# Dynamically dominant excitations of string solutions in the $S$=1/2 antiferromagnetic Heisenberg chain in a magnetic field

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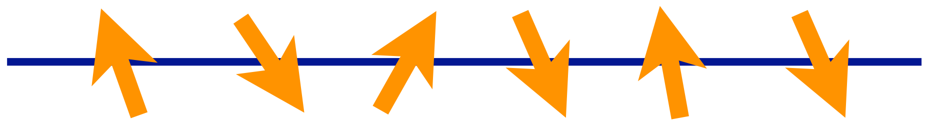
M.K., Phys. Rev. Lett. **102**, 037203 (2009).

# Spin-1/2 antiferromagnetic Heisenberg chain

The **spin-1/2 antiferromagnetic Heisenberg chain in a magnetic field**

$$\mathcal{H} = J\sum_{x} \boldsymbol{S}_x \cdot \boldsymbol{S}_{x+1} - HS^z.$$



It exhibits interesting ***quantum many-body effects***:

*Fractionalization*, *spin liquid*, *quantum criticality*, ...

which have inspired modern concepts for strongly correlated systems.

This system is an excellent platform to make precise comparisons between

- quasi-1D antiferromagnets — ***Experiment***
- Exact solutions using the Bethe ansatz [1]. — ***Theory***

Very long history! But, properties have not been fully understood...

**$S(k,\omega)$ in a magnetic field**

[1] H. Bethe, Z. Phys. **71**, 205 (1931).

# The Bethe ansatz

Bethe wavefunction： $\Phi(x_1, \cdots x_M) = \sum_P \exp\left\{ \mathrm{i} \left( \sum_j k_{Pj} x_j + \sum_{\substack{j<l \\ Pj>Pl}} \phi_{PjPl} \right) \right\}$,

where $k$ and $\phi$ are determined so that this wavefunction becomes an eigenstate of the Hamiltonian under periodic boundary conditions.

Bethe equation：

$$L\theta(\Lambda_j) = 2\pi I_j + \sum_{l \neq j} \theta\left( \frac{\Lambda_j - \Lambda_l}{2} \right), \quad j = 1, \cdots, M,$$

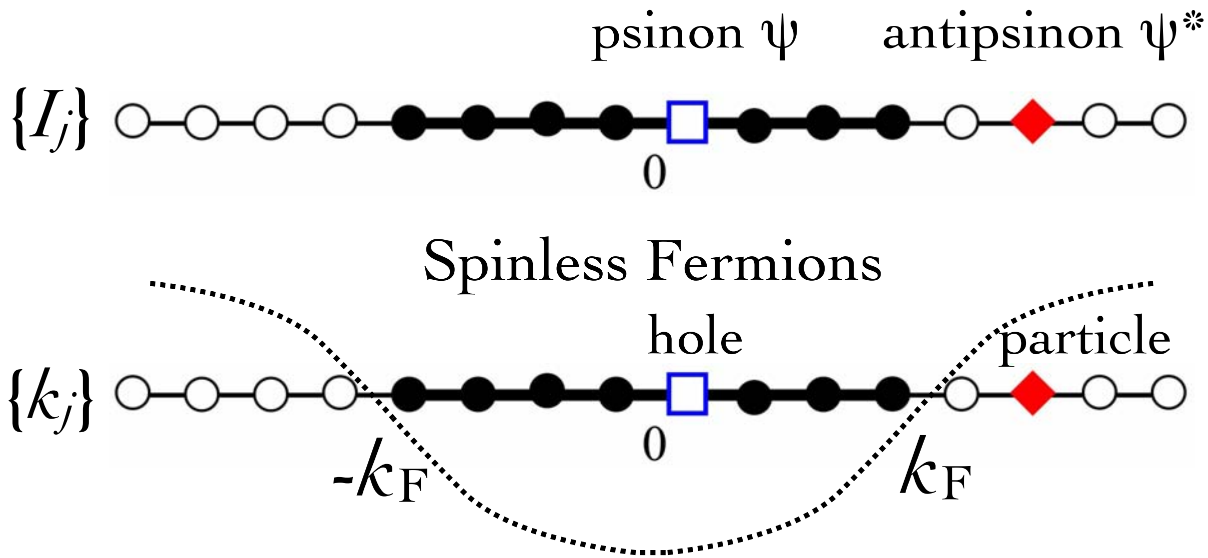
$$\theta(x) \equiv 2\arctan(x),\ \Lambda_j \equiv \cot\left(\frac{k_j}{2}\right),\ \ 2\cot\left(\frac{\phi_{j,l}}{2}\right) = \cot\left(\frac{k_j}{2}\right) - \cot\left(\frac{k_l}{2}\right).$$

$$I_j = \begin{cases} \text{integer} & ,\ \text{if } L-M \text{ is odd} \\ \text{half-odd integer} & ,\ \text{if } L-M \text{ is even} \end{cases}, \quad |I_j| \leq \frac{L-M-1}{2}.$$

Once a set of $\{I_j\}$ is given, an eigenstate is obtained.

[1] H. Bethe, Z. Phys. **71**, 205 (1931).

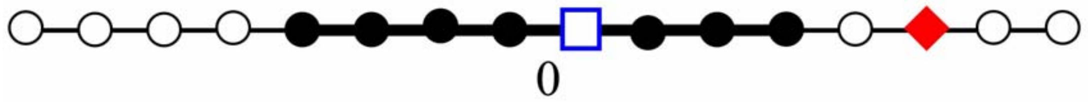
# Dynamically dominant excitations for $S^{zz}(k,\omega)$ and $S^{-+}(k,\omega)$



# Dynamically dominant excitations for $S^{zz}(k,\omega)$ and $S^{-+}(k,\omega)$

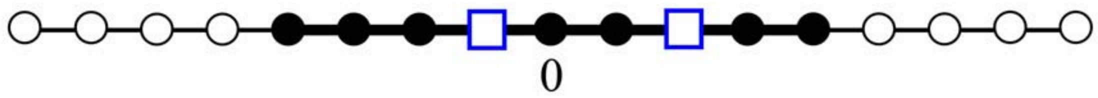
psinon $\psi$ antipsinon $\psi^*$

$S^{zz}(k,\omega)\ \{I_j\}$




$\psi\psi^*$ excitation [2,3]

$S^{-+}(k,\omega)\ \{I_j\}$

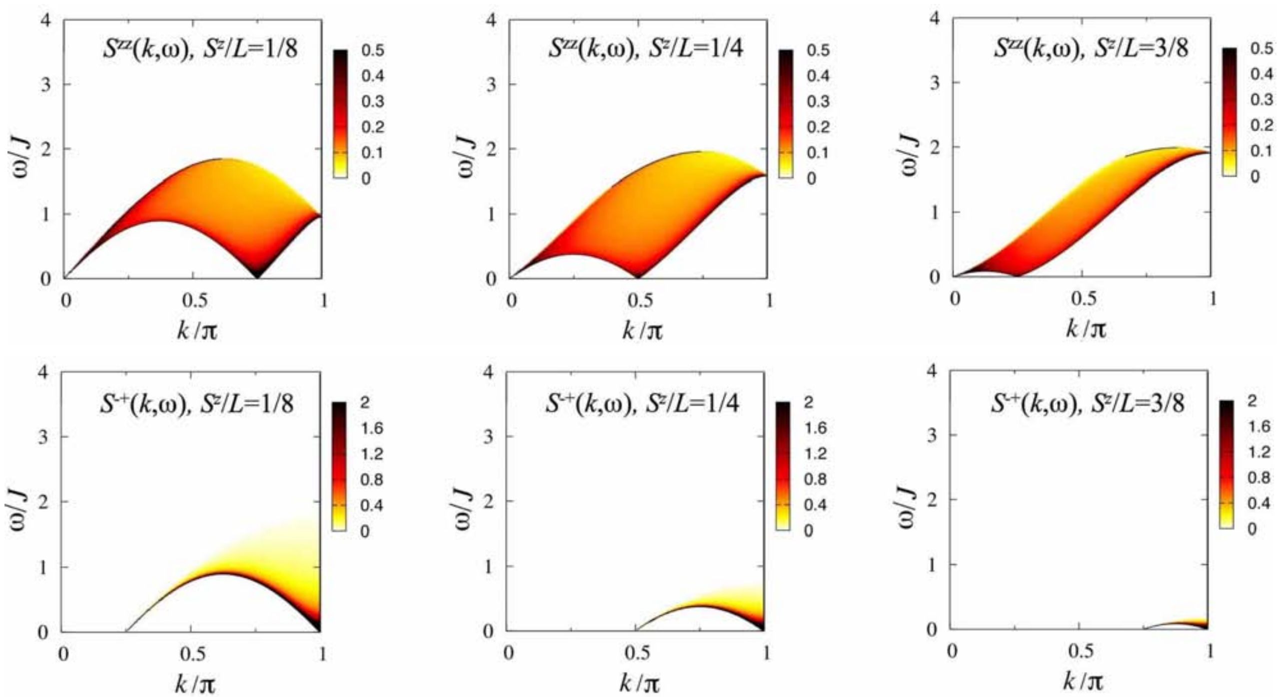



$2\psi$ excitation [3]

$S^z/L=1/8$ $S^z/L=1/4$ $S^z/L=3/8$

$S^{zz}(k,\omega)$
$=\sum_i |\langle k,\varepsilon_i|S_k^z|\mathrm{G.S.}\rangle|^2\delta(\omega-\varepsilon_i)$.

$S^{-+}(k,\omega)$
$=\sum_i |\langle k,\varepsilon_i|S_k^+|\mathrm{G.S.}\rangle|^2\delta(\omega-\varepsilon_i)$.

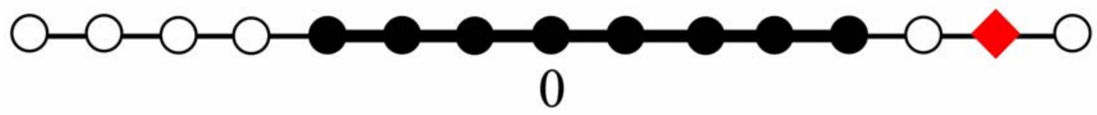



low field $\leftarrow$ $H$ $\rightarrow$ high field

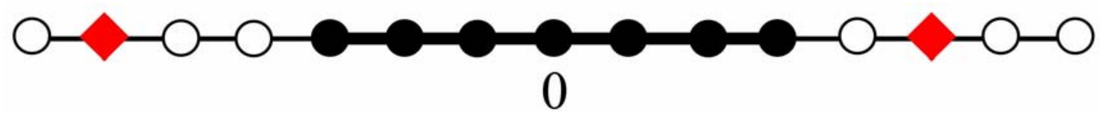
[2] M.Karbach & G.Müller, PRB **62**, 14871 (2000). [3] M.Karbach, D.Biegel & G.Müller, PRB **66**, 054405 (2002).

# Dynamically dominant excitations for $S^{+-}(k,\omega)$

$1\psi^*$ [3-7], $\mathbf{2\psi^*}$ **[8]**: $S^{+-}(k,\omega)=\sum_i|\langle k,\varepsilon_i|S_k^-|\mathrm{G.S.}\rangle|^2\delta(\omega-\varepsilon_i)$.

$\{I_j\}$ 

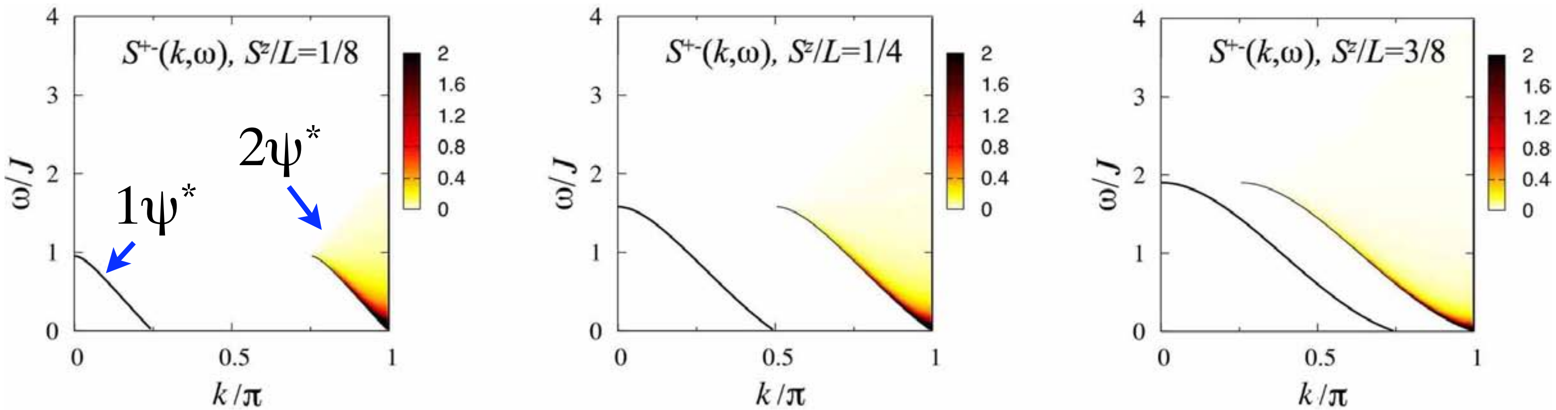
$1\psi^*$ excitation

$\{I_j\}$ 

$2\psi^*$ excitation

$S^z/L=1/8$ $S^z/L=1/4$ $S^z/L=3/8$

$\Delta S^z=-1$




low field ← $H$ → high field

[2] M.Karbach *et al.*, Phys. Rev. B **66**, 054405 (2002).
[4] D.Biegel *et al.*, Europhys. Lett. B **59**, 882 (2002).
[5] G.Müller *et al.*, Phys. Rev. B **24**, 1429 (1981).
[6] K. Lefmann, and C. Rischel, Phys. Rev. B **54**, 6340 (1996).
[7] S. Nishimoto *et al.*, Int. J. Mod. Phys. B **21**, 2262 (2007).
[8] M.K., Phys. Rev. Lett. **102**, 037203 (2009).

# $S^z$ of ψ and ψ*

$$\begin{cases} S^{-+}(k,\omega) \sim |\langle \mathrm{Exc.}(S^z+1)|S^+|\mathrm{G.S.}(S^z)\rangle|^2 & : \Delta S^z = +1 \; \ldots \; 2\psi \text{ excitations} \\ S^{zz}(k,\omega) \sim |\langle \mathrm{Exc.}(S^z)|S^z|\mathrm{G.S.}(S^z)\rangle|^2 & : \Delta S^z = 0 \; \ldots \; \psi\psi^* \text{ excitations} \\ S^{+-}(k,\omega) \sim |\langle \mathrm{Exc.}(S^z-1)|S^-|\mathrm{G.S.}(S^z)\rangle|^2 & : \Delta S^z = -1 \; \ldots \; 2\psi^* \text{ excitations} \end{cases}$$

Psinon (ψ) carries $S^z$=+1/2.

Antipsinon (ψ*) carries $S^z$=−1/2.

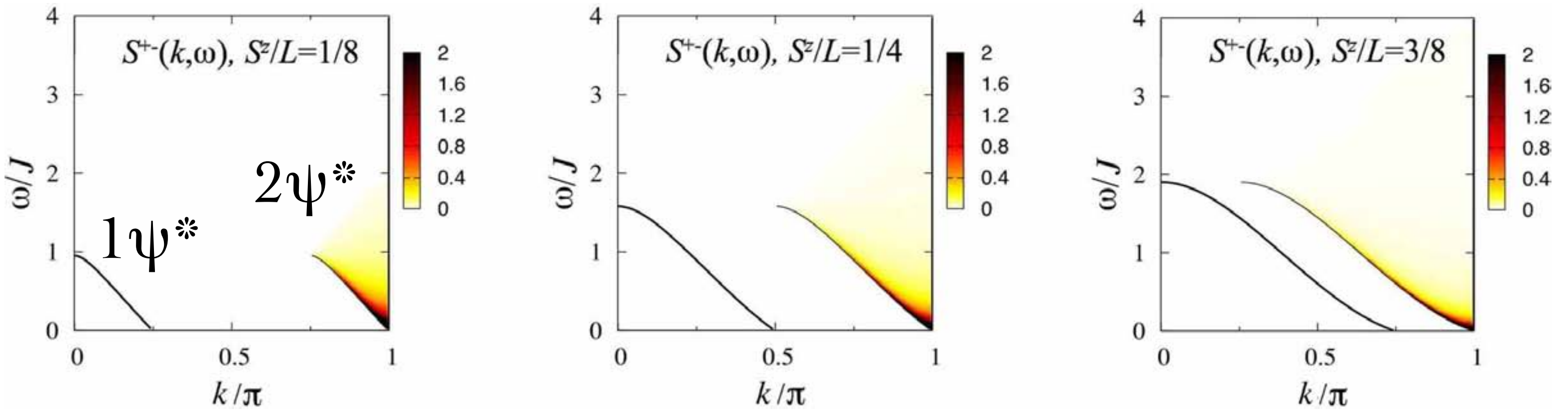
$\xrightarrow{\text{Zero field}}$ Spinon which carries $S^z$=+1/2.

M.K., Phys. Rev. Lett. **102**, 037203 (2009).

# Missing spectral weight in $S^{+-}(k,\omega)$

$S^z/L=1/8$ $S^z/L=1/4$ $S^z/L=3/8$

$\Delta S^z=-1$

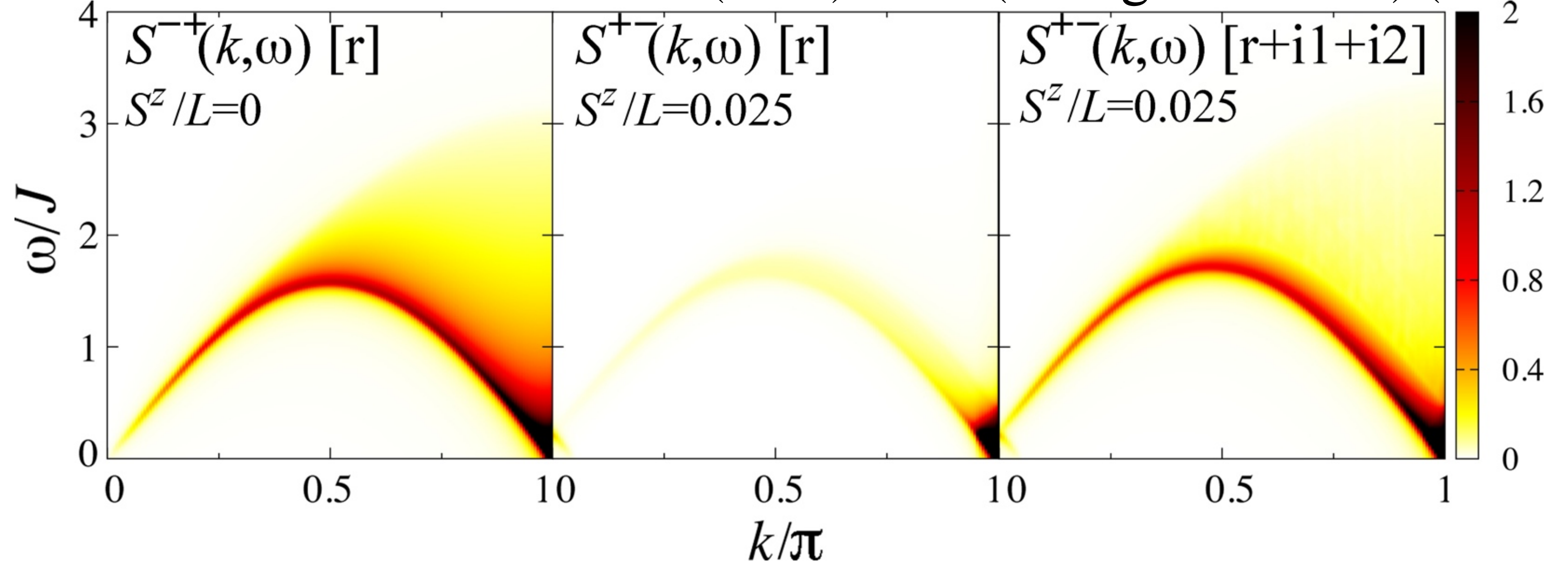



low field ← $H$ → high field

Real-$\Lambda$ solutions ($H\approx0$)

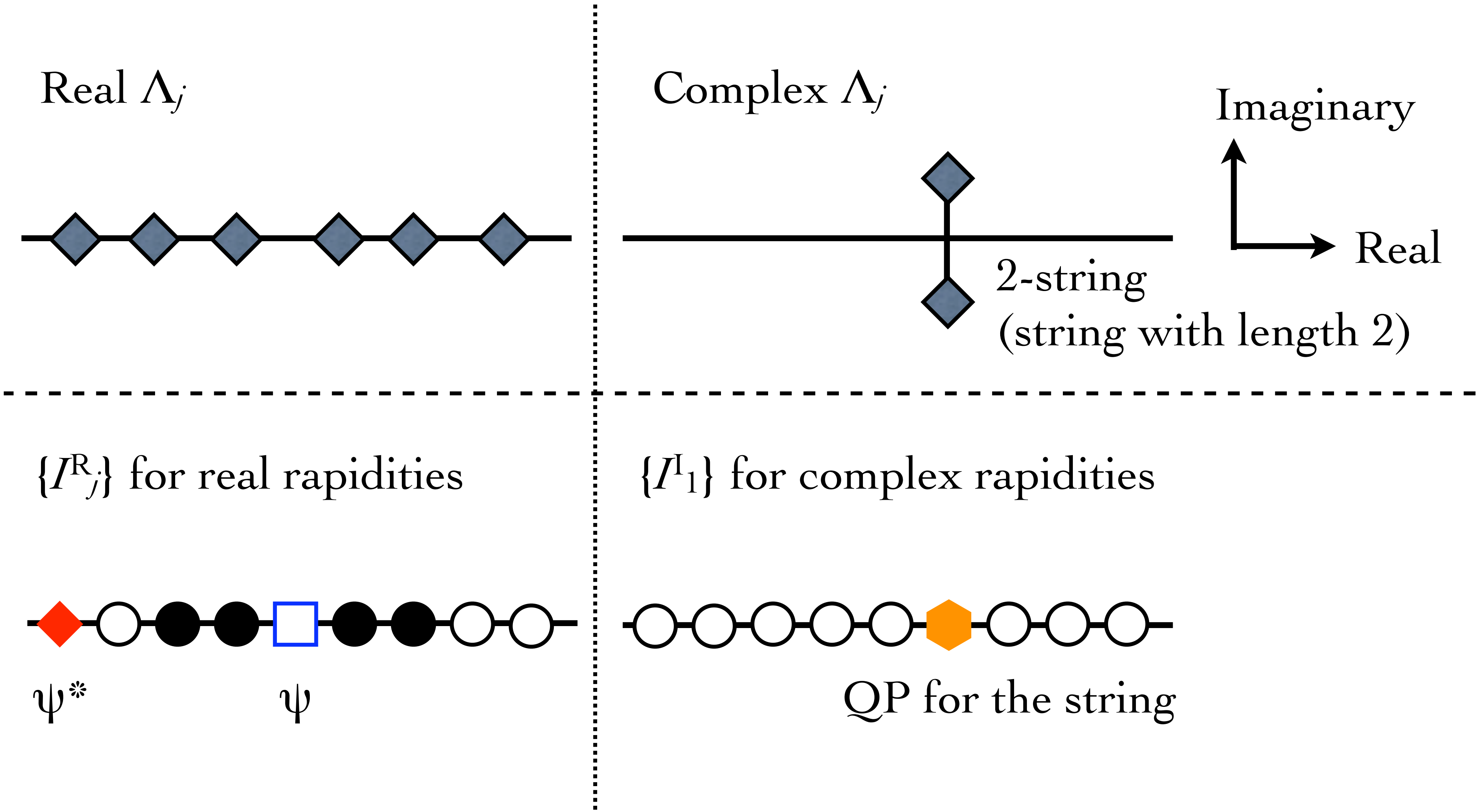
Complex-$\Lambda$ solutions (string solutions) ($H\approx0$)

$S^{-+}(k,\omega)$ ($H=0$)



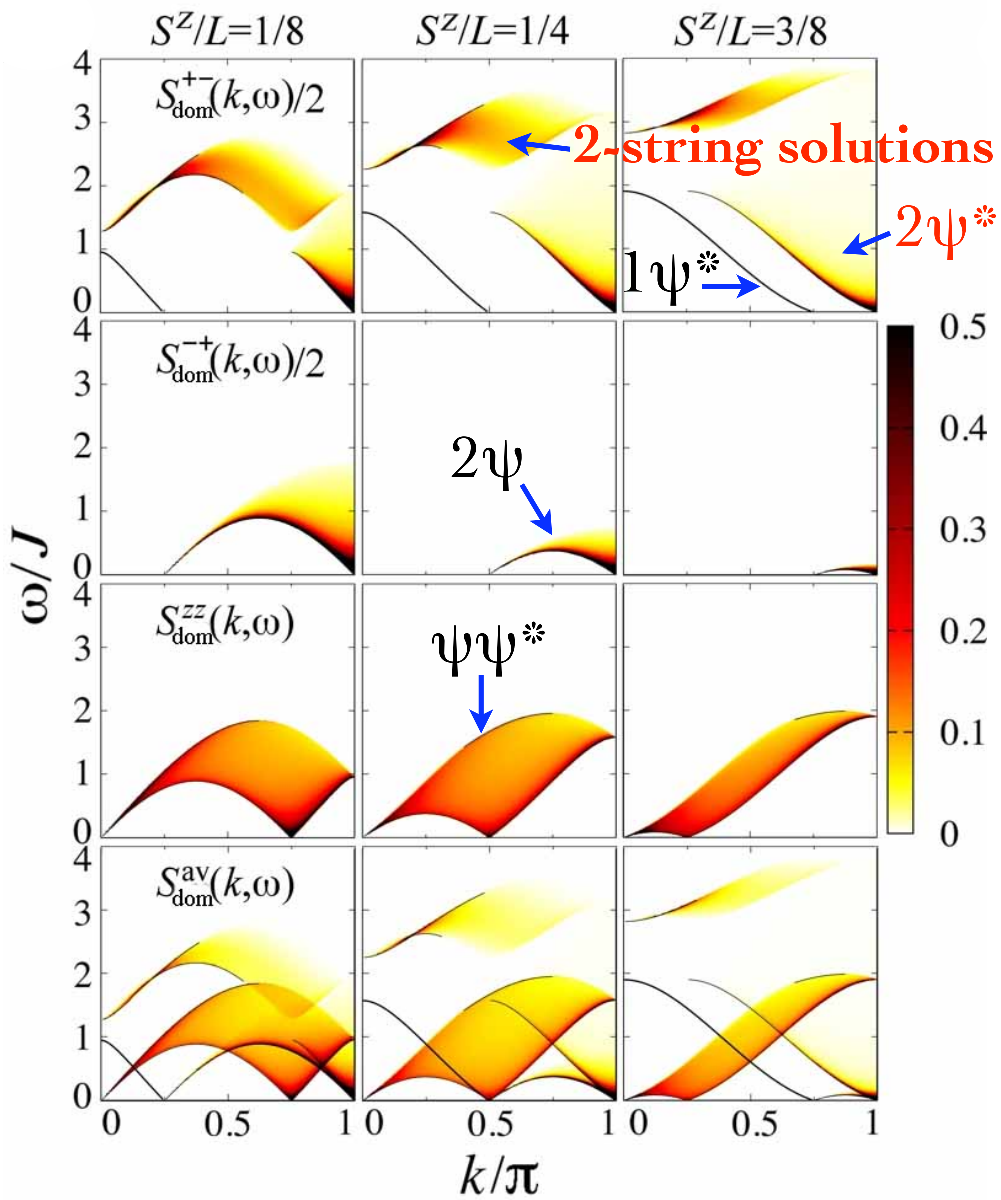
# Solutions with a string

String solutions with one string are specified by two sets of $\{I_j\}$:
$\{I^R_j\}$ for real rapidities and $\{I^I_j\}$ ($j$=1) for complex rapidities.

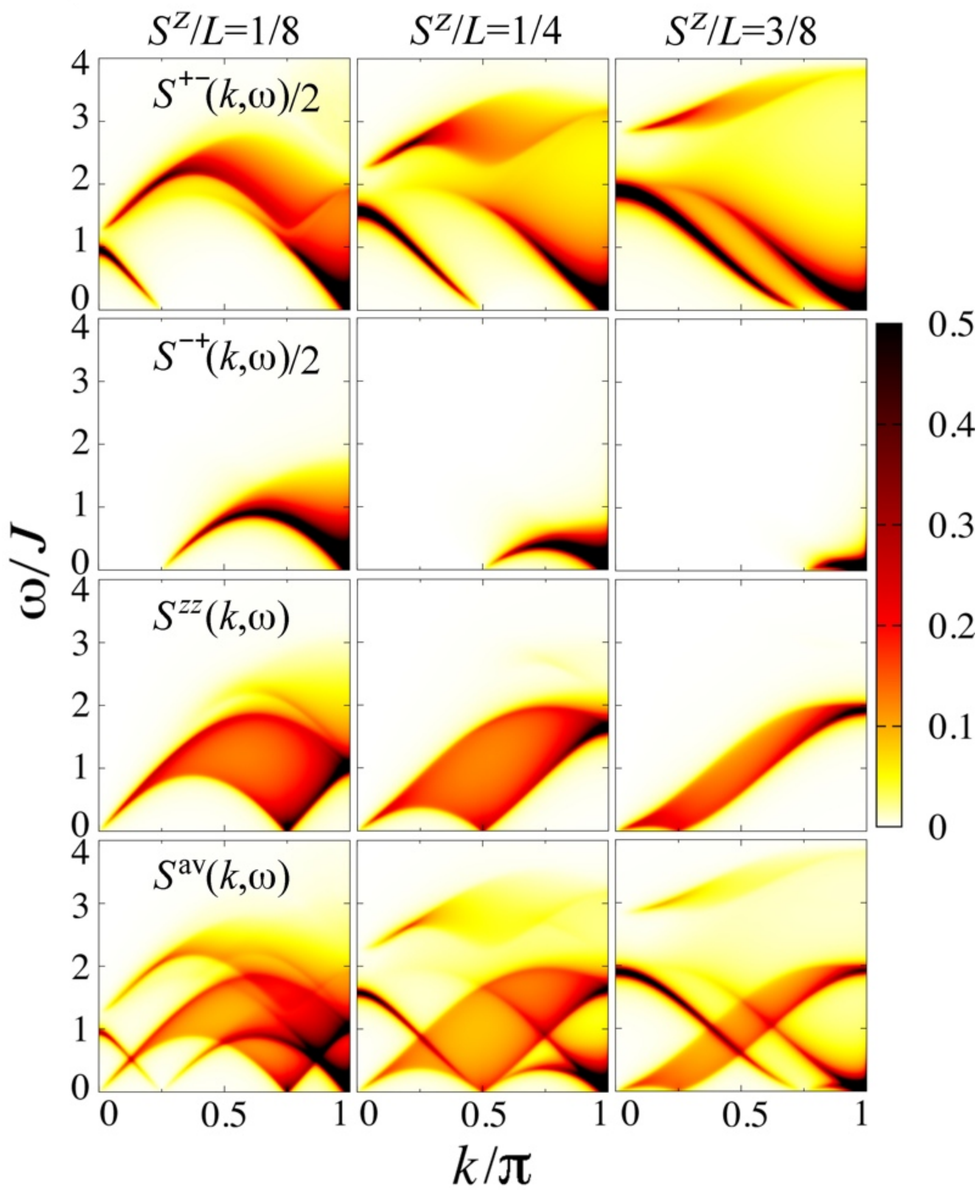


# $S(k,\omega)$ in a magnetic field in 1D

Dynamically dominant excitations in $S(k,\omega)$ in $L$=2240

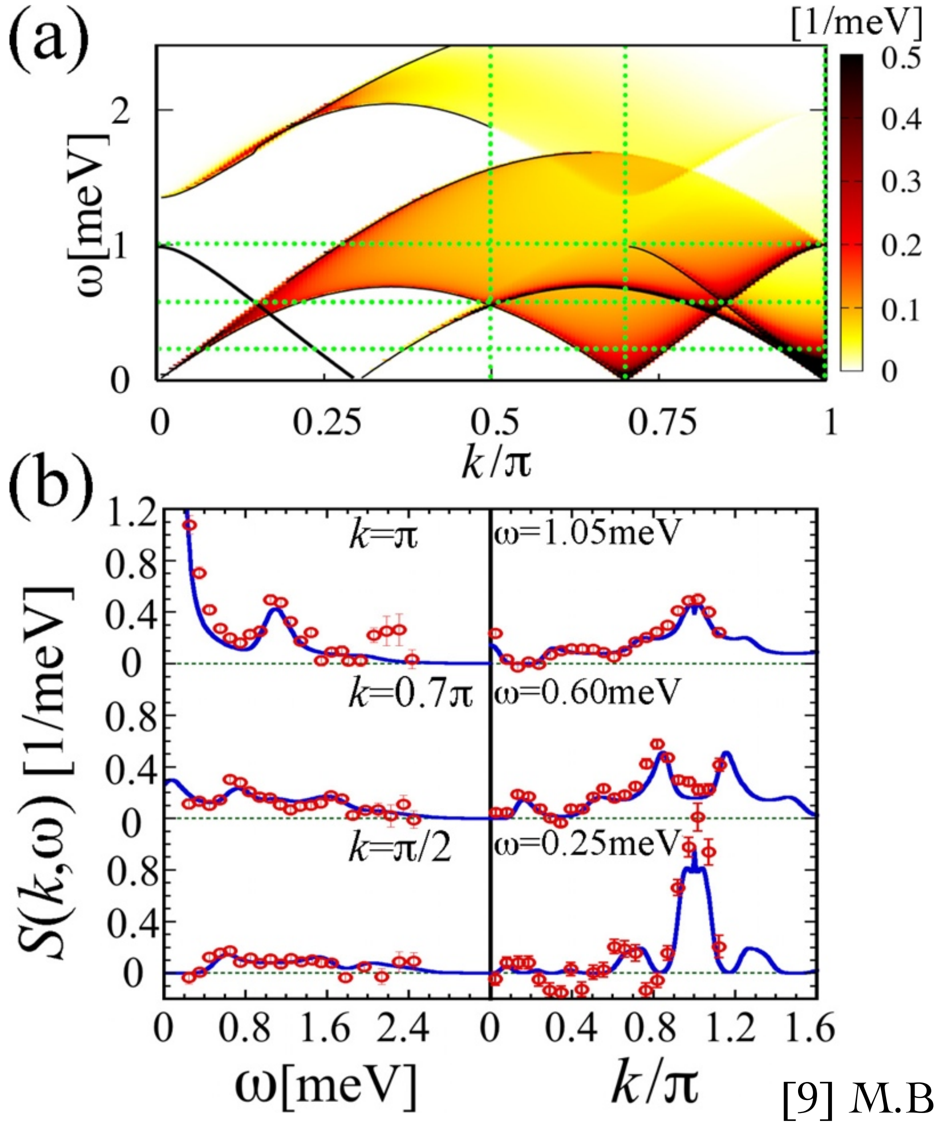



Excitations which satisfy more than 80% of sum rules in $L$=320



# Comparison with experimental results on CuPzN

Experimental results observed in the quasi-one-dimensional antiferromagnet $Cu(C_4H_4N_2)(NO_3)_2$ (CuPzN) in a magnetic field [9] were well explained.



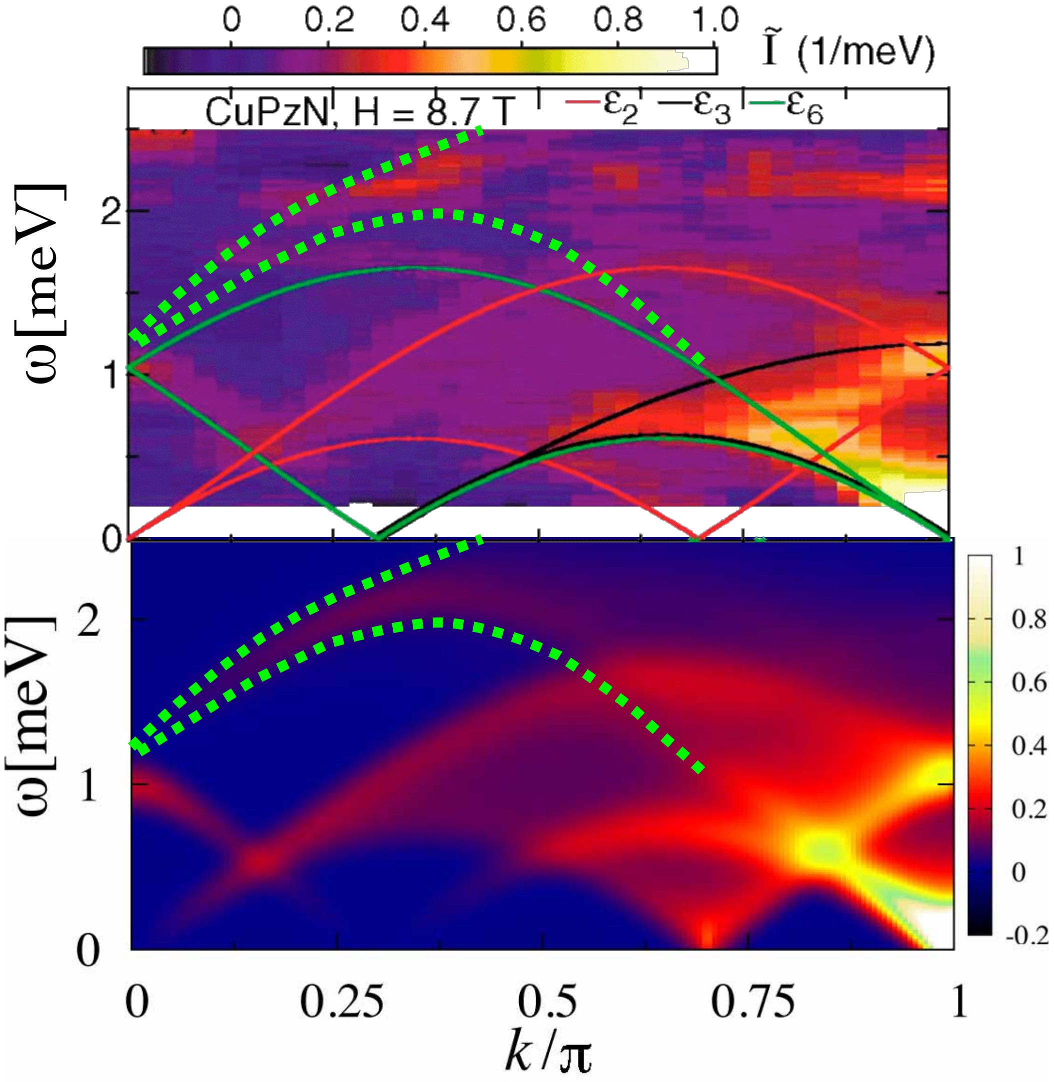

← Present result

— : Present result

○ : Experimental result on CuPzN [9]


[9] M.B.Stone, *et al.*, Phys. Rev. Lett. **91**, 037205 (2003).

# Comparison with experimental results on CuPzN



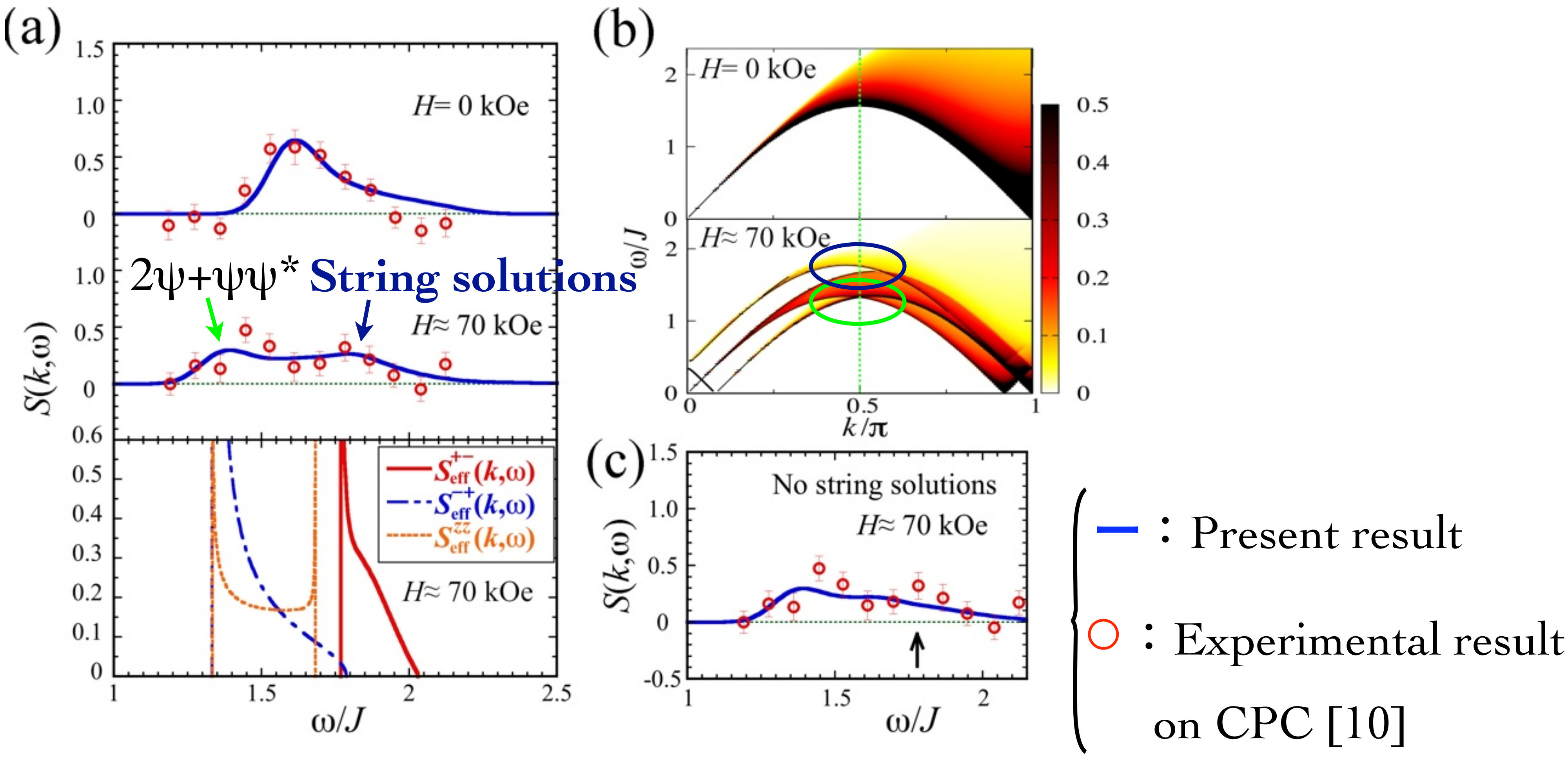

Experimental results on CuPzN [9]

Present result


[9] M.B.Stone, *et al.*, Phys. Rev. Lett. **91**, 037205 (2003).

# Comparison with experimental results on CPC

Experimental results observed in the quasi-one-dimensional antiferromagnet $CuCl_2 \cdot 2N(C_5D_5)$ (CPC) in a magnetic field [10] were also well explained.




[10] I.U. Heilmann *et al.*, Phys. Rev. B **18**, 3530 (1978).

# Summary

Behaviors of dynamical structure factors $S^{+-}(k,\omega)$, $S^{zz}(k,\omega)$, and $S^{-+}(k,\omega)$ of the $S$=1/2 antiferromagnetic Heisenberg chain **in a magnetic field** have been investigated using **exact Bethe-ansatz solutions**.

- **2-string solutions** form a well-defined continuum in $S^{+-}(k,\omega)$.
- This continuum reduces to the **des Cloizeaux-Pearson mode** in the zero-field limit and the **bound states** of overturned spins near the saturation field.
- **Psinon (ψ)** and **antipsinon (ψ*)** can be naturally interpreted as quasiparticles (QPs) in $H$ carrying $\boldsymbol{S^z=+1/2}$ and $\boldsymbol{S^z=-1/2}$, respectively.
- Experimental results on quasi-1D antiferromagnets (CuPzN and CPC) in a magnetic field were reasonably explained.

Not only **ψ** **($S^z$=+1/2)** and **ψ*** **($S^z$=-1/2)** but also QP for a 2-string **($S^z$=-1)** plays an important role for dynamical properties **in a magnetic field**.