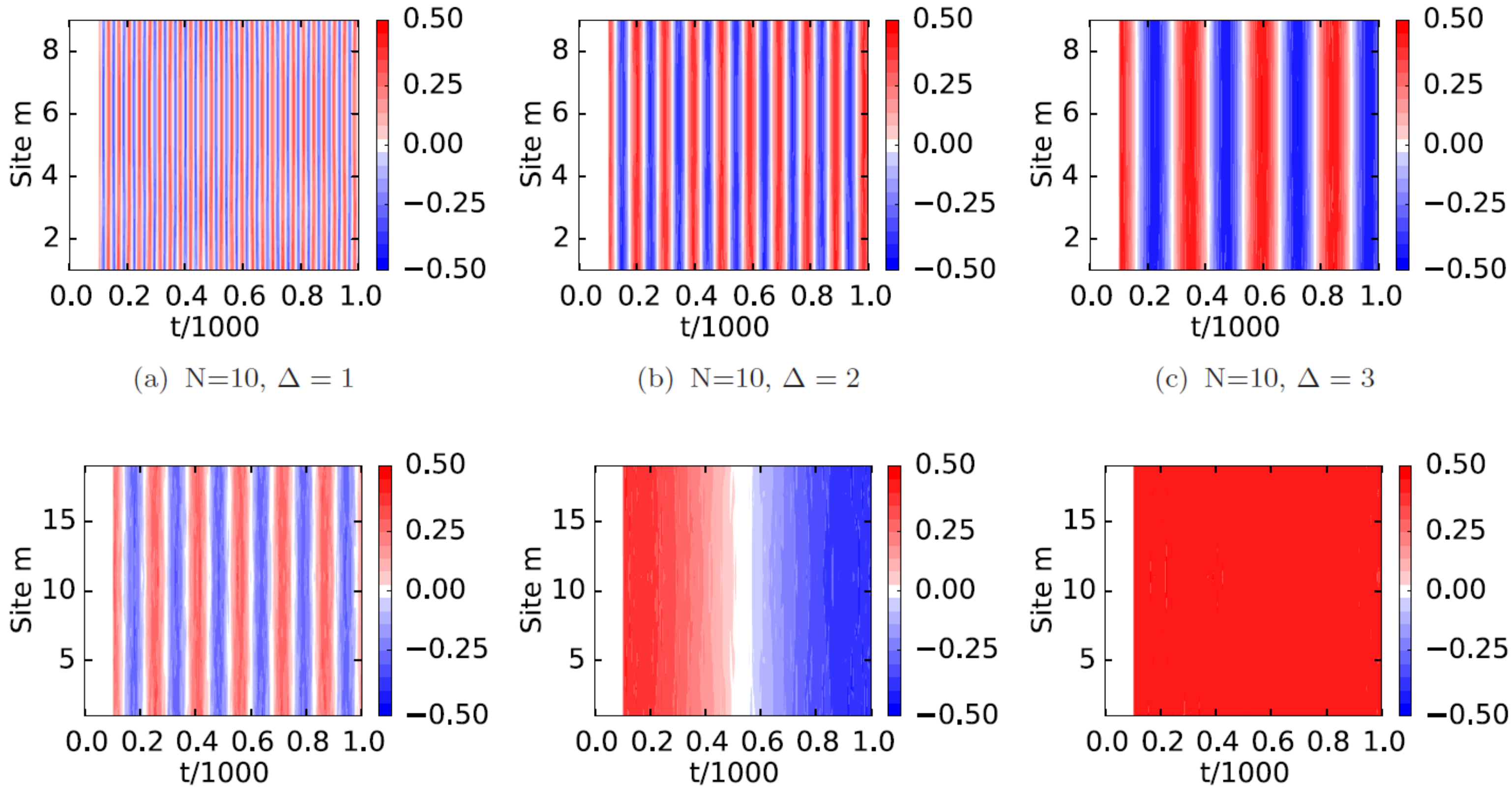


FIG. 7. Magnetization $\langle S_1^z \rangle$ for $N = 20$ and $\Delta = 2$, projections P_1^z are performed at $t = 1$ and $t = 500$. The subsequent measurement (at $t = 500$) restores the sublattice order (close) to the state after the first measurement.

Decoherence waves in AFM for quantum spins V

Oscillations of total magnetization after single local measurement



(a) N=10, $\Delta = 1$ (b) N=10, $\Delta = 2$ (c) N=10, $\Delta = 3$

(d) N=20, $\Delta = 1$ (e) N=20, $\Delta = 2$ (f) N=20, $\Delta = 3$

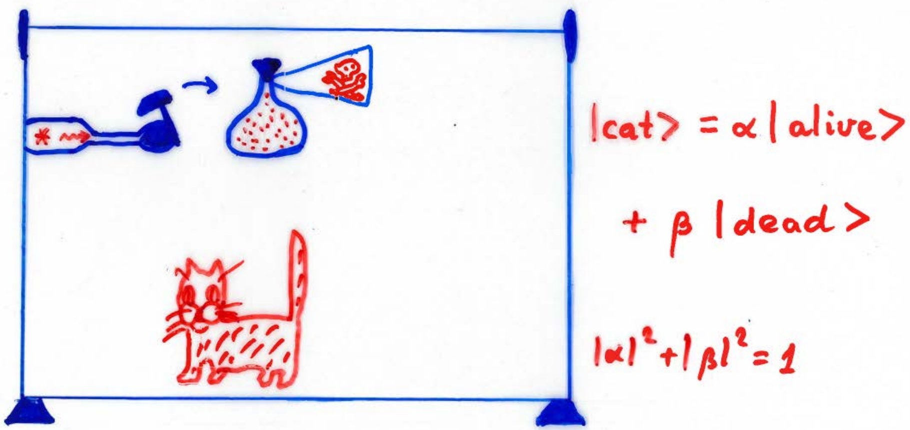
FIG. 9. Magnetization $\langle S_m^z \rangle$ for odd values of m for different values of the anisotropy Δ and chain length N. At $t = 0$, the system is prepared in the ground state, and at $t = 100$ a single measurement is performed on spin 1 along the z direction.

“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”

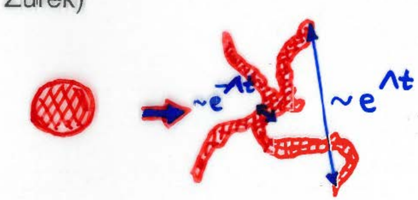
1. Schroedinger cat paradox



2. Unstable systems (W. Zurek)

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

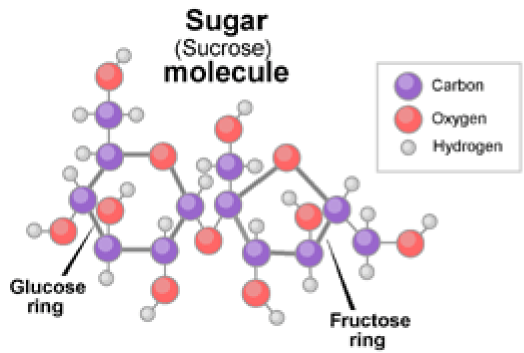
$$\delta p \propto \exp(\Lambda t)$$



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

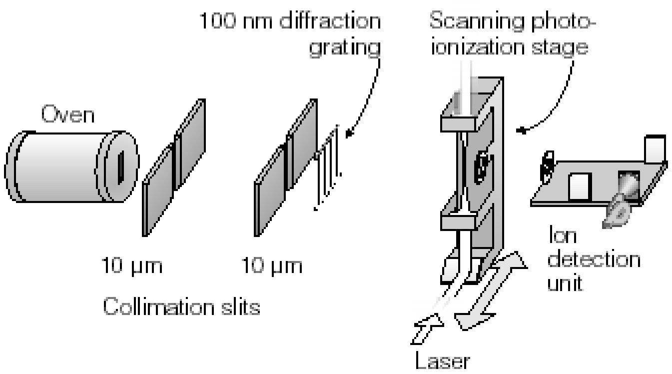
On the other hand: inverse splitting in NH_3 (ammonia maser)

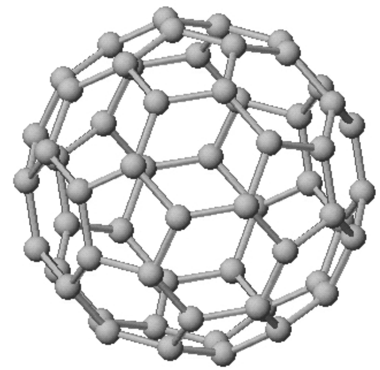
“Decoherence program” III

Wave–particle duality of C_{60} molecules

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

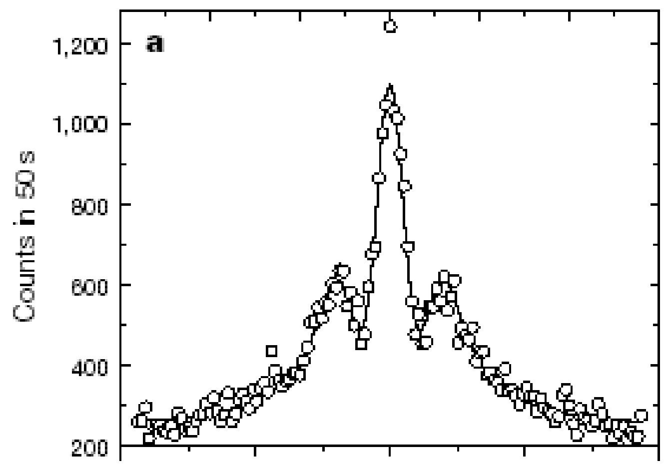
NATURE | VOL 401 | 14 OCTOBER 1999 |





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…

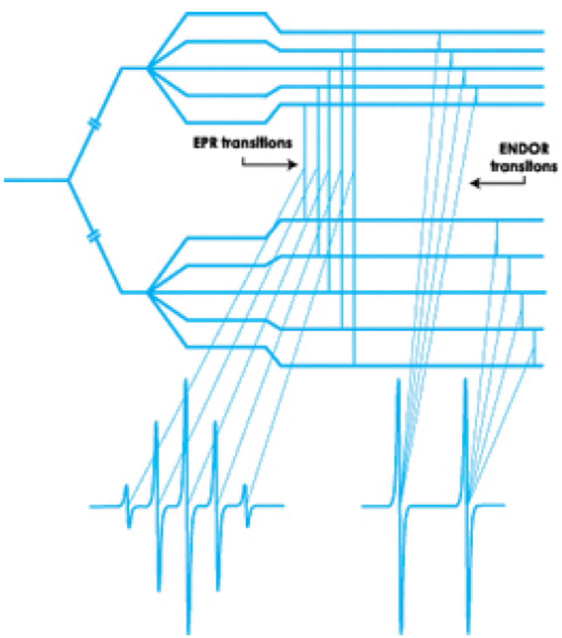
3. Difference between dissipation and dephasing

In terms of NMR: difference between T_1 and T_2.

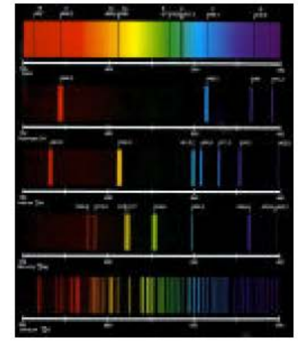
An isolated system is always quantum

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

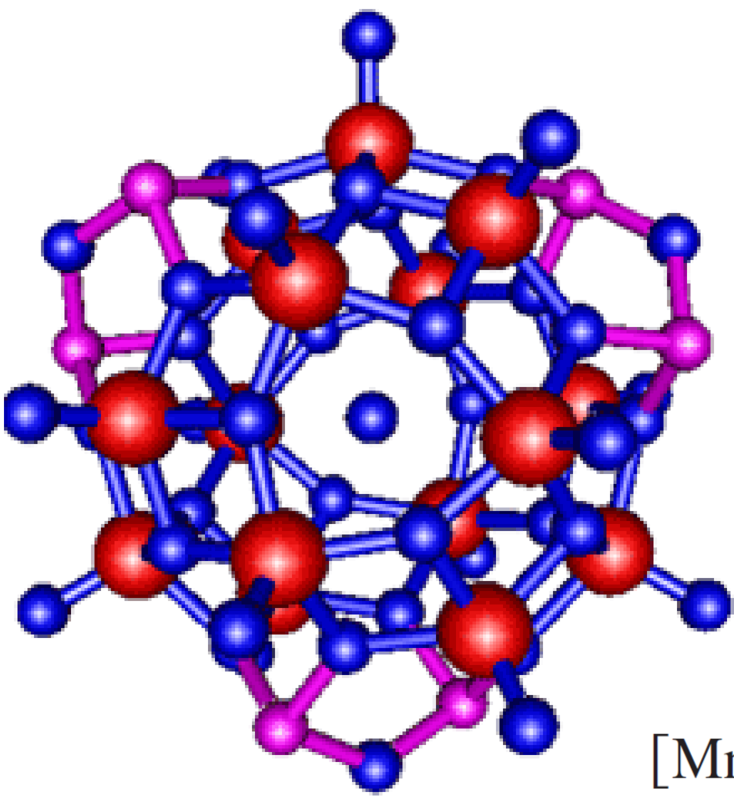
Classical resonance: the spectrum is equidistant $E_n = \hbar\omega_0(n+1/2)$ + selection rules for the coordinate operator $|n\rangle \to |n \pm 1\rangle$:
$\omega = \omega_0$ means nothing

Oscillations in this system are not quantum!

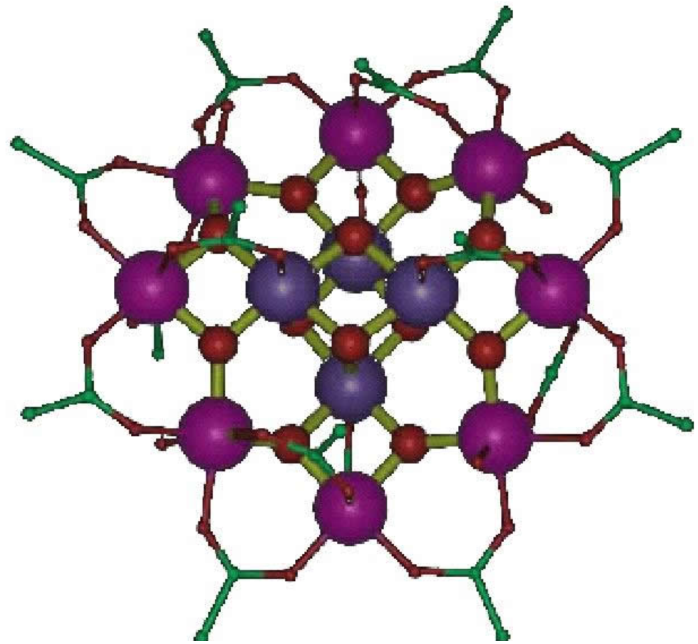
Decoherence in quantum spin systems: Motivation

Molecular magnets

V_{15}



Mn_{12}



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

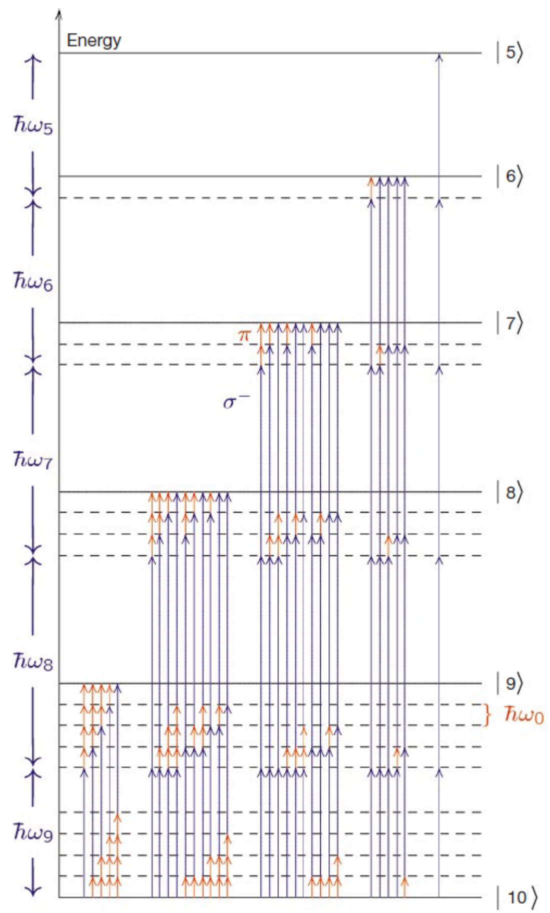
$V_{15}(K_6[V_{15}As_6O_{42}(H_2O)]\cdot 8H_2O)$

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

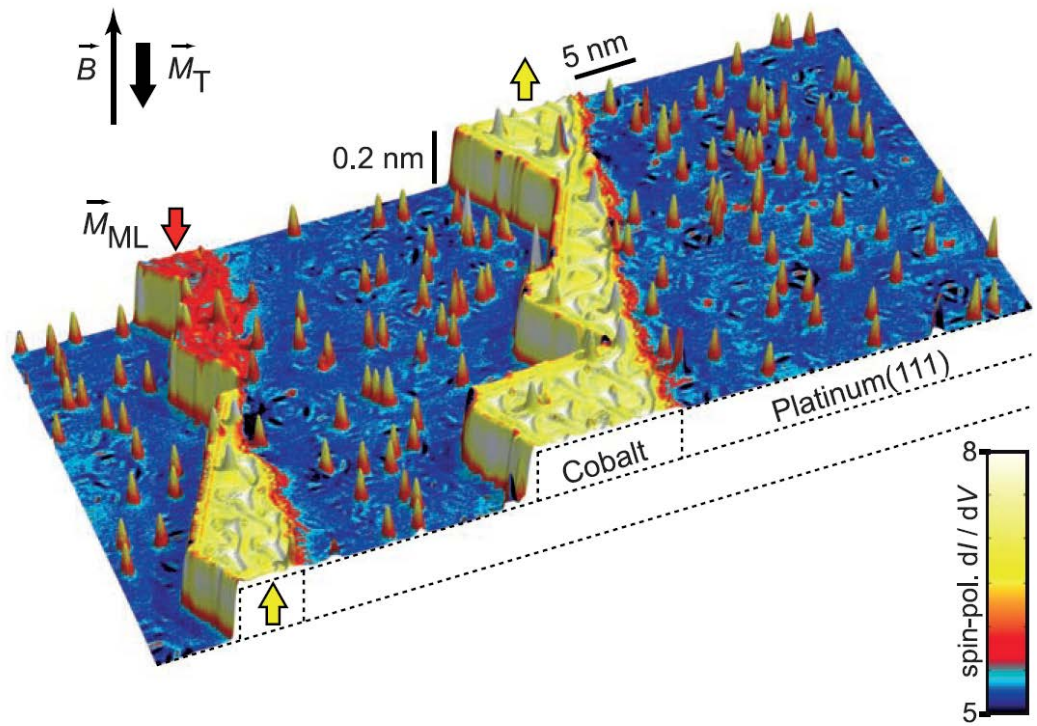
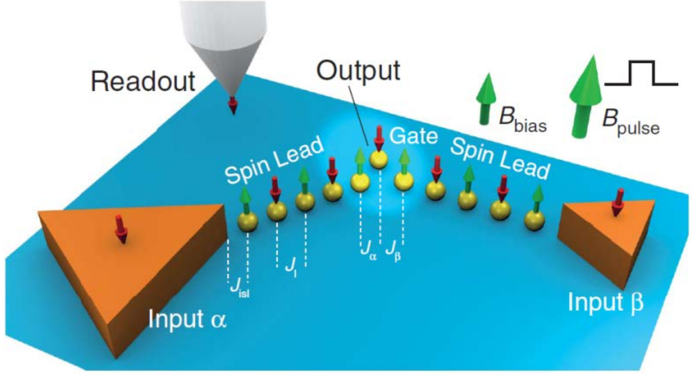


Fig. 1. Overview of the sample of individual Co adatoms on the Pt(111) surface (blue) and Co ML stripes (red and yellow) attached to the step edges (STM topograph colorized with the simultaneously recorded spin-polarized dI/dV map measured with an STM tip magnetized antiparallel to the surface normal). 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

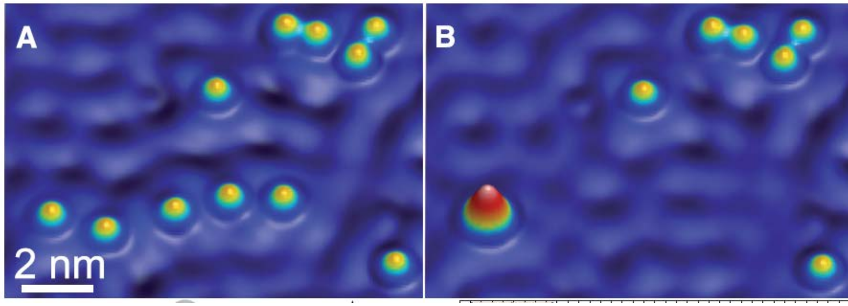
27 MAY 2011 VOL 332 SCIENCE



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

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M. I. Katsnelson
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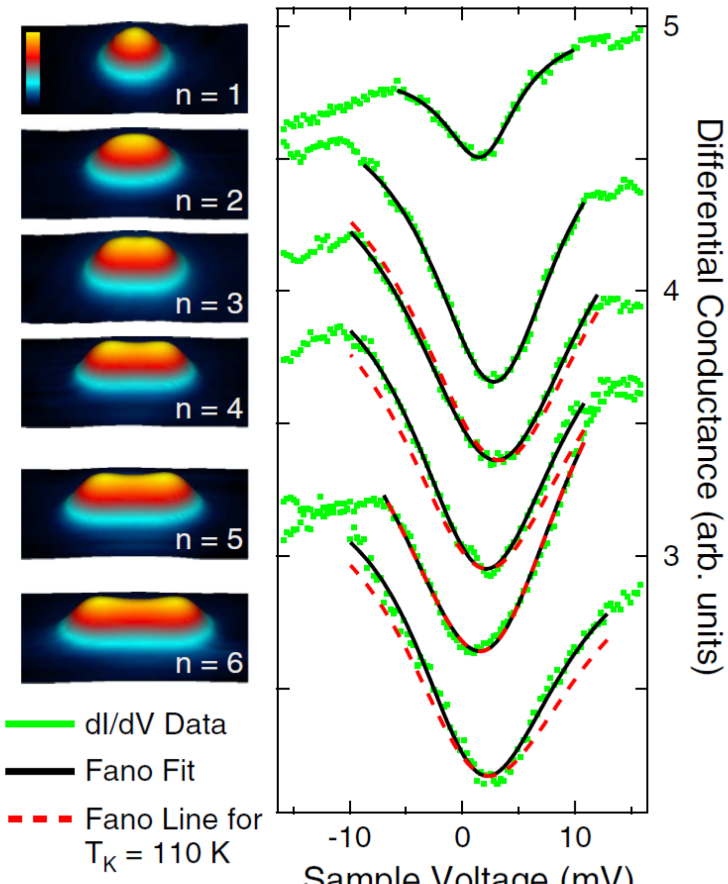
(Received 10 August 2010; published 1 September 2011)



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*
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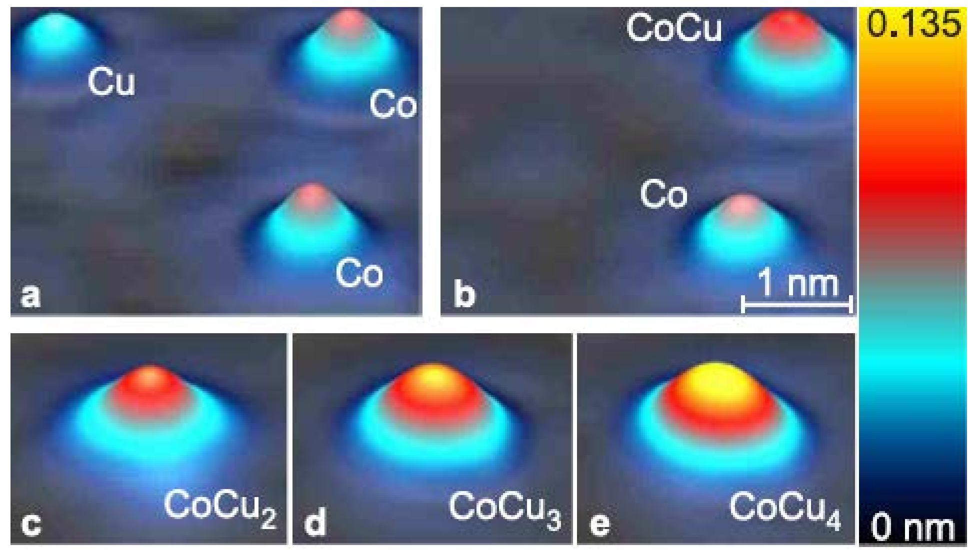
(Received 1 October 2008; published 30 December 2008)

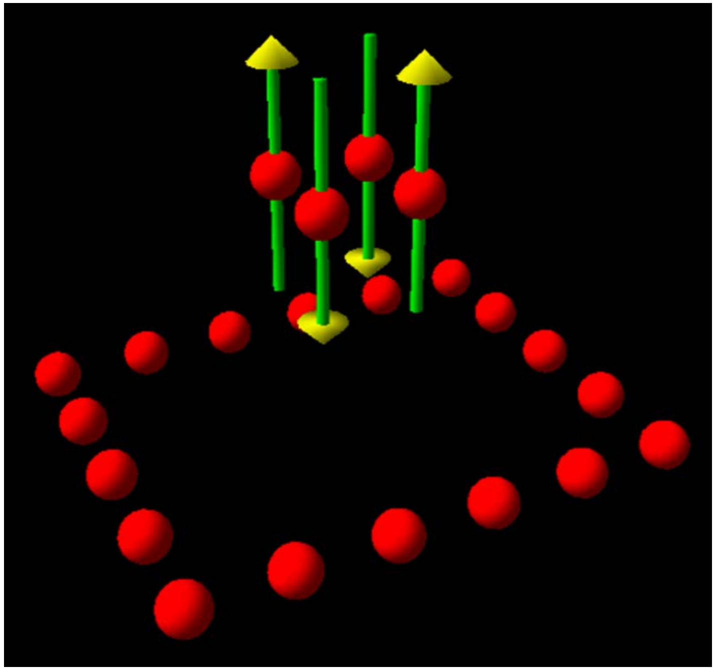
Clusters containing a single magnetic impurity were investigated by scanning tunneling microscopy, spectroscopy, and *ab initio* electronic structure calculations. The Kondo temperature of a Co atom embedded in Cu clusters on Cu(111) exhibits a nonmonotonic variation with the cluster size. Calculations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

Simulations

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)



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

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

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

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

Decoherence depends on symmetry of the Hamiltonians, state of the environment, etc.

Simulations II

- In quantum mechanics, the state of a quantum system is described by a state vector (wave function) in the Hilbert space.

- The time evolution of wave function follows the Time-dependent Schrodinger Equation (TDSE):

$$i\frac{\partial}{\partial t}\left|\phi(t)\right\rangle = H\left|\phi(t)\right\rangle, \hbar = 1$$

Formal solution

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

Operator exponent in calculated via Chebyshev polynom expansion

Density Matrix and Decoherence

- The state of quantum system *S* is determined by its reduced density matrix, which is obtained by tracing out the degree of freedom of the environment *E*.

$$i\hbar \frac{\partial}{\partial t}\left|\phi(t)\right\rangle = H\left|\phi(t)\right\rangle \rightarrow \rho(t) = \left|\phi(t)\right\rangle\left\langle\phi(t)\right| \rightarrow \rho_S(t) = \boldsymbol{Tr}_E\,\rho(t)$$

- Decoherence: the mechanism by which quantum systems interact with their environments to lose the interference (phase relations) and exhibit the feature of "classical" physics.

$$\textbf{\textit{Off - Digonal Terms are Zero}}$$

$$\rho_{ij}(t) \rightarrow \boldsymbol{0} \;\; \textbf{\textit{for}}\; i \neq j$$

Computational results

Currently simluations can be done up to 40 spins ½
(in that time up to 30 spins ½)

ISSN 0021-3640, JETP Letters, 2006, Vol. 84, No. 2, pp. 99–103. © Pleiades Publishing, Inc., 2006.

Giant Enhancement of Quantum Decoherence by Frustrated Environments¶

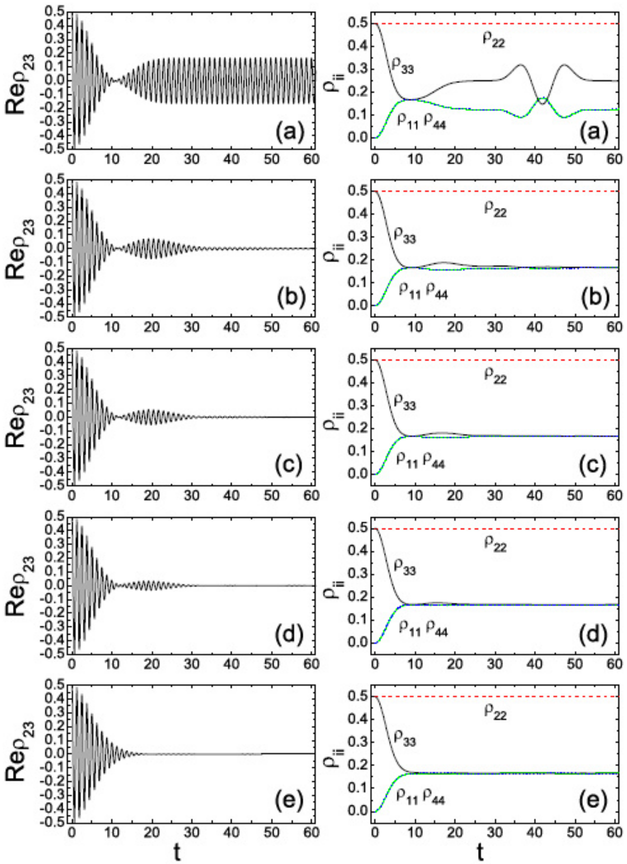
S. Yuan[a], M. I. Katsnelson[b], and H. De Raedt[a]

Important observation: decoherence is very strong if spins in the bath are highly connected and, especially, if their interactions are frustrated (spin-glass-like)

Allows to simulate "thermodynamic limit" for small enough systems!

Examples of Decoherence

The coupling within the spins in the environment is important to the decoherence of the central system



H_S : ***Heisenberg***

H_E : ***Heisenberg - type***

H_{SE} : ***Heisenberg***

$n_S = 2, n_E = 18$

$J_S = -5, \Omega_E = 0.15, \Delta_{SE} = -0.075$

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

a) $K = 0$; b) $K = 2$; c) $K = 4$; d) $K = 6$

e) $K = N - 1$

For $K = 0$:

$$Re[\rho_{23}(t)] = \left[\frac{1}{6} + \frac{1-bt^2}{3}e^{-ct^2}\right]\cos\omega t$$

$b = \frac{N\Delta^2}{4}, c = \frac{b}{2}$ ***and*** $\omega = J - \Delta$

S. Yuan, H. De Raedt, and M. I. Katsnelson, Phys. Rev. B **77**, 184301 (2010).

Canonical Ensemble

- A statistical ensemble in statistical mechanics: representing a probability distribution of microscopic states of the system.
- A basic postulate in statistical mechanics: a generic system that interacts with a generic environment evolves into a state described by the canonical ensemble.
- The probability of finding the system P_n in a particular state n with energy level E_n is given by Boltzmann distribution:

$$\textbf{\textit{Probability Distribution}:}\ P_n = \frac{e^{-\beta E_n}}{\sum_n e^{-\beta E_n}},\ \ \beta = 1/k_B T$$

$$\textbf{\textit{(Reduced) Density Matrix}:}\ \rho_\beta = \frac{e^{-\beta H_S}}{Tr_S e^{-\beta H_S}},\ \ H_S = \sum_n |E_n\rangle\langle E_n|$$

Origin of Canonical Ensemble

- Time-average-approximation: the time average of expectation value of any operator is approximately equal to the value in a canonical ensemble. There is no stationary state.

$$\overline{\langle A \rangle}_t \equiv \lim_{T \to \infty} \frac{1}{T} \int_0^T A(t)dt \approx \langle A \rangle_\beta^{Can}$$

H. Tasaki, *Phys. Rev. Lett.* **80**, 1373 (1998).

- State-average-approximation (*Canonical Typicality):* if the state of the whole system is in the subspace of the whole Hilbert space, with small energy interval, then the subsystem is approximately in the canonical ensemble. There is no dynamics.

S. Popescu, A. J. Short, and A. Winter, *Nature Phys.* **2**, 754-758 (2006).

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

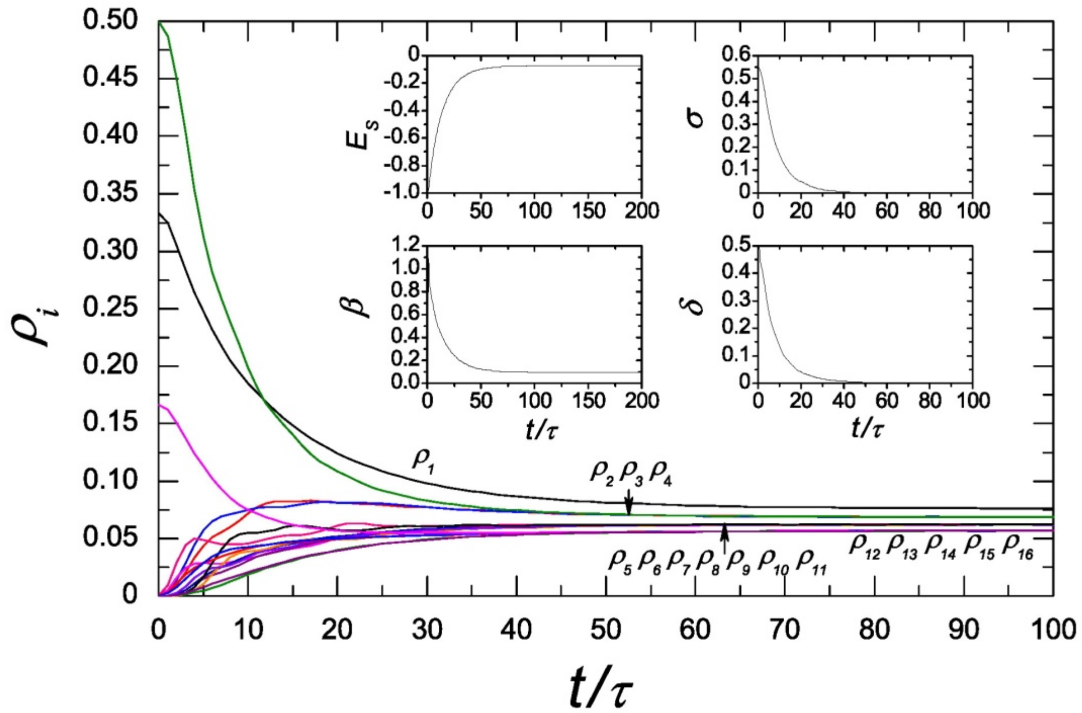
$$\delta(t) \to \boldsymbol{0}$$

$$\sigma(t) \to \boldsymbol{0}$$

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

Dynamical Evolution to Canonical Ensemble II

- For certain types of Hamiltonian and initial states, a quantum spin system can dynamically approach to a stable state which follows canonical distribution.



H_S : ***Heisenberg - ring***

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

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

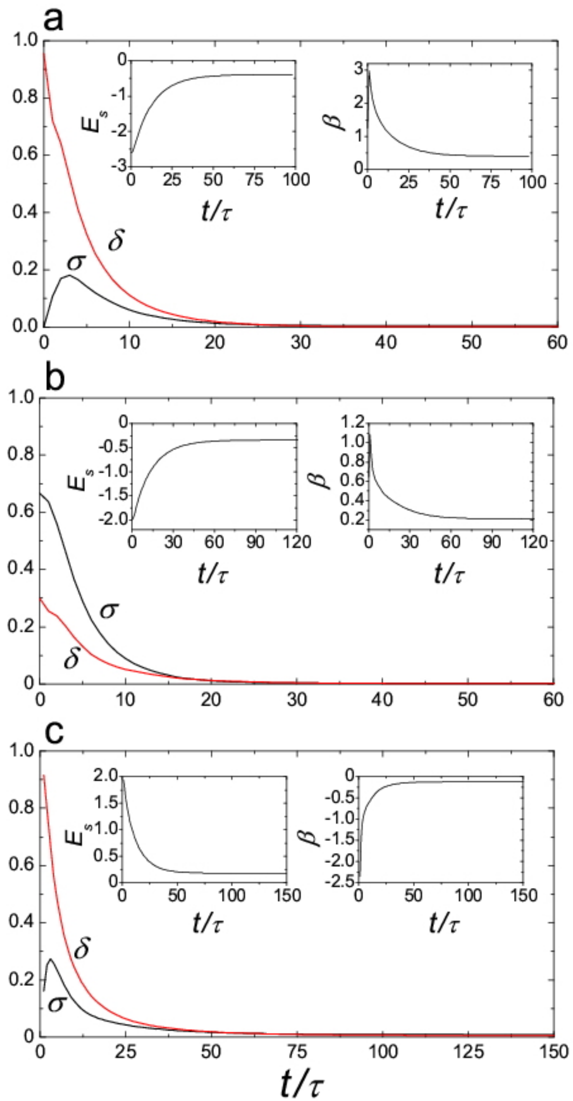
$n_S = 4, n_E = 18$

$J_S = -1, \Omega_E = \mathbf{1}, \Delta_{SE} = \mathbf{0.3}, \tau = \pi/10$

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

S. Yuan, H. De Raedt, and M. I. Katsnelson, J. Phys. Soc. Jpn. **78**, 094003 (2009).

Dynamical Evolution to Canonical Ensemble III



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

(b) Heisenberg - ring

(c) Ising - ring

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

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

$n_S = 8, n_E = 16$

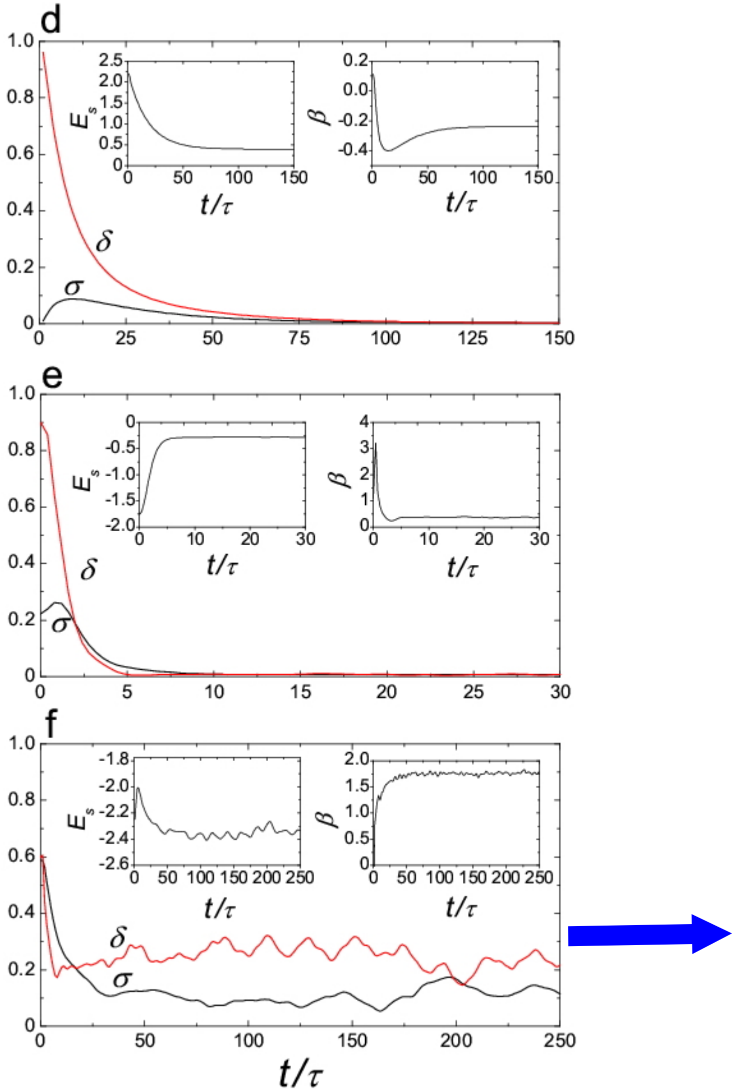
$J = -\mathbf{1}, \Omega = \mathbf{1}, \Delta = \mathbf{0}.3$

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

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

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

Dynamical Evolution to Canonical Ensemble IV



H_S : ***(d) Heisenberg - triangular - lattice***

(e) Heisenberg - type - spin - glass

(f) Heisenberg - ring

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

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

$n_S = 6, n_E = 16$

$J = -1, \Omega = 1, \Delta = 0.3\,(\Delta = 1 \text{ in } e)$

$(d)\,|\phi(0)\rangle = |UUUU\rangle_S \otimes |RANDOM\rangle_E$

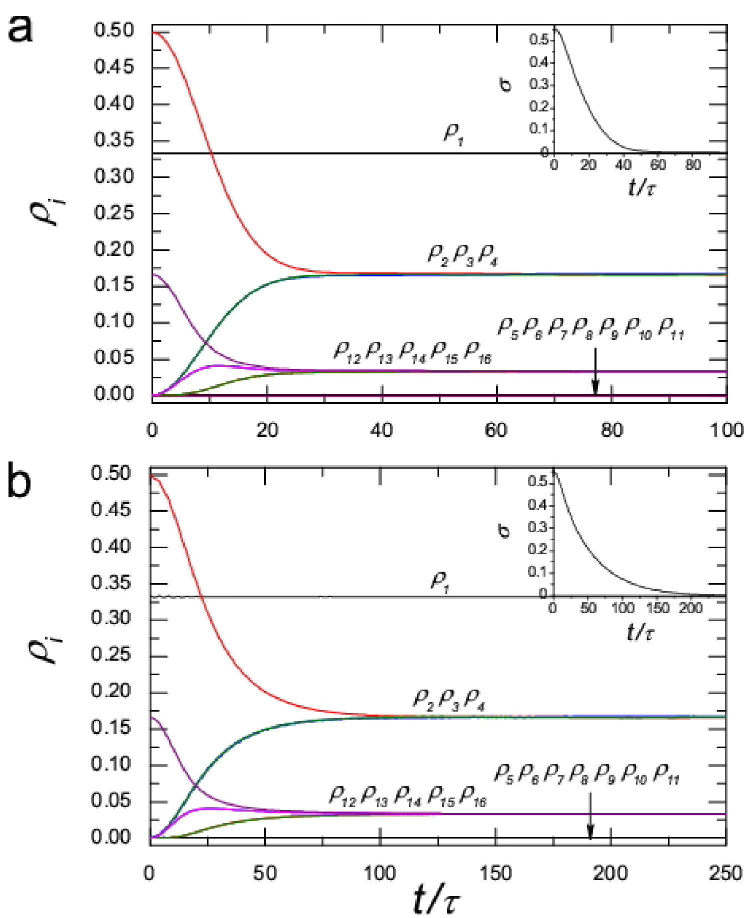
$(e)\,|\phi(0)\rangle = |GROUND\rangle_S \otimes |UDUD\rangle_E$

$(f)\,|\phi(0)\rangle = |UDUD\rangle_S \otimes |GROUND\rangle_E$

Full Decoherence without Canonical Distribution

- A quantum system can approach a state with full decoherence but without canonical distribution if energy exchange is small

e.g. $[H_S, H] = 0$ or $|\Omega| \ll |J|$



H_S : Heisenberg - ring

H_E : Heisenberg - type - spin - glass

H_{SE} : (a) Heisenberg

(b) Heisenberg - type

$n_S = 4, n_E = 16, J = -5, \Omega = 0.15$

(a) $\Delta = 0.075$, (b) $\Delta = 0.15$

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

Conditions for Dynamic Evolution to Canonical Ensemble

- The general conditions under which we observe that a quantum system S dynamically evolves to the canonical distribution are:

I. The system *S* interacts with an environment *E*. The whole system *S*+*E* is a closed quantum system that evolves in time according to the TDSE.

II. The interaction between *S* and *E* must lead to the full decoherence of *S*.

III. The system *S* and *E* can exchange energy and the range of energy distribution of *E* is large compared to the range of energy distribution of *S*.

S. Yuan, H. De Raedt, and M. I. Katsnelson, J. Phys. Soc. Jpn. **78**, 094003 (2009).

Summary from Simulation of Quantum Spin System

- We emphasize that our observations are
  - based on the direct solution of the TDSE;
  - without making any approximation;
  - without performing any time averaging;
  - without making the environment infinitely large;
  - without introducing any special distribution such as the microcanonical ensemble, or a subspace with small energy interval.
- We suggest that the canonical ensemble, being one of the basic postulates of statistical mechanics, is a natural consequence of the dynamical evolution of a quantum system.

Looking for pointer states in quantum spin systems

Sci|Post 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]

What are pointer states?

Density matrix is Hermitian, it can always be diagonalized. The states which diagonalize it should be the most robust and reazonably time independent (if Schrödinger cat is dead it should state dead)

Predictability sieve criterion (Zurek): von Neumann entropy

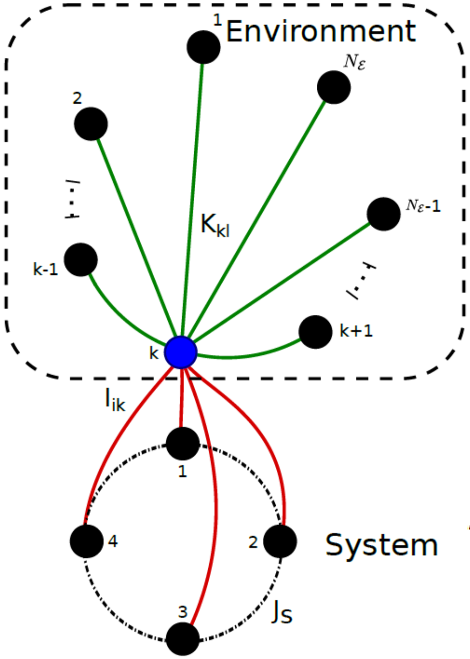
$$S(t) \equiv -\mathrm{Tr}[\rho(t)\ln\rho(t)]$$

should be small (robustness!) and weakly time-dependent

Looking for pointer states in quantum spin systems II

Hypothesis: if interaction Hamiltonian is much larger thn energy distances for the central system PS are eigenstates of the interaction Hamiltonian; in the opposite limit they are eigenstates of the central system Hamiltonian

The first part is supposed to explain von Neumann measurement Prescription, the second part is supposed to explain why we have atomic transitions between discrete well-defined atomic levels



Let us check...

$$H = H_S + H_I + H_\mathscr{E}$$

$$H_S = J_S \sum_{\langle i,j\rangle \in S} \boldsymbol{S}_i \cdot \boldsymbol{S}_j \qquad H_\mathscr{E} = \sum_{k,l\in\mathscr{E}} K_{kl} \boldsymbol{S}_k \cdot \boldsymbol{S}_l$$

Heisenberg

Random, each with each

$$H_I = \sum_{i\in S,\, k\in\mathscr{E}} I_{ik} S_i^z S_k^z$$

Should stabilize classical Neel state (eigenstate of this Hamiltonian)?!

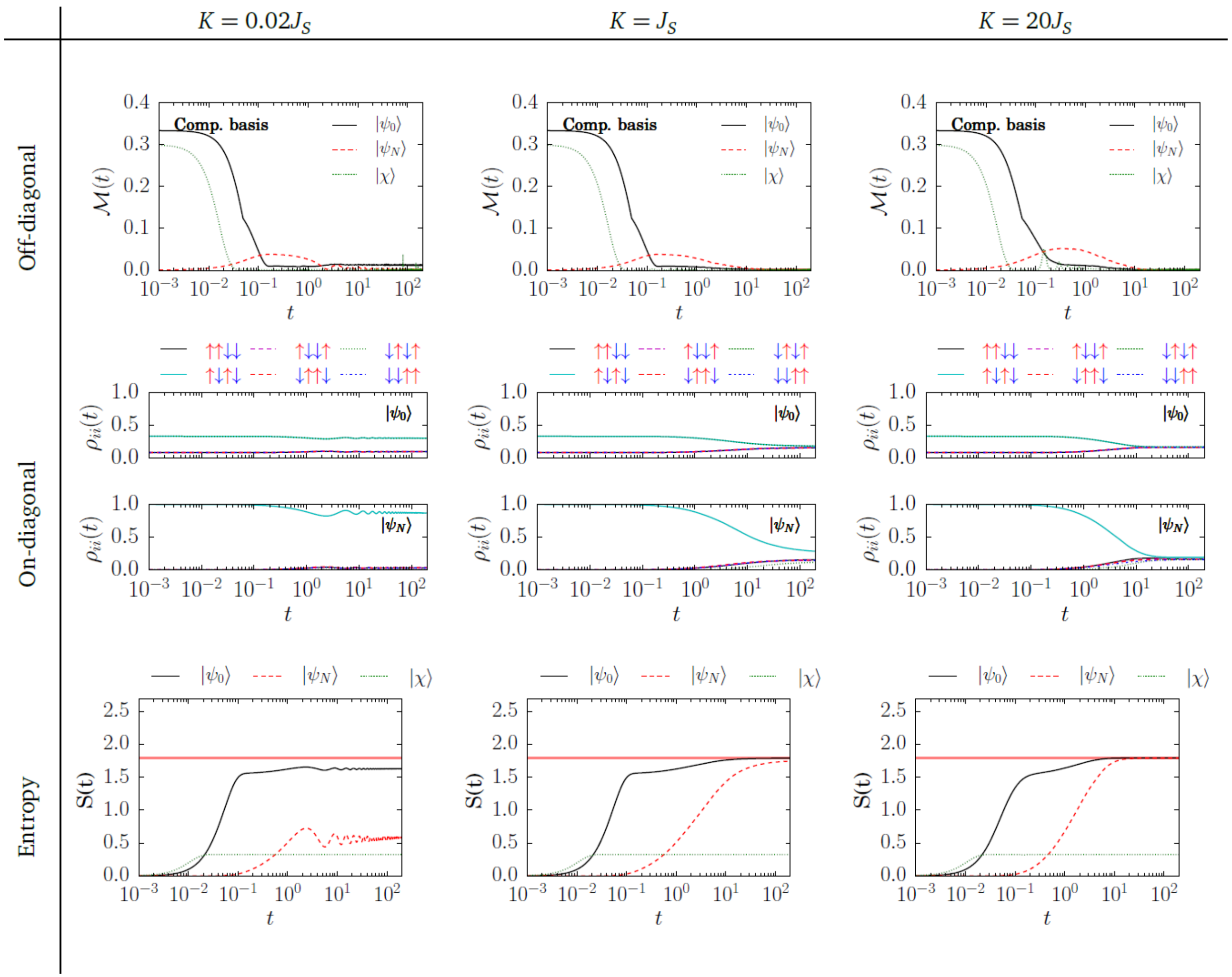
Looking for pointer states in quantum spin systems III

$$I_{ab} = I r_{ab}$$

r_{ab} $\tilde{r}_{ab}$ are uniform random nublers within [0,1)

$$K_{ab} = K \tilde{r}_{ab}$$

Strong interaction, $I = 20J_s$



$$\mathcal{M}(t) \equiv \max[|\rho_{i\neq j}(t)|]$$

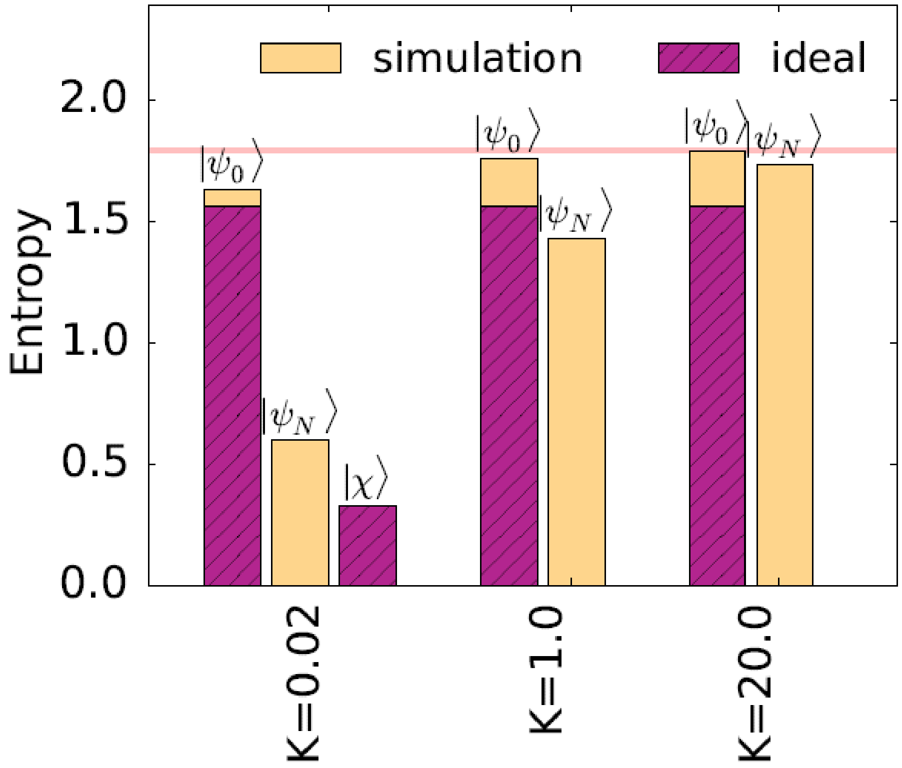
$$|\psi_N\rangle = |\uparrow\downarrow\uparrow\downarrow\rangle$$

$$|\chi\rangle = [|\Uparrow\rangle + 3\,|\Downarrow\rangle]/\sqrt{10}$$

4 spins central system, 16 in ennvironment

Seems to be counterexample to Zurek assumption (you need to go to large time to see it!)

Looking for pointer states in quantum spin systems IV



Neel state is not the most robust!

Figure 3: The von Neumann entropy $S(t = 10)$ extracted from Fig. 2 (indicated by simulation) compared to entropy for the mixed-state that corresponds to pure dephasing in the computational basis (marked by ideal). The simulations have been carried out for a central-system of $N_S = 4$ particles strongly coupled ($I = 20J_S$) to $N_{\mathcal{E}} = 16$ environment particles via random antiferromagnetic Ising coupling. The initial state of the CS and the intra-environment strength (in units of J_S) are indicated in the panel. For initial state $|\chi\rangle$ the simulation and ideal entropy exactly coincide and are identical for all three K values ($K = J_S$ and $K = 20J_S$ have been omitted in the figure). The ideal entropy for state $|\psi_N\rangle$ is zero.

Looking for pointer states in quantum spin systems V

Weak interaction, $I = 0.25 J_s$

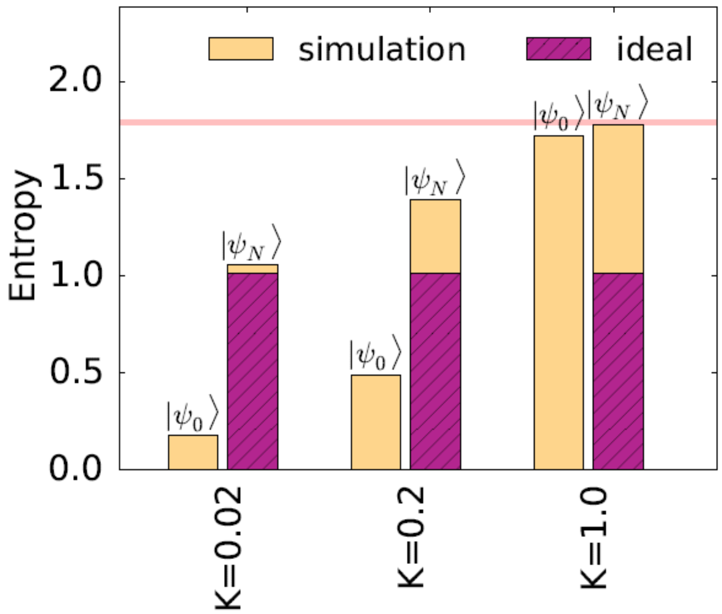


Figure 6: The von Neumann entropy $S(t = 2500)$ extracted from Fig. 5 (indicated by simulation) compared to entropy for the mixed-state that corresponds to pure dephasing in the energy eigenbasis (marked by ideal). The simulations have been carried out for a central-system of $N_S = 4$ particles weakly coupled ($I = 0.25 J_S$) to $N_{\mathcal{E}} = 16$ environment particles via random antiferromagnetic Ising coupling. The initial state of the CS and the intra-environment strength (in units of J_S) are indicated in the panel. The ideal entropy for state $|\psi_0\rangle$ is zero.

Looking for pointer states in quantum spin systems VI

$$D(\rho_1, \rho_2) = \frac{1}{2}\mathrm{Tr}|\rho_1 - \rho_2| \qquad |M| = \sqrt{M^\dagger M}$$

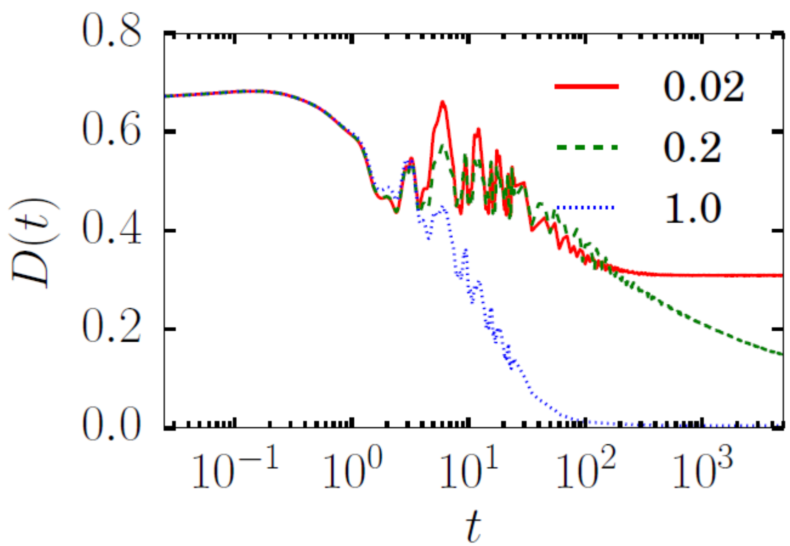


Figure 7: Trace distance [Eq. (19)] between RDMs $\rho_1(0) = |\psi_0\rangle\langle\psi_0|$ and $\rho_2(0) = |\psi_N\rangle\langle\psi_N|$ as a function of dimensionless time t. The antiferromagnetic Ising coupling strength is set to $I = 0.25J_S$ (weak coupling) and the intra-environment K is indicated in the legend (in units of J_S). The system (environment) consists of $N_S = 4$ ($N_{\mathcal{E}} = 16$) particles. Time t has been made dimensionless in units of J_S and $\hbar$, i.e. $t' \to t'J_S/\hbar \equiv t$. Non-monotonicity is a signature of non-Markovian effects.

A LOT OF QUESTIONS
ARE STILL OPEN...

MANY THANKS
FOR YOUR ATTENTION