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On the possibility to detect the bound state of the Heisenberg ferromagnet at intermediate temperatures

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Outline:

- Bound states in a ferromagnet
- Methods used: thermal DMRG and time-dependent thermal DMRG
- Spin-1/2 FM chain
- Spin-1 FM chain
- Conclusions

Bound state: an well documented feature …

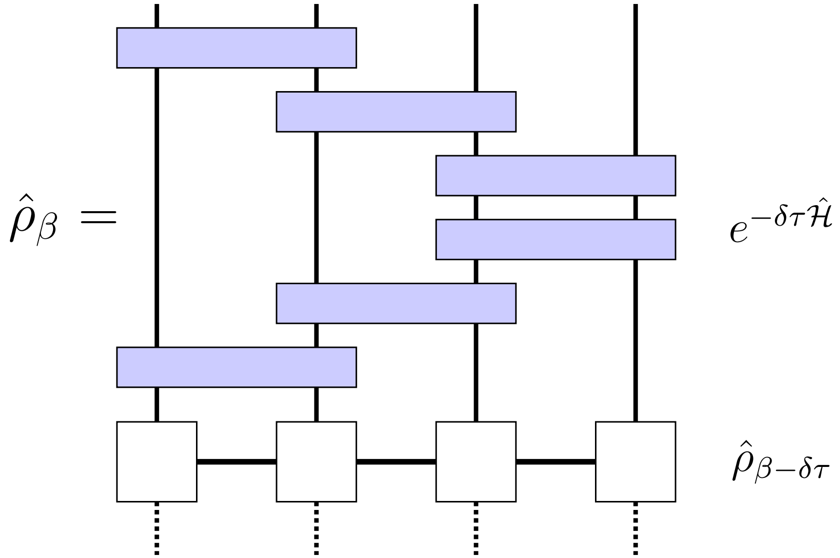
- Already pointed out by Hans Bethe (Journal Z. Physik 71, 205 (1931)),
- Was again revisited with spin wave analysis by F. Dyson (Phys. Rev. 102, 1217(1956))
- A complete bound state computation was done by Wortis (Phys. Rev. 132, 85 (1963))
- Early attempts to observe the bound state by Date, Motokawa (PRL 16,1111(1966)), Torrance and Tinkham (Phys.Rev. 187, 595 (1969)) – but they were indirect detection by studying resonances near k=0.
- Our proposal is to perform the experiment at finite temperature to observe the bound state directly.
- Inelastic Neutron Scattering experiments always observe single spin-flip processes, but are conducted at very low temperatures.
- So finite temperature populates the spin-wave states on which an additional spin-flip results in bound state.

Method

- We start from MPDO ansatz to represent the thermal ensemble where one denotes physical and auxillary degrees of freedom.

$$\rho_\beta = \frac{e^{-\beta\mathcal{H}}}{\mathcal{Z}(\beta)}, \qquad \mathcal{Z}(\beta) = \mathrm{Tr}[e^{-\beta\mathcal{H}}]$$

- From imaginary time evolution Suzuki-Trotter operators, the thermal ensemble is obtained.



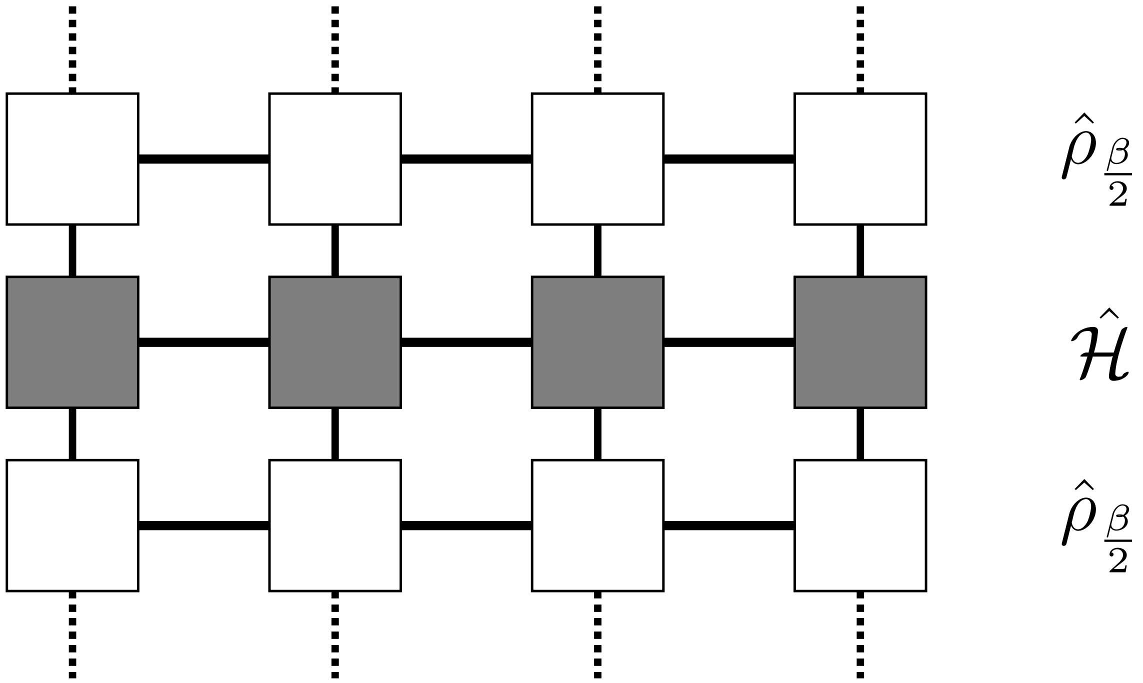
TN diagram showing one iteration of a second order Suzuki Trotter time-evolution scheme

Non exhaustive list of references
F. Verstraete et.al. PRL 93, 207204 (2004)
T. Barthel et. al. PRB 79, 245101 (2009)

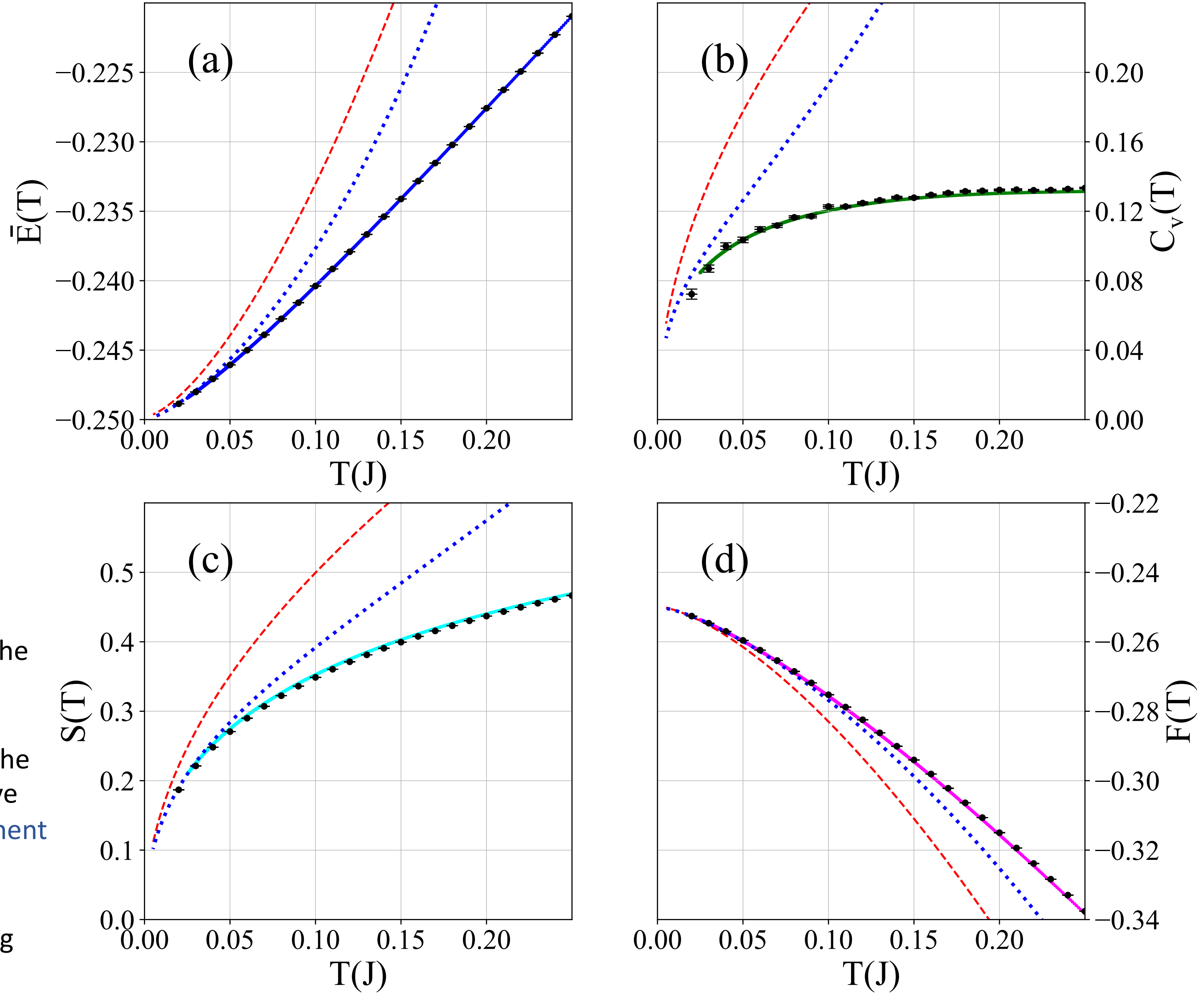
Computing the observables …

- By simply taking the trace over the auxillary indices (dotted legs) , one computes the observables.

$$\langle E \rangle_\beta = \mathrm{Tr}_a \left[\hat{\rho}_\beta \hat{\mathcal{H}} \right] = \mathrm{Tr}_a \left[\hat{\rho}_{\frac{\beta}{2}} \hat{\mathcal{H}} \hat{\rho}_{\frac{\beta}{2}} \right] =$$



Thermodynamics of spin-1/2 Ferromagnet



At low temperatures, the leading order dependency is :

$$S \propto T^{\frac{1}{2}}$$

$$\langle E \rangle - E_0 \propto T^{\frac{3}{2}}$$

$$C_v \propto T^{\frac{1}{2}}$$

*) **Red** dashed line represents the curve due to spin-wave theory.

*) **Blue** dotted line represents the curve due to modified spin-wave theory (Takahashi, PTP supplement 87, 233(1986)).

*) MonteCarlo simulations using ALPS package.

Finite temperature DSF

Dynamical structure factor is fourier transform of time-dependent real space correlations

$$C^{\gamma,\alpha}(i,j;\beta;t) = \mathrm{Tr}\left[\rho_\beta S^\gamma(j;t) S^\alpha(i;0)\right]$$

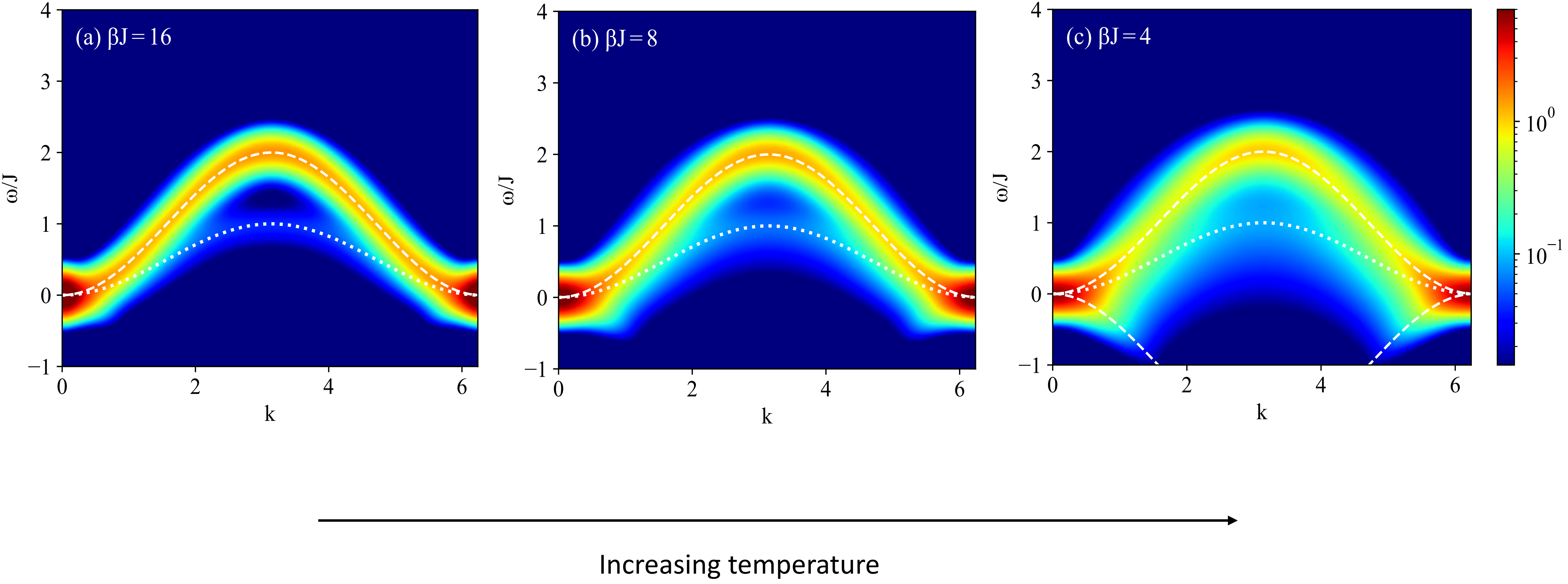
Where, $\gamma, \alpha \in \{z, +, -\}$

Using the cyclicity of Trace and using the Heisenberg picture, one finds it is equivalent to :

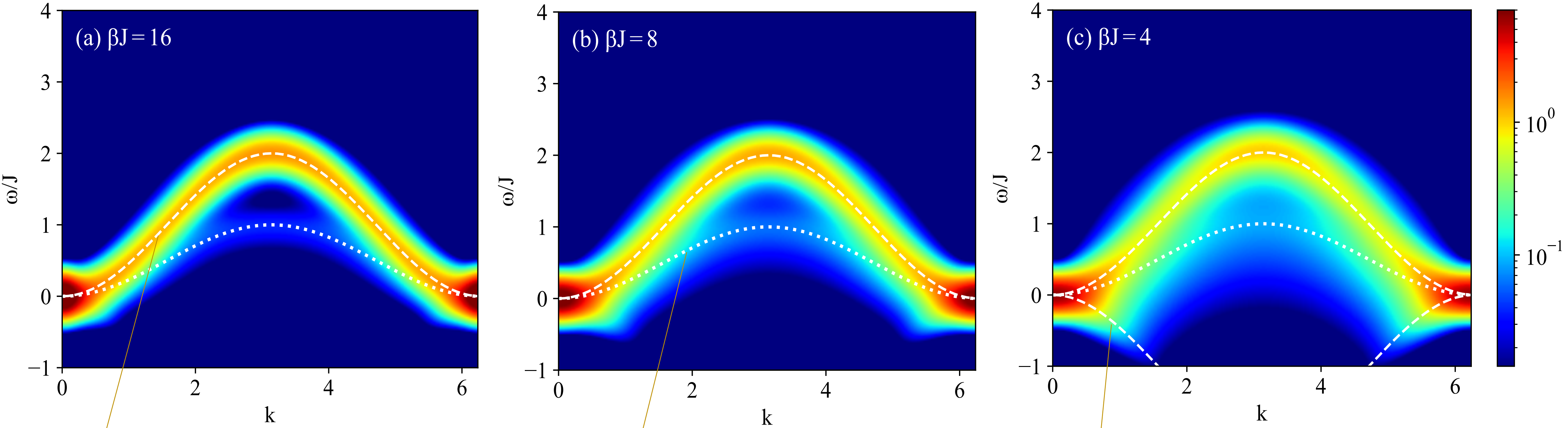
$$C^{\gamma,\alpha}(i,j;\beta;t) = \mathrm{Tr}\left[\rho_{\frac{\beta}{2}} S^\gamma(j) S^\alpha(i) e^{-iHt} \rho_{\frac{\beta}{2}} e^{iHt}\right]$$

So one computes the thermal density matrix upto half the inverse temperature instead of full computation, and one needs then real time evolution

Spin-1/2 FM chain



Spin-1/2 FM chain



$J(1-\cos k)$

Spinwave dispersion

$\frac{J}{2}(1-\cos k)$

Bound state dispersion

$-J(1-\cos k)$

De-excitation from spinwave to aligned state

Characterizing the bound state

- Maximum distance between the bound state and the spinwave excitation is at $k = \pi$.

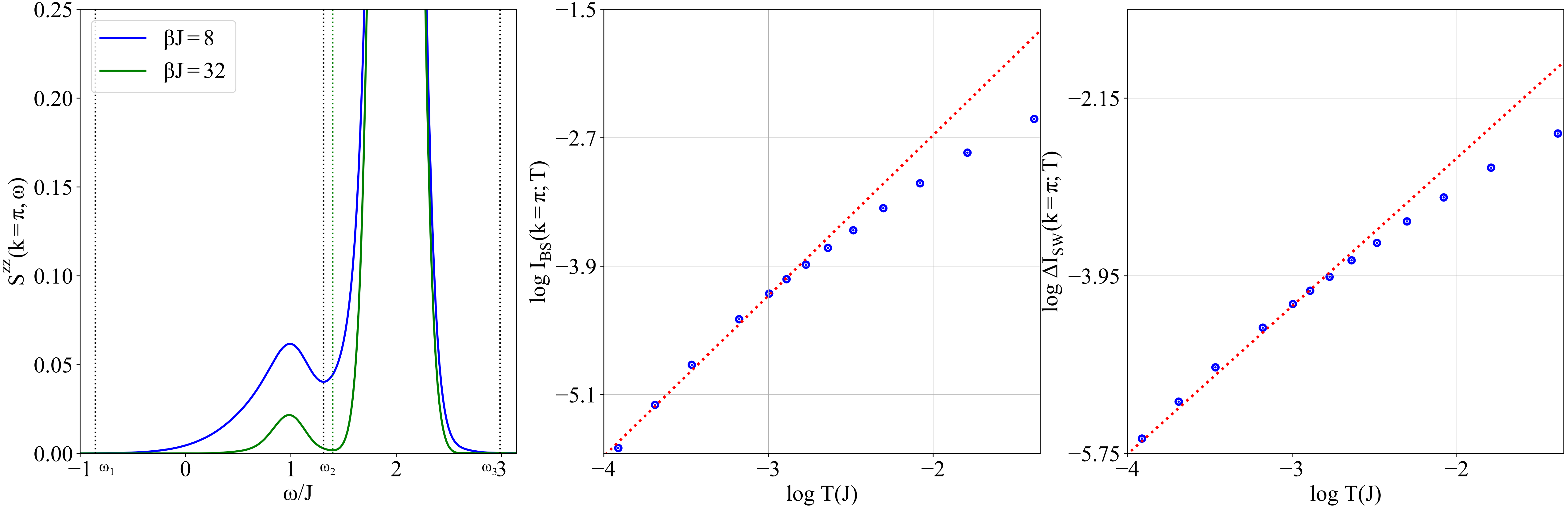
- Finite temperature results in more spectral weights to the bound state but at the same time there is thermal broadening of the mode too.

- We compared the section cuts at $k = \pi$ and decided the lower bound of the temperature when the bound state spectral weight is 5% of the total spectral weight in the DSF section cut.

- Therefore, the best possibility to observe it is between J/12 < T < J/3.

Characterizing the bound state (contd.)

- Varying the temperature shows a dependency of spectral weights of bound state as $T^{3/2}$.



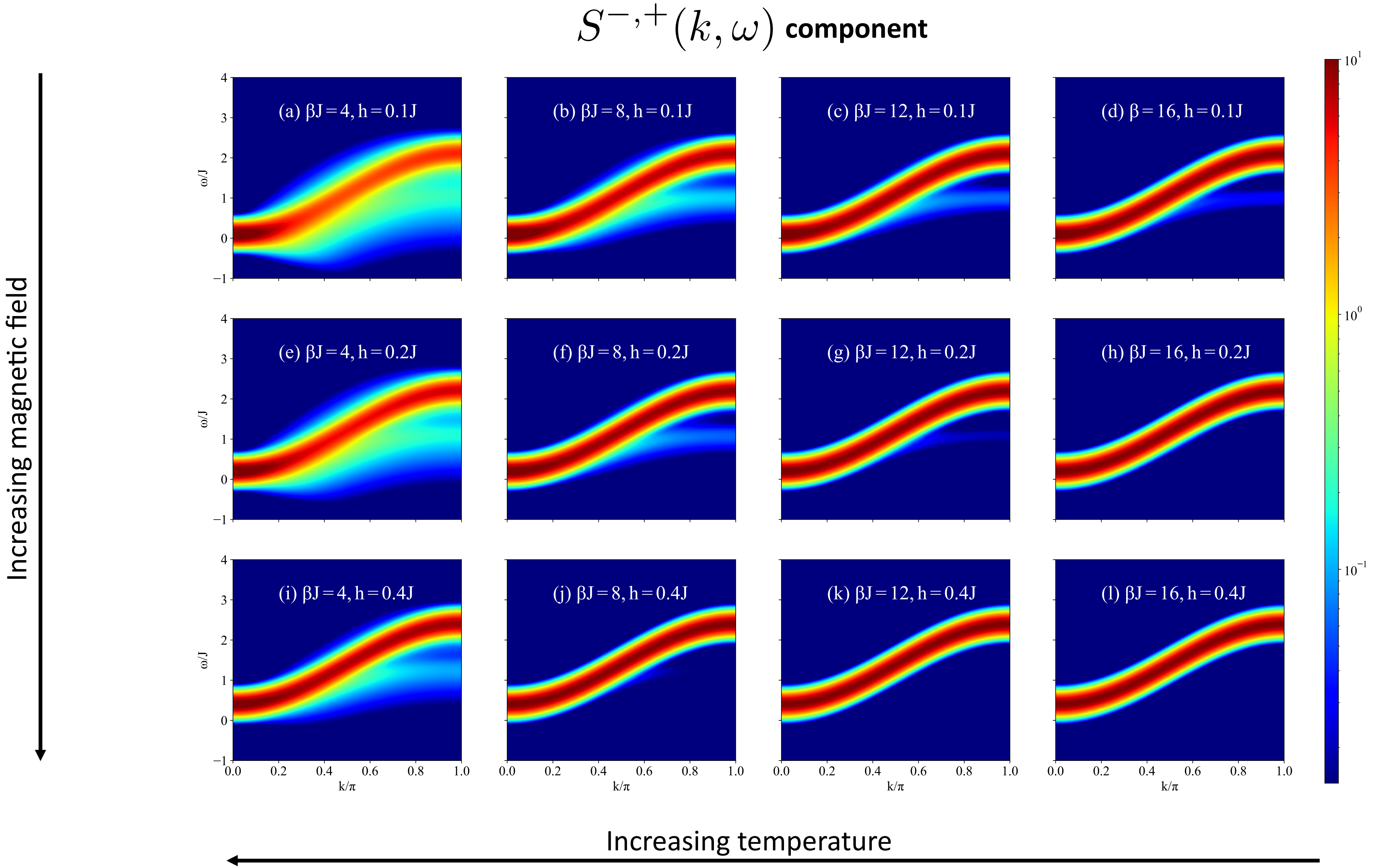
In presence of magnetic field ..

- The model loses its isotropy.

$$H = -J \sum_i \mathbf{S}_i \cdot \mathbf{S}_{i+1} - h \sum_i S_i^z \qquad (J = 1)$$

- Spectral weights of the bound state is present in the transverse component of the DSF.

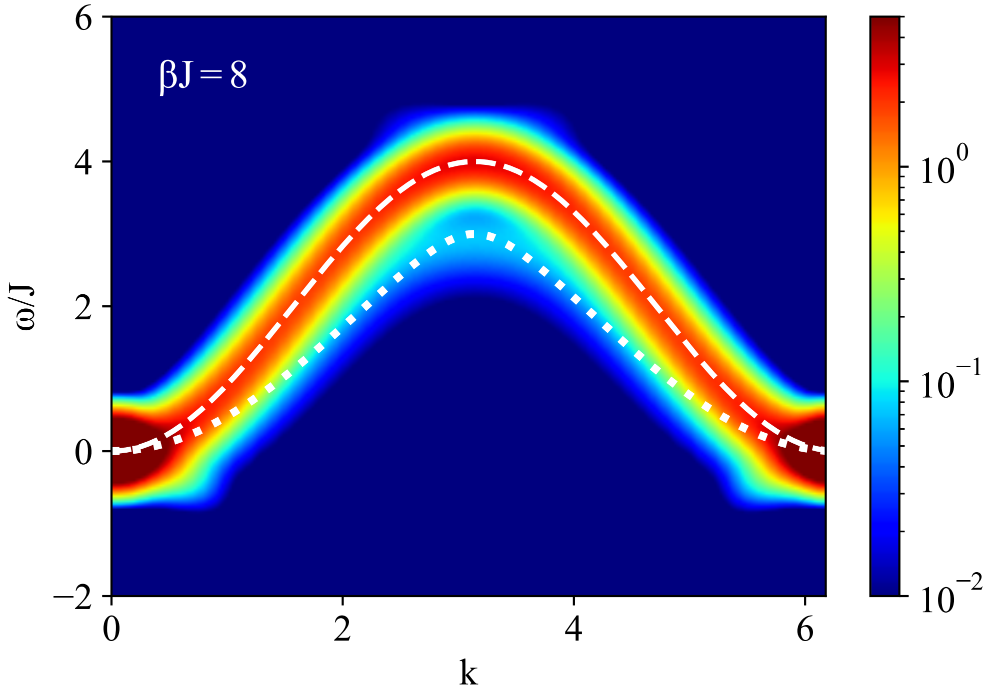
- The spectral weights in the longitudinal component DSF is mostly concentrated at $\mathrm{k} = 0, \omega = 0$.

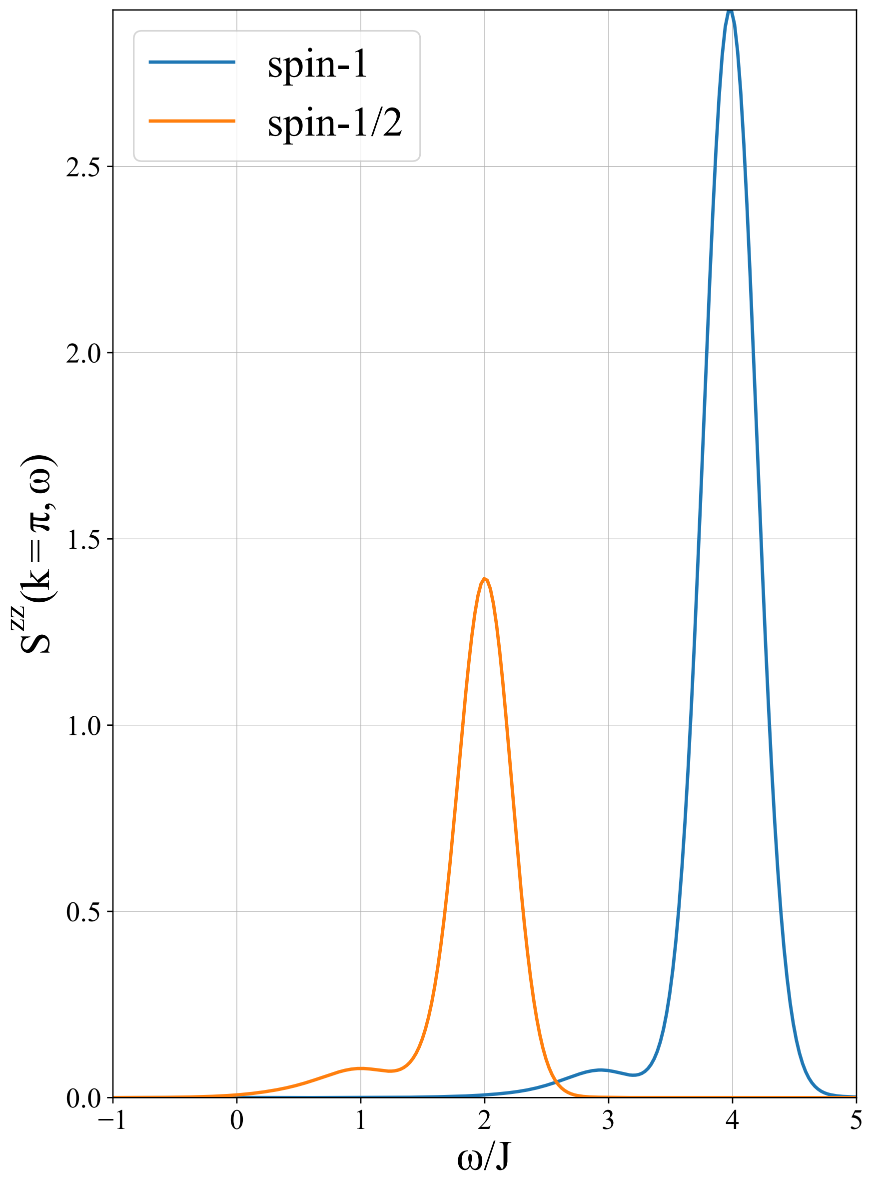


$S^{-,+}(k,\omega)$ component
Increasing magnetic field
Increasing temperature
(a) βJ = 4, h = 0.1J
(b) βJ = 8, h = 0.1J
(c) βJ = 12, h = 0.1J
(d) β = 16, h = 0.1J
(e) βJ = 4, h = 0.2J
(f) βJ = 8, h = 0.2J
(g) βJ = 12, h = 0.2J
(h) βJ = 16, h = 0.2J
(i) βJ = 4, h = 0.4J
(j) βJ = 8, h = 0.4J
(k) βJ = 12, h = 0.4J
(l) βJ = 16, h = 0.4J
ω/J
k/π
10^{1}
10^{0}
10^{-1}

Spin-1 FM chain

- Similar to spin-1/2 FM chain, we also find the bound states in the finite-temperature DSF.
- In the section cut, one can compare the bound state spectral peak sizes as compared to main spin-wave excitation of spin-1/2 and spin-1 FM chain.





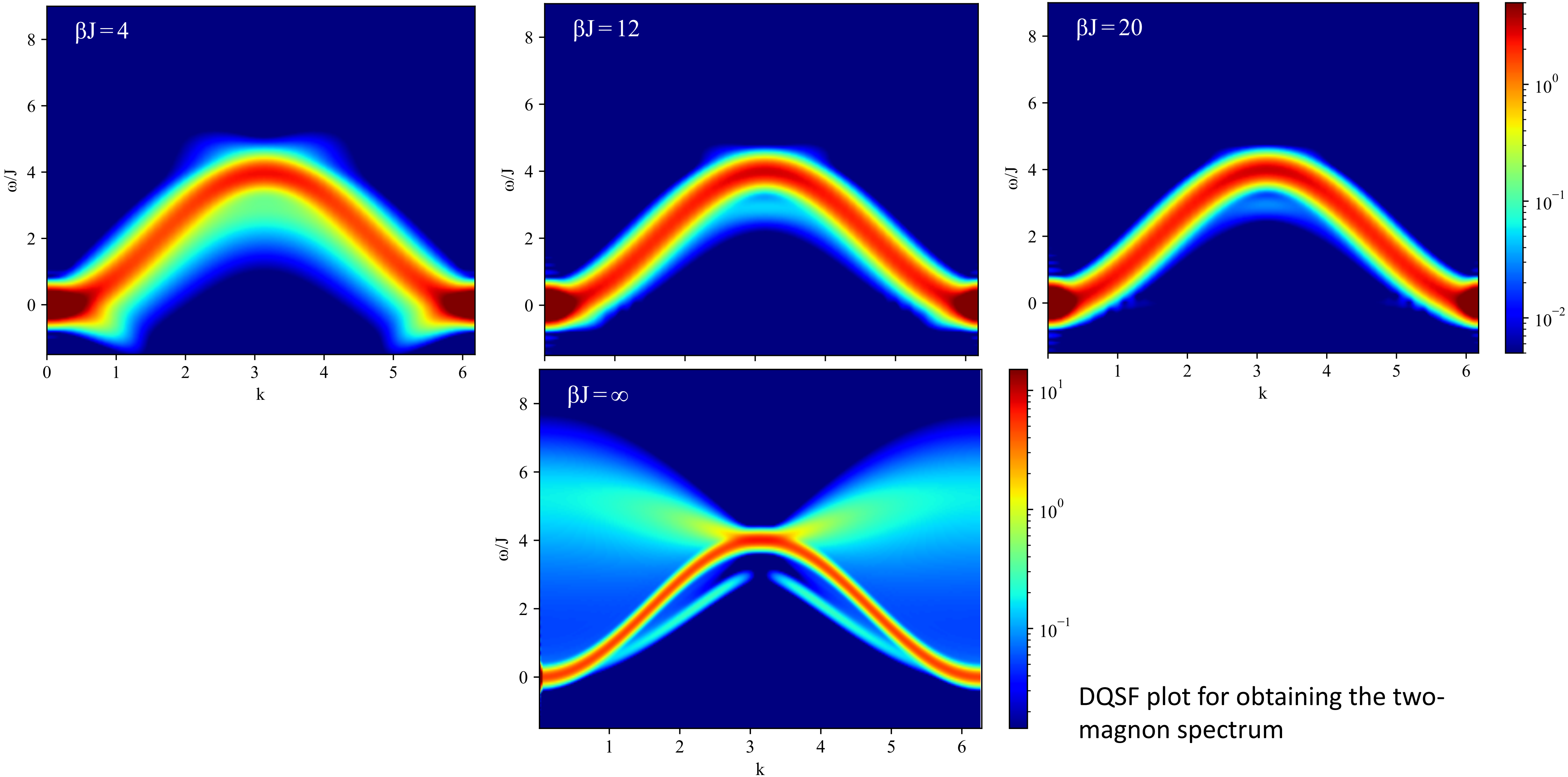
Quadrupolar structure factor (DQSF)

- In order to access the two magnon spectrum (at 0K) of spin-1 FM chain, quadrupolar structure factor should be computed.
- There are 3 components – i) Longitudinal, ii) Transverse , and iii) Pairing component. They are the same in an isotropic model.
- So , we focus only on Pairing component.

$$C_{Q,2}(i,j;t) = \frac{1}{2}\left[\langle \big(S^-(j;t)\big)^2 \big(S^+(i)\big)^2 \rangle + \mathrm{h.c.}\right]$$

- Fourier transform of this component leads to the Quadrupolar Structure Factor.

Comparison between zero and finite temperature

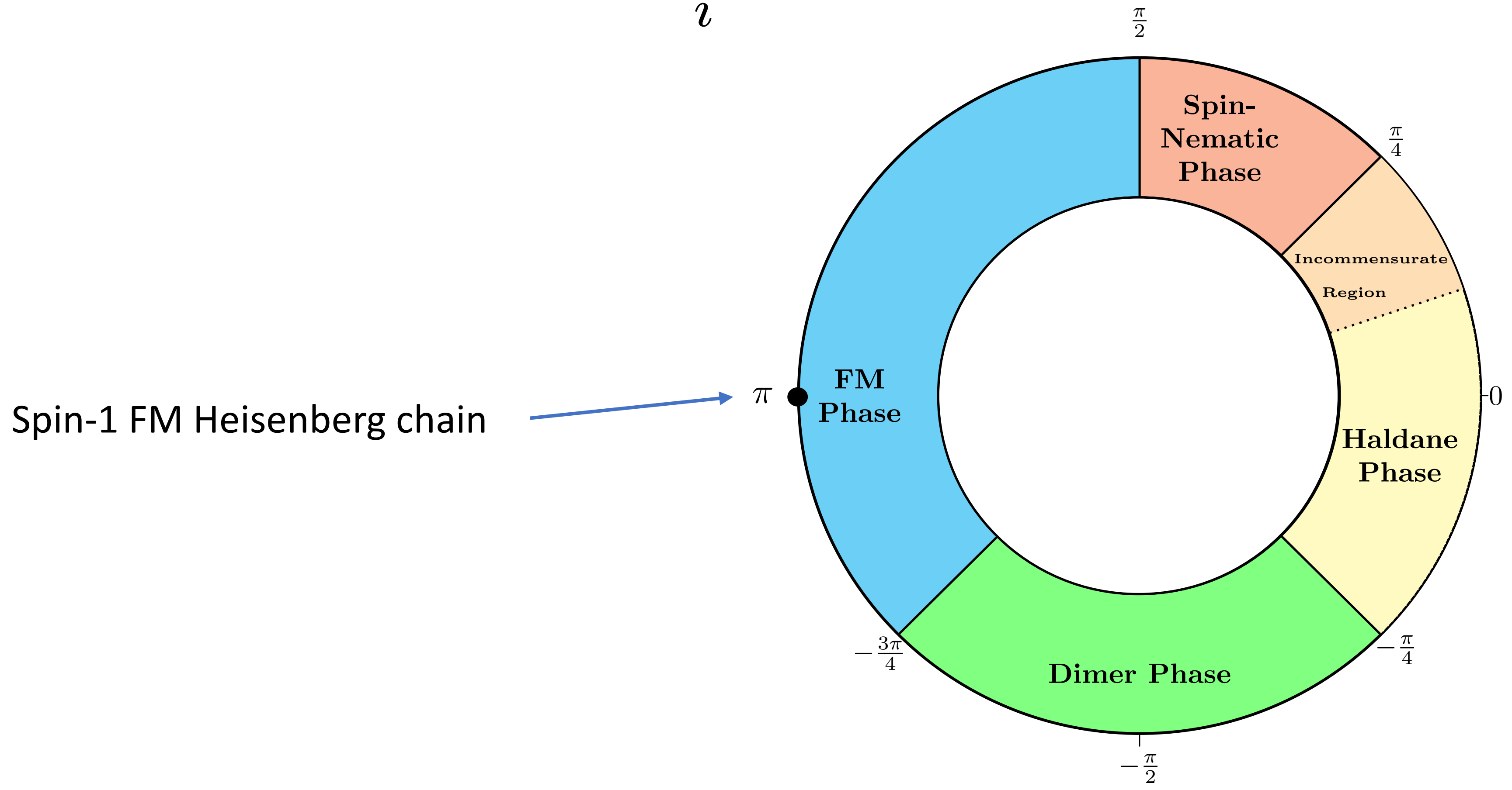


DQSF plot for obtaining the two-magnon spectrum

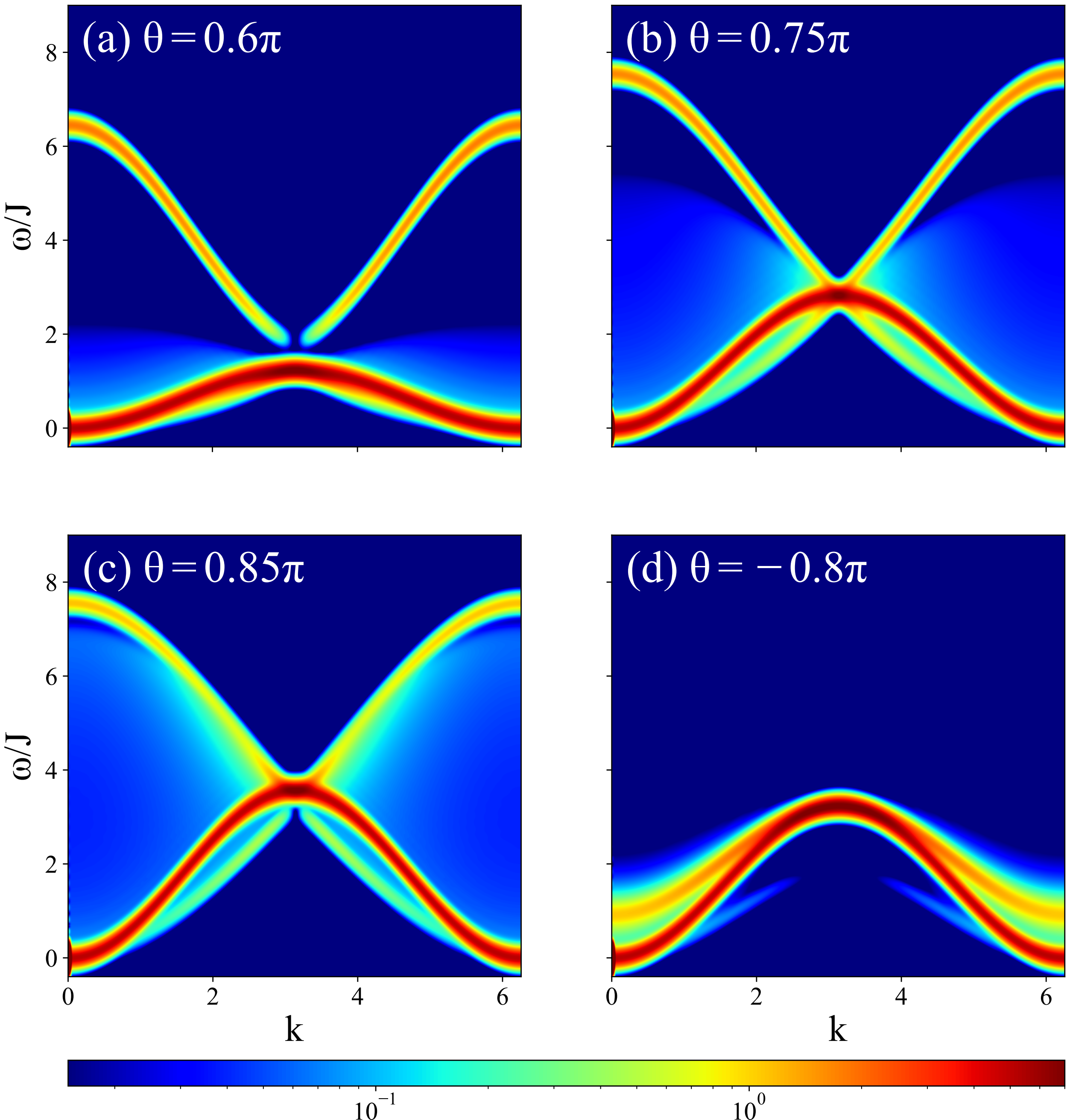
In order to understand the resonance …

- Consider n.n. biquadratic interactions along with the existing Heisenberg interactions

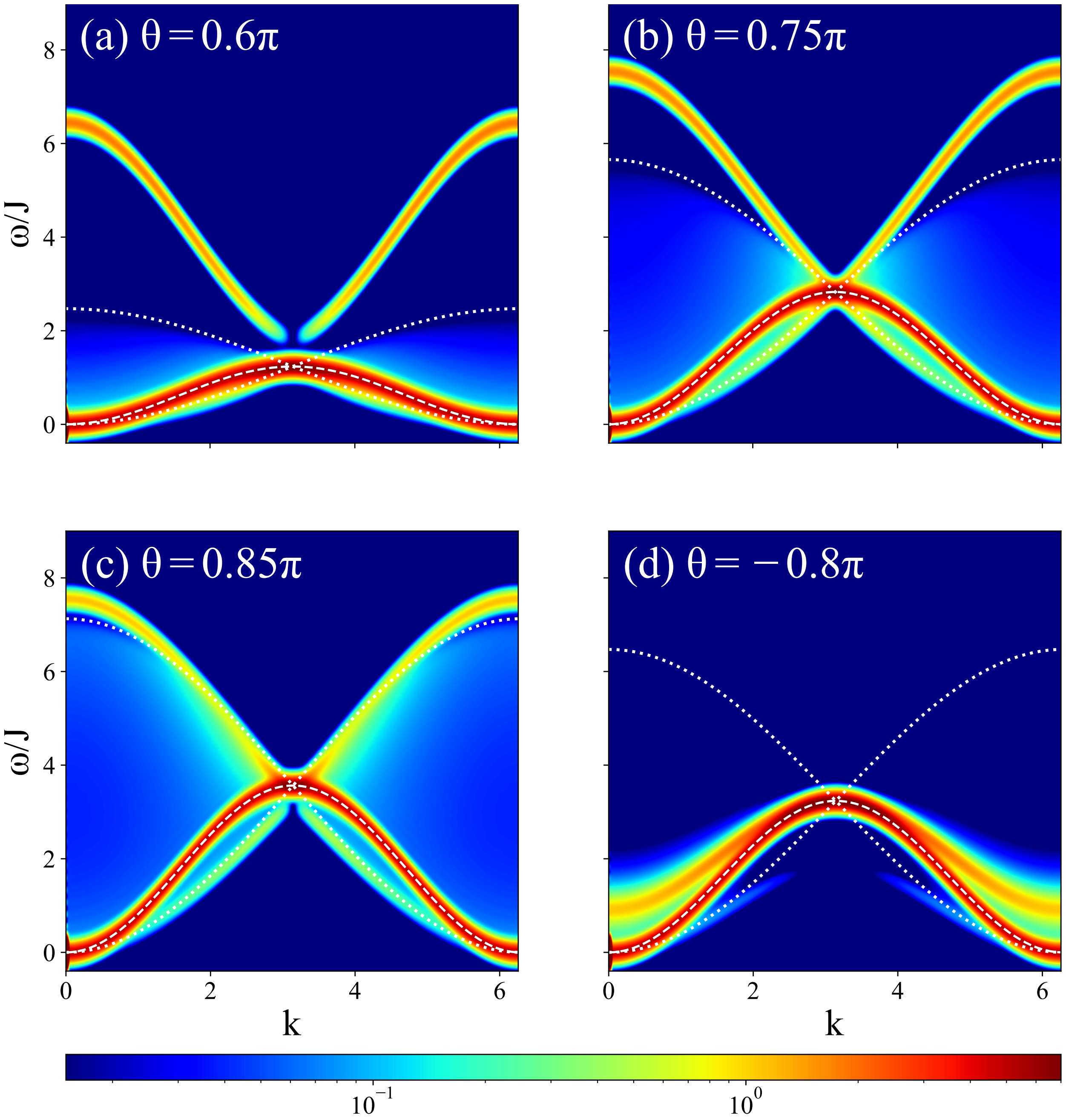
$$\mathcal{H}_{\mathrm{BLBQ}} = J \sum_i \cos\theta \mathbf{S}_i \cdot \mathbf{S}_{i+1} + \sin\theta (\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2$$



Two magnon spectrum of BLBQ chain in FM phase

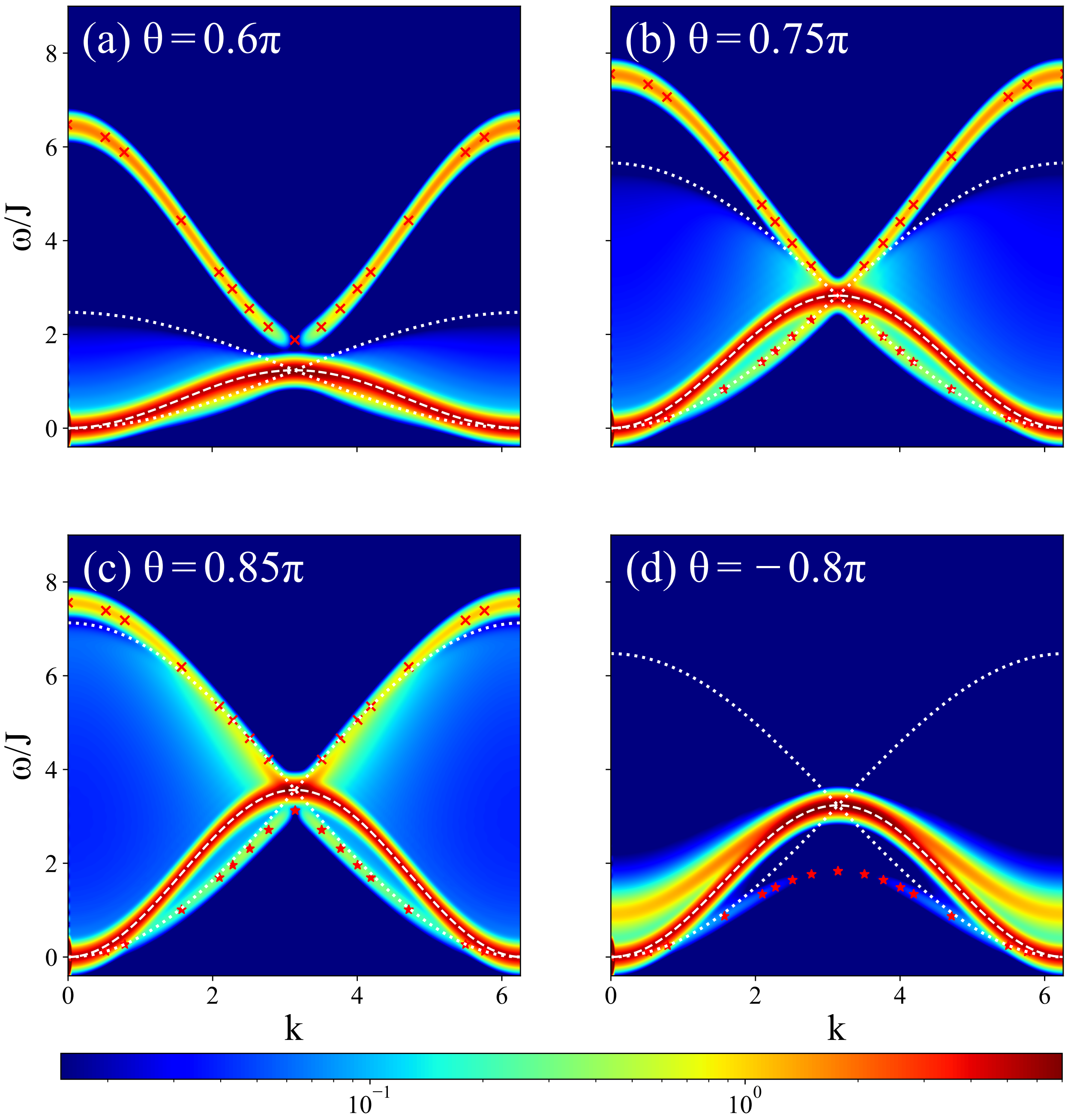


Two magnon spectrum of BLBQ chain in FM phase



Just considering spin-waves on ferromagnets

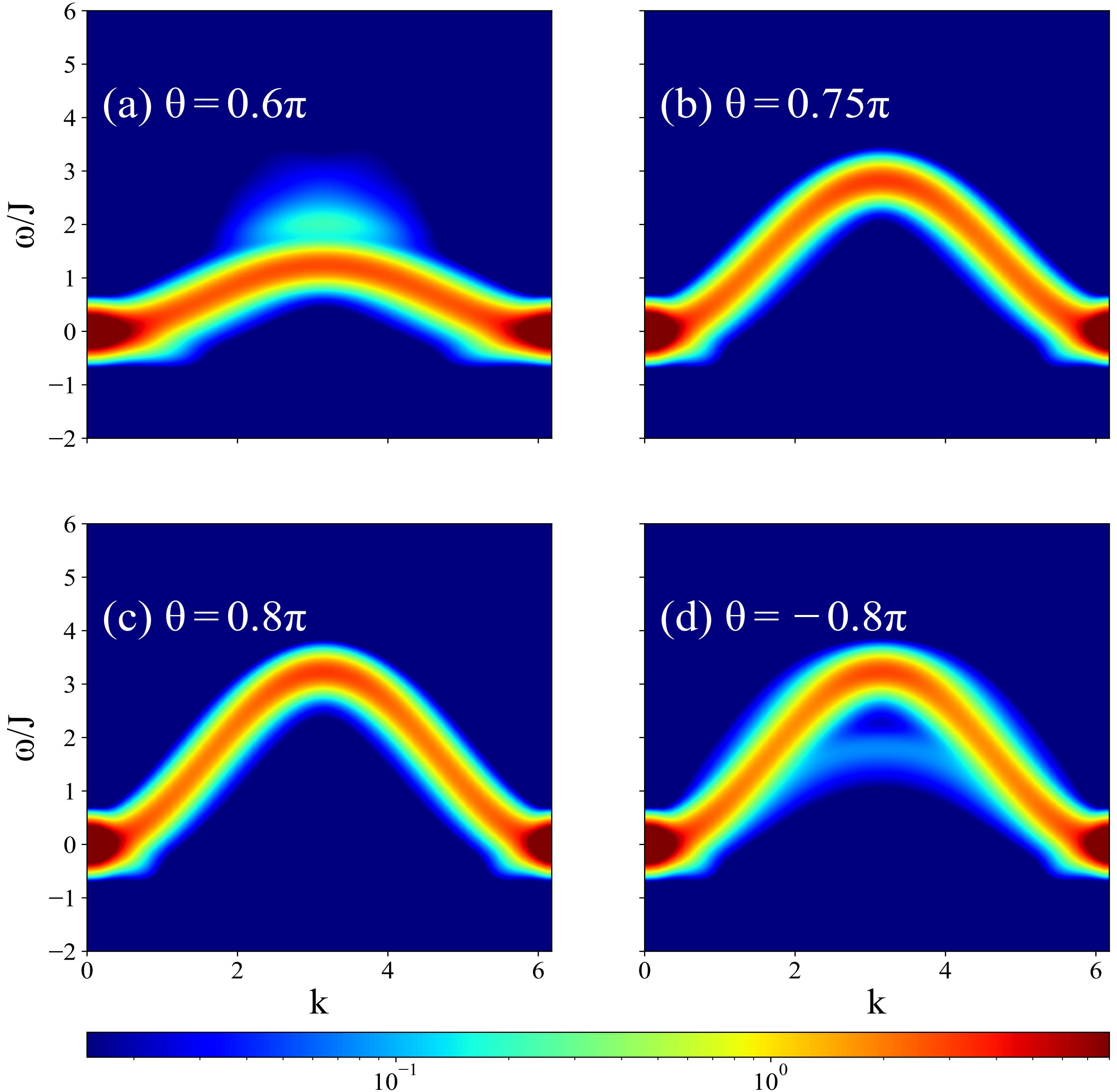
Two magnon spectrum of BLBQ chain in FM phase



Bound states (stars) and anti-bound states (crosses) using Wortis's method (1963)

BLBQ chain's finite temperature simulations

- Just for completeness, note the effect of finite temperature on the BLBQ chain.
- We compare the effect of biquadratic interaction on the the thermal DSF. The finite temperature ensemble is at T = J/10.



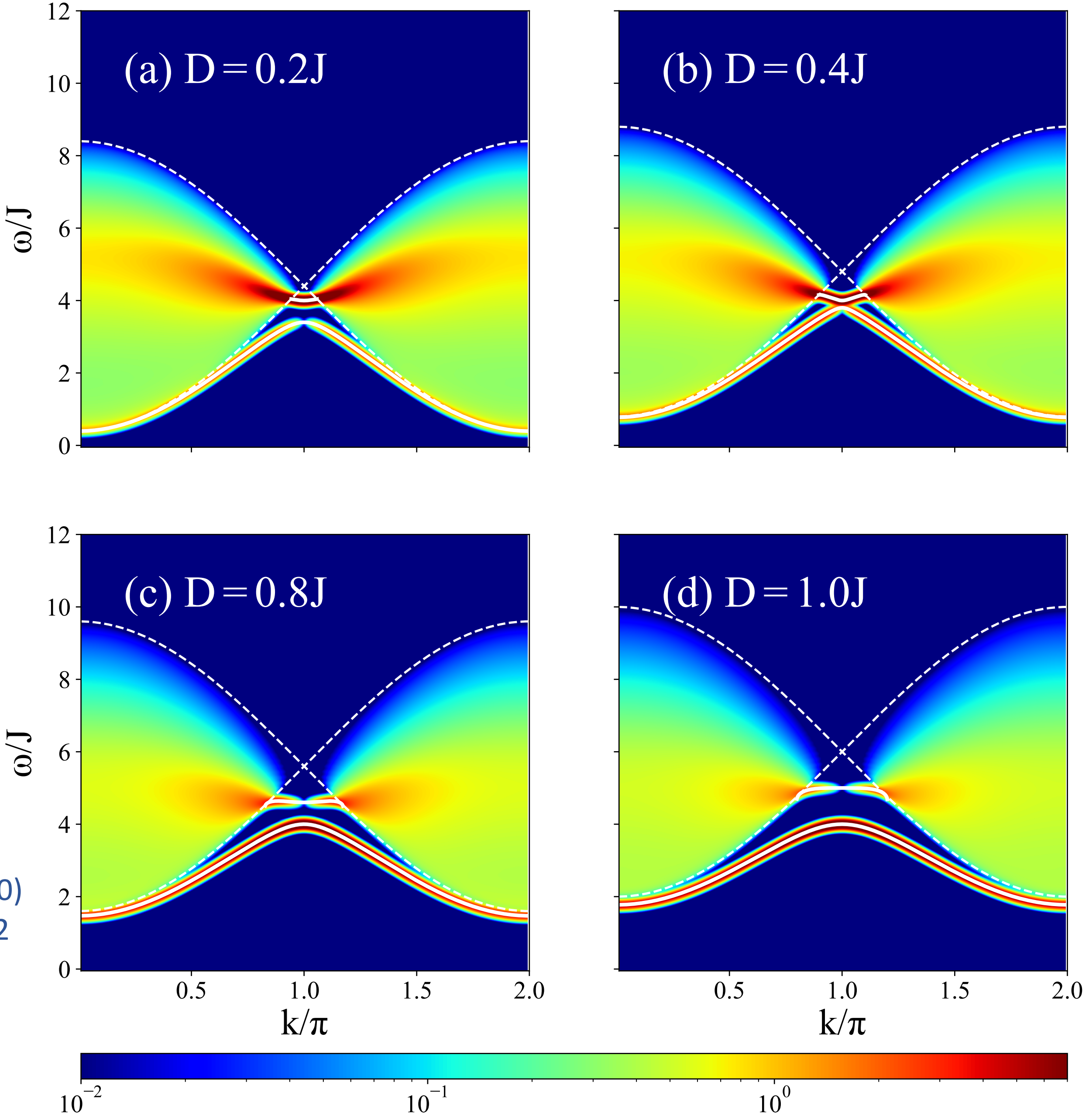
In real materials …

- Often, in real materials that are modelled after spin-1 Heisenberg model also include easy axis single-ion anisotropy interaction.

$$H = -J \sum_i \mathbf{S}_i \cdot \mathbf{S}_{i+1} - D \sum_i (S_i^z)^2 \qquad (J = 1, D > 0)$$

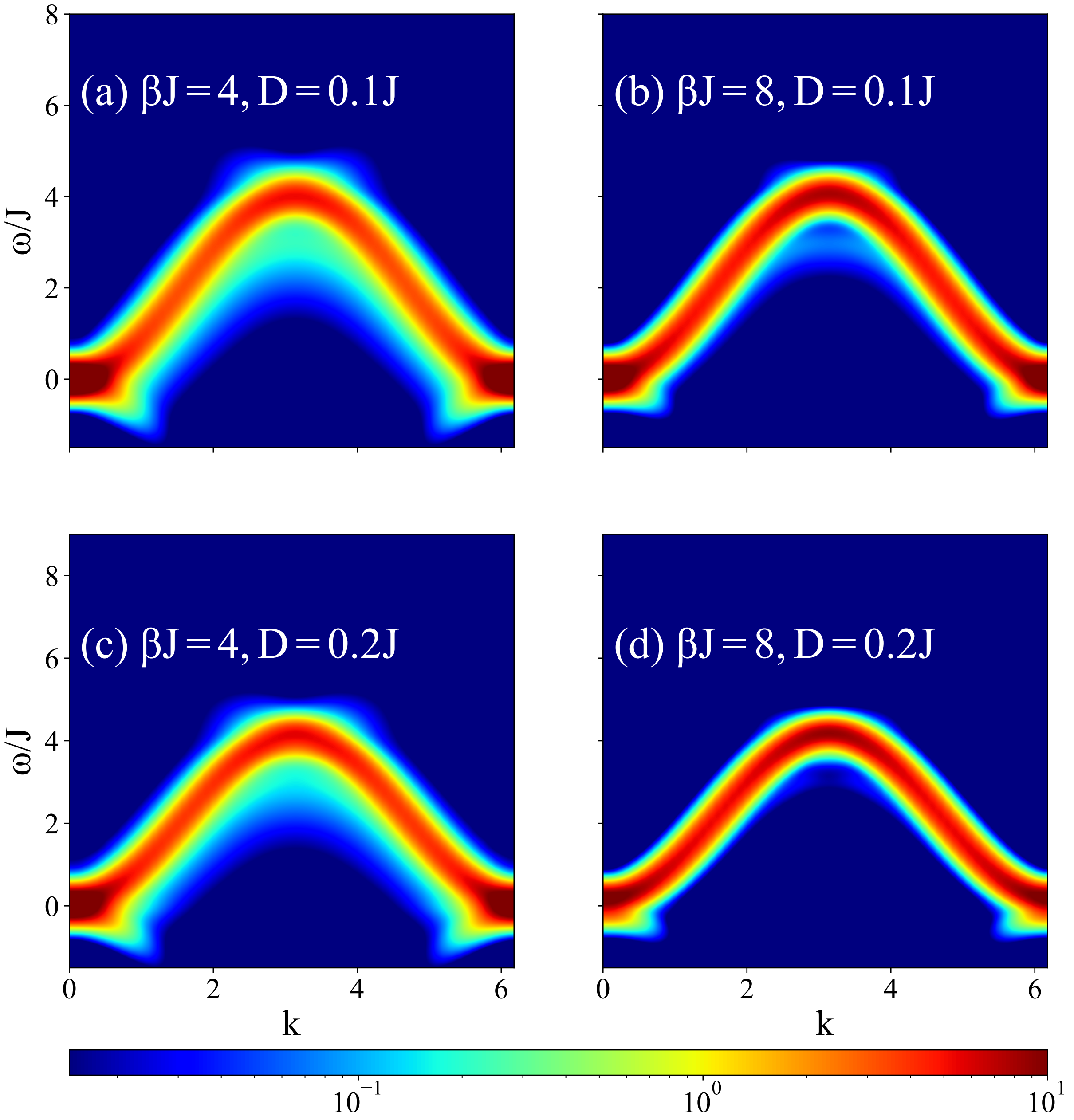
Zero temperature results

The three components of the DQSF are no longer same. We focus on pairing component which captures the spectral weight on the bound states.



R. Silberglitt and J. B. Torrance, PRB 2, 772 (1970)
N. Papanicolaou and G. C. Psaltakis, PRB 35, 342 (1987)

Finite temperature effects



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

Conclusion

- Upon exploring the realistic scenarios of ferromagnetic spin chains, we propose that the best possibility to observe the bound state is in spin-1/2 chain compound.
- The early Neutron Scattering experiments were conducted at low temperatures infact , experiment at T=J/16 had been conducted but our numerical simulations indicate that if an experiment is conducted above T > J/12, the bound state could possibly be detected.

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Short- and long-range correlations in the $S=\frac{1}{2}$ ferromagnetic chain system $(C_6D_{11}ND_3)CuBr_3$

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Thank you