Theory of Electron Spin Resonance

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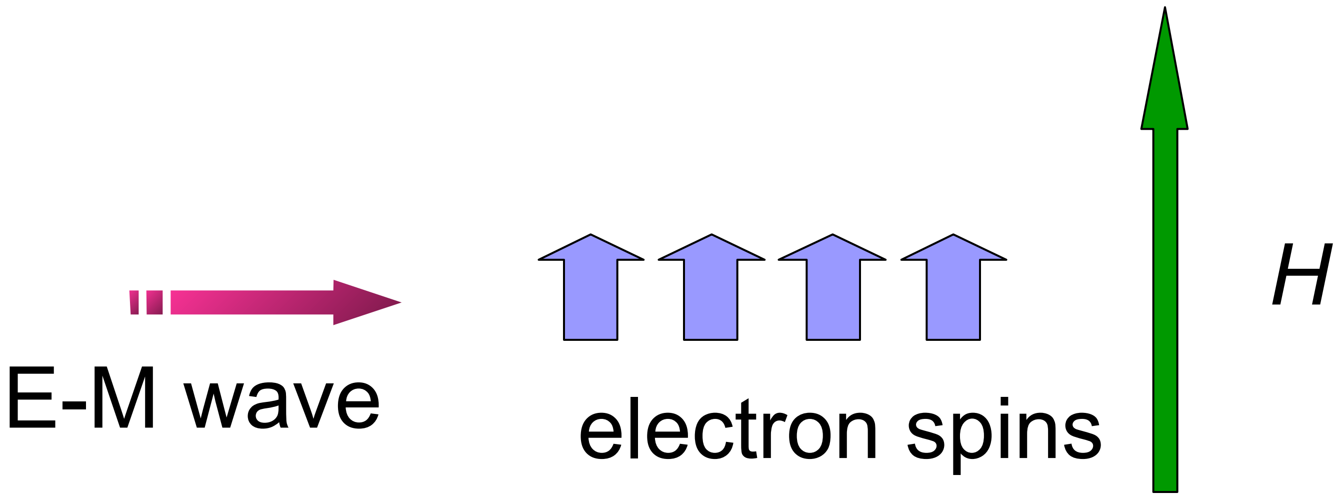
Electron Spin Resonance (ESR)

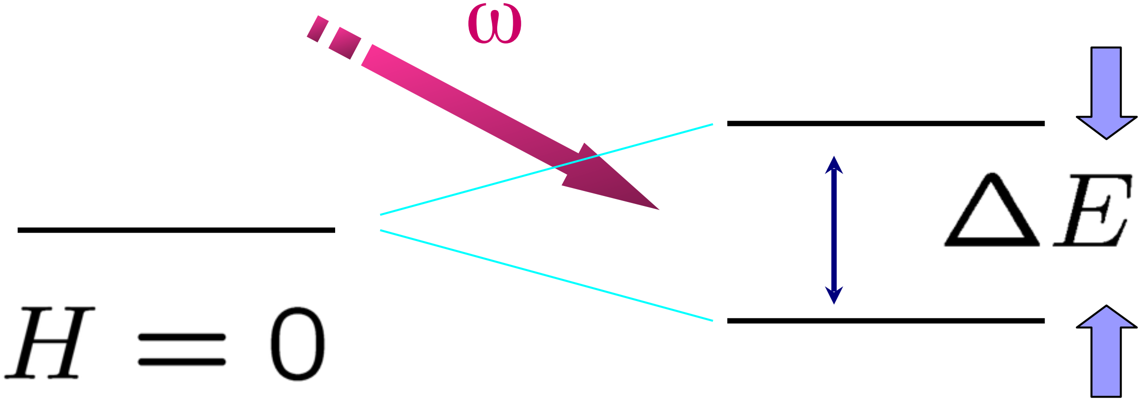


measure the absorption intensity

$$I(\omega) \propto \omega \chi''(\omega)$$

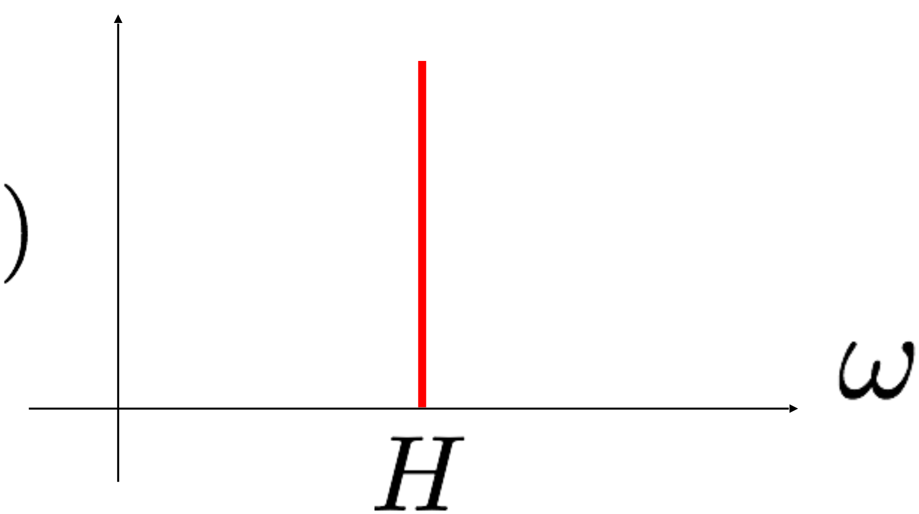
Typically, microwave to milliwave is used:
wavelength >> microscopic scale $\rightarrow q \sim 0$

ESR of a Single S=1/2



$$\Delta E = g\mu_B H$$

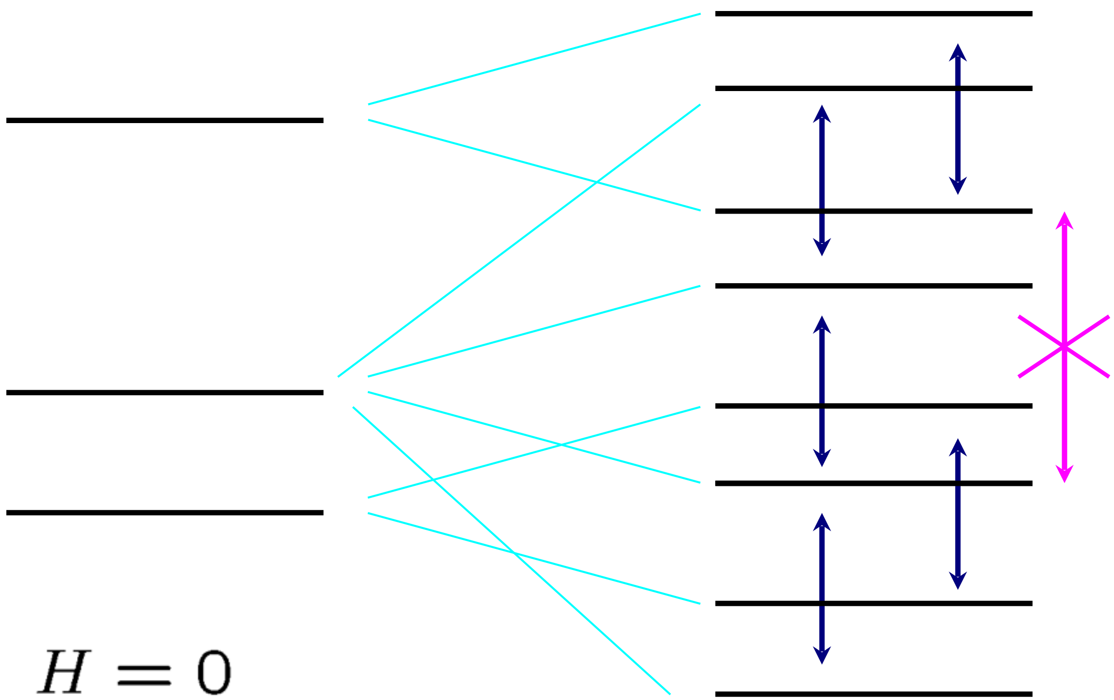
$$I(\omega) \propto \delta(\omega - H)$$



ESR in Heisenberg AFM

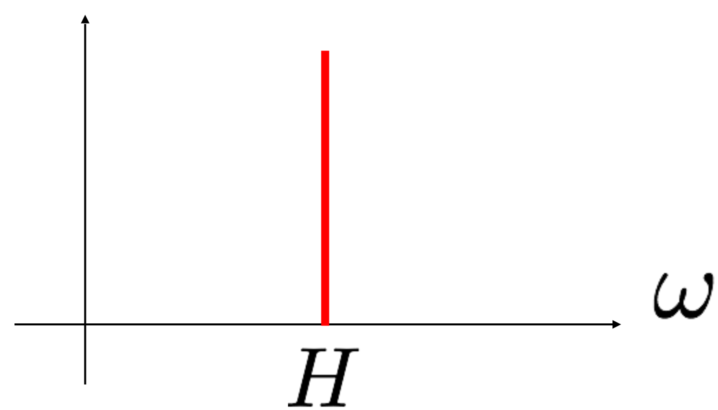
$$\mathcal{H}_0 = J \sum_{\langle j,k \rangle} \vec{S}_j \cdot \vec{S}_k$$ interaction

Eigenstates：labelled by total spin S and total S^z



Transition only occurs when

$$\Delta E = g\mu_B H$$



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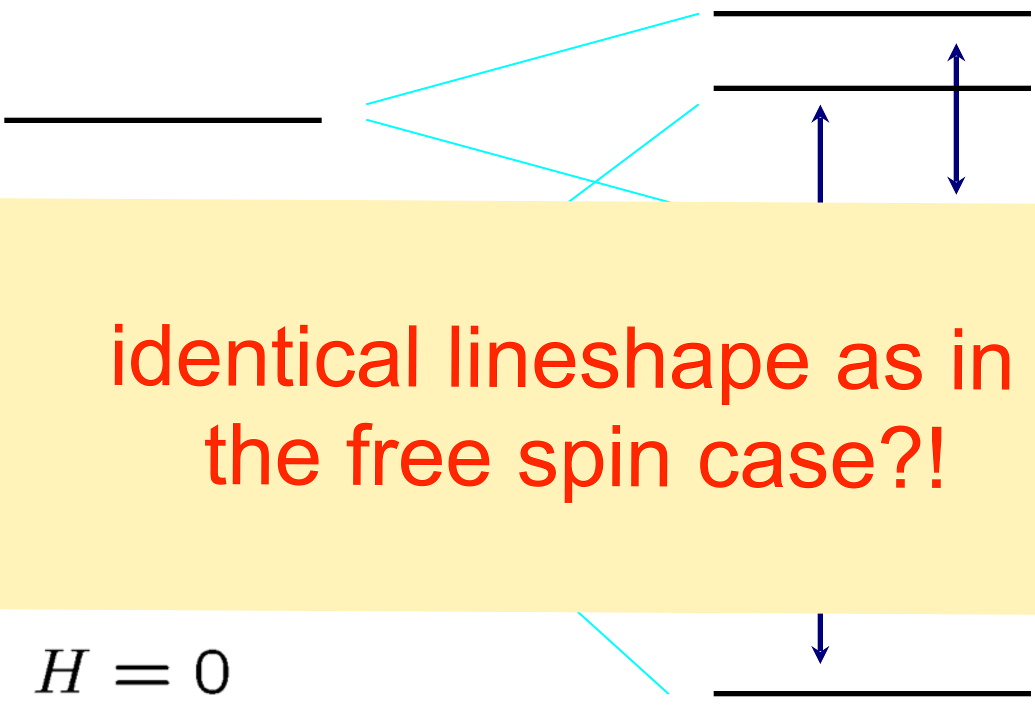
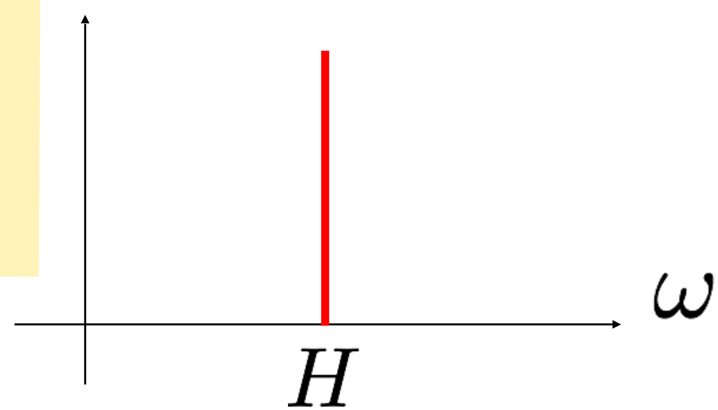


identical lineshape as in the free spin case?!

Transition only occurs when

$$\Delta E = g\mu_B H$$



Why?

Wavelength of the oscillating field
>> lattice spacing etc.

⇨ ESR measures $q \sim 0$

(motion of **total spin** $S^+ \equiv \sum_j S_j^+$ **!**)

$$\frac{dS^+}{dt} = i[\mathcal{H}, S^+] = -iHS^+$$

because $[\mathcal{H}_0, S^+] = 0$

No change
in eq. of motion!

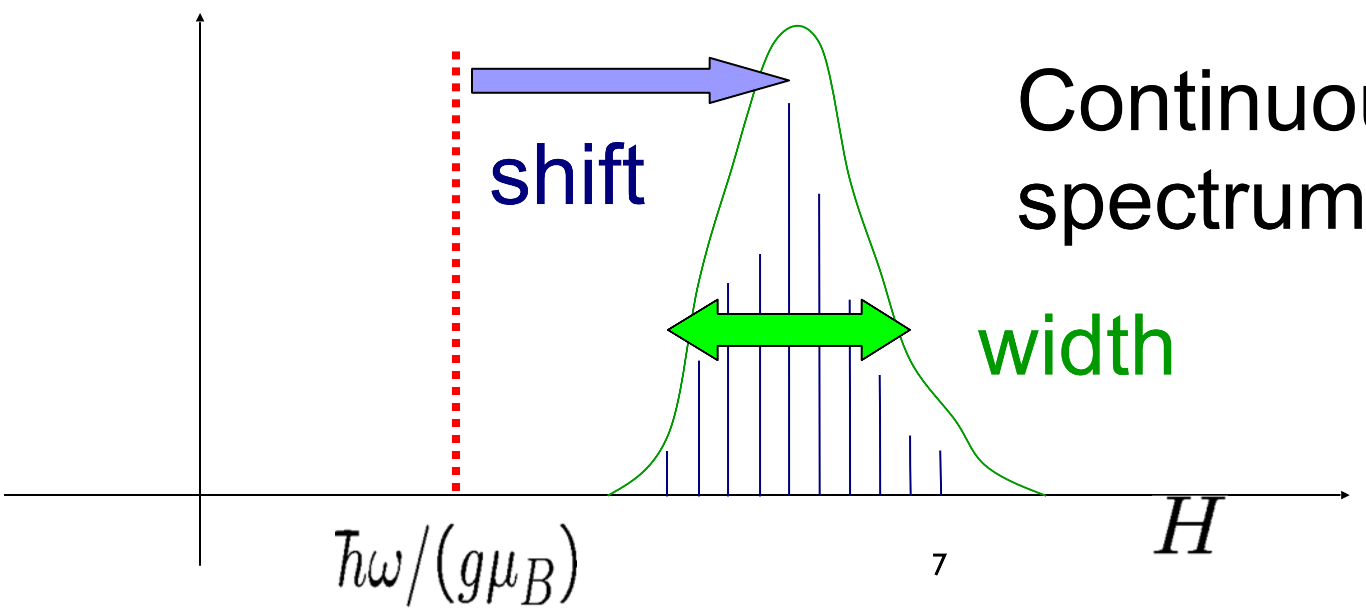
Effects of anisotropy

Real materials: anisotropy exist (often tiny)

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_Z + \mathcal{H}'$$

$$\Delta E = g\mu_B H + \delta$$

Various value for each transition



Continuous absorption spectrum in $N \to \infty$

Effect of anisotropy

(small) anisotropy

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_Z + \mathcal{H}'$$

In the presence of anisotropy, the lineshape does change…. eg. **shift** and **width**

ESR is a unique probe which is sensitive to anisotropies!

e.g.) 0.1% anisotropy in Heisenberg exchange could be detected experimentally with ESR

Pros and cons of ESR

ESR can measure only $q \sim 0$

cf.) neutron scattering

But…..

very precise spectra can be obtained with a relatively small and inexpensive apparatus

highly sensitive to tiny **anisotropies**

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The real problem:

interpretation of the data requires a reliable theory, which is often difficult

Application to frustrated magnets?

$NiGa_2S_4$: S=1 triangular lattice antiferromagnet

[Nakatsuji et al. 2005]

Local 120° structure →
effective theory: non-linear sigma model
with target space = SO(3)?

$\pi_1(SO(3)) = Z_2 \Rightarrow Z_2$ vortex

Phase transition driven by proliferation of
the Z_2 vortices? [Kawamura-Miyashita 1984]

cf.) Z vortices ⇒ BKT transition

ESR linewidth in $NiGa_2S_4$

[Yamaguchi et al. 2008]

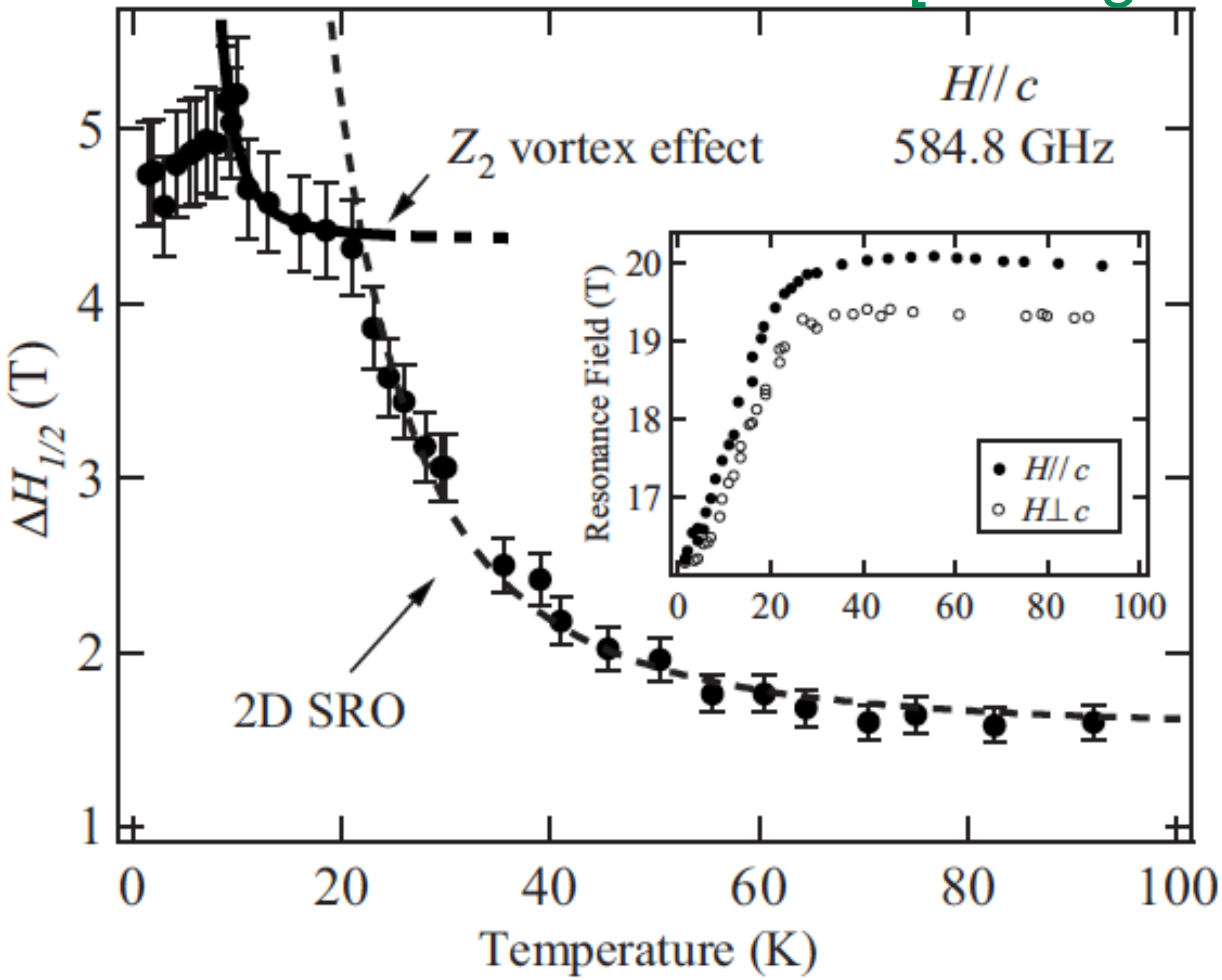
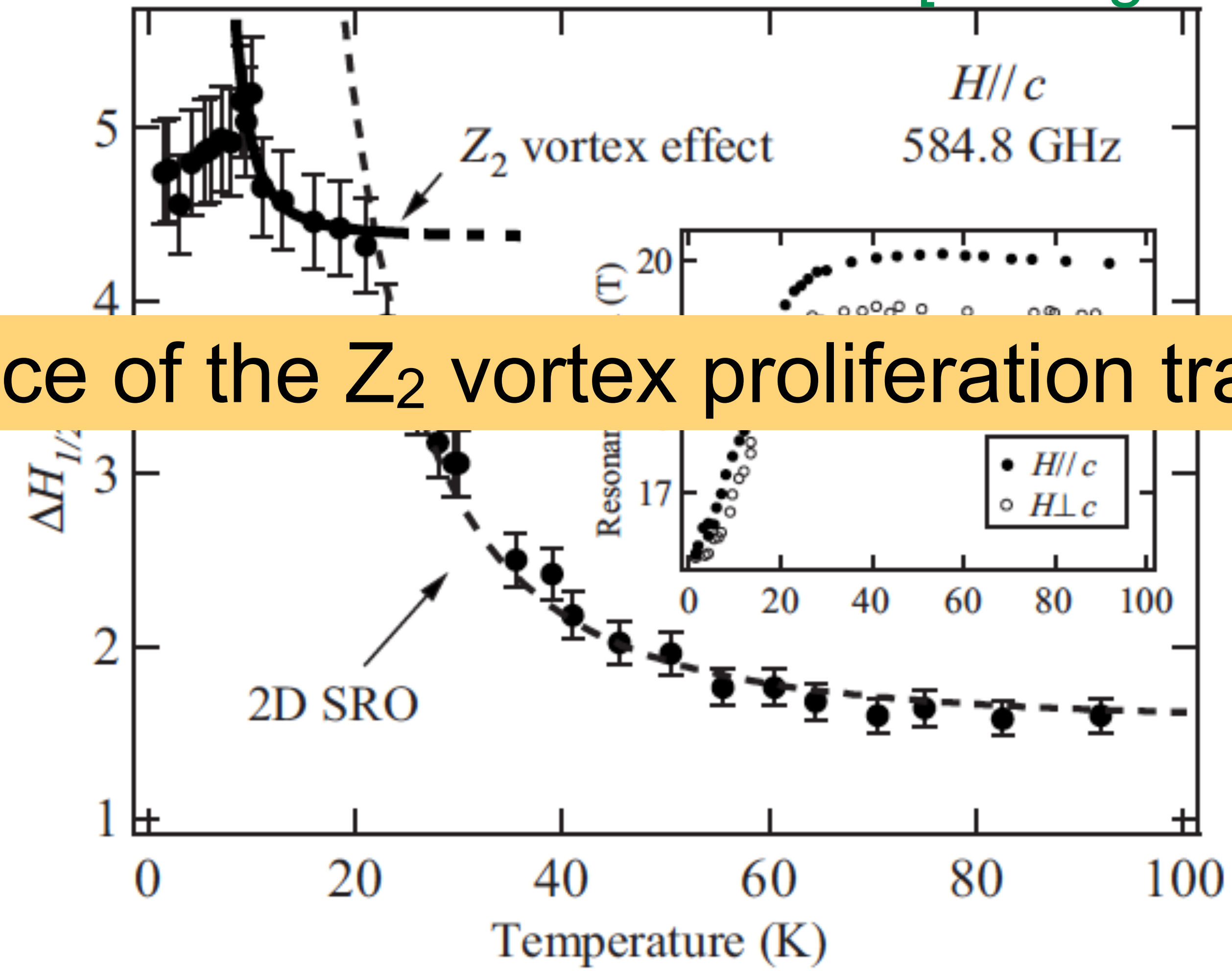


FIG. 2. Temperature dependence of full width at half maximum of the ESR linewidth in $NiGa_2S_4$ for $H \parallel c$ at 584.8 GHz. Solid and

ESR linewidth in $NiGa_2S_4$

[Yamaguchi et al. 2008]



evidence of the Z_2 vortex proliferation transition?

FIG. 2. Temperature dependence of full width at half maximum of the ESR linewidth in $NiGa_2S_4$ for $H \| c$ at 584.8 GHz. Solid and

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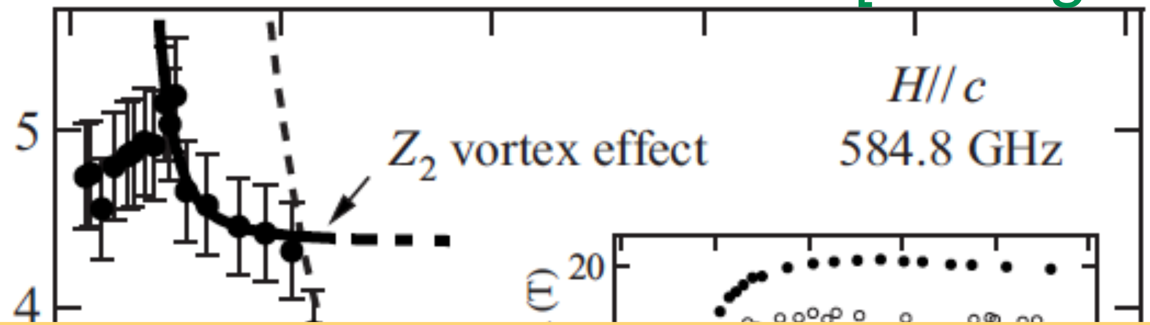

evidence of the Z_2 vortex proliferation transition?

maybe, but not very sure,
because theory is not very well developed (yet)

ESR is a challenging problem for theorists,
even in non-frustrated systems!

FIG. 2. Temperature dependence of full width at half maximum of the ESR linewidth in $NiGa_2S_4$ for $H \| c$ at 584.8 GHz. Solid and


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Shuttle Schedule From Lab
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ESR as a fundamental problem

ESR is a fascinating problem for theorists

Fundamental theories on magnetic resonance：

～ 1960's

J. H. van Vleck, P.W. Anderson

(Nobel Prize 1977) (Nobel Prize 1977)

R. Kubo – K. Tomita

(Boltzmann Medal 1977)

H. Mori – K. Kawasaki

(Boltzmann Medal 2001)

P.W. Anderson

R. Kubo

Journal of the Physical Society of Japan Vol. 9, No. 6, Nov.—Dec., 1954

A General Theory of Magnetic Resonance Absorption*

By Ryogo Kubo

Department of Physics, University of Tokyo

and Kazuhisa Tomita

Department of Physics, Kyoto University

(Received June 26, 1954)

A general expression for the frequency-dependent susceptibility of a magnetic system is derived by a quantum-statistical method based on the linear theory of irreversible process. This fundamental equation provides a physical ground for the so-called Fourier transform method for computing the resonance line contour. The auto-correlation function, or the relaxation function of the magnetic moment, that is the Fourier transform of the absorption intensity distribution, can be expanded in terms of the perturbation energy, which is assumed to be responsible for changes of the resonance spectrum from the

origin of the general "linear response theory"

operators. The customary moment method is examined from this point of view. Introducing a further assumption, we propose a method for computing the contour of resonance lines from the obtained expansion. This may be regarded as the quantum-mechanical formulation of the idea employed by Anderson and Weiss for the exchange narrowing problem of paramagnetic resonance. The problem of

What should we (theorists) do?

Restrict ourselves to linear response regime:
just need to calculate dynamical susceptibility

$$\chi_{+-}(\omega) = -i\int_0^\infty \langle [S^+(t), S^-(0)]\rangle e^{i\omega t}\, dt$$

Anisotropy is often small:
formulate a perturbation theory in the anisotropy $\mathcal{H}'$

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formulate a perturbation theory in the anisotropy $\mathcal{H}'$

This sounds very simple, but not quite !

Difficulty in perturbation theory (I)

If the (isotropic) interaction is strong
(i.e. exchange interaction *J* not small compared to *H*, *T*)
0-th order Hamiltonian $\mathcal{H}_0$ is already nontrivial
(although the ESR spectrum appears trivial…)

ESR probes a **collective motion** of strongly interacting spins, not a single spin

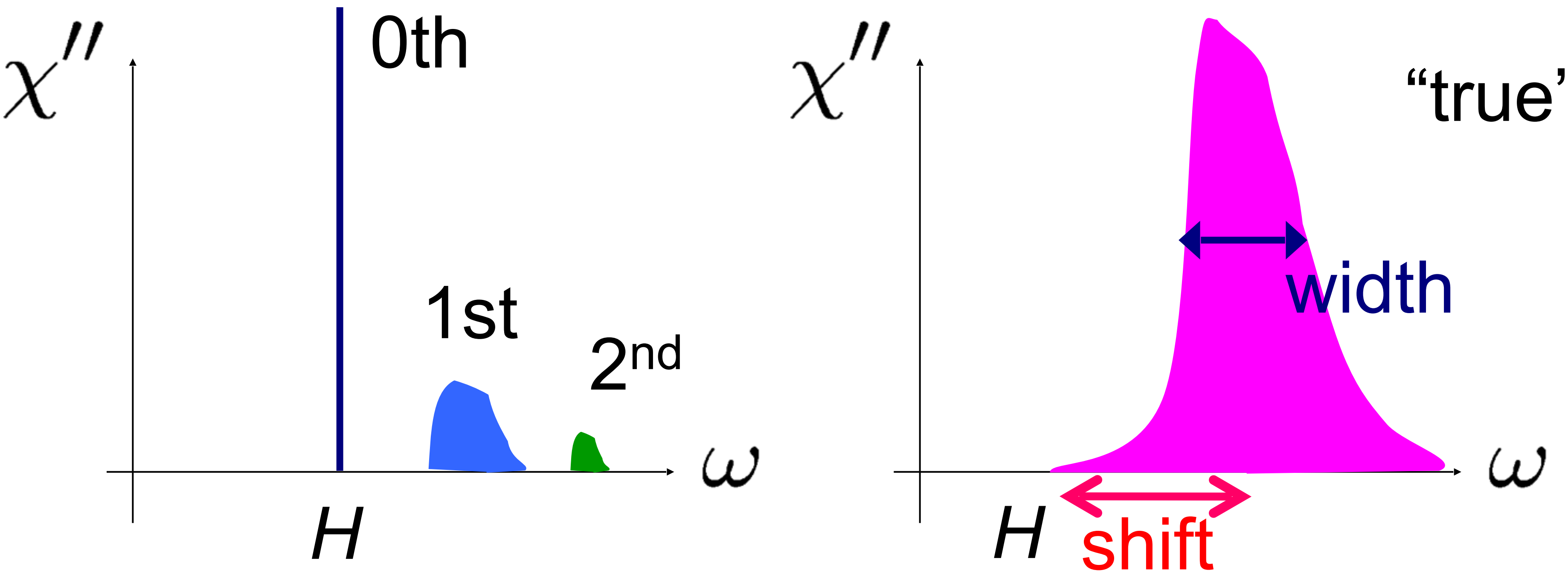
Difficulty in perturbation theory (I)

Any theory of ESR must reproduce
the delta-function spectrum $I(\omega) \propto \delta(\omega - H)$
for $\mathcal{H}_0$, in the absence of anisotropies

A “reasonable” approximation with 1% accuracy
might give a linewidth $\sim$ 0.01 J

already in the absence of anisotropy….
(then it is not useful as a theory of ESR!)

Difficulty in perturbation theory (II)



Any (finite) order of the perturbation series in χ'' is not sufficient…..

We need to sum over infinite series in some way

Phenomenological Theory

H: static magnetic field
r: oscillating magnetic field (e-m wave)

Bloch Equation

$$\frac{dS^x}{dt} = S^y H + S^z r \sin(\omega t) - \frac{S^x - \chi r \cos(\omega t)}{T_2}$$
$$\frac{dS^y}{dt} = -S^x H + S^z r \cos(\omega t) - \frac{S^y + \chi r \sin(\omega t)}{T_2}$$
$$\frac{dS^z}{dt} = -S^x r \sin(\omega t) - S^y r \cos(\omega t) - \frac{S^z - \chi H}{T_1}$$

T_1, T_2 longitudinal/transverse *relaxation* time

phenomenological description of *irreversibility*

Phenomenological Theory

Solving the Bloch eq. up to the first order in *r*
(linear response regime)

$$\chi''(\omega) \sim \frac{\omega T_2}{1+(\omega-H)^2 {T_2}^2} \chi r^2$$

ESR spectrum becomes Lorentzian, with the width $1/T_2$

The ESR width reflects the irreversibility!

Microscopic derivation of the width
= understanding of the irreversibility

Kubo-Tomita theory

The first “microscopic” theory of ESR
(and a precursor of general theory of linear response)

Contains many interesting ideas
but formulated in a different language
from what is common these days
(field theory etc.)

It has been used as a “standard” theory
to interpret experimental results for many years,
although the formulation itself is largely forgotten

(Crude) Review of Kubo-Tomita

$$\mathcal{S}(t) \equiv \langle S^{+}(t) S^{-}(0) \rangle e^{iHt}$$

$\mathcal{S}(t) = 1$ when there is no anisotropy

consider perturbative expansion of $\mathcal{S}$
in terms of the anisotropy $\mathcal{H}'$

2nd order $$\frac{d^2\mathcal{S}}{dt^2}(t) = -f(t) \equiv -\langle \mathcal{A}(t) \mathcal{A}^{\dagger}(0) \rangle e^{iHt}$$

$$\mathcal{A} \equiv [\mathcal{H}', S^{+}]$$

(The 1st order perturbation does not affect the width, and thus ignored here)

$$\mathcal{S}(t) = 1 - \int_0^t dt' \int_0^{t'} dt'' \, f(t'')$$

$$f(t) \equiv \langle \mathcal{A}(t)\mathcal{A}^\dagger(0)\rangle e^{iHt}$$

$$= 1 - \int_0^t d\tau (t-\tau) f(\tau)$$

f(*t*) generally contains oscillatory terms (with frequencies *nH*), which give "satellite peaks" Here we focus on the original resonance peak by considering only the non-oscillatory term $\bar{f}(t)$

Two cases:

1) *J* << *H* (weakly coupled spins)
2) *J* >> *H* (strongly coupled spins)

Weakly Coupled Spins

$$\bar{f}(t) \sim \bar{f}(0) = \text{const.}$$ (at least in the timescale of the Larmor precession)

$$\mathcal{S}(t) \sim 1 - \int_0^t d\tau (t-\tau) \bar{f}(0)$$

$$\sim 1 - \frac{t^2}{2} \bar{f}(0)$$

Crucial assumption: this is the lowest order expansion of the exponential form

$$\mathcal{S}(t) \sim e^{\psi(t)}$$

$$\psi(t) \sim -\frac{t^2}{2} \bar{f}(0)$$

(inclusion of infinite orders!)

Weakly Coupled Spins

$$\langle S^+(t)S^-(0)\rangle \sim \exp\left(-\frac{t^2}{2}\bar{f}(0) - iHt\right)$$

Fourier transform

$$I(\omega) \sim \exp\left(-\frac{(\omega - H)^2}{2\bar{f}(0)}\right)$$

The ESR lineshape is Gaussian!

with the width $\sqrt{\bar{f}(0)} \sim \sqrt{\langle \mathcal{A}\mathcal{A}^\dagger \rangle}$

Strongly Coupled Spins

Generically, we expect f(t) to decay with the characteristic time $\tau_0 \sim 1/J$

$$\mathcal{S}(t) \sim 1 - \int_0^t d\tau (t-\tau) \bar{f}(0)$$

$$\sim 1 - t\tau_0 \bar{f}(0)$$

Making again the same (crucial) assumption that this is the lowest order of $\mathcal{S}(t) \sim e^{\psi(t)}$

$$\psi(t) \sim -|t|\tau_0 \bar{f}(0)$$

Strongly Coupled Spins

$$\langle S^+(t) S^-(0) \rangle \sim \exp\left(-|t|\tau_0 \bar{f}(0) - iHt\right)$$

Fourier transform

$$I(\omega) \propto \frac{\bar{f}(0)\tau_0}{(\omega - H)^2 + (\bar{f}(0)\tau_0)^2}$$

ESR lineshape is Lorentzian!

with the width $\bar{f}(0)\tau_0 \sim \dfrac{\langle \mathcal{A}\mathcal{A}^\dagger \rangle}{J}$

Evolution of the line shape as *J*/*H* is increased:

Gaussian → Lorentzian ("motional narrowing")

“Standard” Theories

Kubo-Tomita (1954) , Mori-Kawasaki (1962) etc.

explain well many (but not all) experiments

Two problems in these “standard” theories

1. based on several **nontrivial assumptions**:
   the fundamental assumptions could break down in some cases.
2. evaluation of correlation functions are done within **classical** or **high-temperature** approximations. not valid with strong quantum fluctuations

A General Theory of Magnetic Resonance Absorption*

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small values of ε. The assumption b) means further that the functions $\psi_\alpha(\varepsilon,t)$ defined by the equation

$$G_\alpha(\varepsilon,t)=G_\alpha(\varepsilon,0)\exp\psi_\alpha(\varepsilon,t)\,, \quad (4.6)$$

are regular in ε and can be calculated in power series of ε from the expansions of $G_\alpha(\varepsilon,t)$ obtained by a perturbation method.

intensity distribution or the line shape. Generally speaking, we cannot decide off hand how close this approximation is to reality, without referring to the detailed nature of the system in question. From a mathematical point of

Exactly Solvable Case

S=1/2 XY chain in a magnetic field

$$\mathcal{H} = \sum_j J(S_j^x S_{j+1}^x + S_j^y S_{j+1}^y) - H S_j^z$$

A “large” anisotropy with respect to the Heisenberg exchange interaction, but the anisotropic interaction as a whole can be regarded as a small perturbation if $J << H$!

(Kubo-Tomita theory should be applicable if $J<<H$, T)

S=1/2 XY chain

Jordan-Wigner transformation

$$S_j^+ = e^{i\pi \sum_{k<j} c_k^\dagger c_k} c_j^\dagger$$

$$S_j^- = e^{i\pi \sum_{k<j} c_k^\dagger c_k} c_j$$

$$S_j^z = c_j^\dagger c_j - \frac{1}{2}$$

The S=1/2 XY chain is mapped to the free fermions on the chain (tight-binding model)

$$\mathcal{H} = -J \sum_j \left(c_{j+1}^\dagger c_j + c_j^\dagger c_{j+1} \right) - H \sum_j \left(c_j^\dagger c_j - \frac{1}{2} \right)$$

Exactly Solvable!

ESR in the S=1/2 XY chain

ESR spectrum is still a nontrivial problem, since it is related to the correlation function of $S^{\pm}$ (with the Jordan-Wigner "string" involving many fermion operators)

Nevertheless, the exact solution is obtained in the infinite T limit [Brandt-Jacoby 1976, Capel-Perk 1977]

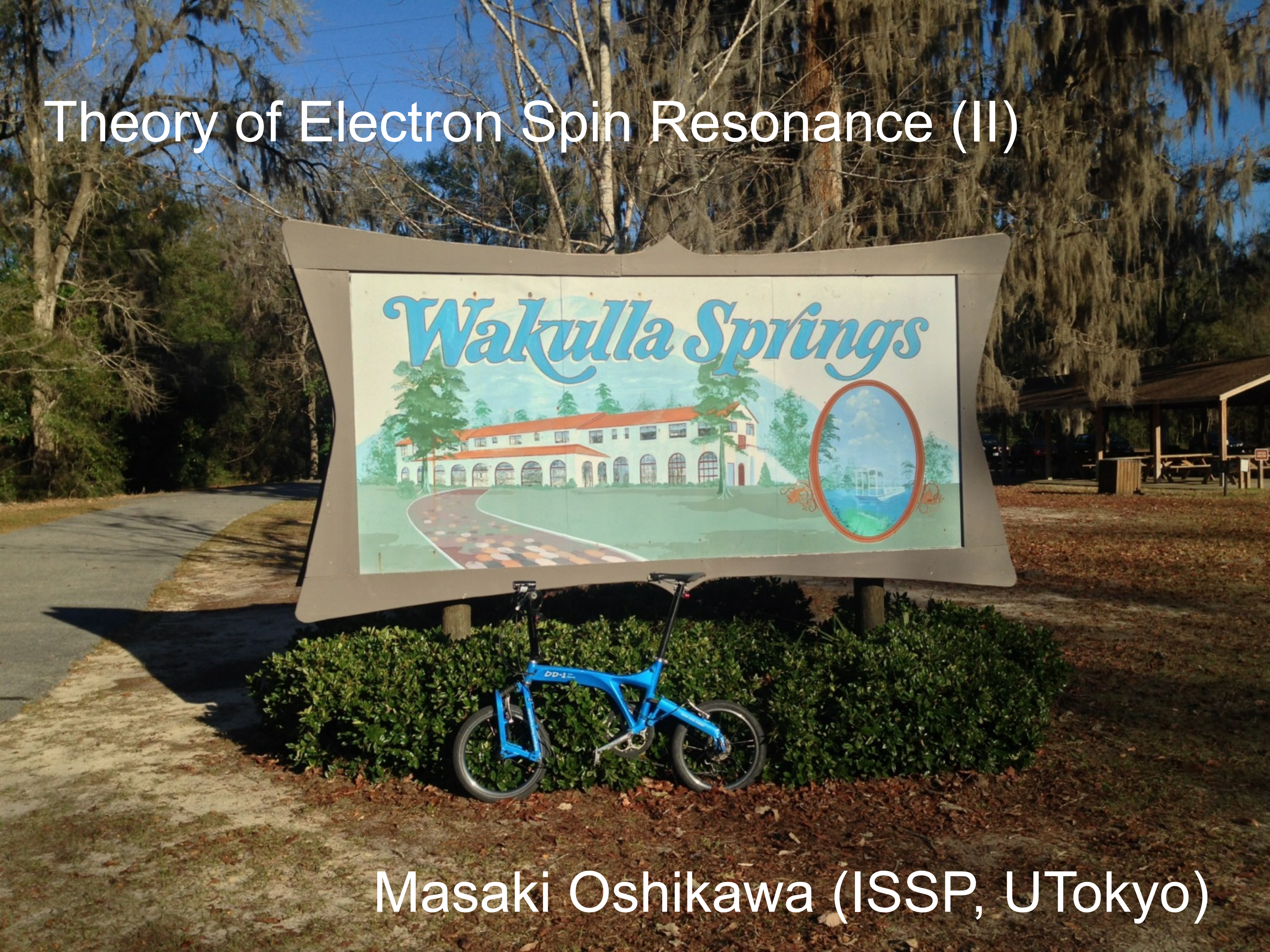
$$I(\omega) \propto \exp\left(-\frac{(\omega - H)^2}{J^2}\right)$$

Gaussian with width $J/\sqrt{2}$

Kubo-Tomita theory is exact in this limit!

Maeda-M.O. 2003

Theory of Electron Spin Resonance (II)



Masaki Oshikawa (ISSP, UTokyo)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S=1/2 Heisenberg AF chain

$$\mathcal{H}_0 = J \sum_j \vec{S}_j \cdot \vec{S}_{j+1}$$

at low temperature: extreme limit of
strong quantum fluctuation

most difficult problem to handle, with
the previous "standard" approaches

However, we can formulate ESR
in terms of field theory (bosonization)

M.O. and I. Affleck, 1999-2002

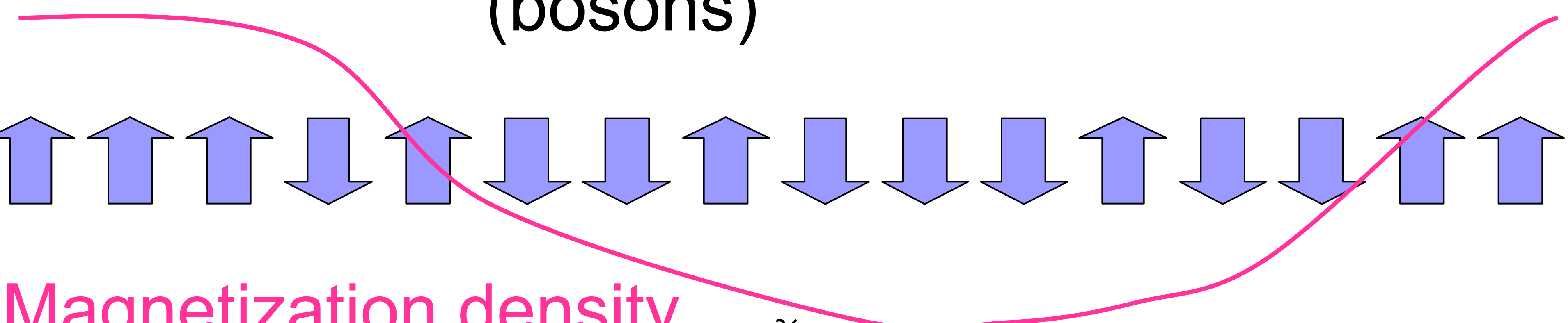
Strongly correlated 1D systems

Difficult to deal with traditional methods
(mean field etc.)

However, the magnetization density propagates very much like a density (sound) wave

↓ quantization

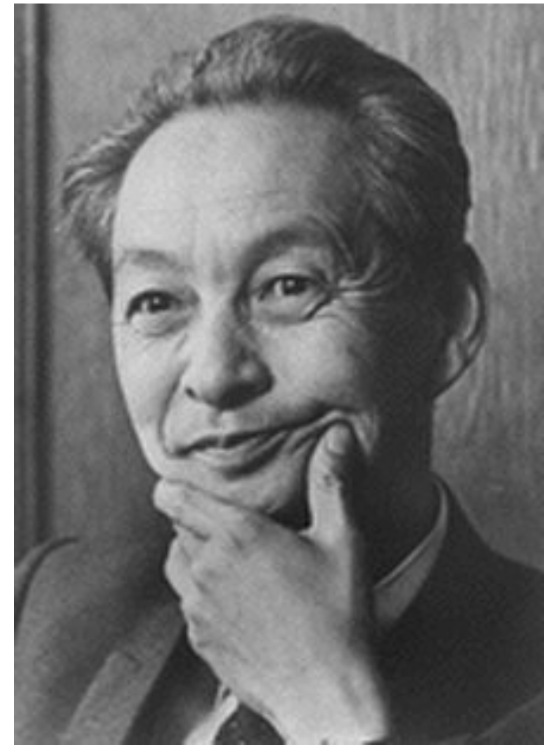
Hypothetical “phonon”
(bosons)



Magnetization density

Tomonaga-Luttinger Liquid

A wide range of 1D quantum many-body systems can be regarded, in the low-energy, low-temperature limit, as hypothetical "phonons" (free bosons)



S.-I. Tomonaga

"bosonization":

asymptotically exact in low-E, low-T limit

Bosonization

S=1/2 (isotropic) Heisenberg AF chain

⇩ low-temperature, low-energy

c=1 free boson $$\mathcal{L}_0 = \frac{1}{2}\int (\partial_\mu \varphi)^2 \, d^2x$$

ESR spectra is given by, within the field theory,

-- Here I skip the subtle derivation! --

$$I(\omega) \propto \chi''_{+-}(\omega, q=0) \propto G^R_{\varphi\varphi}(\omega, q=H)$$

[Green's function of the fundamental boson]

Reminder: What was the problem?

Restrict ourselves to linear response regime:
just need to calculate dynamical susceptibility

$$\chi_{+-}(\omega) = -i \int_0^\infty \langle [S^+(t), S^-(0)] \rangle e^{i\omega t}\, dt$$

Anisotropy is often small:
formulate a perturbation theory in
the anisotropy $\mathcal{H}'$

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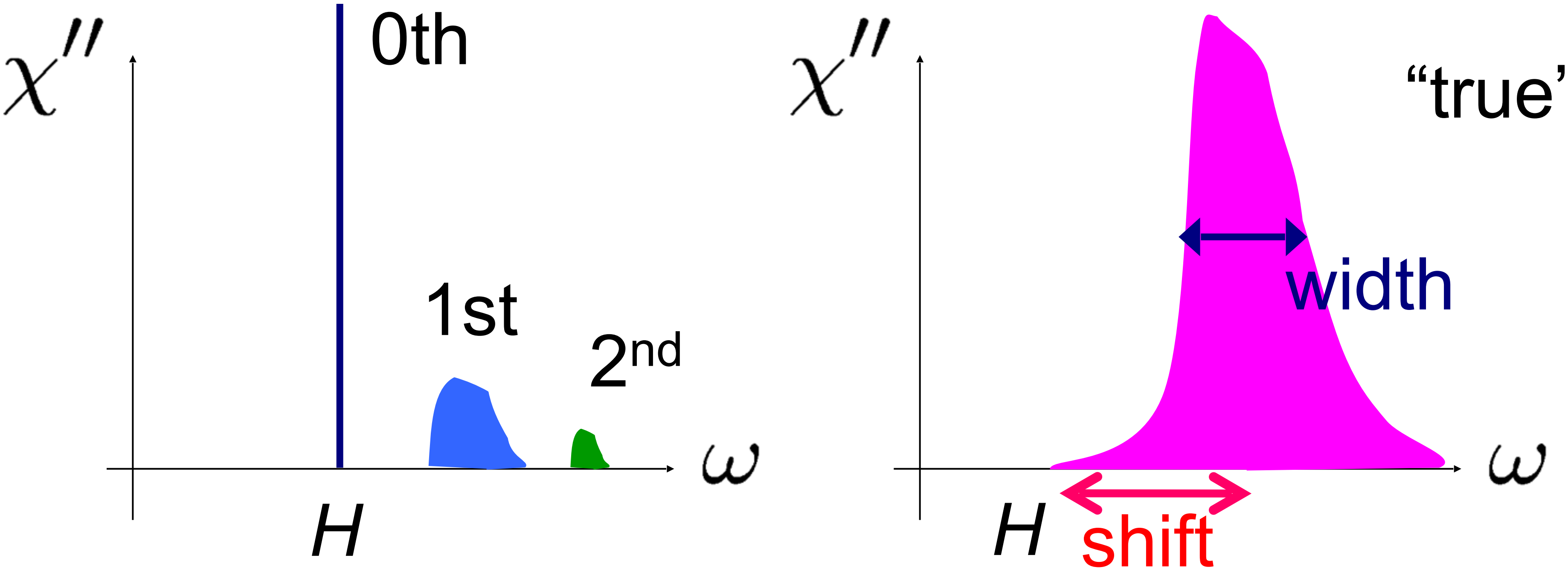
Reminder: Difficulty (II)



Any (finite) order of the perturbation series in χ'' is not sufficient.....

We need to sum over infinite series in some way

ESR spectrum in bosonization

Isotropic Heisenberg chain = free boson

$$\langle \varphi\varphi \rangle \propto \frac{-i}{\omega^2 - q^2} \Rightarrow \chi''(\omega) \propto \delta(\omega - H)$$

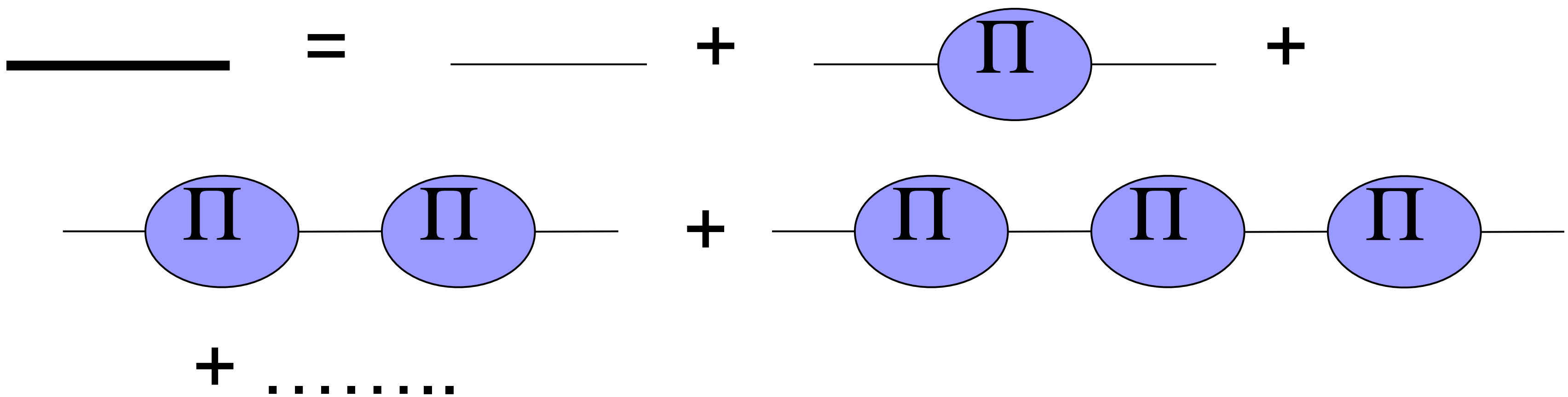
just reproduces the known result, but now
the starting point is the free theory! **(solving Difficulty I)**

Anisotropy: often gives rise to *interaction*

Diagrammatic perturbation theory
can be formulated (Feynman-Dyson)

self-energy summation **solves Difficulty II**

Self-energy formulation



$$\langle \varphi\varphi \rangle \sim \frac{-i}{\omega^2 - q^2 - \Pi(\omega, q)}$$

Shift: $\Delta\omega = \frac{1}{2H}\mathrm{Re}\Pi(H,H)$

Width: $\eta = -\frac{1}{2H}\mathrm{Im}\Pi(H,H)$

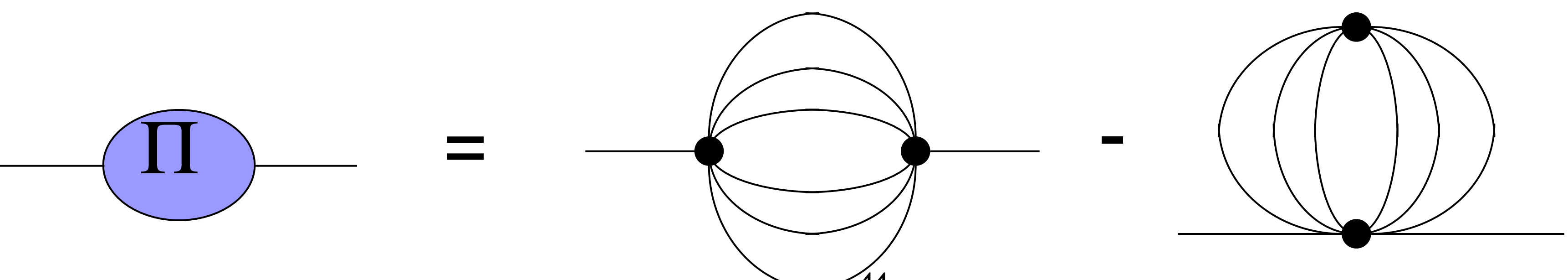
Application: staggered field

$$\mathcal{H}' = h \sum_j (-1)^j S_j^x$$

bosonization

$$\mathcal{L}' \propto h \cos(\sqrt{2\pi}\varphi)$$

The self-energy can be exactly given in the lowest order of perturbation $O(h^2)$



Result for the staggered field

Shift

$$\Delta\omega=\frac{1}{8}\sqrt{\frac{\pi}{2}}\ln\left(\frac{J}{T}\right)\frac{Jh^2}{HT}\left(\frac{\Gamma\left(\frac{1}{4}\right)}{\Gamma\left(\frac{3}{4}\right)}\right)^2 \times\left[1-\frac{\Gamma\left(\frac{3}{4}\right)}{\Gamma\left(\frac{1}{4}\right)}\mathrm{Re}\left\{\frac{\Gamma\left(\frac{1}{4}-i\frac{H}{2\pi T}\right)}{\Gamma\left(\frac{3}{4}-i\frac{H}{2\pi T}\right)}\right\}\right]. \sim 0.344057\frac{Jh^2H}{T^3}\left(\ln\frac{J}{T}\right)^{1/2}$$

Width

$$\eta=\frac{1}{16}\sqrt{\frac{\pi}{2}}\left(\frac{\Gamma(\frac{1}{4})}{\Gamma(\frac{3}{4})}\right)^2\frac{Jh^2}{T^2}\left(\ln\frac{J}{T}\right)^{1/2}\sim 0.68705\frac{Jh^2}{T^2}\left(\ln\frac{J}{T}\right)^{1/2}$$

(up to the leading log)

Diverging shift/width at the low temperature

---- is it observable?

Cu benzoate

very good 1D Heisenberg AF chain with
J =18 K (Neel temperature < 20 mK!)

studied extensively in 1960-70s by Date group but with some “strange” features which were not explained. (including ESR !)

1997: neutron scattering under magnetic field (Dender et al.) found a field-induced gap

an effect of the effective staggered field!

(M.O. and I. Affleck, 1997)

Crystal structure of Cu benzoate

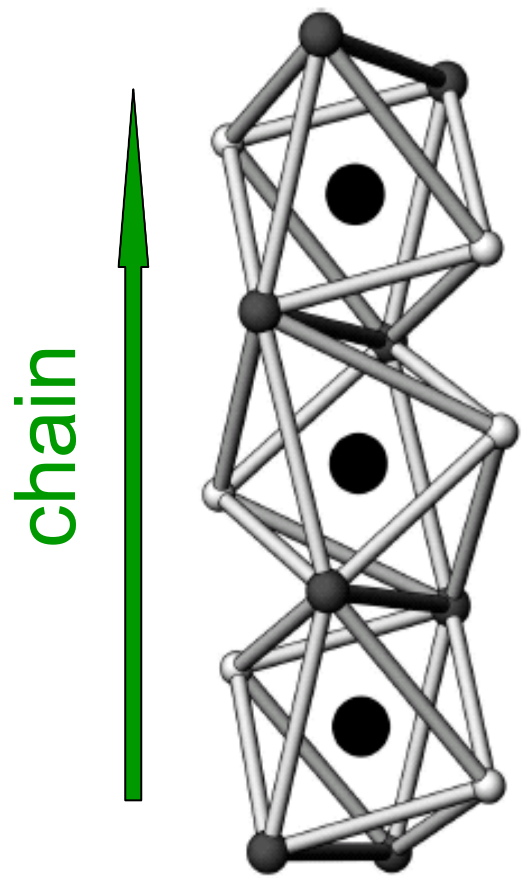


FIG. 2. Enlargement of crystal structure near a Cu (black spheres) chain with O atoms of H_2O (dark spheres) and those of benzoate groups (light spheres). Note that the oxygen octahedra have two different orientations on staggered Cu atoms.

alignment of molecules surrounding Cu^{2+}: alternating along the chain

⇓

staggered *g*-tensor,
staggered Dzyaloshinskii-Moriya int.

⇓

effective staggered field is generated $h \sim cH$

(c) depends on field direction

JOURNAL OF THE PHYSICAL SOCIETY OF JAPAN, Vol. 33, No. 6, DECEMBER, 1972

1972(!)

Electron Spin Resonance in One Dimensional Antiferromagnet $Cu(C_6H_5COO)_2 3H_2O$

Kiichi OKUDA, Hirao HATA and Muneyuki DATE
Department of Physics, Faculty of Science, Osaka University, Toyonaka, Osaka

(Received April 11, 1972)

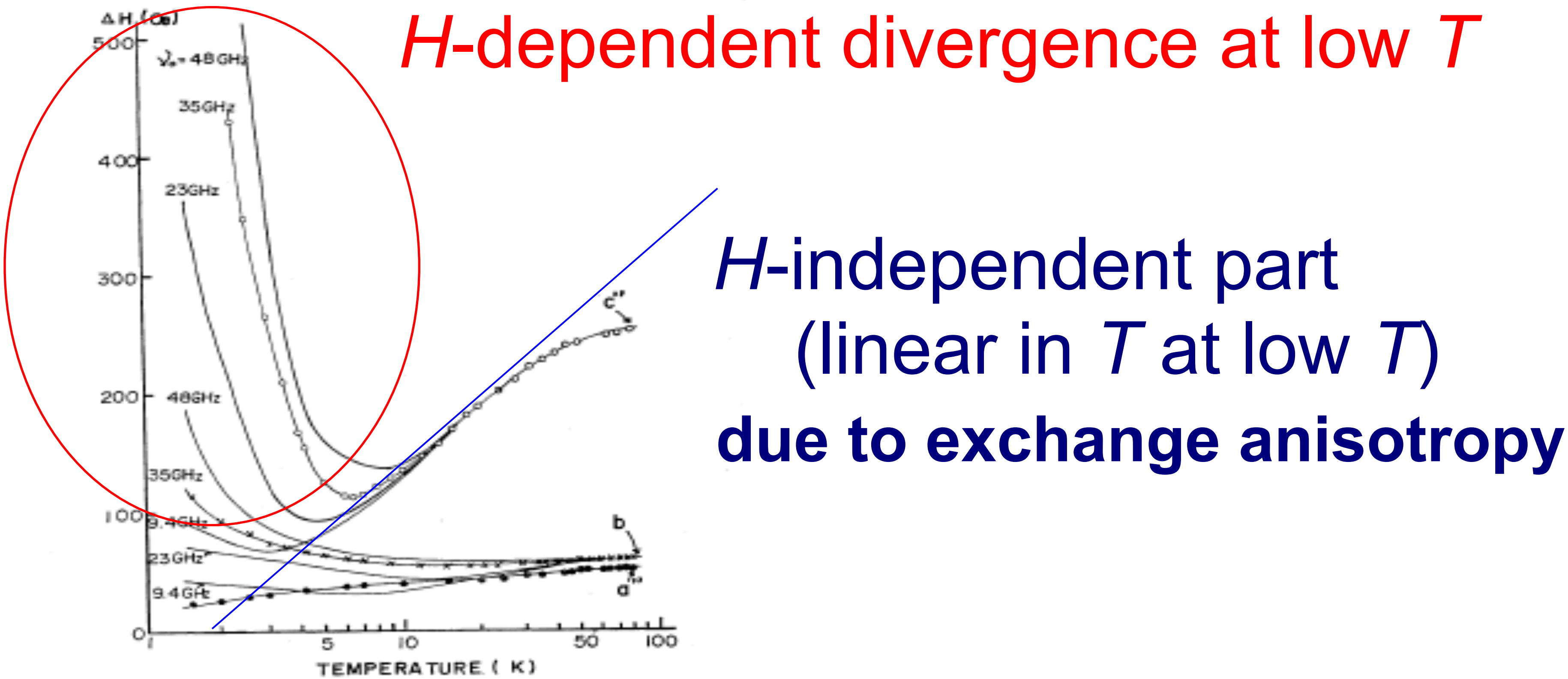
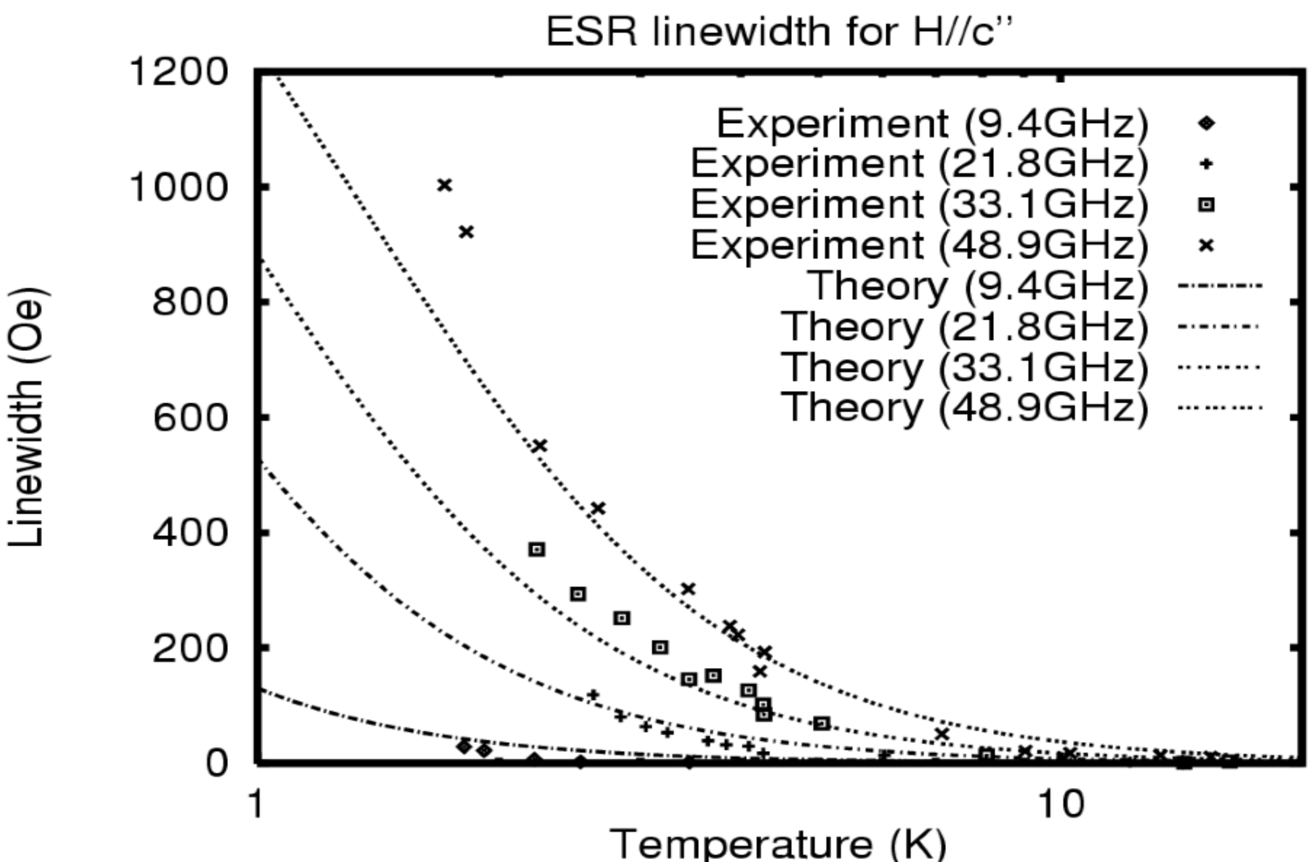


Fig. 6. Temperature dependence of line width in each directions of a''-, b- and c''-axis.

ESR linewidth in Cu benzoate

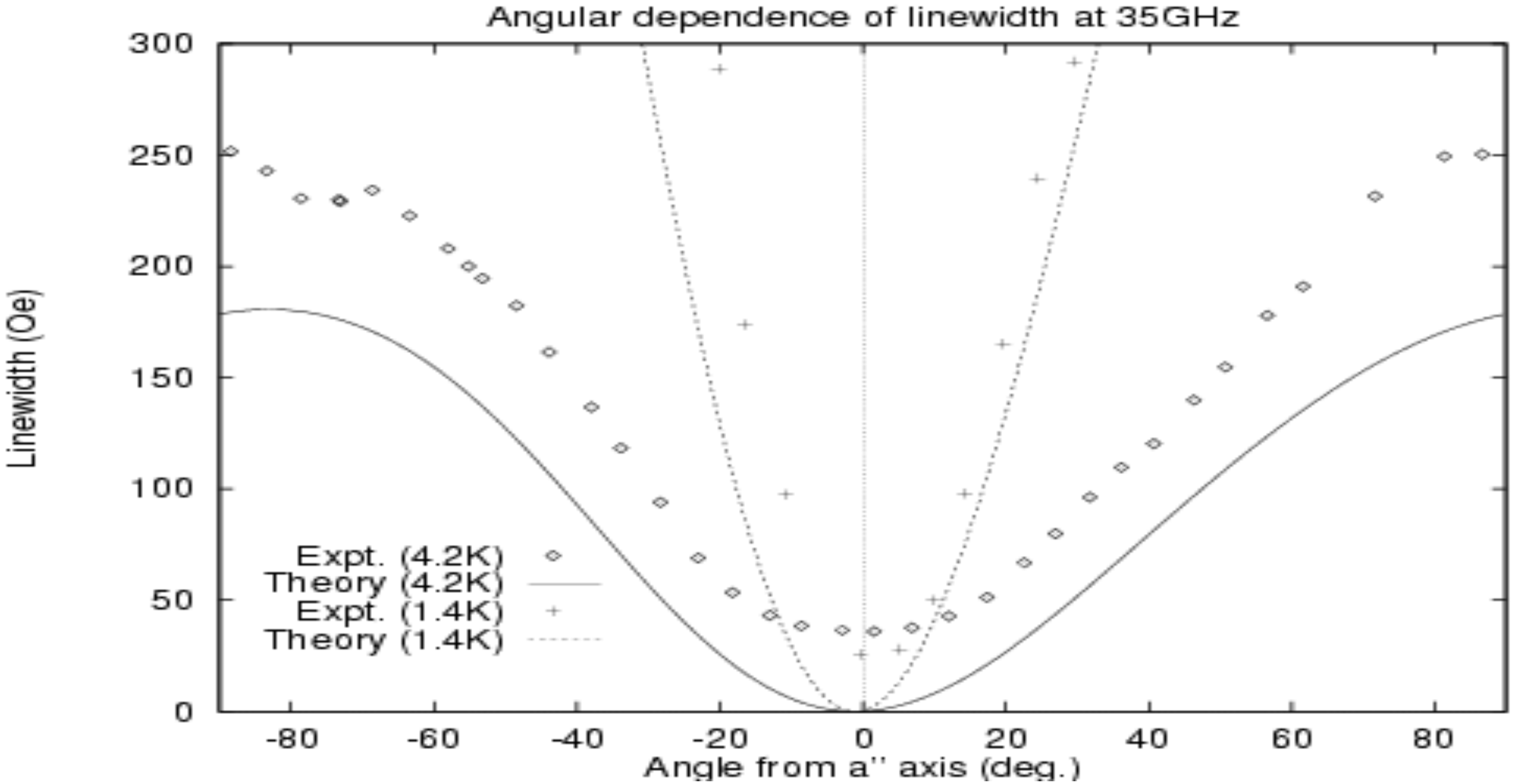
$$\frac{1}{\tau} \propto \frac{Jh^2}{T^2} \propto \frac{c^2 J H^2}{T^2}$$

H / resonance frequency



data from Okuda et al. (1972)
[H-dep.part]

Angular dependence



assumed a DM vector which fits other expt. as well

Exchange anisotropy / dipolar int.

If the crystal symmetry does not allow the staggered field, the most dominant effects on ESR come from

exchange anisotropy / dipolar interaction

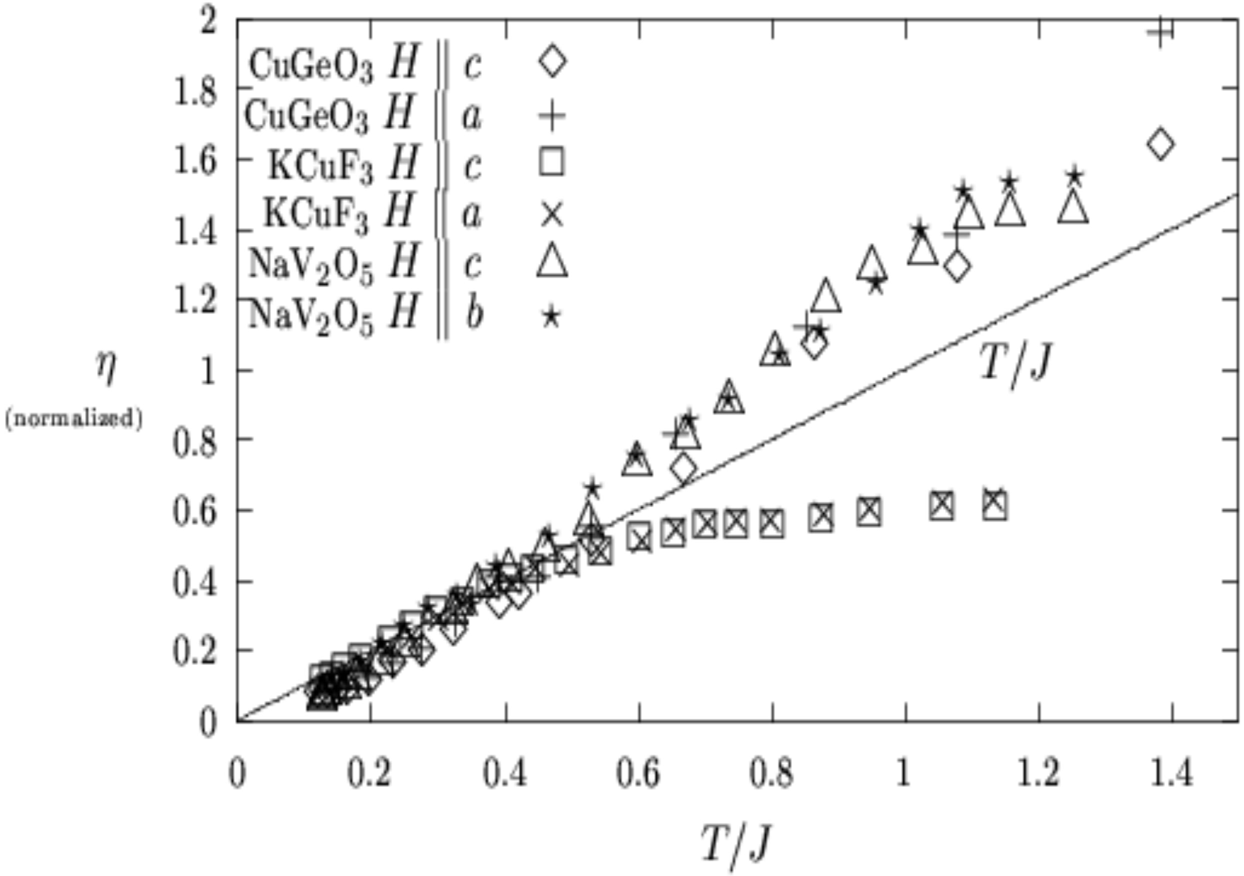
e.g.

$$\mathcal{H}' = \delta \sum_j S_j^\alpha S_{j+1}^\alpha$$

width from our theory:

$$\eta = \frac{2}{\pi^3}\left(\frac{\delta}{J}\right)^2\left(\ln\frac{J}{\max(T,H)}\right)^2 T$$

Comparison with experiments



Reminder: what is the width?

Phenomenologically, the line width is given by the inverse transverse relaxation time $1/T_2$

$$\chi''(\omega) \sim \frac{\omega T_2}{1 + (\omega - H)^2 {T_2}^2} \chi h^2$$

How did we obtain the irreversibility from the field theory approach?

How field theory gives the width

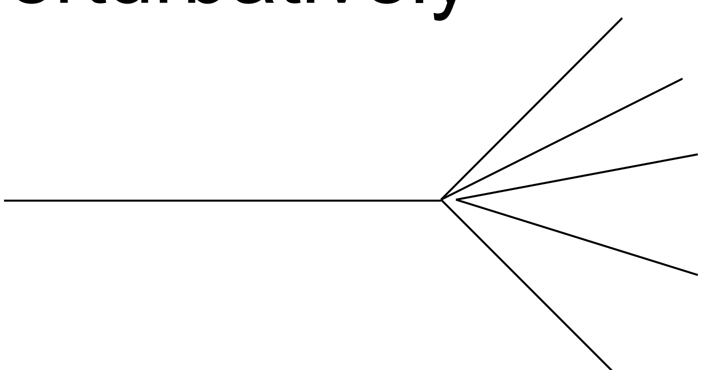
ESR ⇔ creation of a single "boson" with $E \sim H$

Spectrum is delta-function as long as the energy of the boson is unambiguous

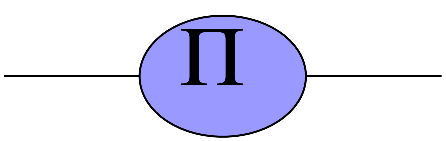
However, once the boson has a finite lifetime τ, its energy has uncertainty $\sim 1/\tau$

$$\Delta E \Delta t \geq \frac{\hbar}{2}$$

The decay rate $1/\tau$ can be calculated perturbatively in field theory

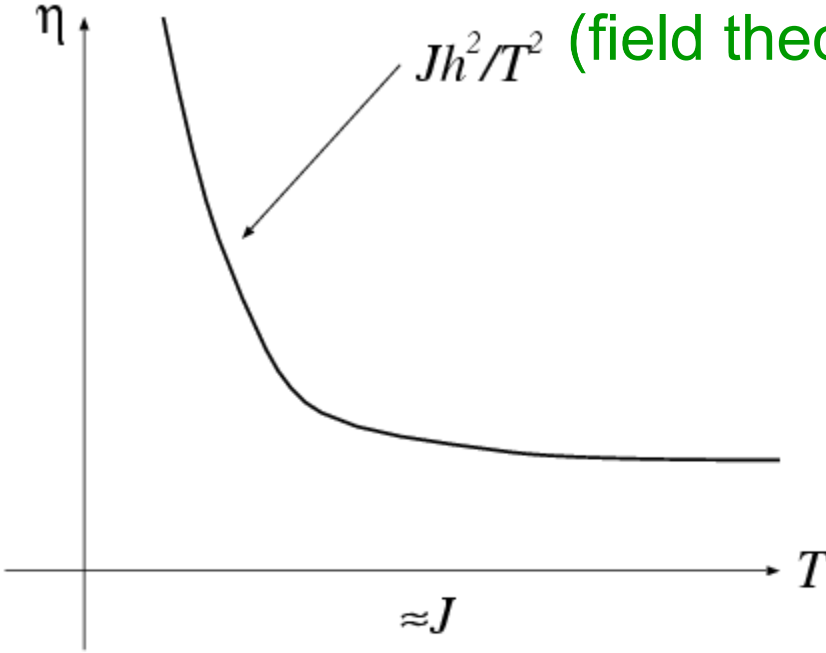


$=$ Im



crossover to high temperatures

conjecture for the linewidth

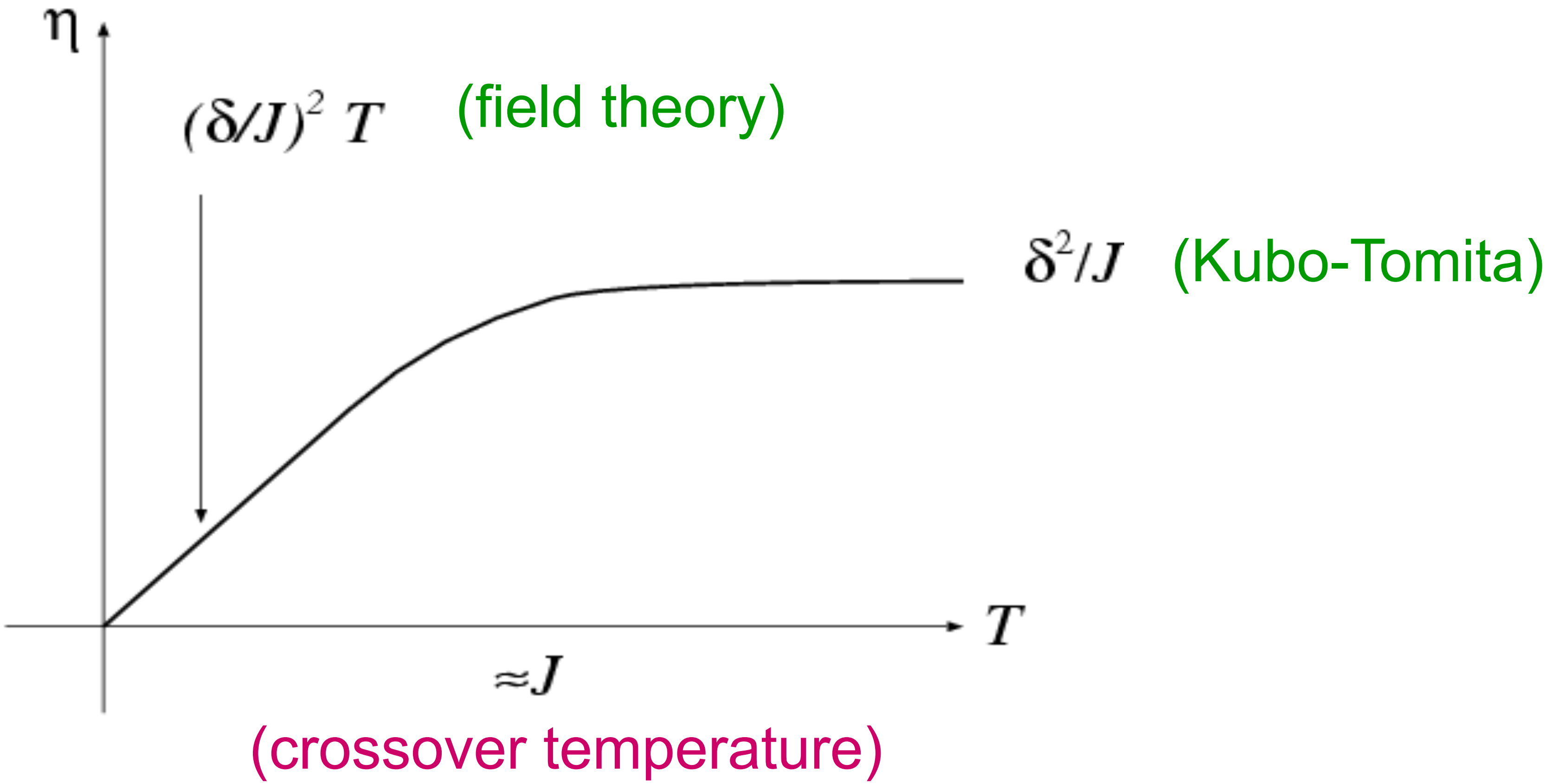


staggered field

(crossover temperature)

crossover of linewidth

exchange anisotropy / dipolar interaction



(Staggered) DM interaction

$$S_j^x S_{j+1}^x + S_j^y S_{j+1}^y = \frac{1}{2}\left(S_j^+ S_{j+1}^- + S_j^- S_{j+1}^+\right)$$

$$S_j^x S_{j+1}^y - S_j^y S_{j+1}^x = \frac{i}{2}\left(S_j^+ S_{j+1}^- - S_j^- S_{j+1}^+\right)$$

$$\vec{D}_j = (-1)^j D\hat{z}$$

$$\vec{H} = H\hat{x}$$

$$\sum_j \left[J\vec{S}_j \cdot \vec{S}_{j+1} + \vec{D}_j \cdot \left(\vec{S}_j \times \vec{S}_{j+1}\right) - \vec{H}\cdot\vec{S}\right] =$$

$$\sum_j \left[\frac{1}{2}\left(J + iD(-1)^j\right) S_j^+ S_{j+1}^- + \frac{1}{2}\left(J - iD(-1)^j\right) S_j^- S_{j+1}^+ + S_j^z S_{j+1}^z - H S_j^x\right]$$

$$\tilde{S}_j^{\pm} = e^{\pm i(-1)^j \alpha/2} S_j^{\pm} \qquad \tan\alpha = \frac{D}{J}$$

$$\sum_j \left[\frac{|\mathcal{J}|}{2}\tilde{S}_j^+ \tilde{S}_{j+1}^- + \frac{|\mathcal{J}|}{2}\tilde{S}_j^- \tilde{S}_{j+1}^+ + \tilde{S}_j^z \tilde{S}_{j+1}^z - H\cos\frac{\alpha}{2}\tilde{S}_j^x - (-1)^j \sin\frac{\alpha}{2}\tilde{S}_j^y\right]$$

Failure of (naive application of) Kubo-Tomita

(staggered) Dzyaloshinskii-Moriya interaction

$$\mathcal{H}' = \sum_j (-1)^j \vec{D} \cdot (\vec{S}_j \times \vec{S}_{j+1})$$

Kubo-Tomita formula ⇓

linewidth in the high *T* limit: $\sim \frac{D^2}{J}$

typically, different by factor 100 !

However, the DM interaction can be eliminated by an exact transformation to give exchange anisotropy and staggered field.

Kubo-Tomita applied after the transformation:

linewidth in the high *T* limit: $\sim \frac{D^4}{J^3} + \frac{D^2 H^2}{J^3}$

correct answer?

(or even smaller)

What happens at lower *T*?

The linewidth due to the staggered field *h* diverges as $T \to 0$, in the lowest order of *h*

i.e. the perturbation theory breaks down at sufficiently low *T*, even for a small *h*

“asymptotic freedom”

Can we say something?

The low-energy effective theory is

$$\mathcal{L} = \frac{1}{2}(\partial_\mu \varphi)^2 + \text{const.}\, h \cos\left(\sqrt{2\pi}\varphi\right)$$

integrable sine-Gordon QFT!

T=0 : excitations from G.S.

At $\beta = \sqrt{2\pi}$ the elementary excitations are

soliton/antisoliton/1st breather : same mass M
and 2nd breather of mass $\sqrt{3}M$

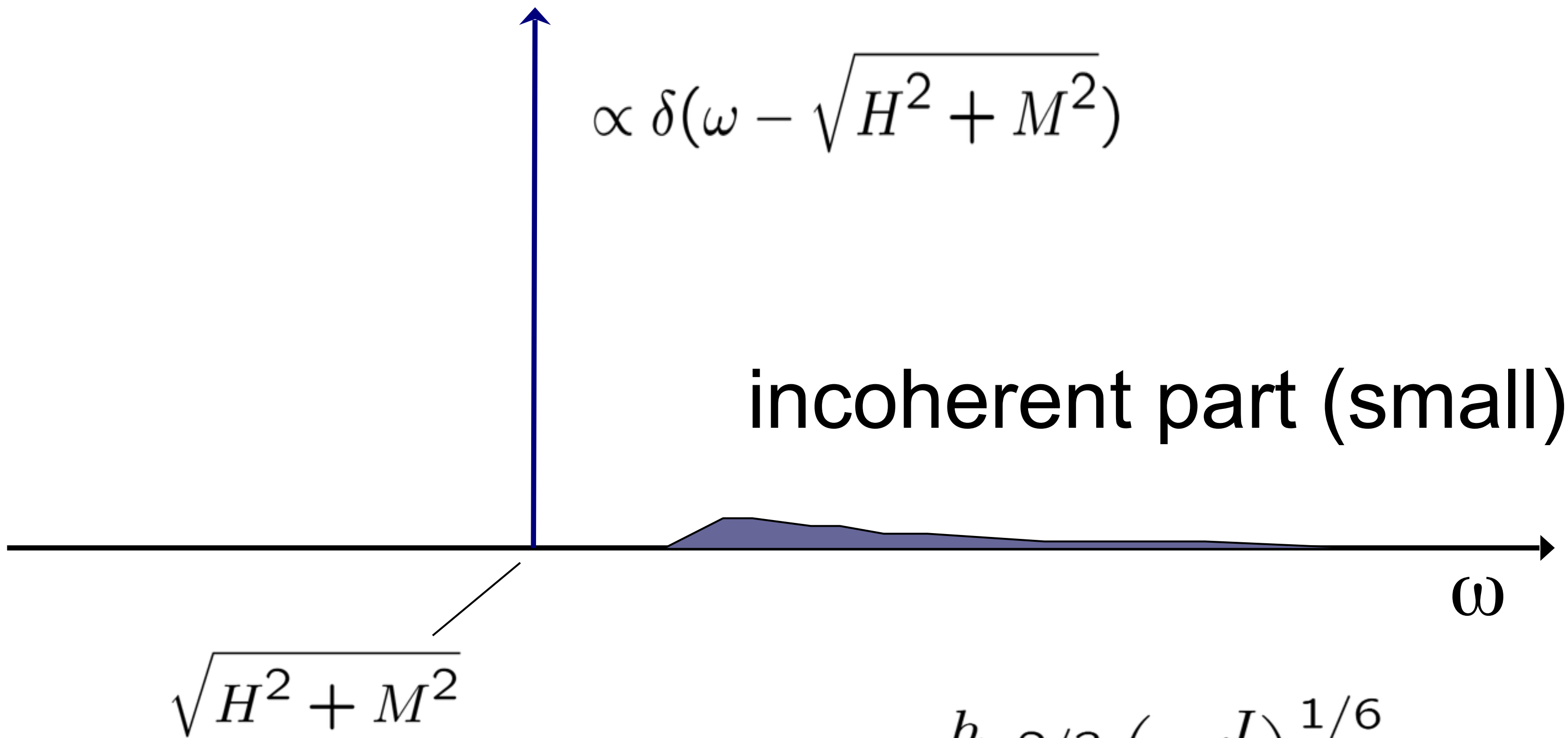
Exact sine-Gordon formfactor **(Karowski-Weisz)**

$$\langle\varphi\varphi\rangle(\omega,q) \sim Z_\varphi \frac{-i}{\omega^2 - q^2 - M^2} + (\text{incoherent multi-particle exc.})$$

$Z_\varphi \sim 0.978689$ ⇨ 1st breather dominant (small incoherent part)

Remember: q=H for ESR spectrum from QFT

Prediction on ESR at T=0



$$M \sim 1.35607 (\frac{h}{J})^{2/3} \left(\ln \frac{J}{h} \right)^{1/6}$$

Huh, didn't I say the linewidth **diverges** as T is lowered?

JOURNAL OF THE PHYSICAL SOCIETY OF JAPAN, Vol. 44, No. 3, MARCH, 1978

1978(!)

Antiferromagnetic Resonance in Copper Benzoate below 1 K

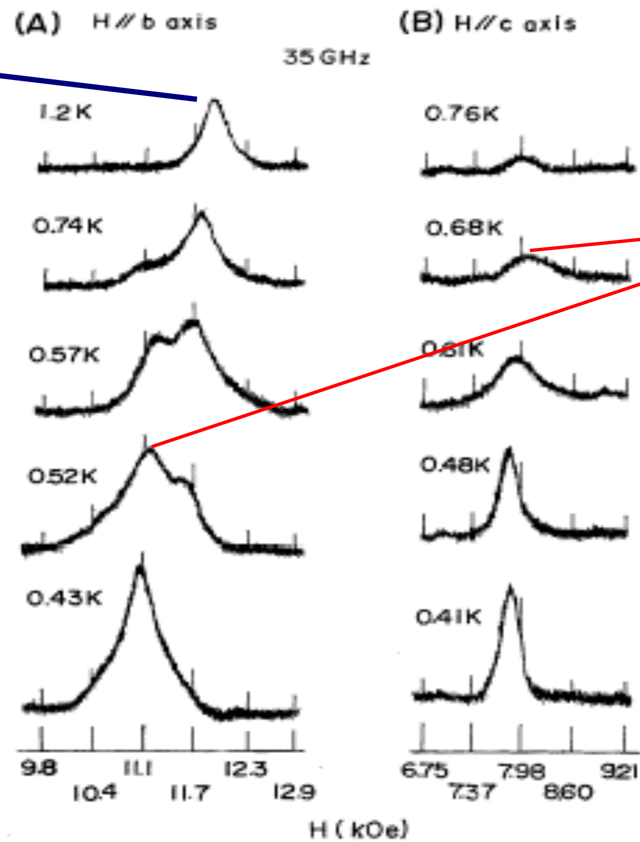
Kokichi OSHIMA, Kiichi OKUDA and Muneyuki DATE

Department of Physics, Faculty of Science, Osaka University Toyonaka, Osaka 560

(Received September 21, 1977)

original "paramagnetic" peak

$\omega \sim H$



"new" peak narrowed as $T \rightarrow 0$

"sG breather"

Testing the sine-Gordon prediction

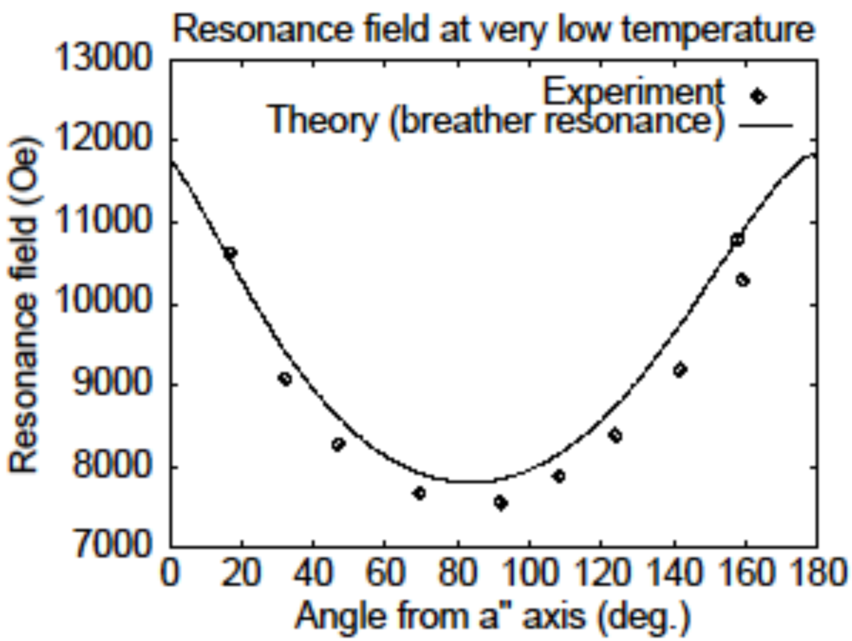


FIG. 3. The resonance field at very low temperature for various field directions in the *ac* plane. The experimental data were taken from the "antiferromagnetic resonance" in Ref. [8] at 0.41 K, and the theory refers to the lowest breather excitation at zero temperature (10).

$$\omega = \sqrt{H^2 + M^2}$$

$$M \sim 1.35607 (\frac{h}{J})^{2/3} \left(\ln \frac{J}{h} \right)^{1/6}$$

Used the **same set of the parameters** as in the perturbative regime

VOLUME 84, NUMBER 25 PHYSICAL REVIEW LETTERS 19 JUNE 2000

ESR Investigation on the Breather Mode and the Spinon-Breather Dynamical Crossover in Cu Benzoate

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(Received 8 November 1999)

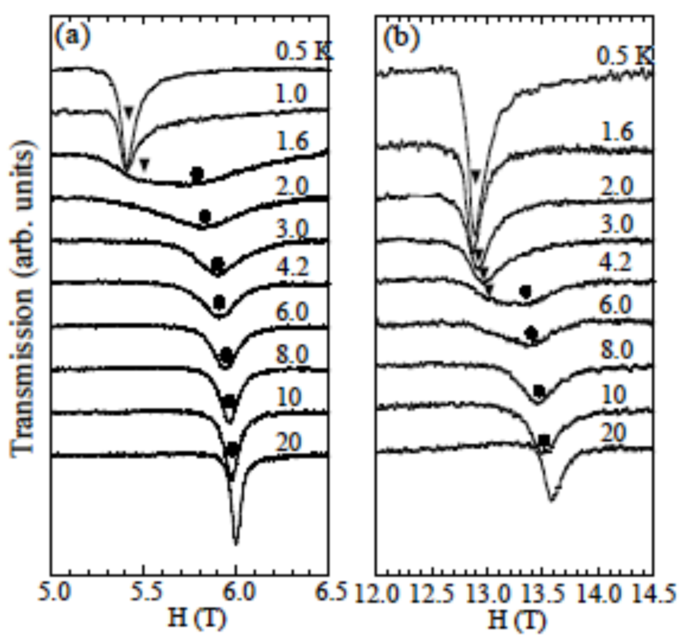
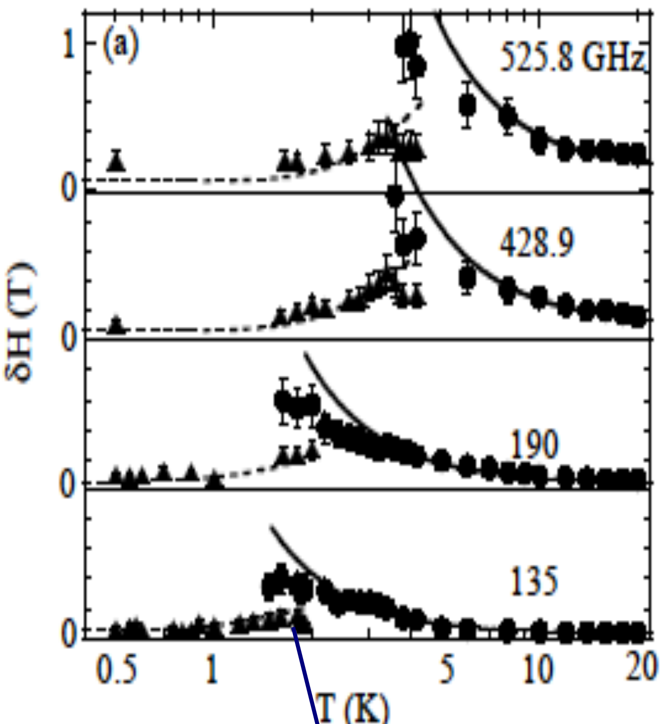


FIG. 1. Examples of ESR spectra at (a) 190 GHz and at (b) 428.9 GHz for $H \parallel c$. The symbols (● and ▼) represent spinon ESR line (S) and the first-breather ESR line (B_1), respectively.

finite-*T* dynamical correlation function in the sG QFT is seen here!!

T-dependence of the width



crossover at T » M

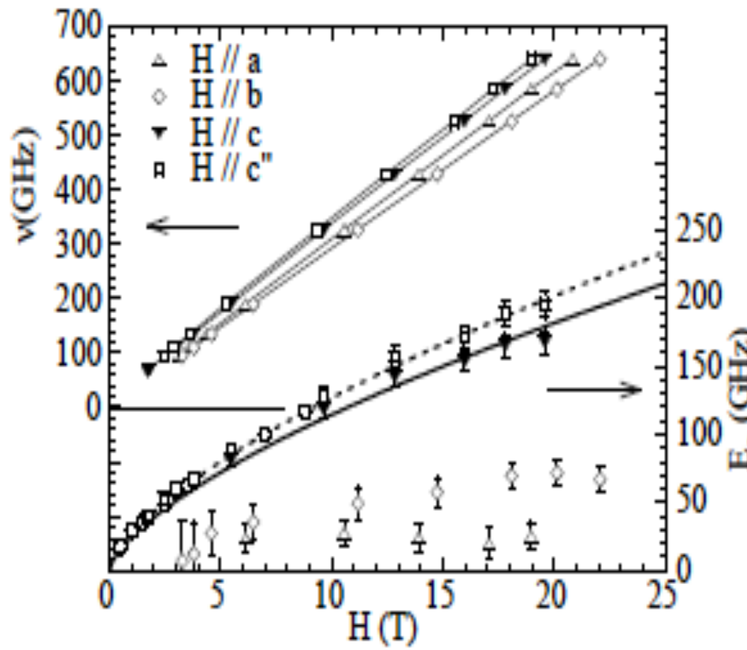


FIG. 3. In the inset panel, a frequency-field plot of the main ESR line for different field orientations is plotted. Solid lines are eye guides. The lower panel, the plot of $E_g(H)$ as a function of external field. Here ○ shows the value determined by the specific-heat measurements taken from Ref. [4]. The dashed line and solid line are the theoretical curves of $E_g(H) \propto H^{2/3}$. The prefactor for $H \parallel c''$ is taken from Ref. [6] and that for $H \parallel c$ is decided in this paper. The c'' axis is in the ac plane and tilts 21° from the a axis (for more detail, see Fig. 1 of Ref. [9]).

VOLUME 92, NUMBER 5 PHYSICAL REVIEW LETTERS week ending 6 FEBRUARY 2004

Electron Spin Resonance in the Spin-1/2 Quasi-One-Dimensional Antiferromagnet with Dzyaloshinskii-Moriya Interaction $BaCu_2Ge_2O_7$

S. Bertaina,[1] V. A. Pashchenko,[2] A. Stepanov,[1] T. Masuda,[3,*] and K. Uchinokura[3,†]

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[2]*Physikalisches Institut, Johann Wolfgang Goethe Universität, FOR412, Postfach 111932, 60054 Frankfurt am Main, Germany*

[3]*Department of Advanced Materials Science, The University of Tokyo, 5-1-5 Kashiwa-no-ha, Kashiwa 277-8581, Japan*

(Received 15 September 2003; published 6 February 2004)

We have investigated the electron spin resonance (ESR) on single crystals of $BaCu_2Ge_2O_7$ at temperatures between 300 and 2 K and in a large frequency band, 9.6–134 GHz, in order to test the predictions of a recent theory, proposed by Oshikawa and Affleck (OA) [Phys. Rev. Lett. **82**, 5136 (1999)], which describes the ESR in a spin-1/2 Heisenberg chain with the Dzyaloshinskii-Moriya interaction. We find, in particular, that the ESR linewidth, ΔH, displays a rich temperature behavior. As the temperature decreases from $T_{max}/2 \approx 170$ to 50 K, ΔH shows a rapid and linear decrease, $\Delta H \sim T$. At low temperatures, below 50 K, ΔH acquires a strong dependence on the magnetic field orientation and for $H \parallel c$ it shows a $(h/T)^2$ behavior which is due to an induced staggered field h, according to OA's prediction.

VOLUME 93, NUMBER 2 PHYSICAL REVIEW LETTERS week ending 9 JULY 2004

Excitation Hierarchy of the Quantum Sine-Gordon Spin Chain in a Strong Magnetic Field

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(Received 15 March 2004; published 6 July 2004)

The magnetic excitation spectrum of copper pyrimidine dinitrate, a material containing $S = \frac{1}{2}$ antiferromagnetic chains with alternating g tensor and the Dzyaloshinskii-Moriya interaction and exhibiting a field-induced spin gap, is probed using submillimeter wave electron spin resonance spectroscopy. Ten excitation modes are resolved in the low-temperature spectrum, and their frequency-field diagram is systematically studied in magnetic fields up to 25 T. The experimental data are sufficiently detailed to make a very accurate comparison with predictions based on the quantum sine-Gordon field theory. Signatures of three breather branches and a soliton, as well as those of several multiparticle excitation modes, are identified.

Bosonization approach does work well for ESR, but remember that it applies only to 1D systems in the low-T, low-energy limit!

Kubo-Tomita theory seems to work in some cases, but its range of validity is not established.

What can we do then?

Let us focus on the shift only

Forget the full lineshape!
-- to avoid the difficulties

Kanamori-Tachiki (1962), Nagata-Tazuke (1972)

single mode approximation

⇨ shift $$\Delta\omega = -\frac{\langle [[\mathcal{H}', S^+], S^-] \rangle}{2\langle S^z \rangle}$$

validity?

Nagata-Tazuke then evaluated this formula in the classical & weak field limit.

more systematic derivation

Maeda-M. O. (2005)

Define the shift by the first moment

$$\Delta\omega \equiv \frac{\int_0^\infty d\omega\ \omega\chi''(\omega)}{\int_0^\infty d\omega\ \chi''(\omega)} - H$$

expand in $\mathcal{H}'$

$$\Delta\omega = -\frac{\langle[[\mathcal{H}', S^+], S^-]\rangle_0}{2\langle S^z\rangle_0} + O(\mathcal{H}'^2)$$

Kanamori-Tachiki formula is generally exact in the first order, but NOT in second and higher orders!

Exchange anisotropy

Antisymmetric exchange (DM interaction) gives the shift only in the second order

So we only consider the symmetric exchange anisotropy between nearest neighbors

$$\mathcal{H}' = \sum_{j,a} J'_a S^a_j S^a_{j+1}$$

(diagonalized by taking principal axes)

Second-order formula

The second-order correction to the width presumably depends on how the width is defined. In a certain definition, we found:

[Maeda-M.O. 2005]

$$\delta\omega_{m,a}(\alpha) = \alpha\omega^{(1)}_{m,a} + \alpha^2\omega^{(2)}_{m,a}$$

$$= -\frac{\langle[A,S_j^-]\rangle_0 + \langle[A,S_j^-]\rangle_1}{2\langle S_j^z\rangle_0} + \frac{\langle[A,S_j^-]\rangle_0}{2\langle S_j^z\rangle_0}\left[\frac{\langle S_j^z\rangle_1}{\langle S_j^z\rangle_0} \pm \frac{\langle[A^\dagger,S_j^-]\rangle_0 - \langle[A,S_j^+]\rangle_0}{4H\langle S_j^z\rangle_0}\right]$$

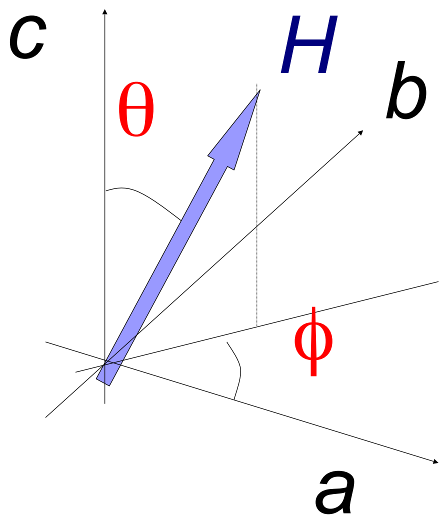
$$-\frac{1}{8\langle S_j^z\rangle_0}\lim_{\epsilon\to 0}[4\chi'_{AA^\dagger} + 2\epsilon\partial_\omega\chi''_{AA^\dagger} \pm \frac{1}{H}\left(\epsilon\left(\chi''_{AA} + \chi''_{A^\dagger A^\dagger}\right) - \epsilon^2\left(\partial_\omega\chi'_{AA} + \partial_\omega\chi'_{A^\dagger A^\dagger}\right)\right)]$$

$$A \equiv [\mathcal{H}', S^+]$$

$$-\frac{1}{8\langle S_j^z\rangle_0}\lim_{\epsilon\to 0}[-\frac{3\epsilon^3}{2H^3}\chi''_{AA^\dagger} + \frac{\epsilon^3}{2H^3}\chi''_{A^\dagger A} - \frac{\epsilon^3}{2H^2}\partial_\omega\chi''_{A^\dagger A} + \frac{\epsilon^4}{2H^3}\partial_\omega\chi'_{AA^\dagger} - \frac{3\epsilon^4}{4H^4}\chi'_{A^\dagger A}$$

$$+\frac{\epsilon^4}{2H^3}\partial_\omega\chi'_{A^\dagger A} \pm \frac{1}{H}\{-\frac{\epsilon^3}{2H}\left(\partial_\omega\chi''_{AA} + \partial_\omega\chi''_{A^\dagger A^\dagger}\right) + \frac{\epsilon^6}{8H^5}\left(\chi'_{AA} + \chi'_{A^\dagger A^\dagger}\right)\}]$$

First-order shift



$$\Delta\omega = -\frac{\langle [[\mathcal{H}', S^+], S^-] \rangle_0}{\langle S^z \rangle_0} = f(\theta, \phi) Y(T, H)$$

$$f(\theta,\phi) = J'_a(1-3\sin^2\theta\cos^2\phi) + J'_b(1-3\sin^2\theta\sin^2\phi) + J'_c(1-3\cos^2\theta)$$

$$Y(T,H) = \frac{\langle S^z_j S^z_{j+1} - S^x_j S^x_{j+1} \rangle_0}{\langle S^z \rangle_0}$$

to be evaluated for S=1/2 Heisenberg AF chain in the field H//z

Static quantity (easier!)

Exact evaluation of *Y(T,H)*

Consider a fictitious XXZ chain in the field *H*

$$\mathcal{H}_{XXZ} = \sum_j (J\vec{S}_j \cdot \vec{S}_{j+1} + \delta S^z_j S^z_{j+1} - H S^z_j)$$

Free energy (per site) *F* is known exactly for arbitrary *H*, δ, *T* by the Quantum Transfer Matrix technique.

$$-\frac{\partial F}{\partial \delta}(\delta = 0, T, H) = \langle S^z_j S^z_{j+1} \rangle_0$$

desired term in *Y*!

Exact solution

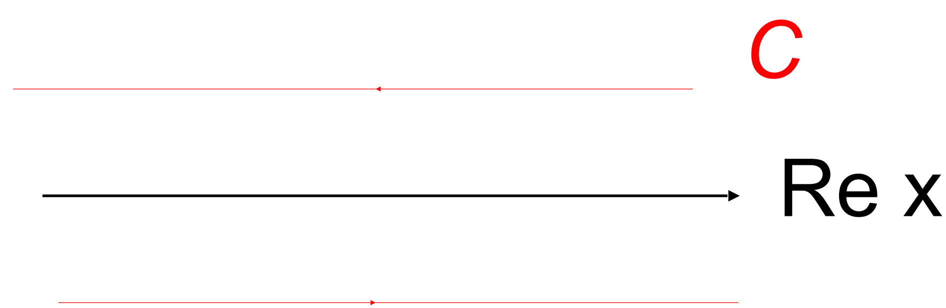
Thanks to the exact solvability of S=1/2 chain!

Maeda-Sakai-M.O. 2005

$$Y(T,H) = \frac{1}{2} - \frac{T}{2\pi J}\oint_C \ln(1+\eta(x+i))\,dx$$

$$\ln\eta(x) = \frac{2\pi J}{T}a_1(x) - \frac{H}{T} - \oint_C a_2(x-y-i)\ln(1+\eta(y+i))\,dy$$

$$a_n(x) = \frac{n}{\pi(x^2+n^2)}$$



g-shift

ESR frequency shift is often proportional to the applied field H (e.g. in Nagata-Tazuke)

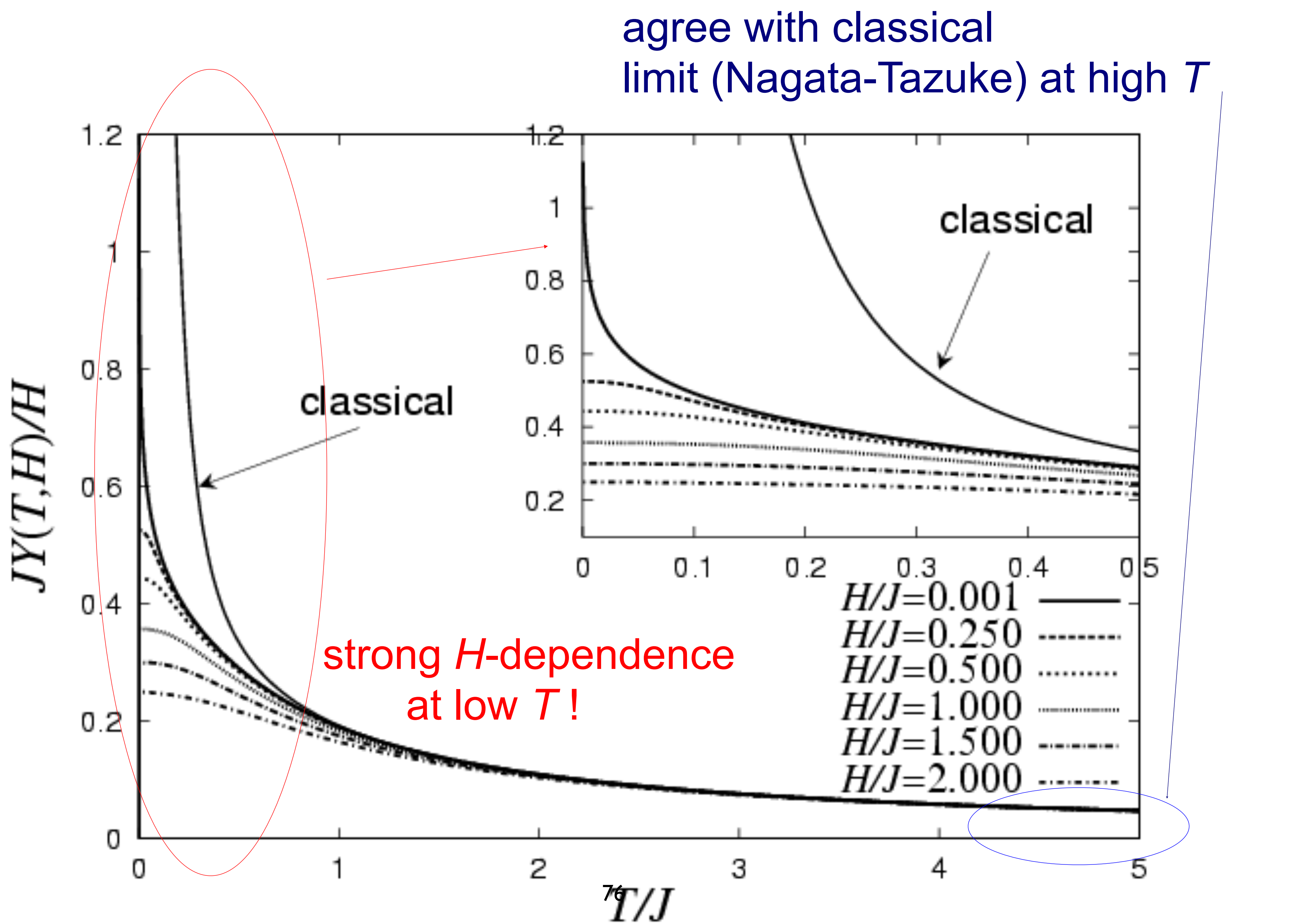
It is thus customary to discuss the shift in terms of effective *g*-factor

$$\hbar\omega = \mu_B g_{eff} H$$

"g shift"

$$\Delta g_{eff} = g_\infty \frac{\Delta\omega}{H}$$

Result...


agree with classical
limit (Nagata-Tazuke) at high T
classical
classical
strong H-dependence
at low T !
H/J=0.001
H/J=0.250
H/J=0.500
H/J=1.000
H/J=1.500
H/J=2.000
JY(T,H)/H
T/J

Comparison with experiments

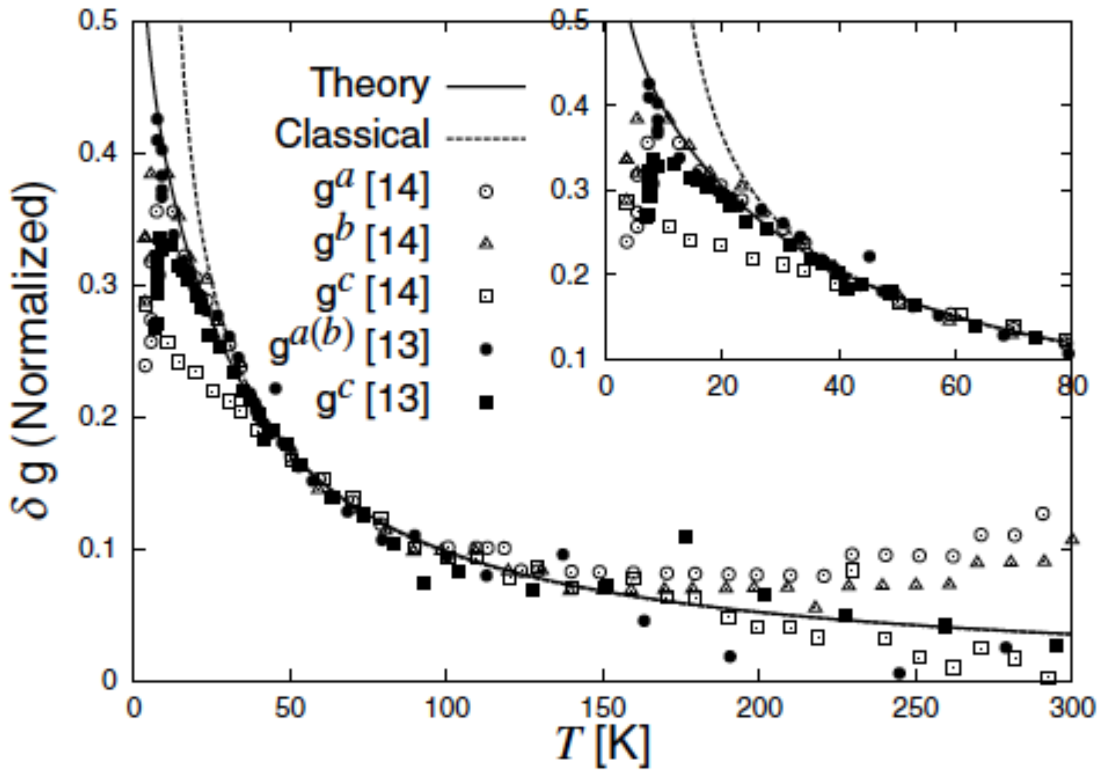
We want "pure" S=1/2 Heisenberg AF chain without the staggered field effect

$KCuF_3$, $CuGeO_3$, NaV_2O_5…..
(no significant *T*-dependence in shift?? (why?))

$LiCuVO_4$ another S=1/2 Heisenberg chain

Vasil'ev et al. (2001)
von Nidda et al. (2002)

ESR shift in $LiCuVO_4$



theory vs.
experiment

FIG. 3. Normalized effective g shift $\delta g/(g_\infty f) = (g_{\rm eff} - g_\infty)/(g_\infty f)$ where f is the direction-dependence factor (9) and is plotted against the temperature T. Points are experimental data for $LiCuVO_4$ [13,14], while the curve is the theoretical result (11) and the classical results (14). Inset: the behavior at low temperatures.

More complicated systems…

PHYSICAL REVIEW B **82**, 054431 (2010)

Anisotropy of magnetic interactions in the spin-ladder compound $(C_5H_{12}N)_2CuBr_4$

E. Čižmár,[1,2] M. Ozerov,[1] J. Wosnitza,[1] B. Thielemann,[3] K. W. Krämer,[4] Ch. Rüegg,[5] O. Piovesana,[6] M. Klanjšek,[7,8] M. Horvatić,[7] C. Berthier,[7] and S. A. Zvyagin[1]

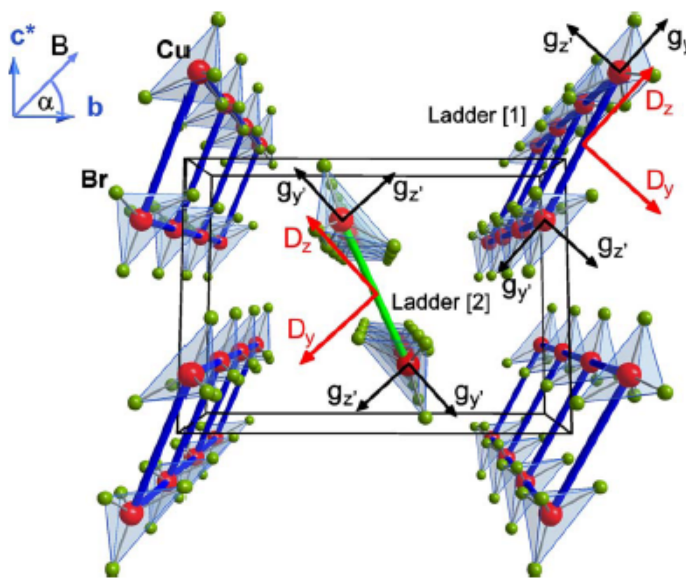


FIG. 1. (Color online) Schematic view of the crystal structure of BPCB along the *a* axis (Ref. 22). The ladders [1] and [2] are highlighted by thick blue and green lines, respectively. Black arrows define the directions of the principal axes of the *g* tensors while the red arrows define the vectors of the effective anisotropy (see text for details). Piperidinium groups are omitted for clarity.

BPCB: *S*=1/2 ladder system

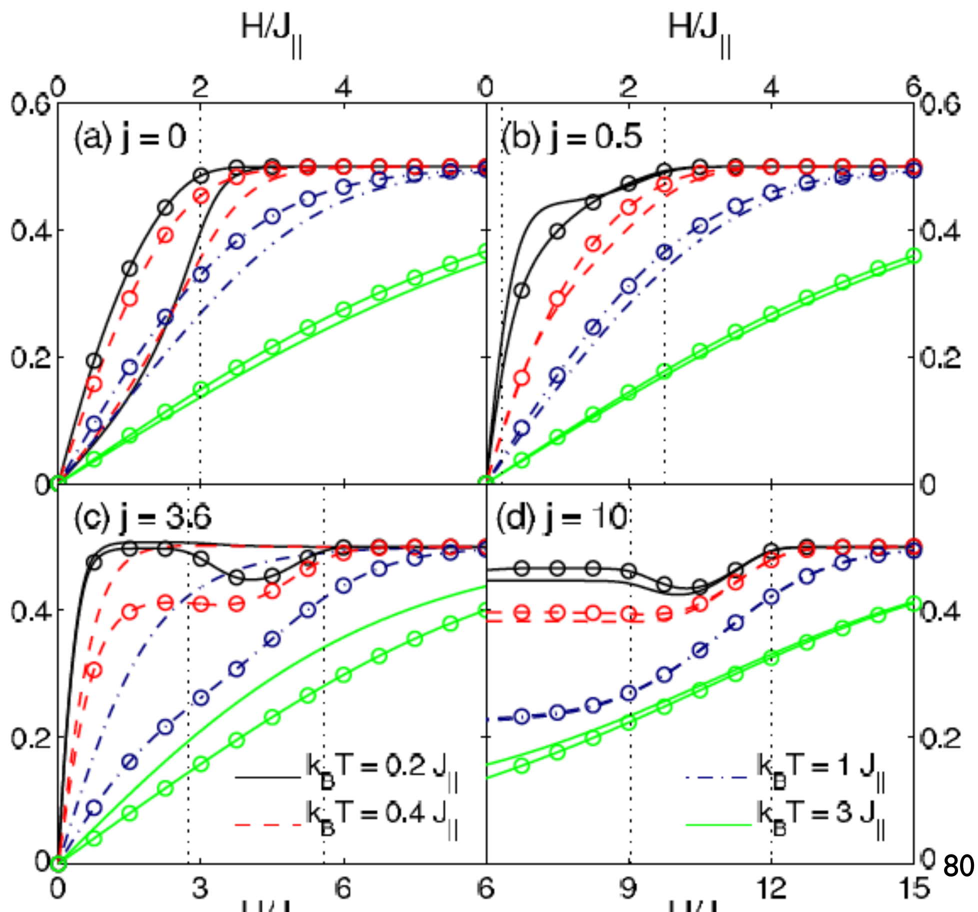
two different orientation
of ladders in the compound!

$$Y_{\parallel}(T,H) = \frac{\langle S^z_{i,1} S^z_{i+1,1} - S^x_{i,1} S^x_{i+1,1} \rangle_0}{\langle S^z_{i,1} \rangle_0},$$

ESR shift due to anisotropy along the legs

$$Y_{\perp}(T,H) = \frac{\langle S^z_{i,1} S^z_{i,2} - S^x_{i,1} S^x_{i,2} \rangle_0}{\langle S^z_{i,1} \rangle_0}.$$

ESR shift due to anisotropy along the rungs



Furuya-Bouillot-Kollath-M.O.-Giamarchi 2012

The spin ladder is not exactly solvable.

Nevertheless, they can be numerically evaluated very precisely with DMRG!

$$j = J_{\perp}/J_{\parallel}$$

Electron Spin Resonance Shift in Spin Ladder Compounds

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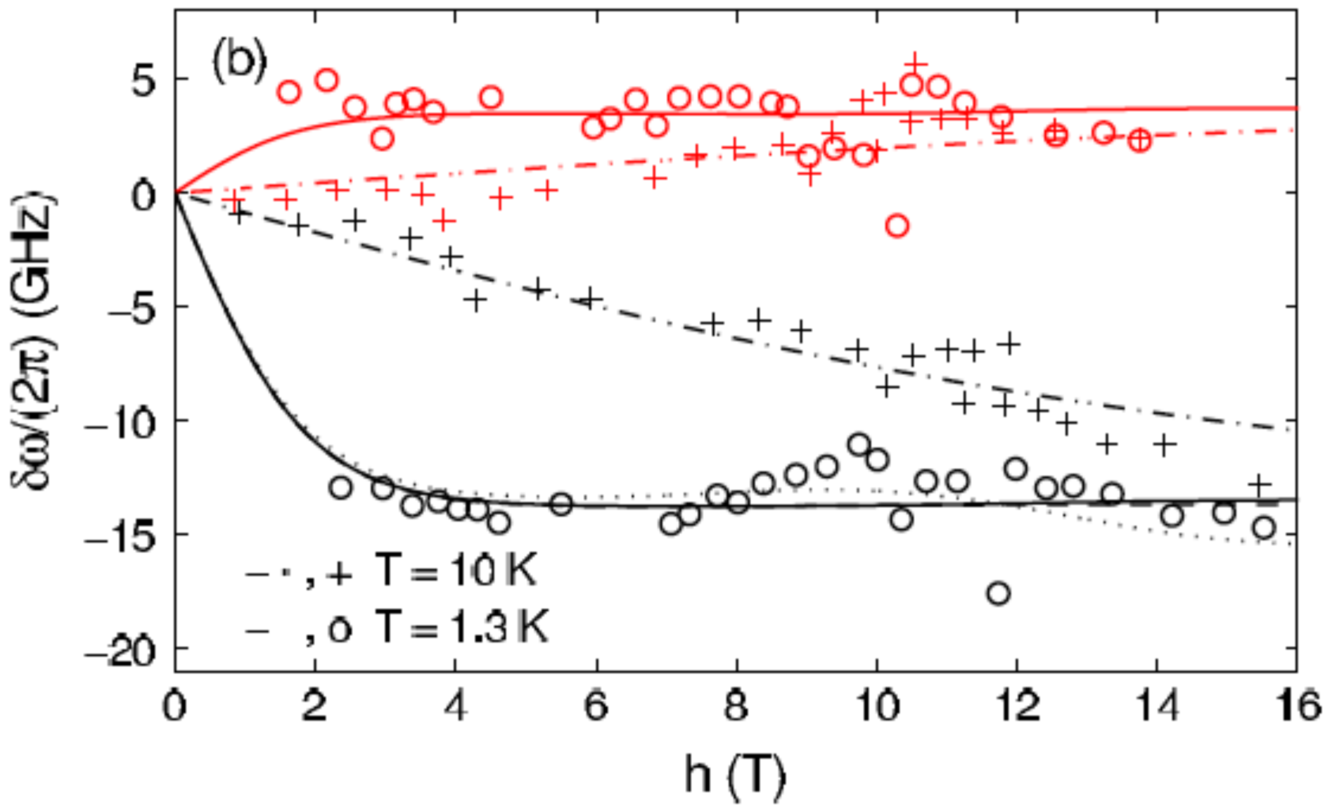


We can fit the ESR shift and its temperature- and field-dependences in the two differently oriented ladders at the same time!

Single-ion anisotropy

In S=1 systems, single-ion anisotropies

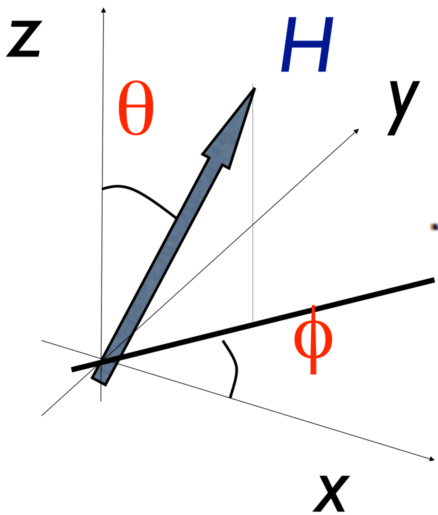
$$D(S_j^z)^2 + E\left[(S_j^x)^2 - (S_j^y)^2\right]$$

generally exist;

they can be written as

$$\mathcal{H}'_D = \sum_j \sum_\alpha D_\alpha (S_j^\alpha)^2$$

Factorization of the shift



$$\delta\omega = f_D(\theta,\phi) Y_D(T,H),$$

$$f_D(\theta,\phi) = D_z(1-3\cos^2\theta) + D_x(1-3\sin^2\theta\cos^2\phi) + D_y(1-3\sin^2\theta\sin^2\phi)$$

$$Y_D(T,H) = \frac{\sum_j \langle 2(S_j^z)^2 - (S_j^x)^2 - (S_j^y)^2\rangle_0}{2\langle S_\mathrm{T}^z\rangle_0}.$$

T- and *H*- dependence is contained

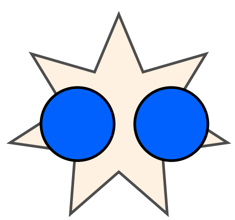
Theoretical Evaluation

$\left(S_j^\alpha\right)^2$ creates two magnons in the *S*=1 chain

In the low-temperature limit, the density of thermally excited magnons is very low. So, naively we expect that the magnons can be regarded as free particles.

However, the "free magnon" approximation does not work!

$\left(S_j^\alpha\right)^2$ creates/annihilates two magnons at the same point

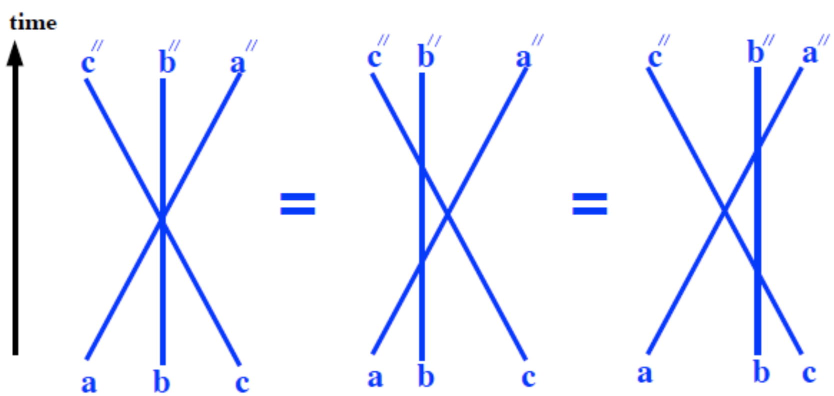


These magnons do interact, even if the average density is low!

Field Theory for S=1 Chain

In the low-energy limit, scatterings of magnons can be described by factorizable *S*-matrix (Zamolodchikov[2] 1979)

$$S_{a_1 a_2}^{a_3 a_4}(\theta) = \delta_{a_1 a_2}\delta_{a_3 a_4}\sigma_1(\theta) + \delta_{a_1 a_3}\delta_{a_2 a_4}\sigma_2(\theta) + \delta_{a_1 a_4}\delta_{a_2 a_3}\sigma_3(\theta)\,;$$



$$\sigma_1(\theta) = \frac{2\pi i\theta}{(\theta + i\pi)(\theta - i2\pi)}\,;$$

$$\sigma_2(\theta) = \frac{\theta(\theta - i\pi)}{(\theta + i\pi)(\theta - i2\pi)}\,;$$

$$\sigma_3(\theta) = \frac{2\pi i(i\pi - \theta)}{(\theta + i\pi)(\theta - i2\pi)}\,.$$

exactly solvable field theory
"O(3) Nonlinear Sigma Model"

Form Factors

$$f^{\mathcal{O}}_{a_1\cdots a_n}(\theta_1,\cdots,\theta_n) = \langle \mathcal{O}(0,0) A_{a_n}(\theta_n)\cdots A_{a_1}(\theta_1)\rangle.$$

Matrix elements with *n*-magnon states

Can be determined by consistency with the S-matrix, and a few additional axioms

$$F_{S^a}(\theta_1, a_1) = \sqrt{Z}\,\delta_{a,a_1},$$

1-magnon form factor of single spin operator (same as the free magnon approx.)

Explicit 2-Magnon Form Factor

Balog-Weisz 2007
Furuya-Suzuki-Takayoshi-Maeda-M.O. 2011, 2013

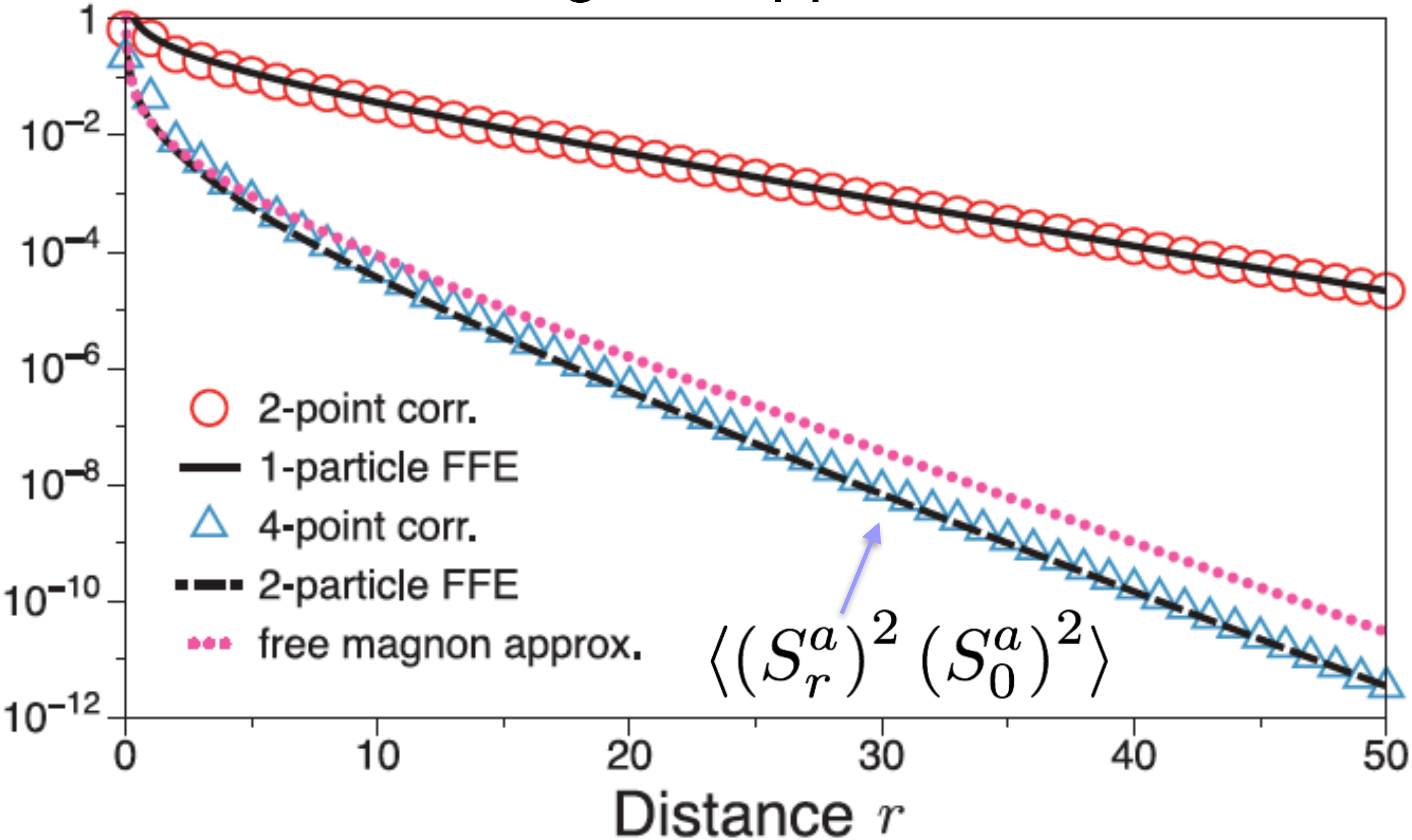
$$F_{(S^a)^2}(\theta_1, a_1; \theta_2, a_2) = -iZ_2\, \delta_{a_1,a_2}(3\delta_{a,a_1} - 1)\psi_2(\theta_1 - \theta_2).$$

$$\psi_2(\theta) = \sinh\frac{\theta}{2} \exp\left[\int_0^\infty \frac{d\omega}{\omega} e^{-\pi\omega} \frac{\cosh[(\pi + i\theta)\omega] - 1}{\sinh(\pi\omega)}\right].$$

$$= \frac{i}{2}(\theta - \pi i)\tanh\frac{\theta}{2}.$$

Nontrivial, reflecting the magnon-magnon interaction!

Exact 2-particle form factor fits the numerical result on $\langle (S_r^a)^2 (S_0^a)^2 \rangle$ correlation better than the free magnon approximation!



Form-factor approach

$$P_1 \sum_j [3(S_j^z)^2 - 2] P_1$$
$$= \int \frac{d\theta}{4\pi} \frac{3Z_2 v}{2\Delta_0 \cosh\theta} \Big[2|\theta,0\rangle\langle\theta,0| - |\theta,+\rangle\langle\theta,+| - |\theta,-\rangle\langle\theta,-| \Big].$$

Dilute magnon limit:

$$Y_D(T,H) = -\frac{3Z_2}{4}\tanh\left(\frac{H}{2T}\right) \frac{\int \frac{d\theta}{4\pi} \frac{v}{\Delta_0\cosh\theta} e^{-\Delta_0 \cosh\theta/T}}{\int \frac{d\theta}{4\pi} e^{-\Delta_0\cosh\theta/T}}.$$

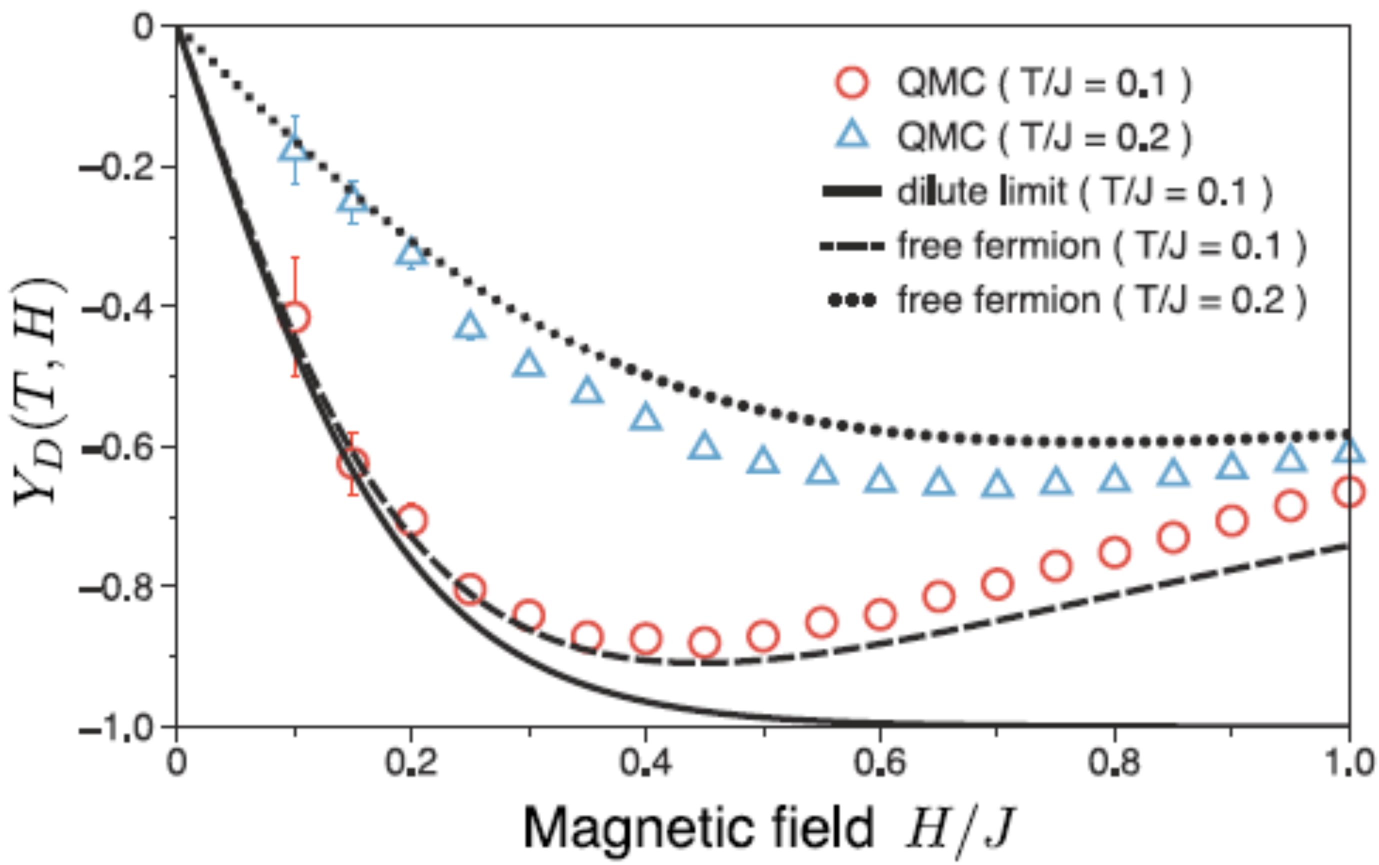
$Z_2 = 0.24.$ determined from the numerical result on the correlation function of $(S^z)^2$

Valid for low-*T* and low-*H*

On the other hand, Y_D can be numerically evaluated very precisely using Quantum Monte Carlo or DMRG

Comparison with numerics

The theory indeed works well at low-*T* and low-*H*, but breaks down at around the critical field *H*=0.41 *J*



Comparison w/ experiments

Furuya-Suzuki-Takayoshi-Maeda-M.O. 2011, 2013

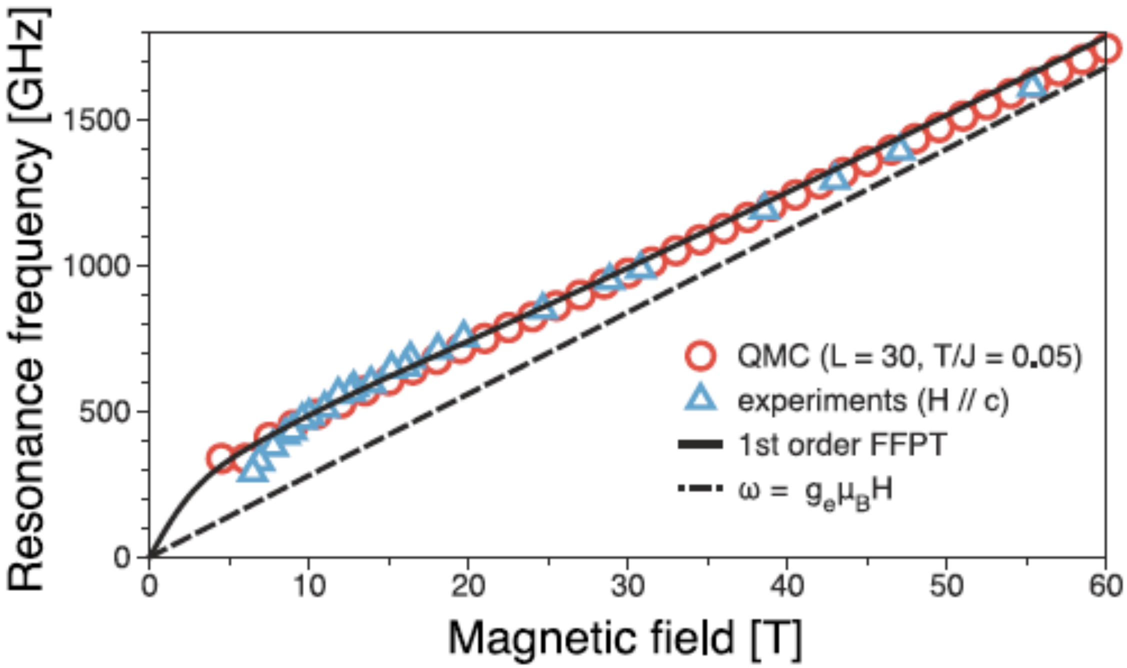


Figure 4. (color online) Comparison of the resonance frequency $\omega_r = g_e\mu_B H + \delta\omega$ by QMC (circles) with experimental data [28] (triangles). We performed QMC calculations with $L = 30$ sites. We used $D = 0.25J$ and $H \parallel c$ ($\Theta = \Phi = 0$). The solid curve is obtained from (19) and the dashed line represents the paramagnetic resonance $\omega = g_e\mu_B H$.

Kanamori-Tachiki Formula

$$\Delta\omega = -\frac{\langle [[\mathcal{H}', S^{+}], S^{-}] \rangle_0}{2\langle S^z \rangle_0} + O(\mathcal{H}'^2)$$

Gives the ESR shift in the 1st order of the anisotropy perturbation;

can be used for more complicated systems (frustrated etc.), as long as you can evaluate the static expectation value in the RHS

Conclusions

ESR provides challenging and fundamental problems in statistical physics

Plethora of experimental data,
yet to be understood

Numerical approaches: similar difficulties as in analytical ones, but will be more important

Many open problems = exciting opportunities?!