Title: Quantum Critical Dynamics in Two Quantum Magnets

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Abstract: <p>Quantum phase transitions arise at zero temperature when ground state energy meets non-analyticity upon tuning a non-thermal parameter.</p>

<p>Physical properties around quantum critical points (QCPs) are of extensive current interests because the fierce competition between critical quantum and thermal fluctuations near the QCPs can strongly affect dynamics and thermodynamics, leading to unconventional physics.</p>

<p>Despite of its great interests, however, it remains challenge to analytically understand such real frequency dynamics in strongly-correlated quantum systems, even for the dynamics in the quantum systems of one spatial dimension.</p>

<p> </p>

<p>In the talk, motivated by recent experimental progresses, we shall take the challenge via analytically exploring finite temperature dynamics at the QCP of 3(space)+1(time) quantum Ï†^4 model, and zero-temperature spin dynamics in the quantum critical regime of XXZ Heisenberg model.</p>

<p> </p>

<p>During the exciting excursion, sophisticated but powerful theoretical tools were introduced, and a bunch of new physics beyond conventional pictures were discovered. At the end we shall also discuss the implication of our results for experiments in relevant materials and suggest proper future experimental setups to test our theoretical findings.</p>

Quantum Critical Dynamics in Quantum Magnets

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11/25/2016@Perimeter Institute

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Outline

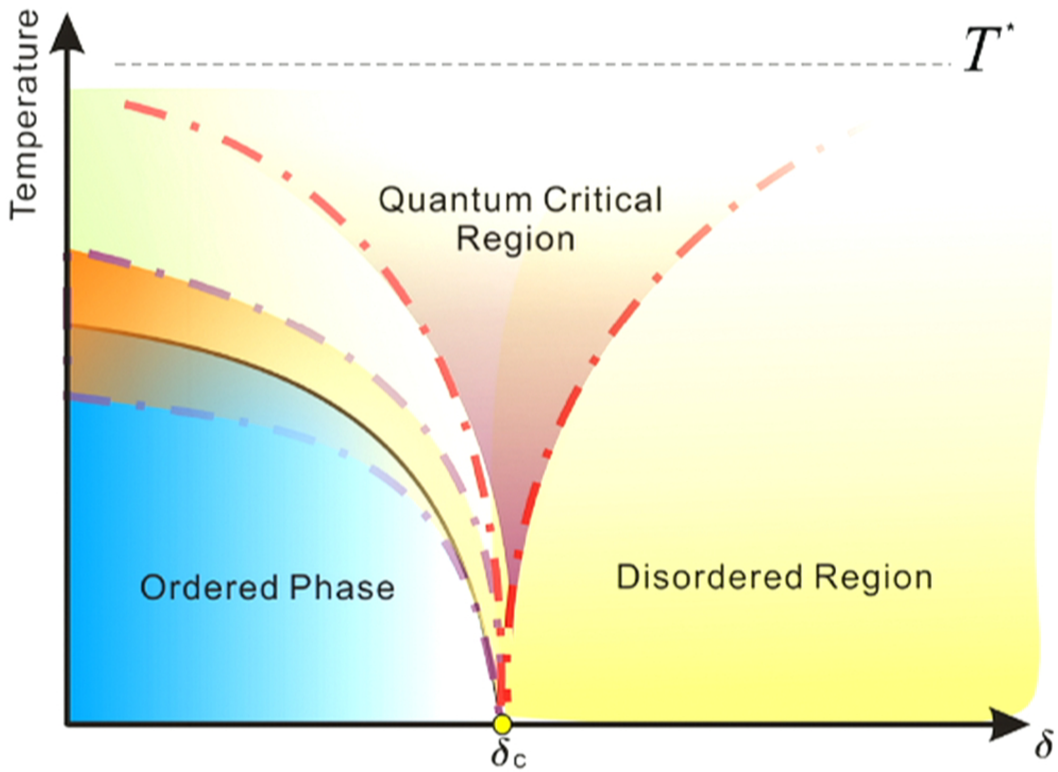
I. Introduction

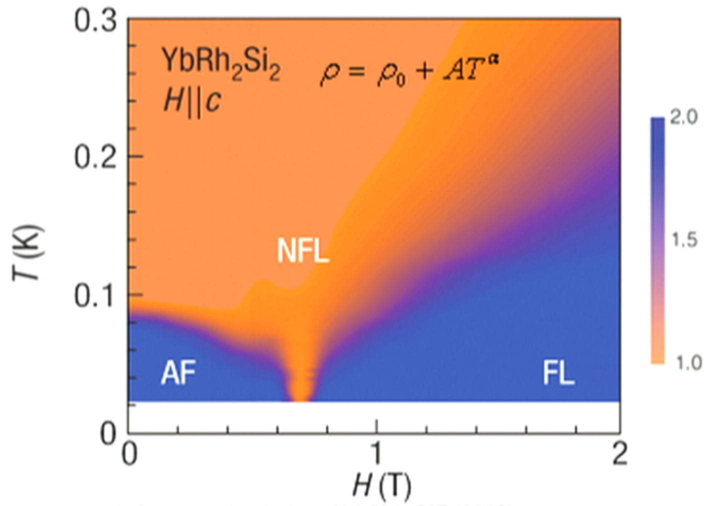
II. Critical marginal dynamics in a model for quantum insulator

III. Spin dynamics in XXZ chain with an external field

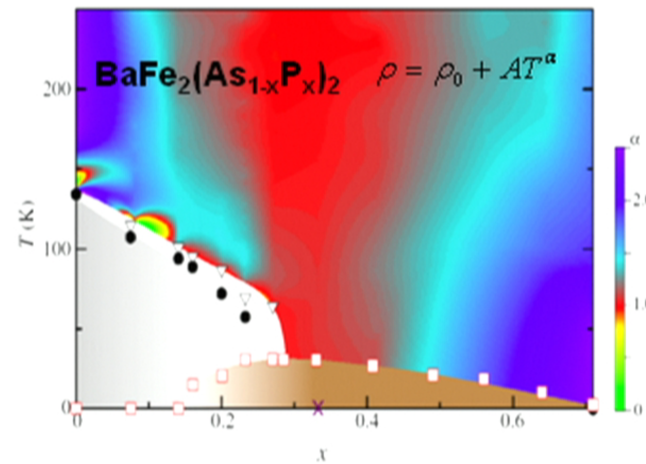
IV. Outlook

A typical phase diagram for quantum phase transition

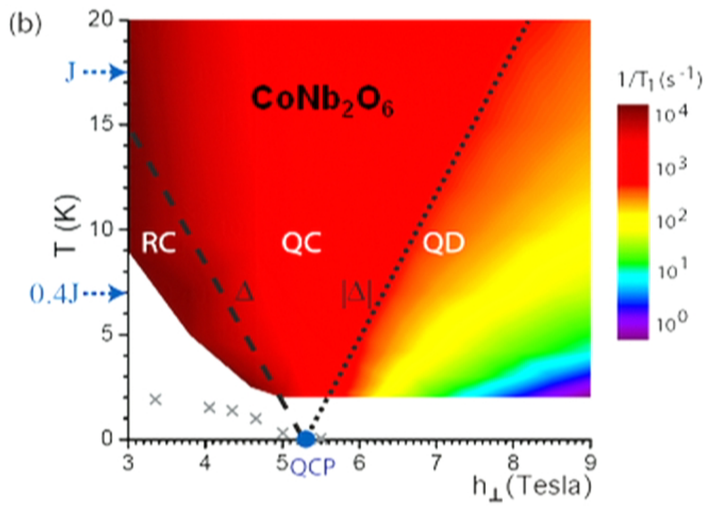




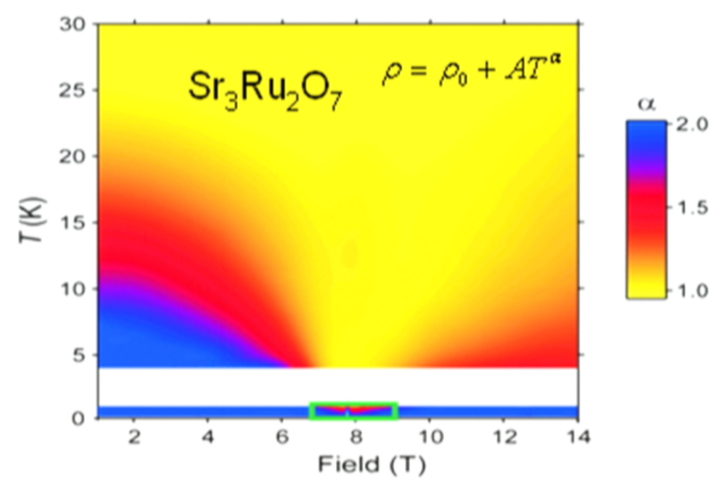
J. Custers, etc. *Nature* **424**,524–527 (2003).
P. Gegenwart, Q. Si and F. Steglich, Nat. Phys. 4, 186 (2008)



Y. Nakai, etc. Phys. Rev. Lett, 105, 107003(2010)
K. Hashimoto etc. *Science* 336, 1554 (2012)



A. W. Kinross, etc. Phys. Rev. X 4, 031008 (2014)



S.A. Grigera et al., Science **306**, 1155 (2004)

- **Challenge**

Despite of its great interests, describing the dynamics of quantum criticality remains to be challenge.

None of the analytic, semi-classical, or numerical methods of condensed-matter physics yield accurate (exact) results, except for some special systems in one spatial dimension at special situations.

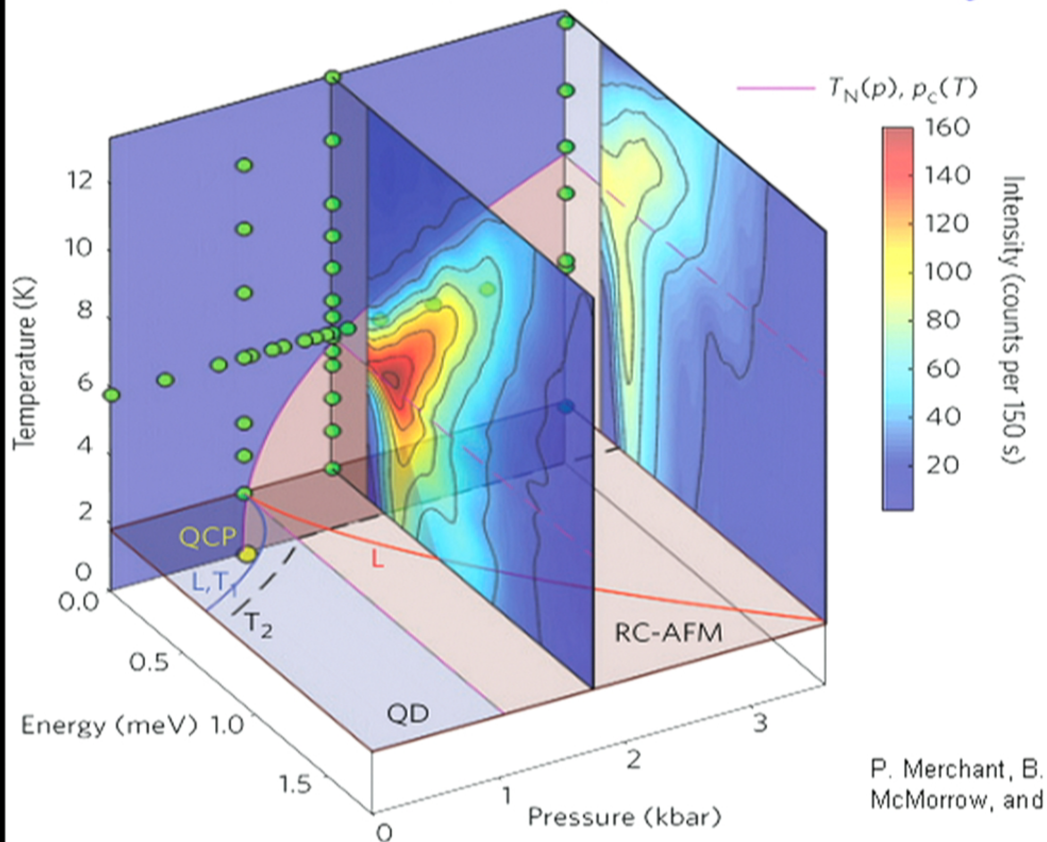
- **Main Goals**

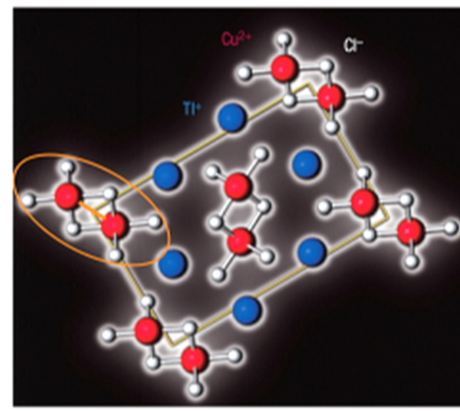
Trying to understand the zero and finite temperature dynamics near quantum critical points in strongly correlated quantum systems via a bunch of powerful analytical tools.


Linear response measurements can provide us useful dynamic information in many body systems at both zero and finite temperatures.

II. Critical marginal dynamics in a model for quantum insulator

Inelastic Neutron Scattering Experiment on 3D Insulating Magnet $TlCuCl_3$

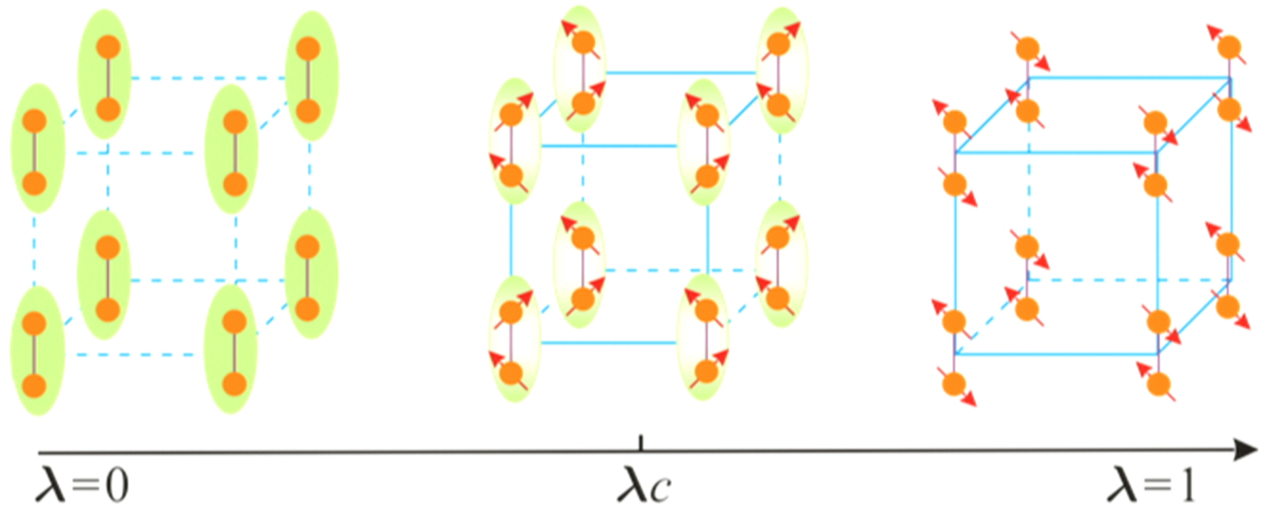




$TlCuCl_3$

P. Merchant, B. Normand, K. Krämer, M. Boehm, D. McMorrow, and C. Rüegg, Nat. Phys. **10** 373 (2014).

A model and a quantum phase transition



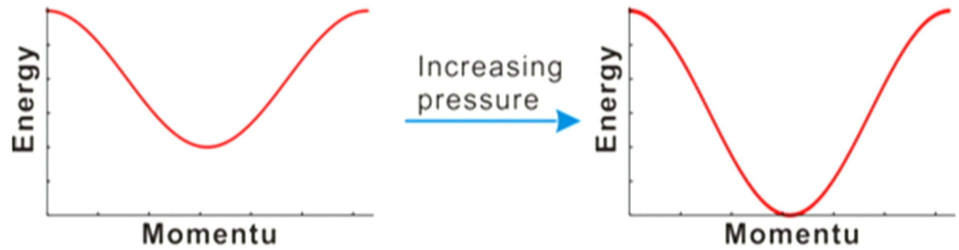
- A simplified description: J_1-J_2 model

$$H = J \sum_{\mathbf{r}} \mathbf{S}_{\mathbf{r},1} \cdot \mathbf{S}_{\mathbf{r},2} + \lambda J \sum_{\langle \mathbf{r},\mathbf{r}' \rangle;\, l=1,2} \mathbf{S}_{\mathbf{r},l} \cdot \mathbf{S}_{\mathbf{r}',l}$$

- Quantum phase transition emerges when λ is tuned to a critical value.

Projection and effective field theory

- **Project to singlet-triplet space via bond operators**
- **Increasing pressure leads to a quantum phase transition.**



- **Effectively described by a relativistic 3(space) + 1(time) *O*(3) invariant quantum φ^4 theory.**

$$\mathcal{L}_0 = \chi(\partial_\tau \phi_\alpha)^2 + \rho_s(\nabla \phi_\alpha)^2 + m^2\phi_\alpha^2 + u\phi_\alpha^2\phi_\beta^2$$

$$\chi \approx 1/J,\ \rho_s \approx 2za^2\lambda J,\ m^2 \approx J(1-4z\lambda),\ u \approx 2za^d\lambda J$$

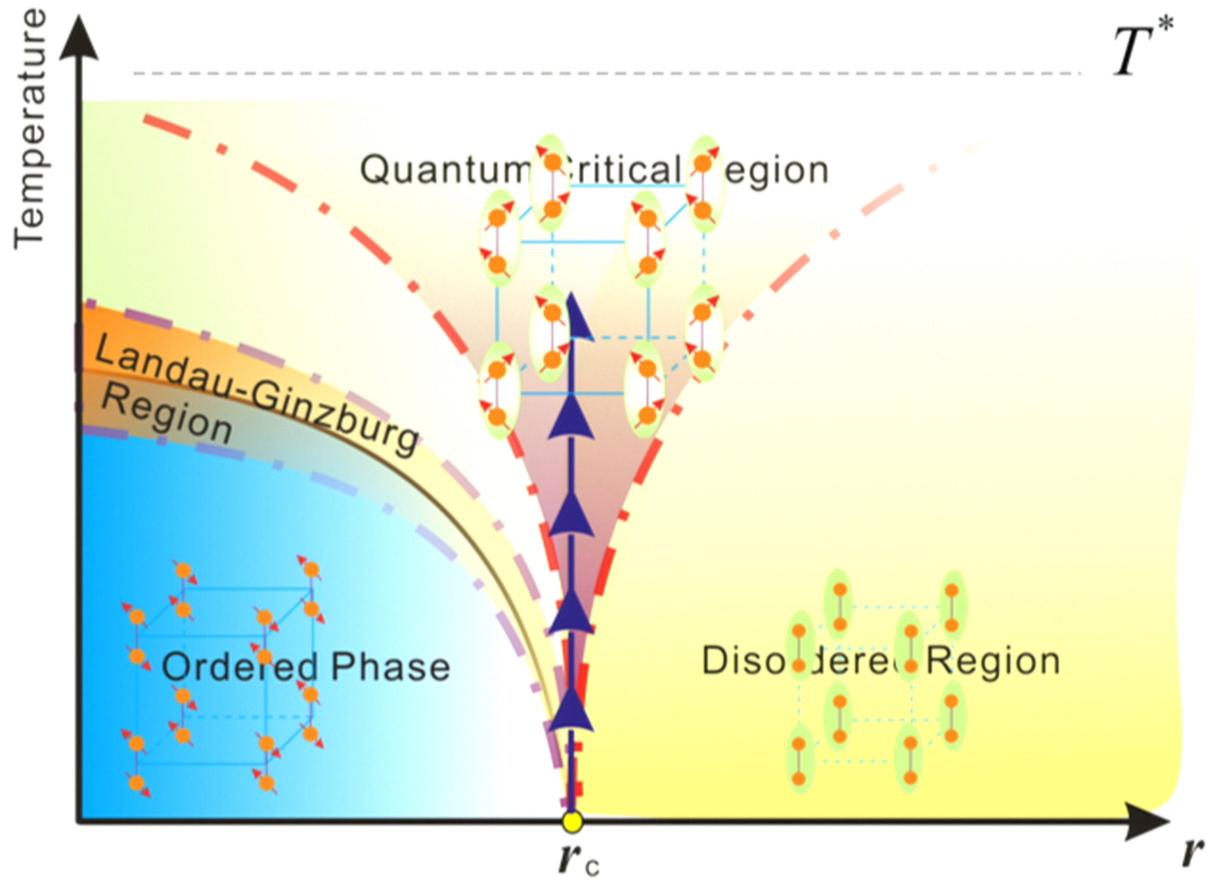
S. Chakravarty, B. I. Halperin, and D. R. Nelson, Phys. Rev. B **39** 2344 (1989);
A. V. Chubukov, S. Sachdev, and J. Ye, Phys. Rev. B **49** 11919 (1994).

Motivations

- **Theoretical motivation: (Exact) Finite temperature dynamics of relativistic quantum φ^4 theory is waiting for exploring.**

- **Experimental reason: A large part of the finite-temperature dynamic experiments on the material of $TlCuCl_3$ remains puzzled.**

Quantum hot soup



Relativistic (D - 2ε) $O(N)$ Quantum φ^4 Theory

$$\mathcal{L}_0 = \frac{1}{2}\left(\partial_\nu \varphi_i(\tau,\bar{x})\right)^2 + \frac{g^2}{4!}\mu^{2\varepsilon}\varphi_i^2(\tau,\bar{x})\varphi_j^2(\tau,\bar{x})$$

- **Renormalizable**
- **Contains infinite series of counter terms**
- **Right at QCP with zero renormalized mass**
- **Counter terms determined by Braaten-Pisarski (BP) re-summation program**

Basic Facts on BP Re-Summation Program

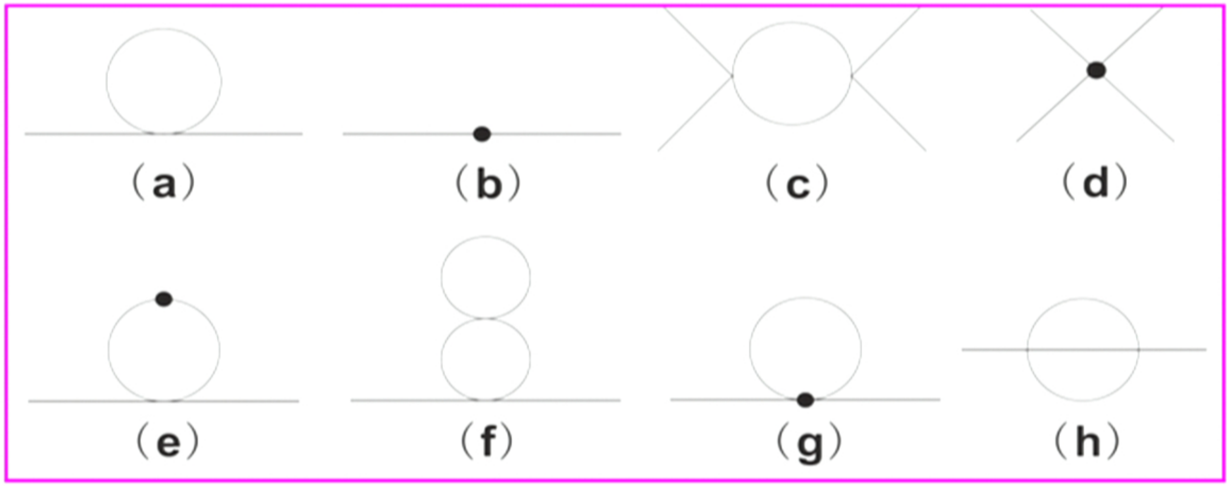
- A calculation machinery combines powerful techniques of ε - expansion and re-summation
- ε - expansion takes care UV divergences
- Re-summation takes care IR divergences
- Carry out systematically order by order

Direct implication for a renormalized theory at QCP

- Strictly resides on the QCP at finite temperature.
- Only gains a finite thermal mass.

R. D. Pisarski, Nucl. Phys. B **309** 476 (1988); Phys. Rev. Lett. **63** 1129 (1989); Nucl. Phys. A **525** 175 (1991).
E. Braaten and R. D. Pisarski, Nucl. Phys. B **337**, 569 (1990).

Updated Lagrangian to Two Loops



$$\mathcal{L}_3 = \frac{1}{2}\left[\left(\partial_\nu \phi_i\right)^2 + m_T^2 \phi_i^2\right] + \frac{g^2}{4!}\mu^{2\varepsilon}\phi_i^2\phi_j^2 - \frac{1}{2}m_T^2\phi_i^2 + \frac{g^2\mu^{2\varepsilon}}{4!}\frac{N+8}{6}\frac{g^2}{(4\pi)^2}\frac{1}{\varepsilon}\phi_i^2\phi_j^2$$

with $m_T^2 = (N+2)g(\mu)^2 T^2 / 72.$

JW, W. Yang, C. Wu and Q. Si, arXiv:1605.07163

•The damping rate comes from the sunset diagram (Fig.h).

Mass and Damping Rate for on-Shell Scattering

- **For on-shell scattering $\omega^2 = M(\mu)^2$ at long-wavelength limit with a specific energy scale μ, to two loops,**

$$M^2(\mu) = m_T^2 \left\{\left[1 + b_N g^2(\mu)\ln(T/\mu)\right] + c_1 g(\mu) + c_2 g^2(\mu)\ln g^2(\mu) + c_3 g^2(\mu)\right\}$$

$$\gamma(\mu) = g(\mu)^2 m_T/(64\pi)$$

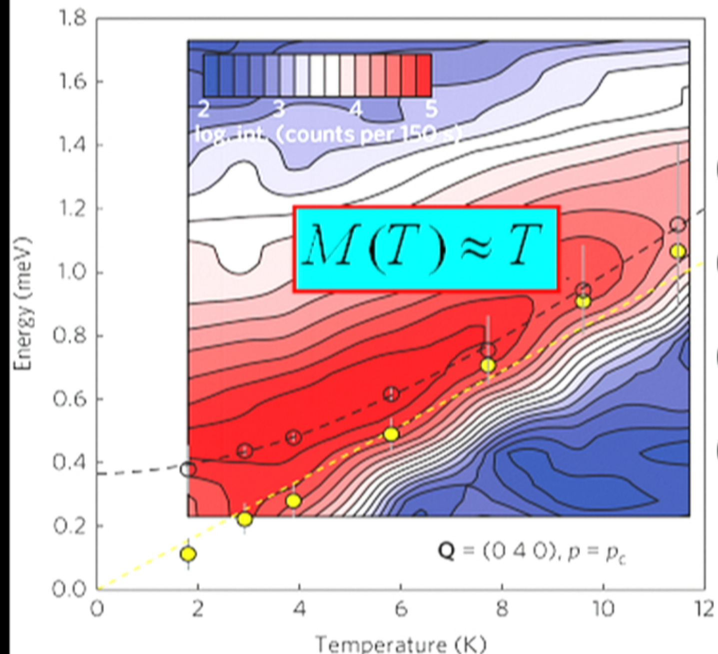
$$m_T^2 = (N+2)g(\mu)^2 T^2/72$$

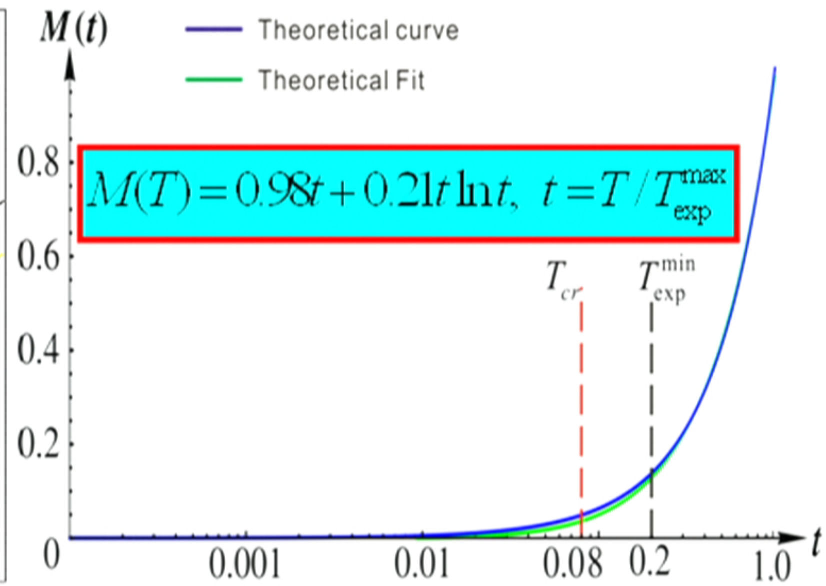
$$g^2(\mu) = g^2(\mu_0)/[1 + b_N g^2(\mu_0)\ln(\mu_0/\mu)]$$

- **Setting $N = 3$, we can determine the corresponding on-shell thermal mass and damping rate, and compare with experimental results.**

JW, W. Yang, C. Wu and Q. Si, arXiv:1605.07163

Mass comparison





JW, W. Yang, C. Wu and Q. Si, arXiv:1605.07163

- **Quantitatively agree with experiments in the experimental relevant region.**
- ***t*** **ln(*t*) behavior is expected to be dominant when further decreasing temperature !**

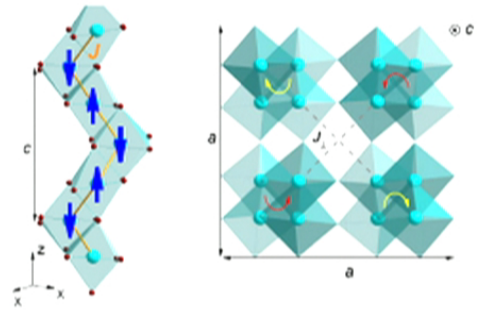
Part II conclusions

- We studied finite temperature spectral function at the QCP of relativistic $O(N)$-invariant quantum φ^4 model.
- We calculate the temperature dependence of the energy and damping rate of the spin excitations in the quantum critical regime.
- We demonstrate good agreements with the experimental results, and determine the parameter regime of the field theory that is appropriate for $TlCuCl_3$.
- We expect the $t\ln(t)$ behavior will be dominant at low temperature, verifiable by future experiments.

III. Spin dynamics in XXZ chain with an external field

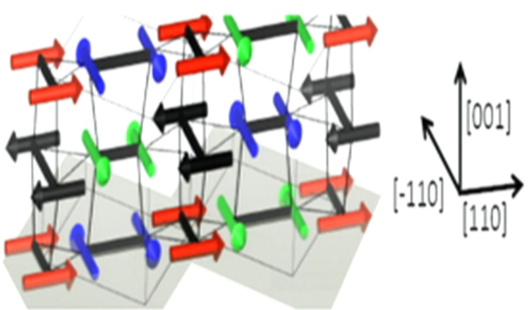
XXZ chain with an external field

$$H = \sum_i \left(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta S_i^z S_{i+1}^z \right) - h \sum_i S_i^z$$

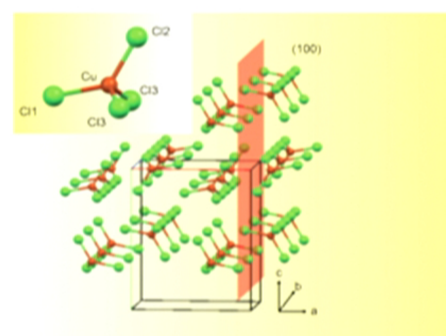


$SrCo_2V_2O_8 : \Delta \approx 2$

$CuSO_4.5D_2O: \ \Delta \approx 1$



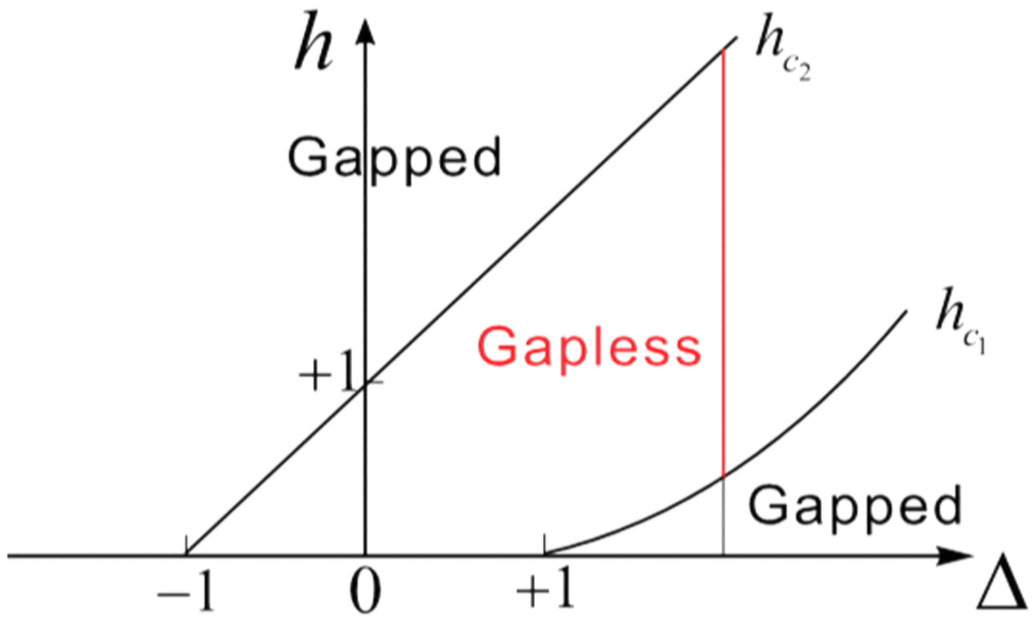
$Yb_2Pt_2Pb : \Delta \approx 4$



$Cs_2CuCl_4, \ \Delta \approx 1$

Phase diagram of XXZ model

$$H = \sum_i \left(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta S_i^z S_{i+1}^z \right) - h \sum_i S_i^z$$



Dynamical Structure Factor

- **Zero Temperature Dynamical Structure Factors (DSF):**

(Fourier transform of $\langle GS|S_j^{\alpha}(t)S_{j'}^{\bar{\alpha}}(t')|GS\rangle$)

$$S^{\alpha\bar{\alpha}}(q,\omega) = 2\pi\sum_{\mu}\left|\left\langle\mu\left|S_q^{\bar{\alpha}}\right|GS\right\rangle\right|^2 \delta\left(\omega - E_{\mu} + E_{GS}\right)$$

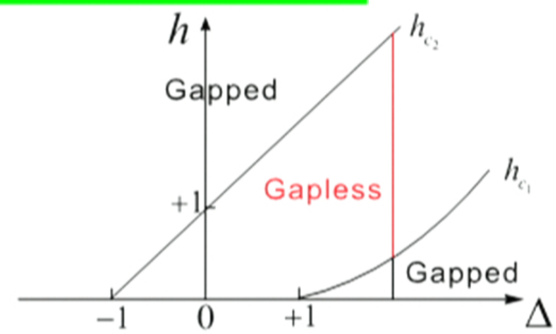
Proportional to differential cross section;
Experimentally relevant, inelastic neutron scattering, ESR, NMR.....

In this talk we focus on the transverse dynamical structure factors:

$$S^{-+}(q,\omega),\ S^{+-}(q,\omega).$$

Dominant excitations

$$S^{\alpha\bar{\alpha}}(q,\omega) = 2\pi \sum_{\mu} \left| \langle \mu | S_q^{\bar{\alpha}} | GS \rangle \right|^2 \delta\left(\omega - E_\mu + E_{GS}\right)$$



Dominant excitations:

S^{-+} real states: psinons $(1\psi\psi, 2\psi\psi)$

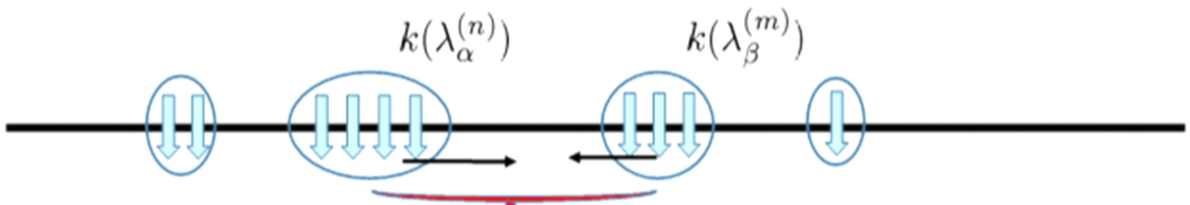
S^{+-} { real states: psinon anti-psinons $(1\psi\psi^{*}, 2\psi\psi^{*})$
string states: 2-string states $(1\chi^{(2)}R)$, 3-string states $(1\chi^{(3)}R)$

Reference State: All Spins Aligning up

W. Yang, **JW***, S. Xu, Z. Wang and C. Wu*, submitted to PRL
*: corresponding author

String ansatz and Bethe-Gaudin-Takahashi (BGT) equations

String state with $M = \sum_n \alpha_n n$ **reversed spins:**
(*n*: string length, α_n**: # of length-n strings)**



Interaction: phase shift

$$N\theta_n(\lambda_\alpha^{(n)}) = 2\pi I_\alpha^{(n)} + \sum_{(m,\beta)\neq(n,\alpha)} \Theta_{nm}(\lambda_\alpha^{(n)} - \lambda_\beta^{(m)})$$

$\lambda_\alpha^{(n)}$: rapidity $\quad I_\alpha^{(n)}$: Bethe quantum number
Θ_{nm} : phase shift due to interacation

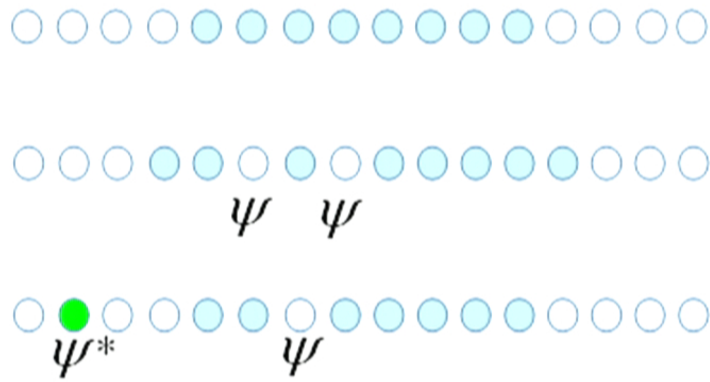
Simple Picture of Dominant Excitations I

Bethe quantum numbers for system of N=32, M=8.

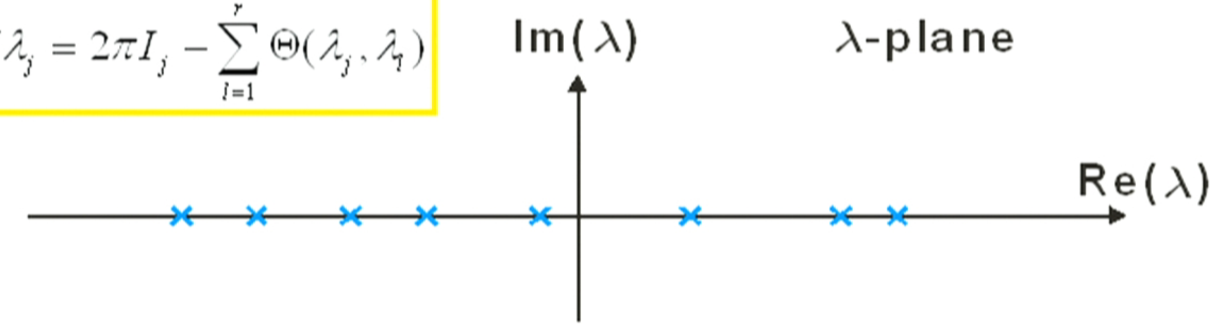
Ground state:

$1\psi\psi$ state:

$1\psi\psi^*$ state:



$$N\lambda_j = 2\pi I_j - \sum_{l=1}^{r} \Theta(\lambda_j, \lambda_l)$$

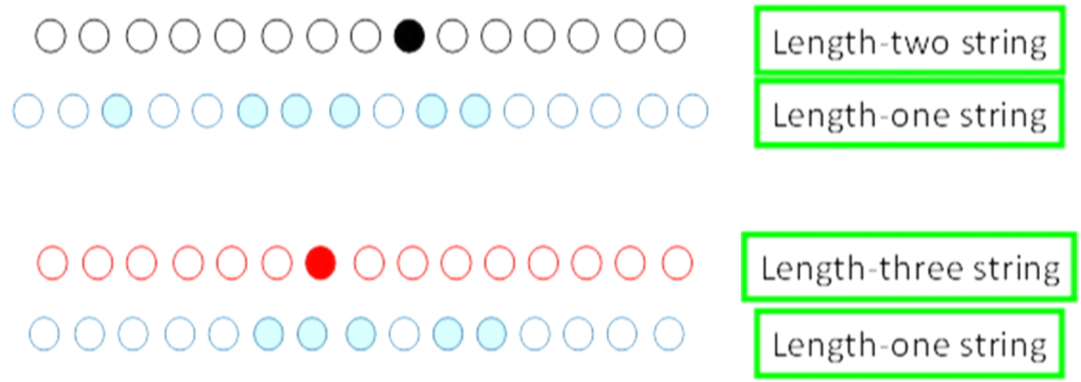


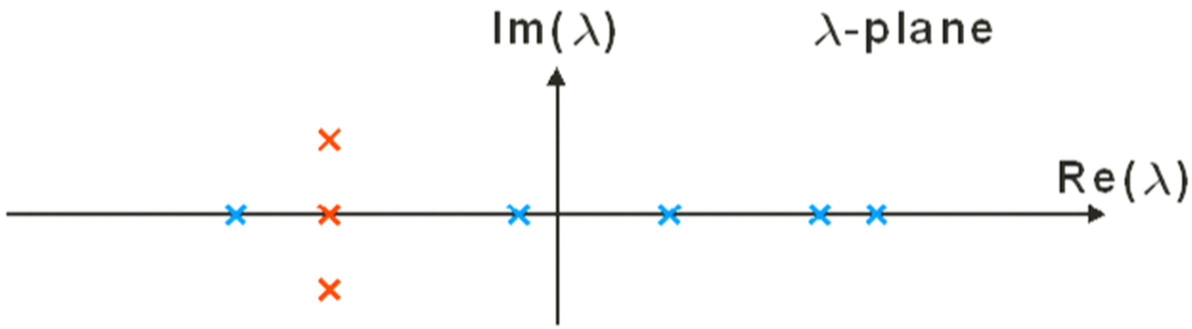
Above pictures do not include all possible range of Bethe quantum numbers.

Simple Picture of Dominant Excitations II

$1\chi^{(2)}R$ **state:**

$1\chi^{(3)}R$ **state:**





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Proportional to differential cross section;
Experimentally relevant, inelastic neutron scattering, ESR, NMR.....

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$$S^{-+}(q,\omega),\ S^{+-}(q,\omega).$$

Algebraic Bethe Ansatz

Yang-Baxter Equation:

$$R_{12}(\lambda_1,\lambda_2)R_{13}(\lambda_1,\lambda_3)R_{23}(\lambda_2,\lambda_3) = R_{23}(\lambda_2,\lambda_3)R_{13}(\lambda_1,\lambda_3)R_{12}(\lambda_1,\lambda_2)$$

Monodromy matrix:

$$\mathcal{T}(\lambda) = R_{0n}(\lambda, i\frac{\eta}{2})...R_{02}(\lambda, i\frac{\eta}{2})R_{01}(\lambda, i\frac{\eta}{2}) = \begin{pmatrix} A(\lambda) & B(\lambda) \\ C(\lambda) & D(\lambda) \end{pmatrix}_{[0]}$$

Yang-Baxter algebra

$$R(\lambda,\mu)\ \ \mathcal{T}(\lambda)\otimes\mathcal{T}(\mu) = \mathcal{T}(\mu)\otimes\mathcal{T}(\lambda)\ \ R(\lambda,\mu)$$

Magnon (Renormalized) creation operator:

$$\Psi(\lambda_1,\lambda_2,...,\lambda_r) = B(\lambda_1)B(\lambda_2)...B(\lambda_r)|\uparrow\uparrow...\uparrow\rangle$$

Hamiltonian:

$$H = \sin(i\eta)\frac{d}{d\lambda}\ln T(\lambda)|_{\lambda=i\eta/2} + \text{const.}$$

$$T(\lambda) = \text{Tr}\mathcal{T}(\lambda)$$

L. A. Takhtadzhan and L. D. Faddeev *Russ. Math. Sur.* 34,11 (1979)

Determinant Formulas for Form Factors

$$
\begin{aligned}
|\langle\mu|S_q^-|\lambda\rangle|^2 \;=\; & N\delta_{q,q\{\lambda\}-q\{\mu\}}|\sin(i\eta)|\frac{\Pi_{j=1}^{M+1}|\sin(\mu_j - i\eta/2)|^2}{\Pi_{j=1}^{M}|\sin(\lambda_j - i\eta/2)|^2} \\
& \Pi_{j>k=1}^{M+1}|\sin^2(\mu_j-\mu_k)-\sin^2(i\eta)|^{-1}\Pi_{j>k=1}^{M}|\sin^2(\lambda_j-\lambda_k)-\sin^2(i\eta)|^{-1} \\
& \frac{|\det H^-|^2}{|\det\Phi(\{\mu\})|\;|\det\Phi(\{\lambda\})|}
\end{aligned}
$$

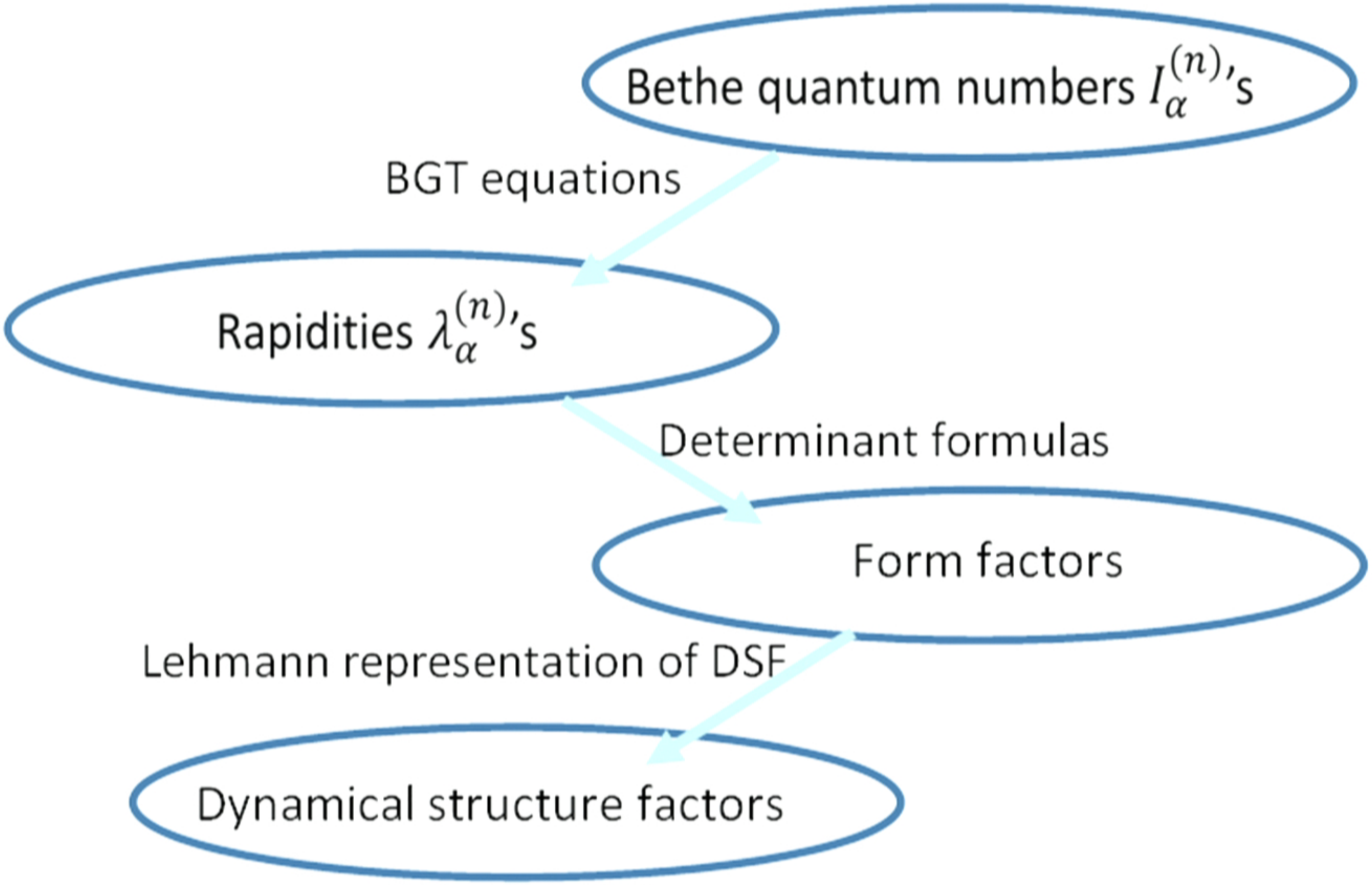
V. E. Korepin *Commun. Math. Phys.* 86, 391 (1982)
J. M. Maillet and J. Sanchez De Santos *arXiv: q-alg/9612012* (1996)
N. Kitanine, J. M. Maillet and V. Terras *Nucl. Phys. B* 554, 647 (1999)

For string states, the formulas need to be regularized.

J. Mossel, and J-S Caux *New Journal of Physics* 12.5 (2010)

Coordinate Bethe Ansatz: 10^1 sites
Determinant formulas: 10^3 sites with finite density of magnons
10^6sites with dilute magnons

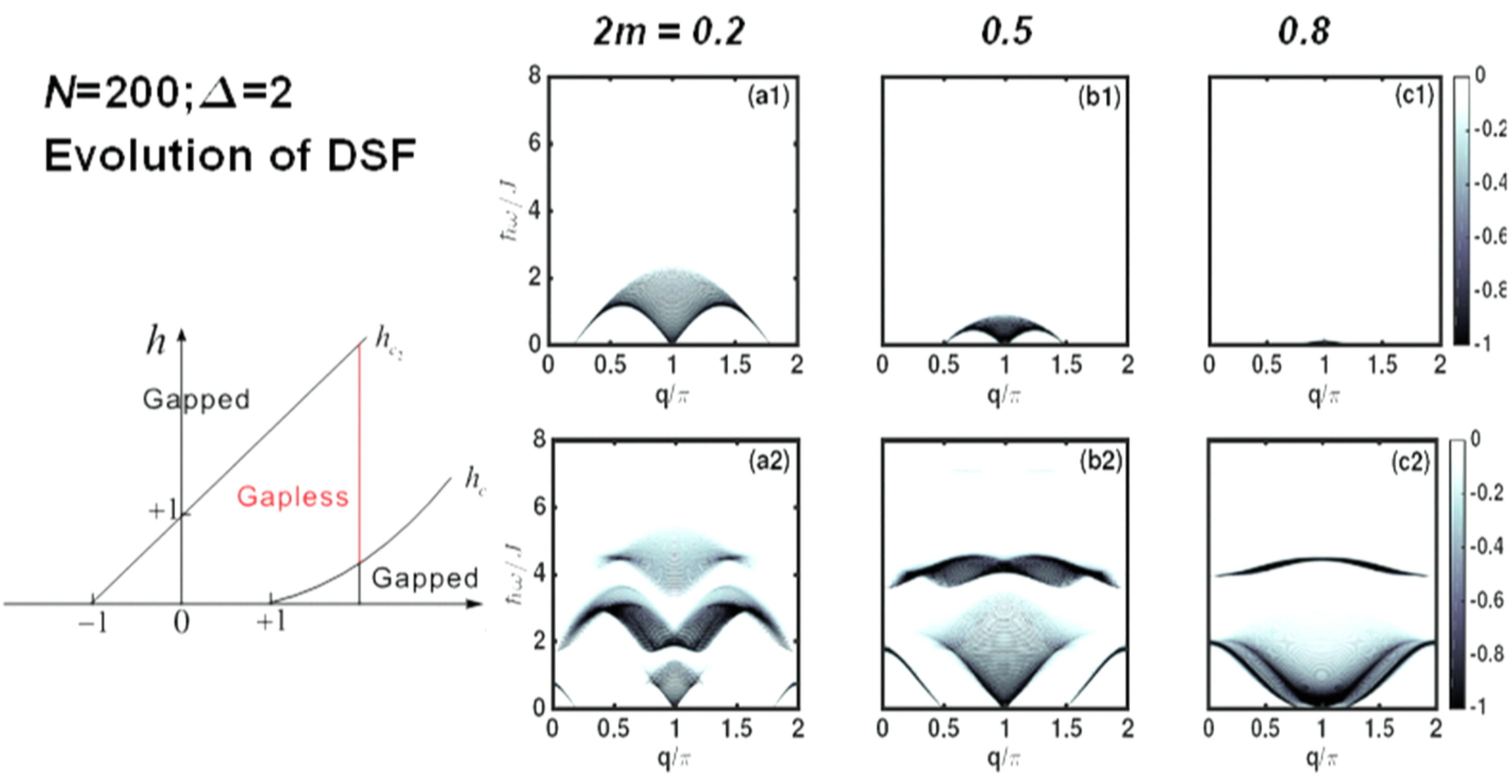
Sketchy Computation of DSF



DSF and physics beyond Luttinger Liquid

N=200; Δ=2

Evolution of DSF



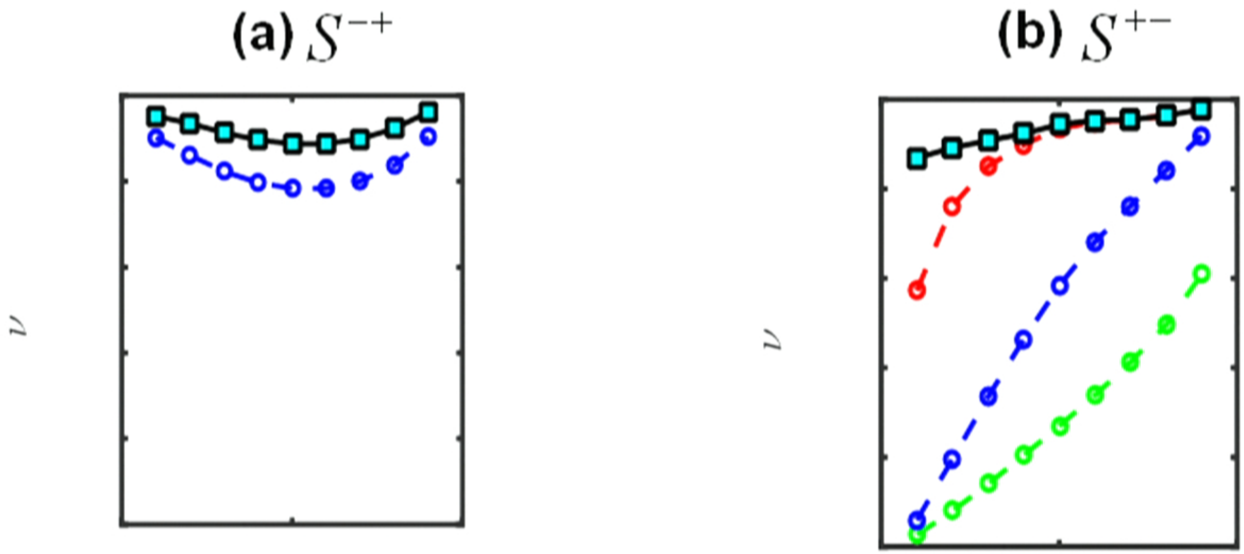
Turning on temperature:

Quantum hot soup => Quantum hot porridge/noodle ?

W. Yang, **JW***, S. Xu, Z. Wang and C. Wu*, submitted to PRL

Sum ratios of integrated intensity

$$R_{a,-a} = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{1}{N} \sum_q S^{a,-a}(q,\omega) = \frac{1}{2} + am$$



Blue: $1\psi\psi$

Black : $2\psi\psi$

Green: $1\psi\psi^*$

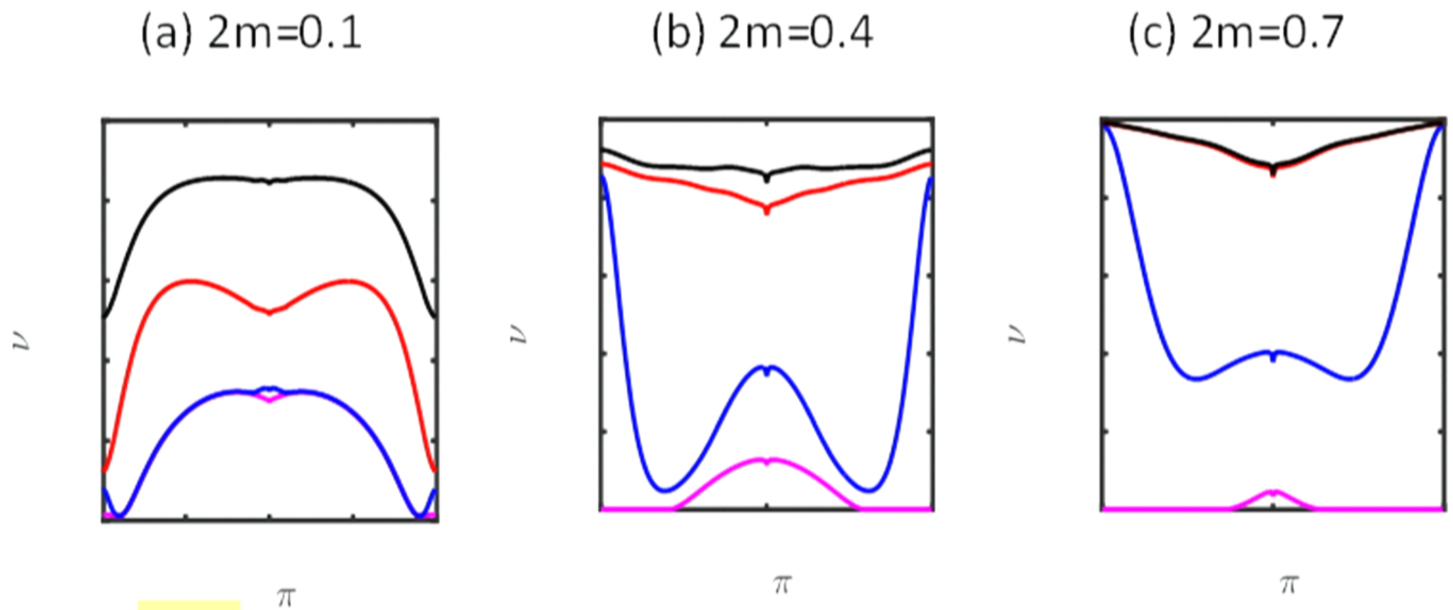
Blue: $2\psi\psi^*$

Red: two-string states

Black: three-string states

W. Yang, **JW***, S. Xu, Z. Wang and C. Wu*, submitted to PRL

Sum ratios of first frequency moment



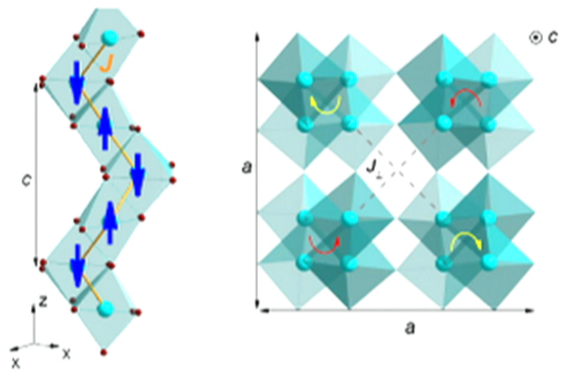
Pink: S^{-+}
Blue: real states in S^{+-}
Red: two-string states in S^{+-}
Black: three-string states in S^{+-}

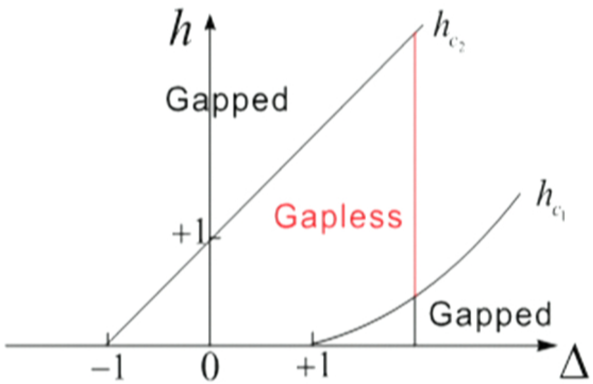
$$W(q) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega\,\omega\left[S^{+-}(q,\omega) + S^{-+}(q,\omega)\right]$$

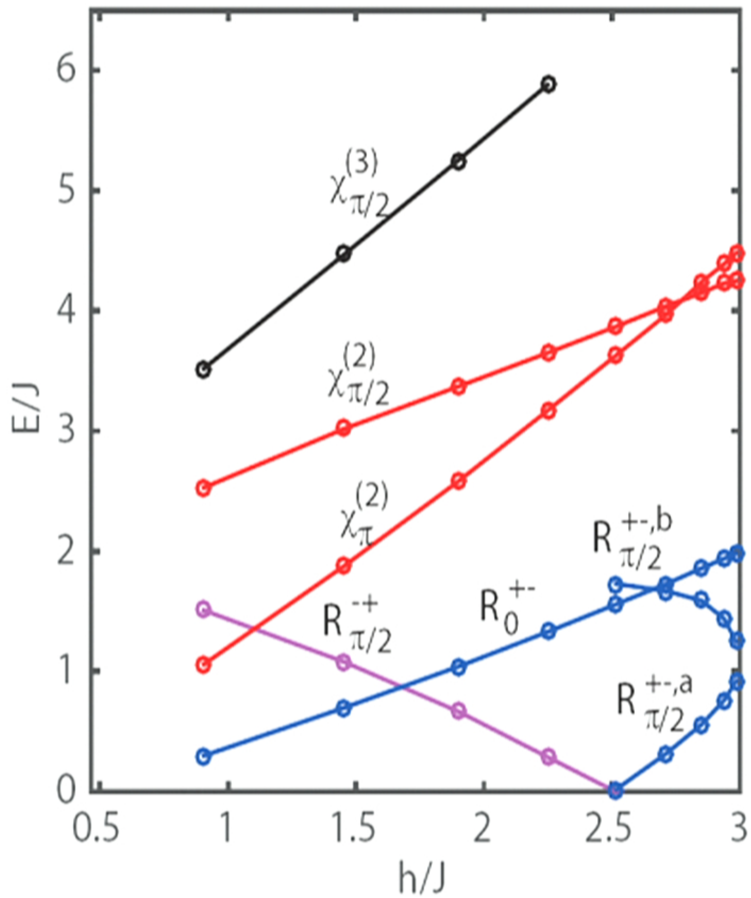
$$= \left(E_0 + \Delta\partial E_0/\partial\Delta - m\partial E_0/\partial m\right) + \left[(\Delta^2 - 2)\partial E_0/\partial\Delta - \Delta E_0\right]\cos q$$

W. Yang, **JW***, S. Xu, Z. Wang and C. Wu*, submitted to PRL

Theoretical Predictions







A collaboration paper with experimentalists was submitted to Science

Part III Conclusions

- We calculated transverse DSF in XXZ model with a longitudinal field.
- We found dominant string excitations in the gapless regime, well beyond conventional Luttinger-liquid paradigm and psinon/spinon picture.
- We demonstrate good agreement with sum rules, laying down a concrete support for the identification of the excitations in XXZ model.
- We proposed proper spin dynamics experiments to probe the novel string excitations.

IV. Outlook

1. An extended finite temperature dynamics study near the transition line of the quantum φ^4 model can be further compared with experiments.

2. A study for the entanglement structure of the string excitations in the XXZ model may reveal deeper secrets in the XXZ model.

3. An extended study on the evolution of dynamical-dominant excitations for the full regime of Δ would provide us a deeper and systematic understanding about the XXZ model, which should have broad theoretical and experimental impacts.

Thanks !