Dynamics of 1D Quantum Magnets: High Field Fractionalization, BEC, and Transport

Wolfram Brenig

S. Grossjohann, WB, Phys. Rev. B 79, 094409 (2009)
H. Kühne, WB, et al., Phys. Rev. B 80, 045110 (2009)

Acknowledgements

Theory:

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H. Kühne	Dresden
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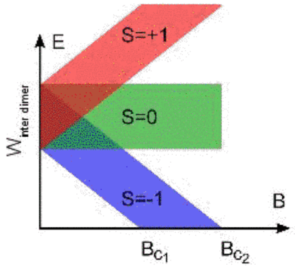
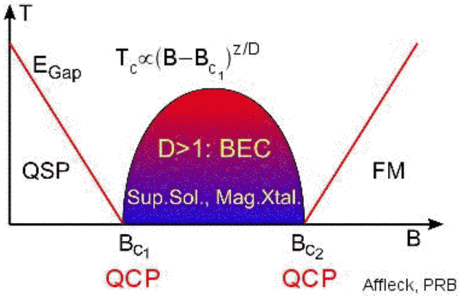
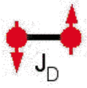
Field Induced BEC in Quantum Spin Systems



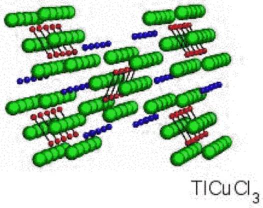


Affleck, PRB (90,91)
Sorensen, et al. PRL (93)
Giamarchi, et al., PRB (99)

S=1/2



AFM
Dimers



- D~3 S=1/2 dimer-systems $TlCuCl_3$
  Oosawa, et al., J.Phys., (99)
  Nikuni, et al., PRL (00)
  Ruegg, et al., Nature (03)
- D~2 S=1/2 dimer-systems $BaCuSi_2O_6$
  Sebastian, et al., Nature (06)

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Festkörpertheorie

Mapping

Giamarchi, et al. PRB (99)
Nikuni, et al. PRL (00)

- Bose liquids

$$H_{S^z=1}=\sum_l (J_D - g\mu_B B) b_l^+ b_l + \sum_{lm} t_{lm} b_l^+ b_m + \sum_{lm} U_{lm}^{HC} b_l^+ b_m^+ b_m b_l$$

$\longleftrightarrow$

- Quantum magnets

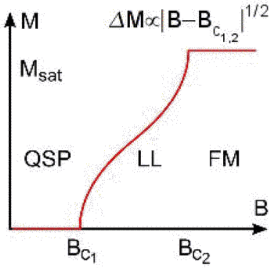
$$H=\sum_l J_D \vec{S}_{l1}\cdot\vec{S}_{l2} - \sum_l g\mu_B B S_l^z + \sum_{lm,ij} \vec{S}_{li}\cdot\vec{S}_{mj}$$

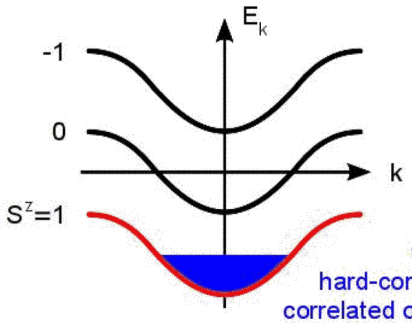
bosons:	n	μ	U(1)	$\langle\psi\rangle$	ρ_S	$\partial n/\partial\mu=\infty$
triplets:	$\langle S^z\rangle$	B	$O(2)_{\perp B}$	$\langle S^\pm\rangle$	$\langle S^\pm S^\mp\rangle$	$\partial\langle S^z\rangle/\partial B=\infty$

cold atoms:	μ-canonical	U(1) exact	low-T_c~nK (low dens., heavy)
quant. mag.:	canonical	O(2) ?	high-T_c~10...300K (high dens., light)

Demokritov, et al. Nature 443, (06)

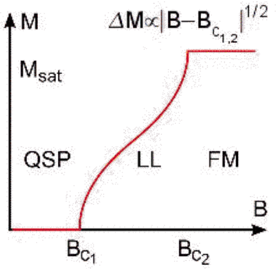
One Dimension

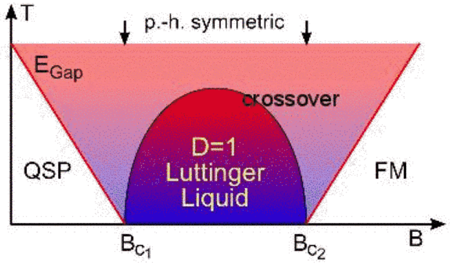




1D:
hard-core bosons =
correlated σ-less fermions

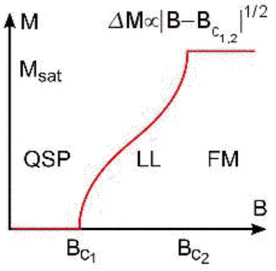
One Dimension

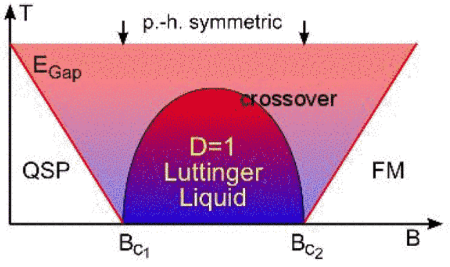




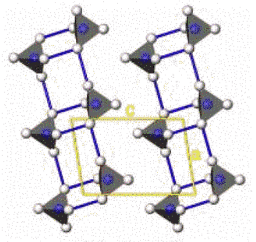
- BEC → fractionalization

One Dimension





- BEC → fractionalization



$(C_5H_{12}N)_2CuBr_4$

- S=1/2 ladders $(C_5H_{12}N)_2CuBr_4$

  Watson, et al., PRL (01)
  Lorenz, et al., PRL (08); Rüegg, et al. PRL (08) & (09)

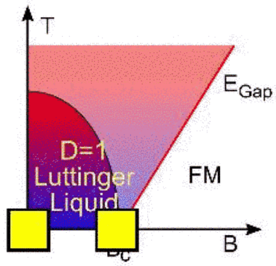
- S=1/2 chains $Cu(C_4H_4N_2)(NO_3)_2$

  Stone, et al., PRL (03)

- S=1 chains $Ni(C_5H_{14}N_2)_2N_3(PF_6)$, $NiCl_2$-$4SC(NH_2)_2$

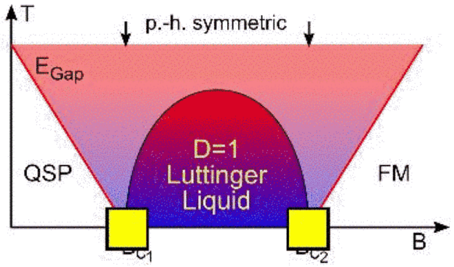
  Honda, et al., PRL (98);
  Zapf, et al., PRL (06); Zvyagin, et al., PRL (07)

Outline



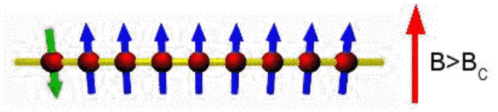
- Field induced critical dynamics of S-1/2 chain
- Transport and spin diffusion in in Spin-1/2 chain

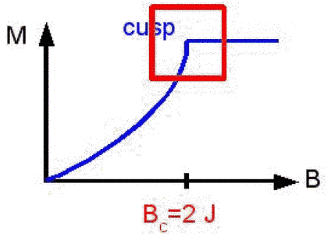
Outline



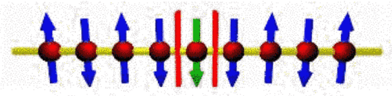
- Field induced critical dynamics of S-1/2 chain
- Transport and spin diffusion in in Spin-1/2 chain
- Fractionalization in S-1 chains

Fractionalization of Ising-Bosons

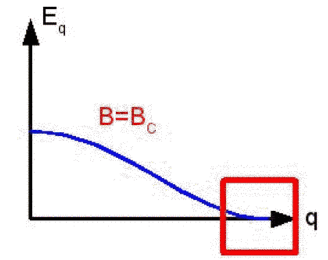




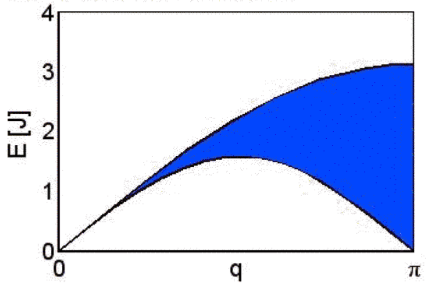
$H=J\sum_{mn}\vec{S}_m\vec{S}_n\ ,\ J>0$



- One boson mode



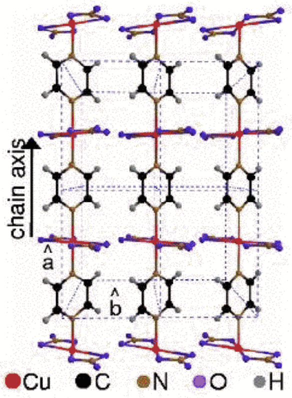
- Two fermion continuum



Copper Pyrazine Dinitrate $Cu(C_4H_4N_2)(NO_3)_2$

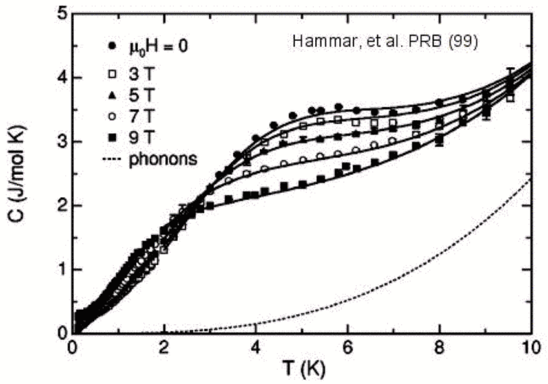
- CuPzN: AFM S=1/2 chain

Losee et al., J. Chem. Phys. (73)



- Thermodynamics

$$H=\sum_{ij} J_{a,ij} \mathbf{S}_i \mathbf{S}_j + J_{r,ij} \mathbf{S}_i \mathbf{S}_j$$



$J/k_B \simeq 10.6K$

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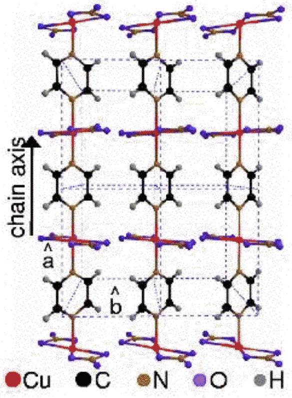

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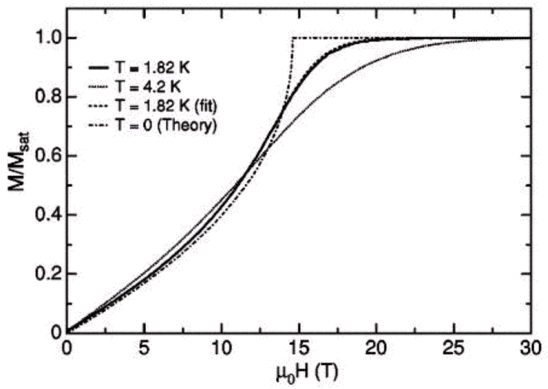

- Saturation B_c=14.5 T accesible

$J/k_B \simeq 10.6K$

Copper Pyrazine Dinitrate $Cu(C_4H_4N_2)(NO_3)_2$

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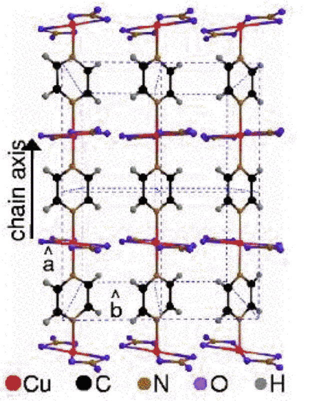

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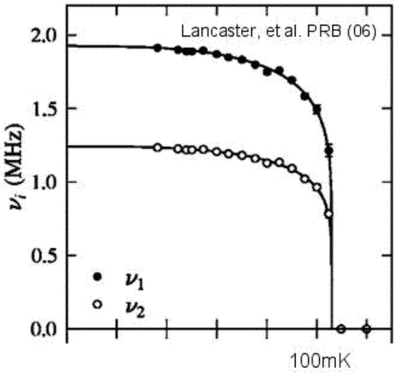


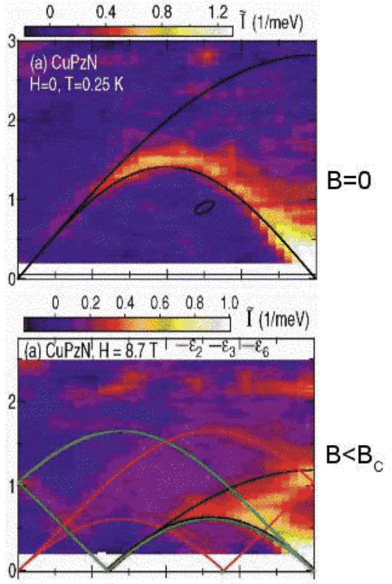
- Saturation B_c=14.5 T accesible

$J/k_B \simeq 10.6\,K$ $|J_{inter}/J_{intra}| \sim 10^{-3}$ $T_N \simeq 0.11\,K$

Copper Pyrazine Dinitrate Spin Dynamics

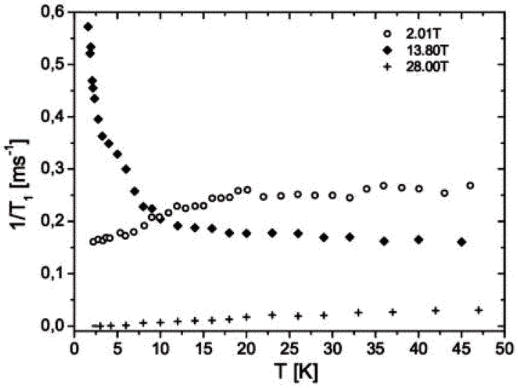
- INS

Stone, et al. PRL (03)



- NMR

H. Kühne, WB, et al., PRB 80, 045110 (2009)



fields $0<B<2B_c$

temperatures $0.25\,J<T<5\,J$

- Dynamical structure factor

$$S^{\alpha\beta}(q,\omega)=\int_{-\infty}^{\infty} e^{i\omega t}\langle S_q^{\alpha}(t)S_{-q}^{\beta}\rangle dt$$

for spin-1/2 chain in B-field

$$H=J\sum_l\left[S_l^z S_{l+1}^z+\Delta\left(S_l^x S_{l+1}^x+S_l^y S_{l+1}^y\right)-BS_l^z\right]$$

at finite T and B

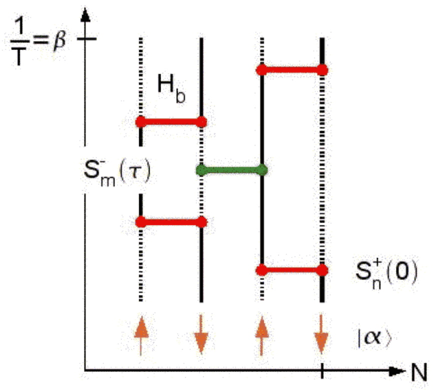
➢ Bethe (n-spinon)	$S^{zz(xx)}(q,\omega)$, $B\neq 0$, $T=0$
➢ Bosonization	$q\ll 1/a$
➢ ED	$N\leqslant 22...28$
➢ T(D)MRG	$S_{00}^{zz}(t)$, $t<\sim 1/J$ or $T=0$
➢ QMC	$S^{zz(xx)}(q,\omega)$, $T,B\neq 0$

Quantum-Monte-Carlo

Sandvik, PRB 59, (99)

- Expand partition function

$$Z=\mathrm{Tr}\exp(-H/T)$$
$$=\sum_{n,b}\mathrm{Tr}[-H_b^n/n!T^n]$$



- Typ.: $N\leq 10^{5...}$, $\beta\leq 1000/J$

- Spin dynamics

$$S_{mn}(\tau)=\langle S_m^-(\tau)S_n^+(0)\rangle$$

Temperature exp(−H/T)

Time exp(−itH)

Frequency ω

$$S_{mn}(\tau)=\int d\omega K(\tau,\omega)S_{mn}(\omega)$$

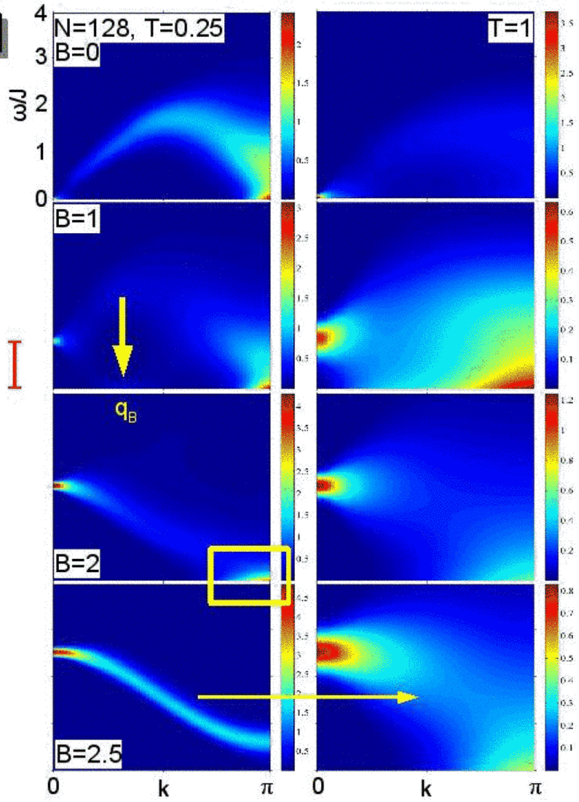
Maximum Entropy Methods

- Typ.: $N\leq 10^{2...3}$, $\beta\leq 10...50/J$

Transverse Dynamical Structure Factor

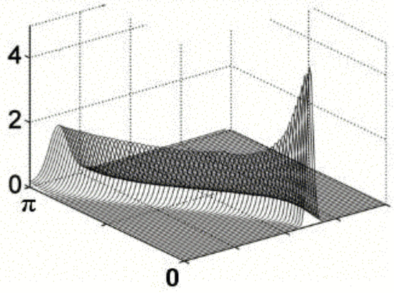
$\langle S^x_q S^x_{-q} \rangle(\omega)$

- B=0: continuum
  $B>B_C$: sharp mode
- q~0, B≠0: gap
- B≠0, $q=q_B$: zone folded zero-mode
- $B=B_C$: critical dynamics
- T ↑: smearing



Thermal Population of Multimagnon States

- Momentum dependence of spectral weight
- 2-magnon contribution

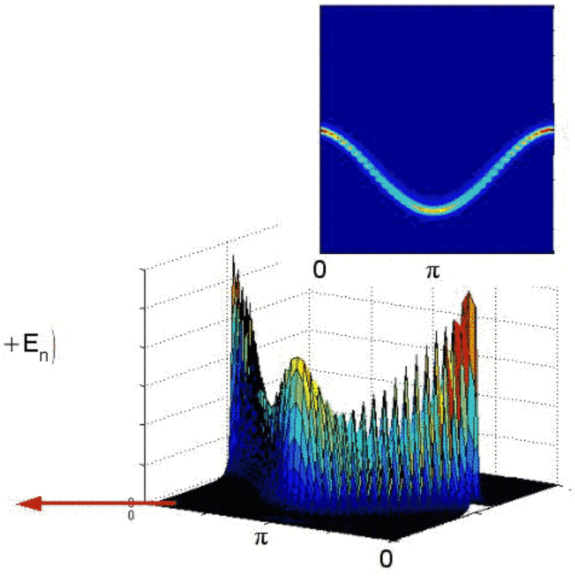


$$S^{xx}(q,\omega)=\sum_{mn}\frac{e^{-\beta E_m}}{Z}\left|\langle m|S^x_q|n\rangle\right|^2\delta(\omega-E_m+E_n)$$

$=1\ \times$ n=1-mag. sector

$+e^{-\beta\Delta_B}\times$ n=2-mag. sector

$+e^{-2\beta\Delta_B}\times\dots$



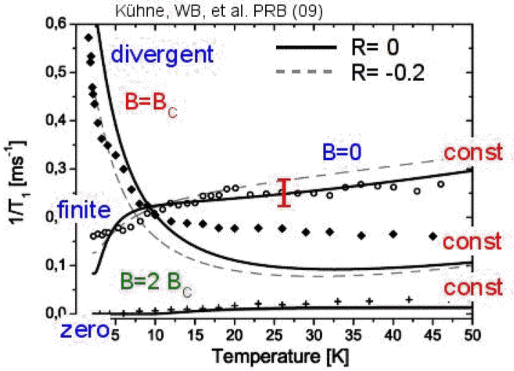
Nuclear Magnetic Resonance: Critical Dynamics

- T_1-relaxation

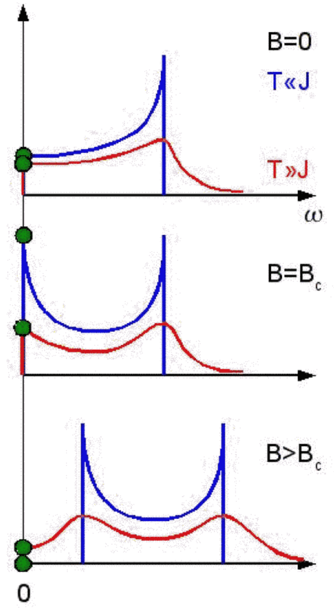
$$\frac{1}{T_1} = 2\sum_q |A(q)|^2 S^{\pm}(q,\omega)\Big|_{\omega\to 0}$$
$$= \left\langle S_0^+(\tau) S_0^-\right\rangle\Big|_{(\tau\to\omega,\ \omega\to 0)}$$

~contact

- Expm. vs. QMC



- Spin-DOS vs. B & T



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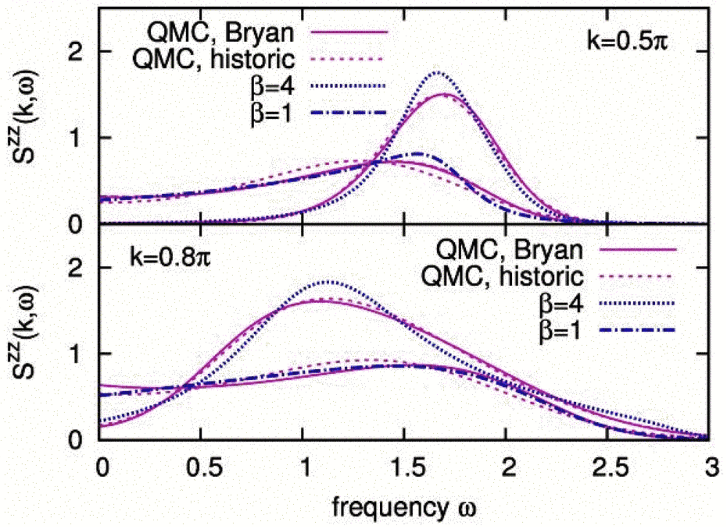
Comparing QMC and t-T-DMRG



QMC
Grossjohann, Brenig
PRB 79, 094409 (09)

t-T-DMRG
Barthel,Schollwöck, White
PRB 79, 245101 (09)

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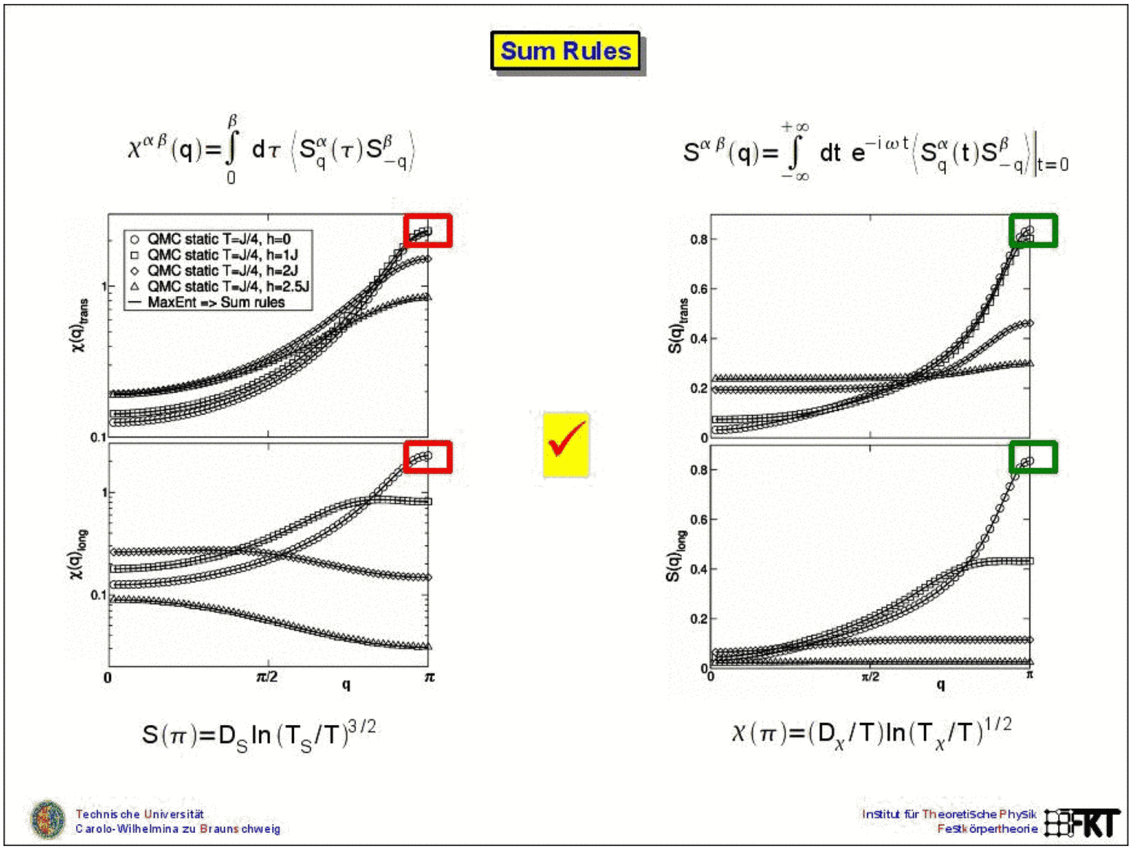

Sum Rules

$$\chi^{\alpha\beta}(q)=\int_0^\beta d\tau \left\langle S_q^\alpha(\tau)S_{-q}^\beta\right\rangle$$

$$S^{\alpha\beta}(q)=\int_{-\infty}^{+\infty} dt\ e^{-i\omega t}\left\langle S_q^\alpha(t)S_{-q}^\beta\right\rangle\Big|_{t=0}$$

$$S(\pi)=D_S \ln(T_S/T)^{3/2}$$

$$\chi(\pi)=(D_\chi/T)\ln(T_\chi/T)^{1/2}$$

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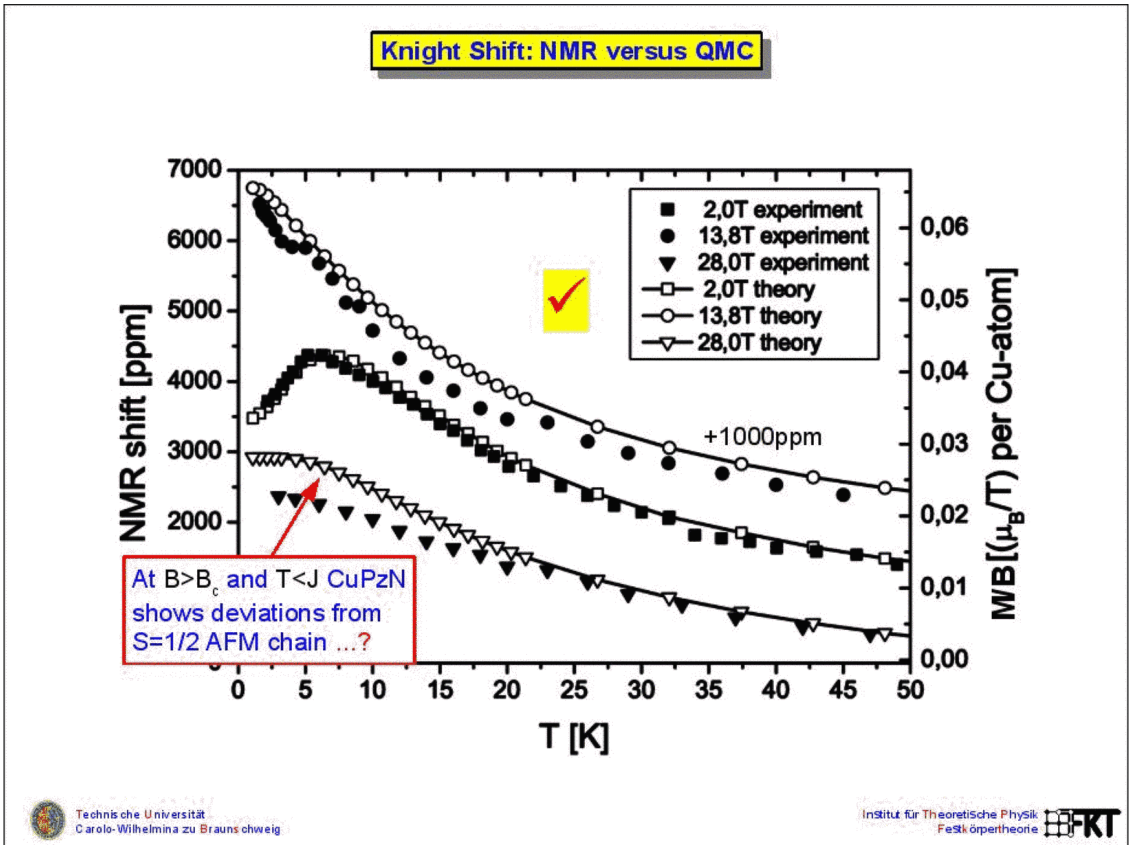

Knight Shift: NMR versus QMC

At $B>B_c$ and T<J CuPzN shows deviations from S=1/2 AFM chain ...?

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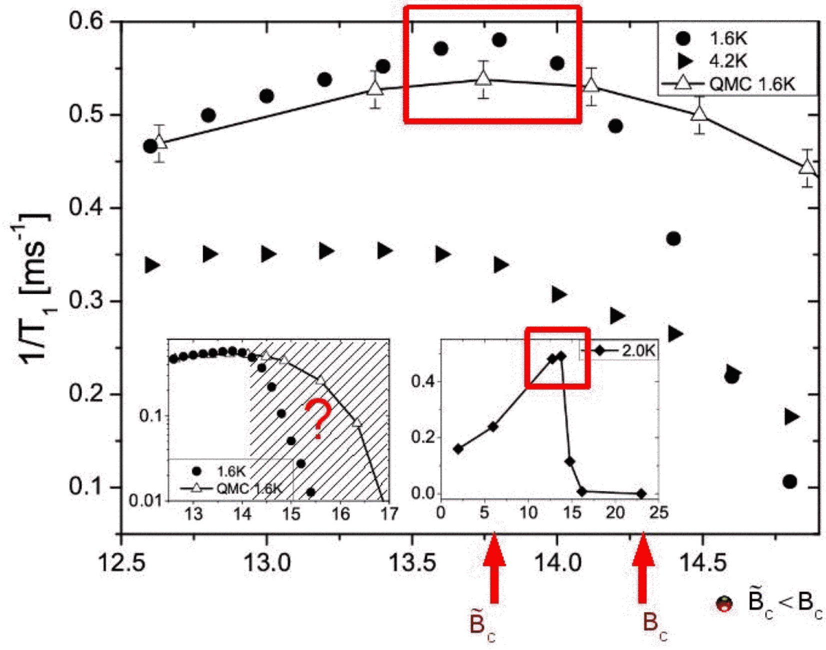
Scanning the B-Field

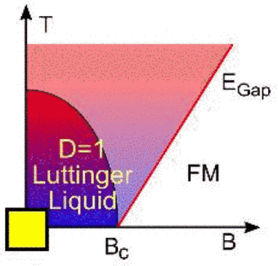
- Pronounced low-T maximum



- NMR rate drops 'too fast' between B_c and ~28T ?

  field induced gap ?

- $\tilde{B}_c < B_c$ = finite-T effect ✓



- Field induced critical dynamics of S-1/2 chain
- Transport and spin diffusion in in Spin-1/2 chain
- Fractionalization in S-1 chains

Conductivity

- spin current

$$\vec{j}_s(q) \sim J \sum_{\langle lm \rangle} e^{iq} \vec{S}_l \times \vec{S}_m$$

↔ conductivity of strongly interacting spinless particles

$$H = J\sum_l [-\tfrac{1}{2}(c^+_{l+1} c_l + h.c.) + \Delta(n_l n_{l+1} - n_l + \tfrac{1}{4})] - B\sum_l n_l$$

$$\Delta = J_\perp / J$$

$$n_l - \tfrac{1}{2} = S^z_l$$

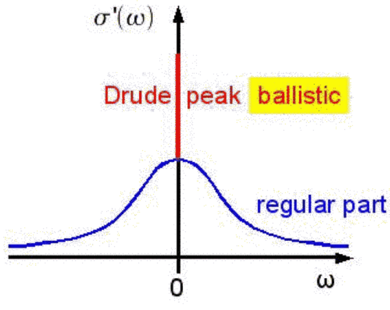
$$e^{i\pi\phi_l} c^+_l = S^+_l$$

Jordan-Wigner

- Optical conductivity

$$\sigma'(\omega) = D\delta(\omega) + \chi_{jj}''(\omega)/\omega$$

Drude regular



- regular ↔ longitudinal structure factor

$$\frac{1}{\omega}\chi_{jj}''(\omega) = \lim_{q\to 0} \frac{\omega}{q^2} \chi_{zz}''(q,\omega)$$

Transport Coefficients: Drude Weight

- transport coefficient

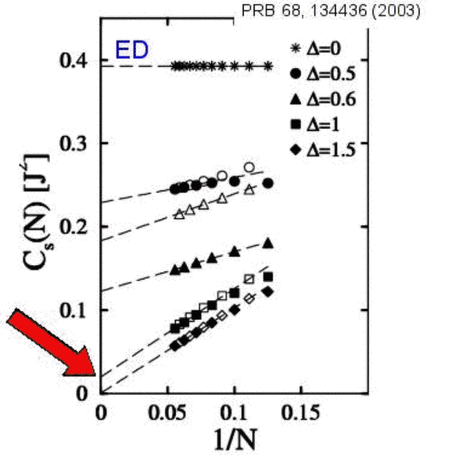
Drude

$$D \sim \frac{1}{ZT} \sum_{E_m = E_n} e^{-E_n/T} |\langle m|j|n\rangle|^2$$

regular

$$\frac{\chi_{jj}''(\omega)}{\omega} \sim \frac{s(\omega)}{ZT} \sum_{E_m \neq E_n} [e^{-E_n/T} \times |\langle m|j|n\rangle|^2 \delta(\omega - \Delta E)]$$

- D: high-T residue [j,H]≠0 !

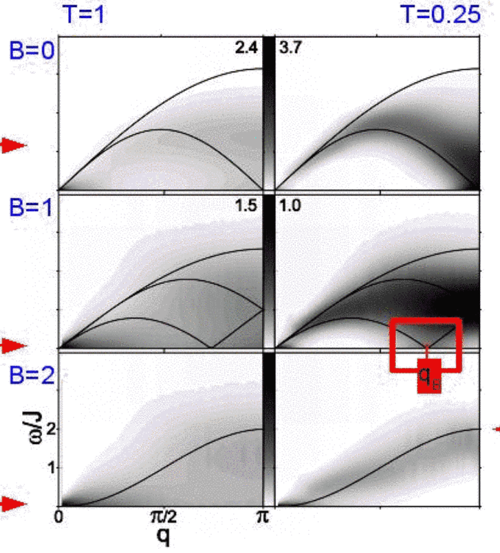


Heidrich-Meisner, WB, et al. PRB 68, 134436 (2003)

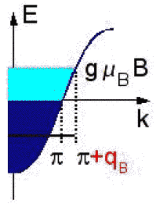
T=0, |Δ|<1 → D≠0 Shastry, Sutherland PRL (90)
T≠0, " BA: D(T)=?
T≠0, |Δ|=1 BA: D=? Lan, Shi-Jian, Chin.PL (07); Benz, et al. EPJ (06); Zotos, PRL 82, 1764 (99)
ED: D≠0 Alvarez, Gros PRL (02), Heidrich-Meisner, WB; et al. PRB (03), Mukerjee, Shastry PRB (08), ...
tDMRG " S. Langer, et al. PRB (09)
MEQN " Michel, et al. PRB (08), Prosen, et al. J.StatM (09)

Longitudinal Dynamical Structure Factor

$\langle S^z_q S^z_{-q} \rangle(\omega)$



- spinon continuum
- $\langle S^z_0 S^z_0 \rangle(\omega)$ removed
- q=q_B: folded zero mode

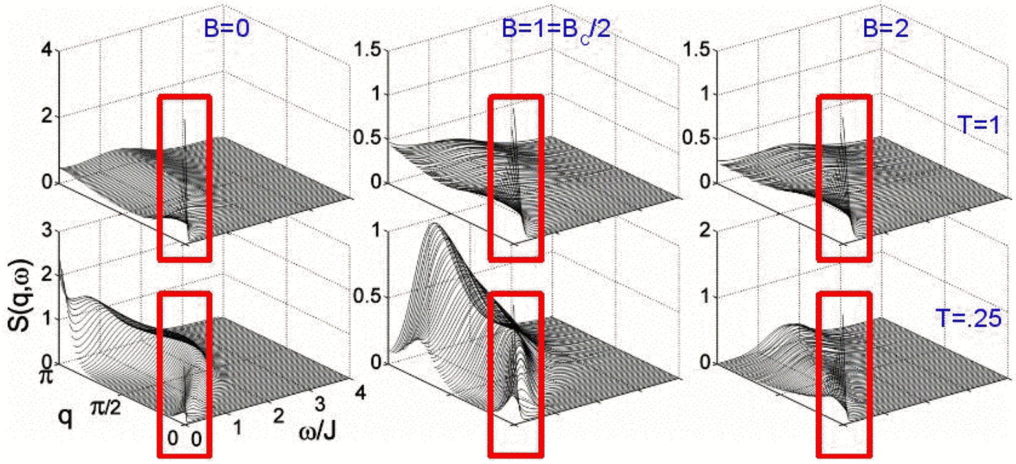


- zone boundary gap

T smears

Longitudinal Dynamical Structure Factor

Diffusion ?



Spin Diffusion and Susceptibility

- Bosonization, 1st irrelevant perturbs umklapp & curvature, $|\omega \pm vq| \ll T$

Sirker, Pereira, Affleck
arXiv:0906.1978v1

$$\chi(q,\omega) \approx \frac{Kvq^2/2\pi}{\underset{\uparrow}{(1+b)}\omega^2 - \underset{\uparrow}{(1+c)}v^2q^2 + i\underset{\uparrow}{\pi g^2}T\omega}$$

$O(g^2)$ $g+\ln(g)/2 \sim \ln(J/T)$

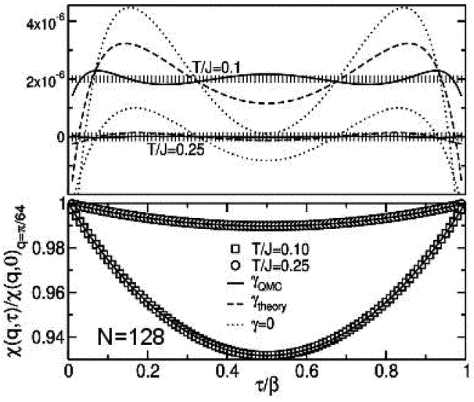
Lukyanov, NucPB
522, 533 (1998)

diffusive for $\omega \ll v^2q^2$

$$\Gamma = (1+c)v^2/(\pi g^2 T)$$

- Compare to QMC

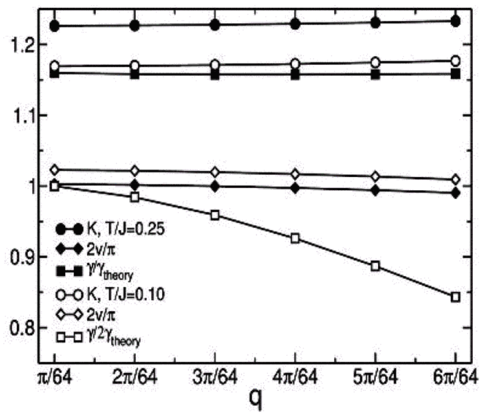
$$\chi(q,\tau) = T\sum_n e^{i\omega_n\tau}\chi(q,\omega_n)$$



$\pi g^2 T[J]$

T[J]	QFT	DMRG	QMC
0.1	0.0096		0.0191
0.2	0.0297	0.0190	
0.25	0.0440		0.0507

- momentum dependence

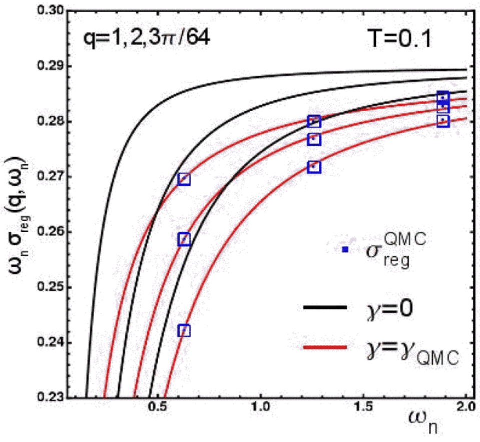


K/v consistent with χ(T) from BA ✓

v~π/2, decreasing ✓

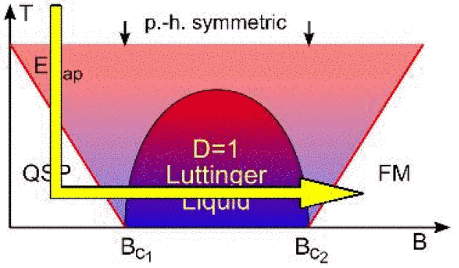
$\gamma=\gamma(q) \rightarrow \Gamma=\Gamma(q) \leftrightarrow$ diff. to DMRG ?

- ...regular optical conductivity



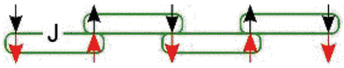
compare QMC $\rightarrow \sigma_{reg}^{QMC}(q,\omega_n)$ with

$$\sigma_{reg}(q,\omega_n) = \frac{\omega_n(Kv)/(2\pi)}{(1+b)\omega_n^2 + (1+c)v^2q^2 + 2\gamma|\omega_n|}$$



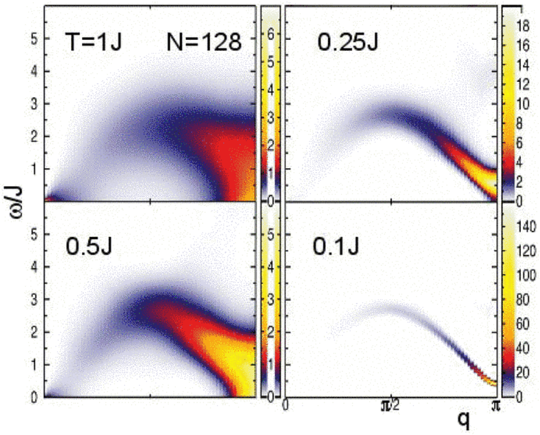
- Field induced critical dynamics of S-1/2 chain
- Transport and spin diffusion in in Spin-1/2 chain
- **Fractionalization in S-1 chains**

Cooling down at B=0

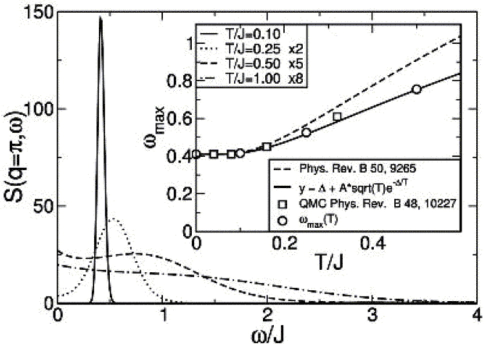


AKLT

- Transverse dynamic structure factor



- T-dependence of S(q,ω)-max



- Haldane gap Δ_0~ 0.41J
- Two-pt. continuum $q<\pi/3$
- consistent with INS Stone, et al. Nature (06)

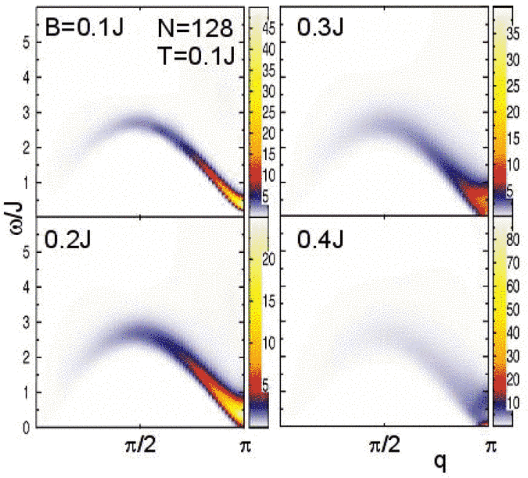
- consistent with NLσ-model Jolicoeur, et al. PRB (94).

$$\Delta(T)\approx\Delta_0+\sqrt{2\pi\Delta_0 T}e^{-\Delta_0/T}$$

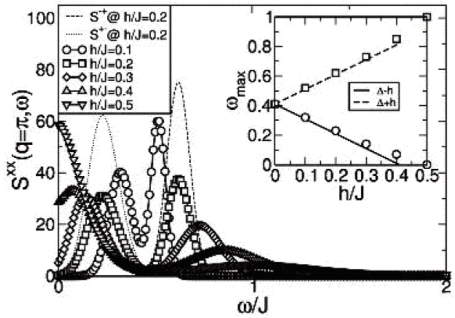
and B=0 QMC Deiz, et al. PRB (93)

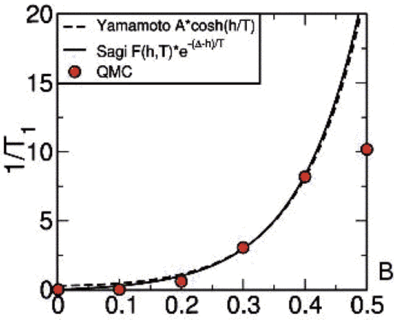
Finite Magnetic Fields $B < B_{c1} \approx 0.41J$

- Transverse dynamical structure factor



- gap closure at B/J=Δ

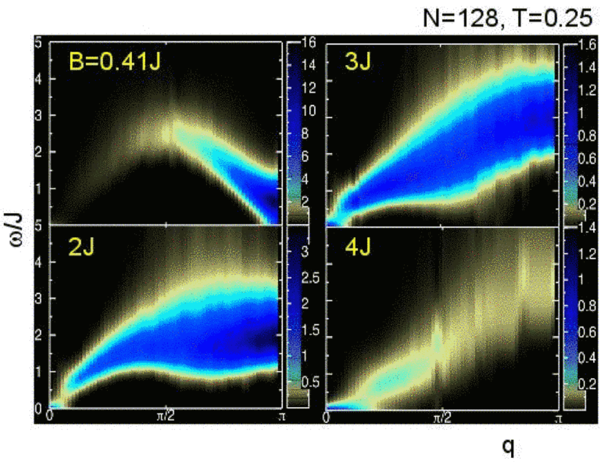


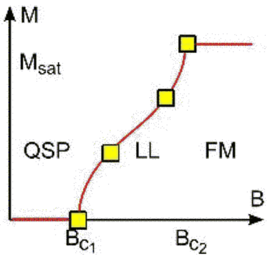


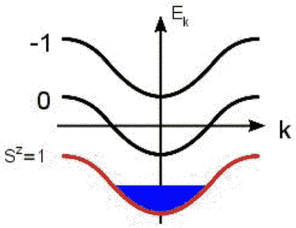
- NMR rate

$B_{c1} \approx 0.41J < B < B_{c2} = 4J$ … Fractionalization …?

- Longitudinal dynamic structure factor







- broad continua ✓
- incommensurate modes ?
- low intensity

Conclusion

- Evidence for field-induced critical dynamics of the AFHC material CuPzN due to triplet fractionalization.
- Regular part of spin conductivity is consistent with hydrodynamic limit with relaxation rate << T.
- First QMC results for the field induced fractionalization in the Haldane chain.