Magnetic and Charge response of Kitaev's spin liquid

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Topological Materials Science

トポロジーが紡ぐ物質科学のフロンティア

M. Udagawa, in preparation

S. Takayoshi, T. Oka and M. Udagawa, in preparation

Outline:

I. Introduction

– Kitaev's honeycomb model

II. Model & Method

– Classical Monte Carlo simulation with parity fixing

– Analytical solution of the real-frequency dynamical correlation

III. Results

– Dynamical magnetic structur efactor of chiral spin liquid phase

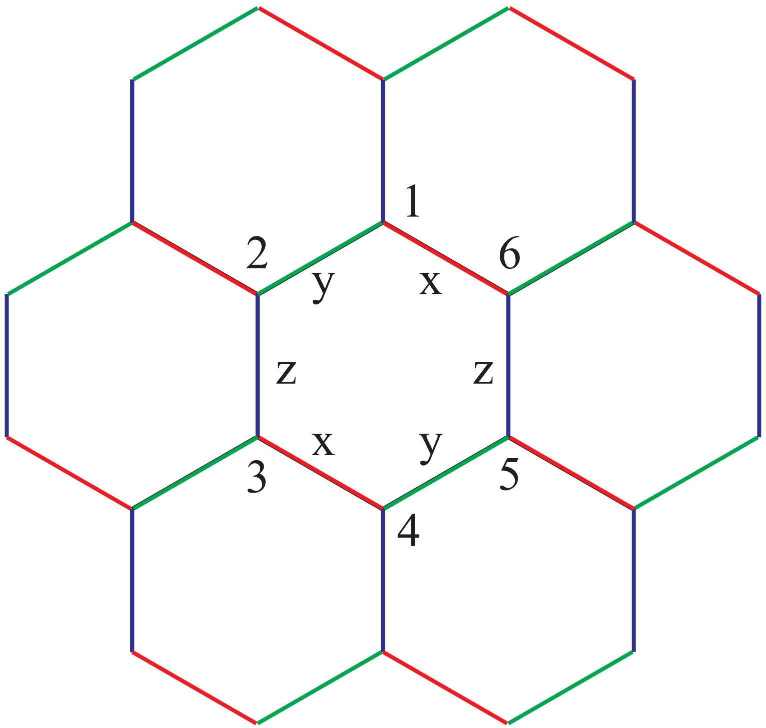
– Detection and control of Visons with local charge probe

IV. Discussions & Summary

Introduction

Introduction: Kitaev's honeycomb model

$$\mathcal{H} = -J_{\mathrm{K}} \sum_{i \in A-\mathrm{sub.}} s_i^x s_{i+x}^x + s_i^y s_{i+y}^y + s_i^z s_{i+z}^z$$



Introduction: Energy level of Kitaev's model

$$\mathcal{H} = \frac{i}{4} J_{\rm K} \sum_{i \in A} (u_i^x c_i c_{i+x} + u_i^y c_i c_{i+y} + u_i^z c_i c_{i+z}).$$

– Z_2 flux $W_p = \pm 1 \to$ gauge fields $u_i^\alpha = \pm 1$

– Ground state

$W_p = +1$ everywhere

c.f. E. Lieb, Phys. Rev. Lett. **73**, 2158 (1994).

– Two types of excitations

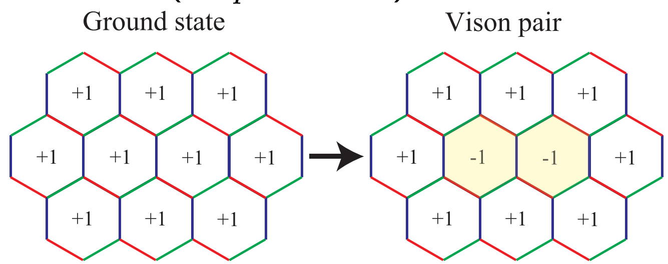
(Bogoliubov) fermion: $c_i \to \gamma_m$

Vison: $W_p = -1$ (π-vortex)

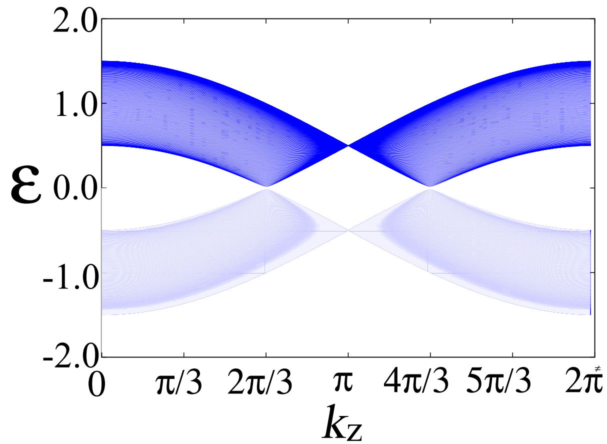
– fermionic spectrum

half of Graphene

– Vison ($W_p = -1$)



– fermion (flux free sector)

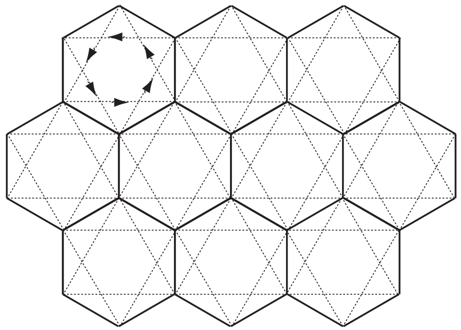


Introduction: Chiral spin liquid phase

– Kitaev's model under magnetic field ∥ [111] ($\kappa \propto H^3$)

$$\mathcal{H} = \mathcal{H}_{\text{Kitaev}} - h \sum_i (\sigma_i^x + \sigma_i^y + \sigma_i^z)$$

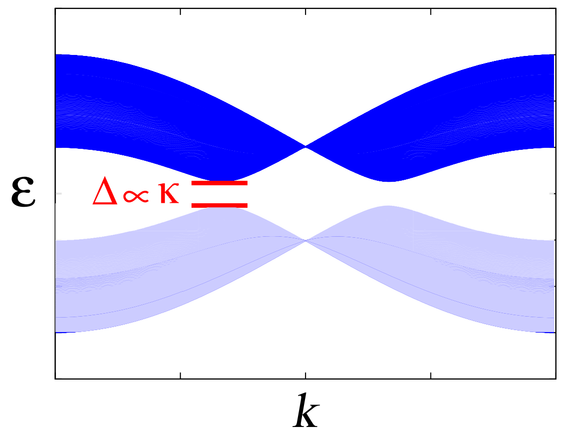
$$\rightarrow \mathcal{H}_{\text{eff}} = \frac{i}{4} J \sum_{n.n.} c_i c_j + \frac{i}{4}\kappa \sum_{n.n.n.} c_i c_j. \quad (\kappa \propto h^3)$$

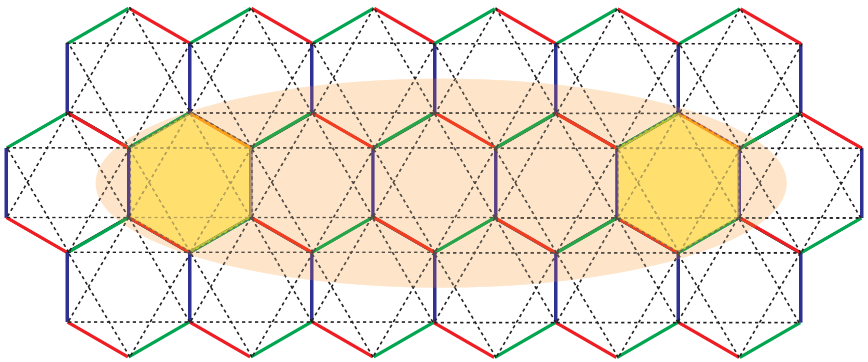


– Majorana Haldane model → Chiral spin liquid

half-integer quantized κ_{xy}

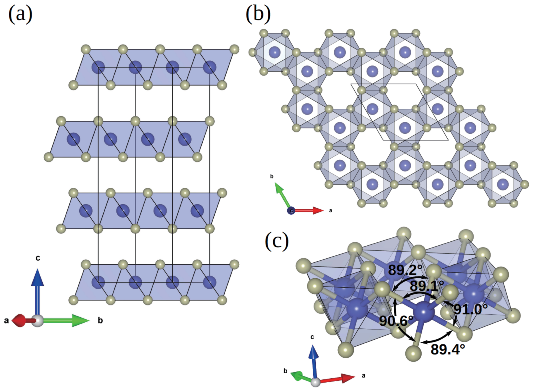
one zero mode shared by two distant Visons !



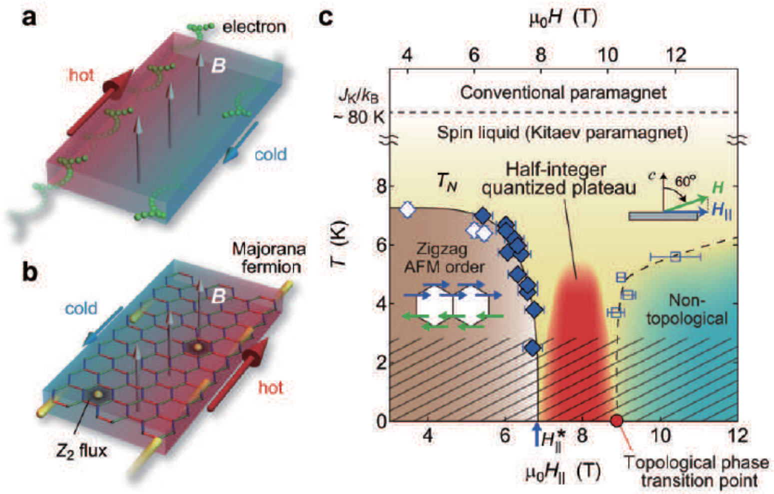


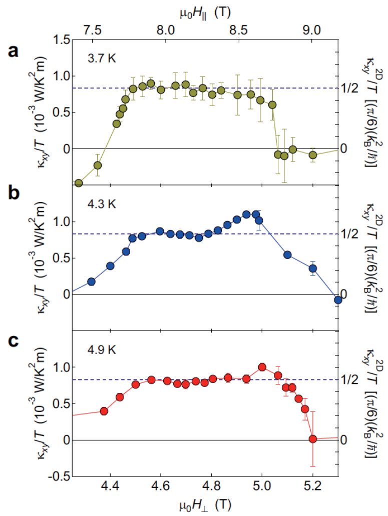
Introduction: Thermal Hall conductivity

– Half-integer quantization of thermal Hall conductivity: $\kappa_{xy}/T = \frac{\pi^2}{6}\frac{k_B^2}{h}$



K. W. Plumb et al., PRB (2014)





K. Kasahara et al. (2018)

– Integer quantum Hall effect + Wiedemann-Franz law

$$\sigma_{xy} = \frac{e^2}{h} \rightarrow \kappa_{xy}/T = \frac{\pi^2}{3}\left(\frac{k_B}{e}\right)^2 \sigma_{xy} = \frac{\pi^2}{3}\frac{k_B^2}{h}$$

Motivation:
– direct evidence of excitation desirable → Majorana zero mode

Model & Method

Model & Method: Classical Monte Carlo method

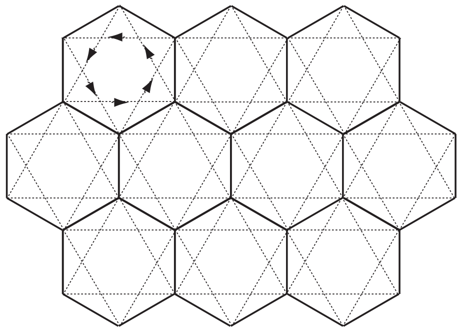
– Kitaev's model on a honeycomb lattice ($2 \times N \times N$ sites)

$$\mathcal{H}[\{W_p\}] = \frac{i}{4} J_{\rm K} \sum_{i \in A} (u_i^x c_i c_{i+x} + u_i^y c_i c_{i+y} + u_i^z c_i c_{i+z}) + \frac{i}{4}\kappa \sum_{\langle i,j \rangle_{2nd}} c_i c_j$$

$$(J_{\rm K} = 1 : \text{ferromagnetic})$$

– Sampling $N^2 + 1$ conserved Z_2 fluxes: $\{W_p\}$:

$$\langle \mathcal{O} \rangle = \sum_{\{W_p\}} \frac{{\rm Tr}_{\rm c}[e^{-\beta \mathcal{H}[\{W_p\}]}]}{Z} \frac{{\rm Tr}_{\rm c}[e^{-\beta \mathcal{H}[\{W_p\}]}\mathcal{O}]}{{\rm Tr}_{\rm c}[e^{-\beta \mathcal{H}[\{W_p\}]}]}.$$



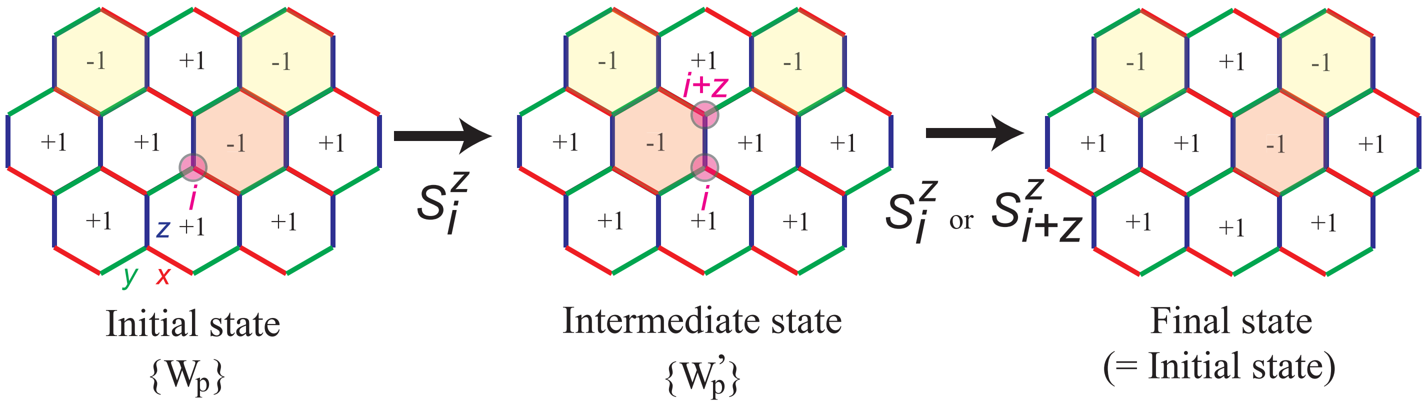
c.f. MC based on Jordan-Wigner transformation

J. Nasu, M. U. and Y. Motome, Phys. Rev. Lett. **113**, 197205.

Model & Method: Dynamical spin correlation

$$\mathcal{C}_{ij}^{\alpha\beta}(\omega) = \int_0^\infty dt\ e^{(i\omega-\delta)t}\langle s_i^\alpha(t) s_j^\beta(0)\rangle$$

$$= \frac{1}{4}\delta_{\alpha\beta}(\delta_{i,j} - iu_i^\alpha \delta_{i+\alpha,j}) \int_0^\infty dt\ e^{(i\omega-\delta)t}\langle e^{iH[\{W_p\}]t} c_i e^{-iH[\{W_p'\}]t} c_{i+\alpha}\rangle.$$



– s_i^α changes fluxes on the both sides of α-bond from site i

– Spin correlation finite at most to nearest-neighbor

Model & Method: Analytical expression

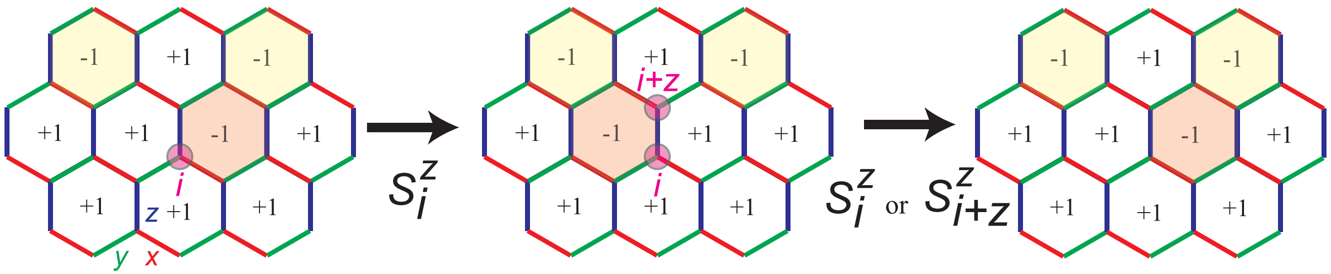
$$\langle s_i^\alpha(t) s_j^\beta(0)\rangle = \frac{1}{4}\delta_{\alpha\beta}(\delta_{i,j} - iu_i^\alpha \delta_{i+\alpha,j})\langle e^{iH[\{W_p\}]t} c_i e^{-iH[\{W_p'\}]t} c_j\rangle.$$

$$= \frac{1}{2\sum_{\{W_p\}} Z[\{W_p\}]} \sum_{\{W_p\}} \Big(\sqrt{\det(1 + e^{-(\beta-it)\cdot iA} e^{-it\cdot iA'})}\Big[\frac{1}{1 + e^{-(\beta-it)\cdot iA} e^{-it\cdot iA'}} e^{-(\beta-it)\cdot iA}\Big]_{ji}$$

$$- (-1)^F \sqrt{\det(1 - e^{-(\beta-it)\cdot iA} e^{-it\cdot iA'})}\Big[\frac{1}{1 - e^{-(\beta-it)\cdot iA} e^{-it\cdot iA'}} e^{-(\beta-it)\cdot iA}\Big]_{ji}\Big)(\delta_{ij} - iu_j^\alpha \delta_{ji+\alpha})$$

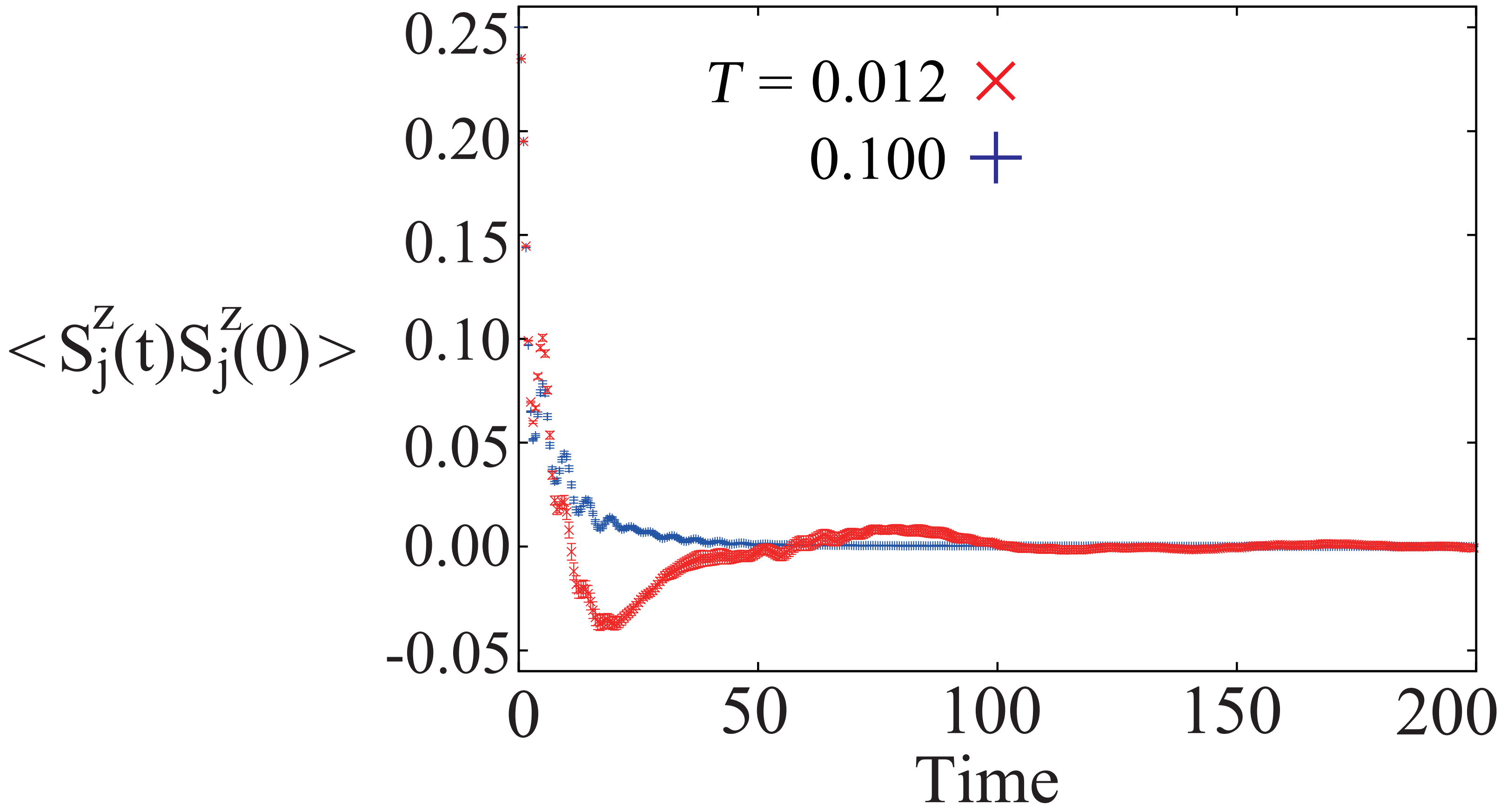
M. Udagawa, Phys. Rev. B 98, 220404(R) (2018)

$$\mathcal{H}[\{W_p\}] = \frac{i}{4} J_K \sum_{i\in A}(u_i^x c_i c_{i+x} + u_i^y c_i c_{i+y} + u_i^z c_i c_{i+z}) = \frac{i}{4} c_k A_{kk'} c_{k'}, \quad \mathcal{H}[\{W_p'\}] = \frac{i}{4} c_k A'_{kk'} c_{k'}$$



Initial state {Wp} — Intermediate state {Wp'} — Final state (= Initial state)

Model & Method: Time dependence, $2 \times 12 \times 12$ sites ($J_K = 1$)

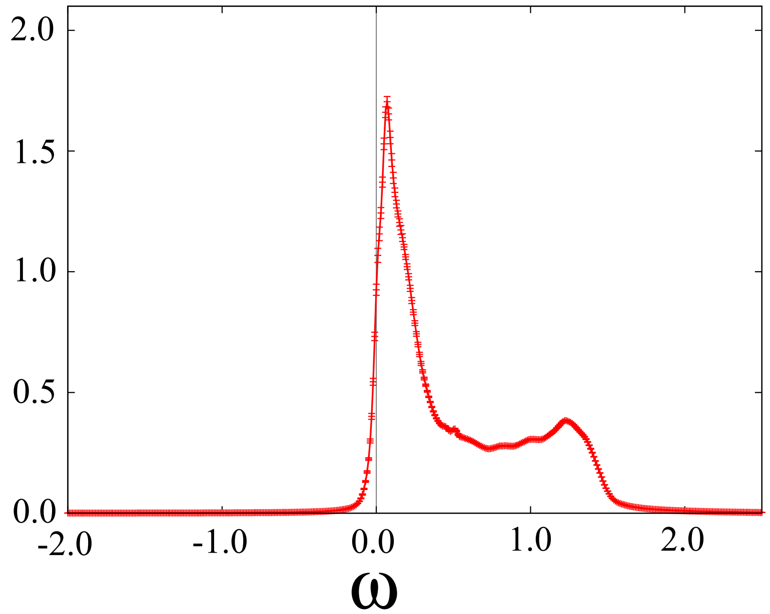


Model & Method: Magnetic response @ $T = 0.02$ ($J_K = 1$), $2 \times 12 \times 12$ sites

On-site correlation

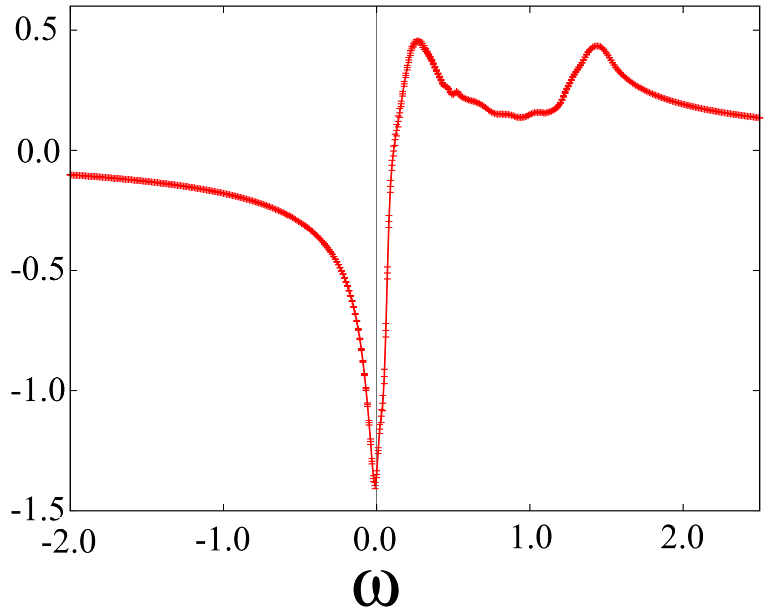
$$\mathcal{C}^z_{jj}(\omega) = \int_0^\infty dt\ e^{(i\omega-\delta)t} \langle S^z_j(t) S^z_j(0) \rangle$$

Real part



$$(1/T_1)_j \propto \frac{\mathrm{Im}\chi_{jj}(\omega_0)}{\omega_0} \propto \mathrm{Re}\ \mathcal{C}^z_{jj}(0)$$

Imaginary part

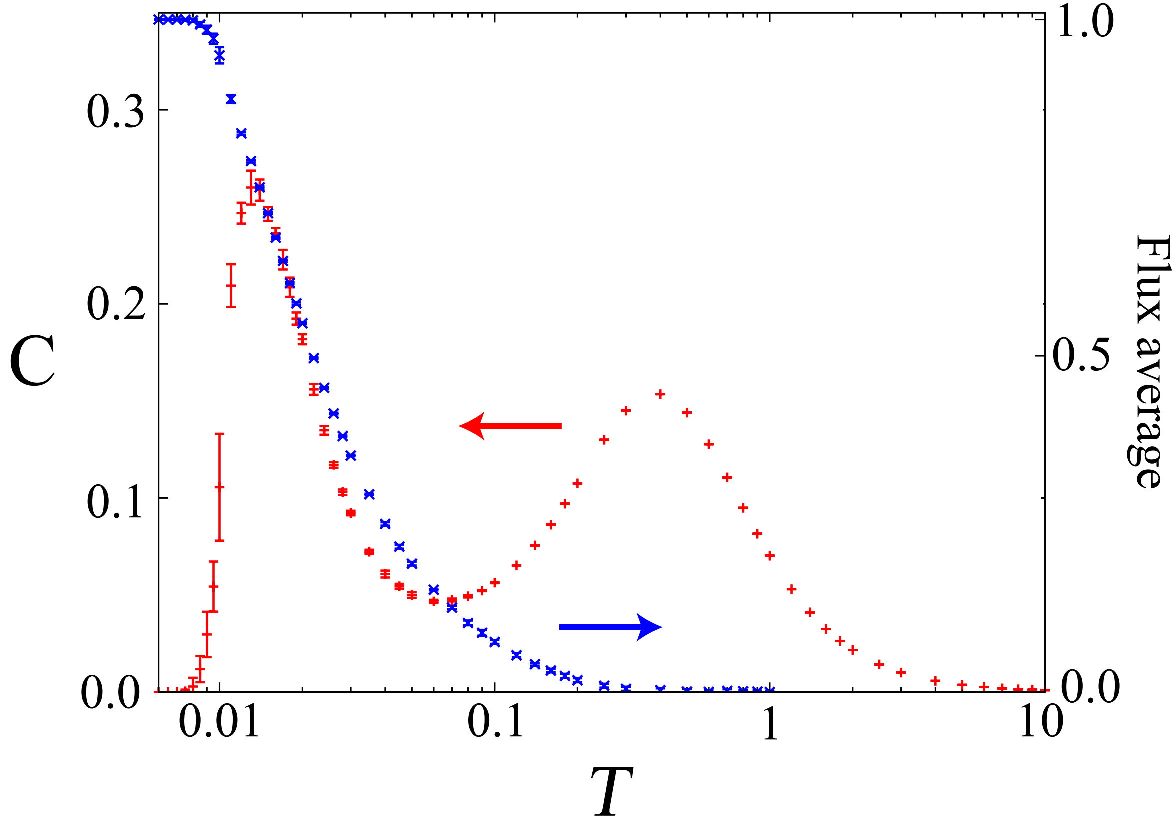


$$\chi_j = -\frac{2}{3} \sum_\alpha \mathrm{Im}(\mathcal{C}^\alpha_{jj}(0) + \mathcal{C}^\alpha_{jj+\alpha}(0))$$

Results

– Dynamical response in chiral spin liquid phase –

Results: Specific heat and flux@ $\kappa = 0.0$



– $J_K = 1.0 \sim 100\text{K} \sim 10\text{meV}$, typically

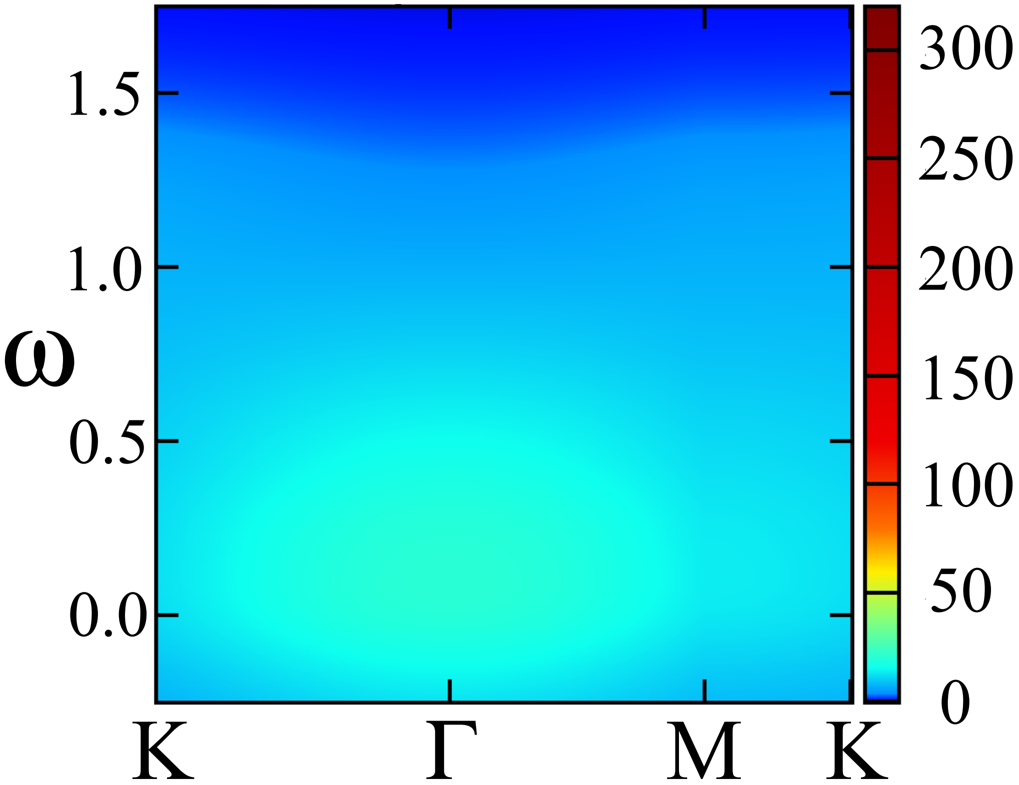
A. Banerjee et al., Nat. Mater. **15** 733 (2016)

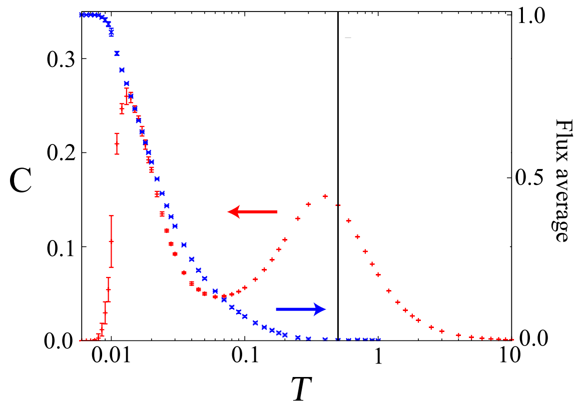
– Low-T peak: Vison, high-T peak: fermion

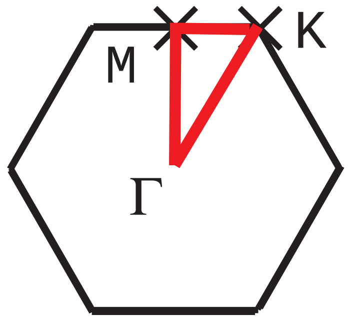
J. Nasu, M. U. and Y. Motome, Phys. Rev. B **92**, 115122 (2015)

Results: $\mathcal{S}(\mathbf{q},\omega)$ @ $\kappa = 0.0$

$T = 0.5$



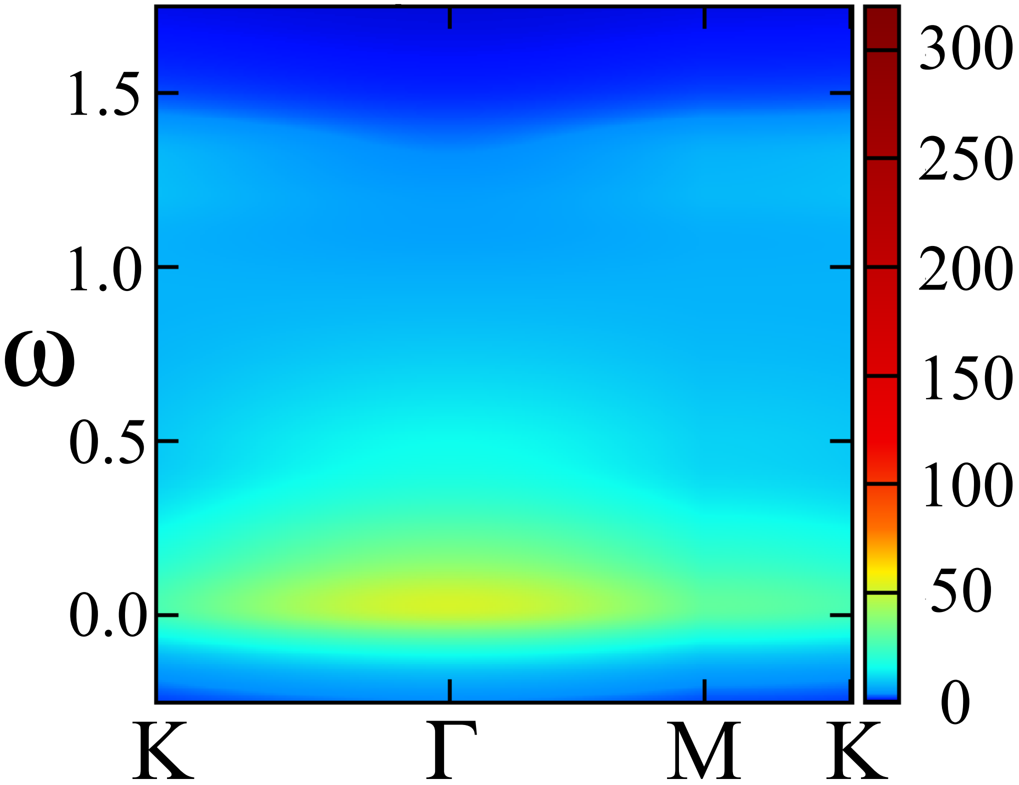


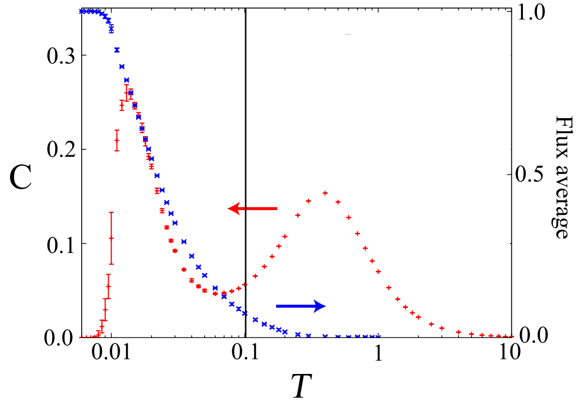


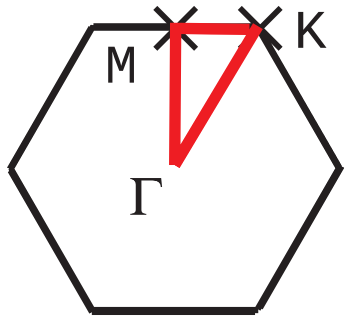
$$\mathcal{S}(\mathbf{q},\omega) = \mathcal{S}^{xx}(\mathbf{q},\omega) + \mathcal{S}^{yy}(\mathbf{q},\omega) + \mathcal{S}^{zz}(\mathbf{q},\omega)$$

Results: $\mathcal{S}(\mathbf{q},\omega)$ @ $\kappa = 0.0$

$T = 0.1$



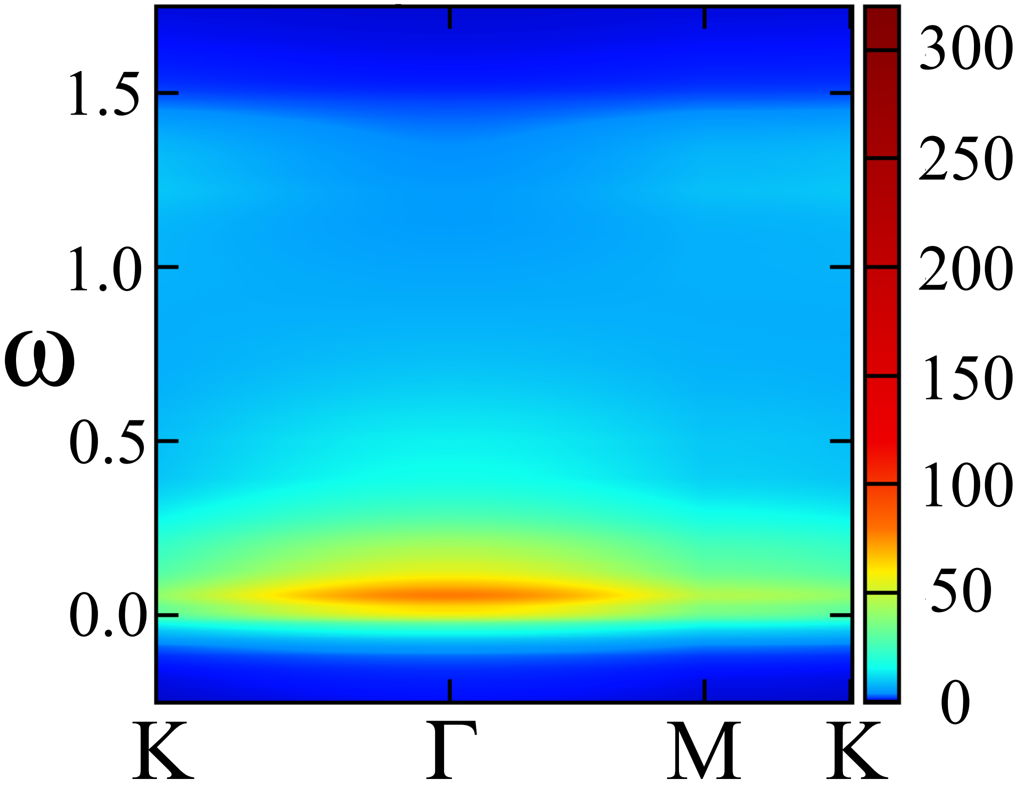


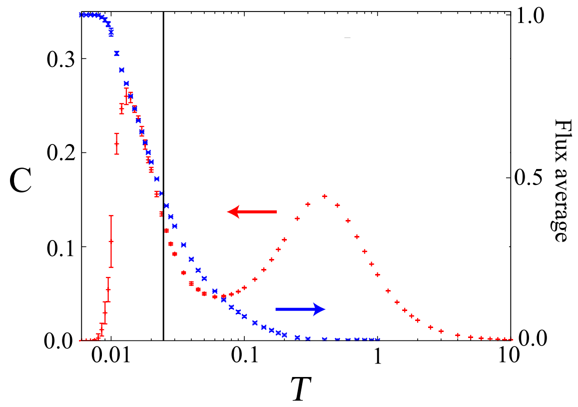


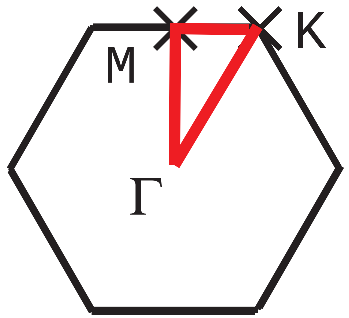
$$\mathcal{S}(\mathbf{q},\omega) = \mathcal{S}^{xx}(\mathbf{q},\omega) + \mathcal{S}^{yy}(\mathbf{q},\omega) + \mathcal{S}^{zz}(\mathbf{q},\omega)$$

Results: $\mathcal{S}(\mathbf{q},\omega)$ @ $\kappa = 0.0$

$T = 0.025$



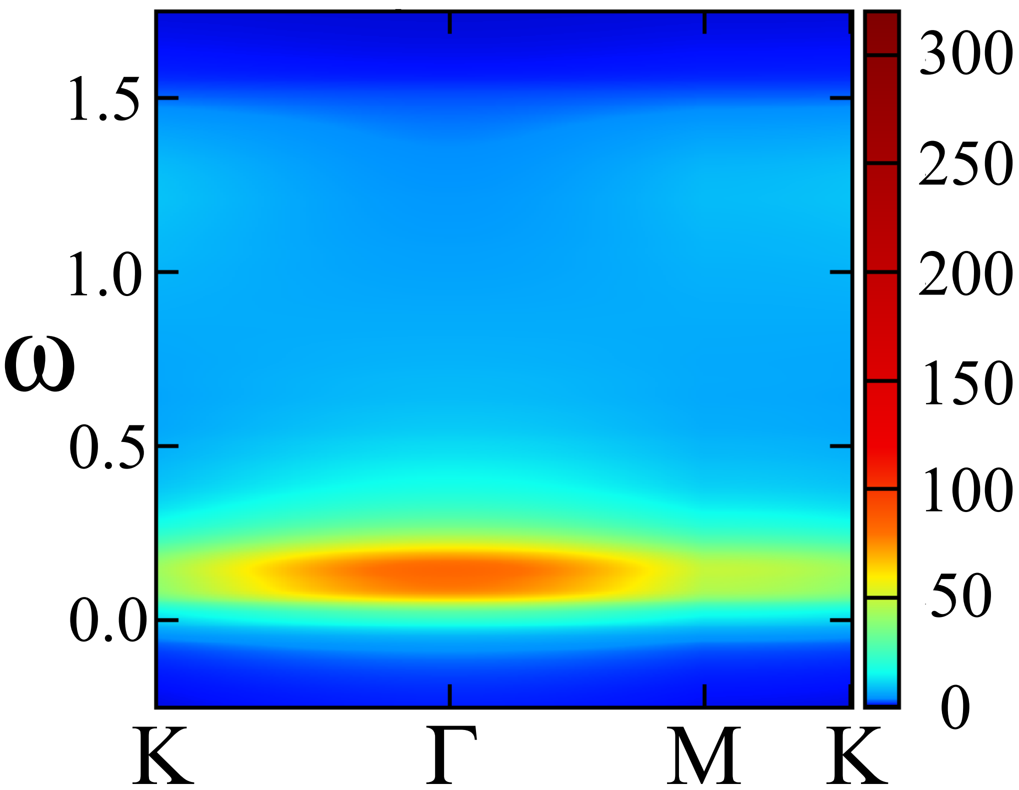


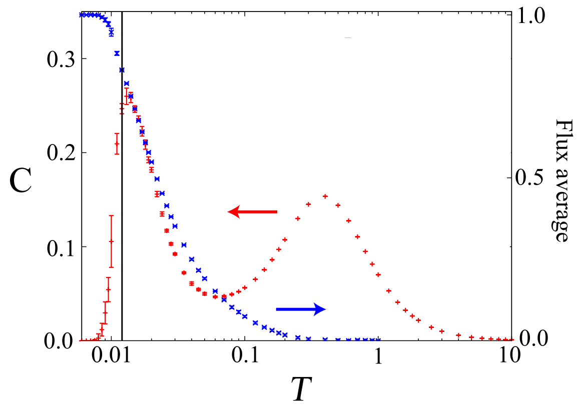


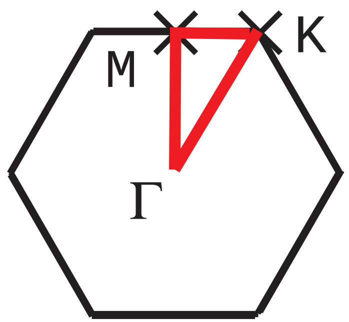
$$\mathcal{S}(\mathbf{q},\omega) = \mathcal{S}^{xx}(\mathbf{q},\omega) + \mathcal{S}^{yy}(\mathbf{q},\omega) + \mathcal{S}^{zz}(\mathbf{q},\omega)$$

Results: $\mathcal{S}(\mathbf{q},\omega)$ @ $\kappa = 0.0$

$T = 0.012$



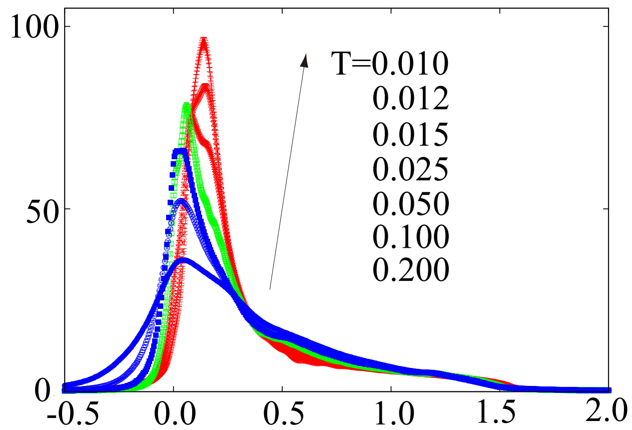




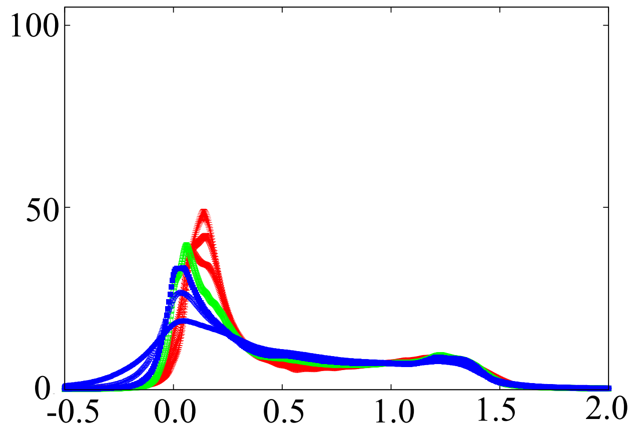
$$\mathcal{S}(\mathbf{q},\omega) = \mathcal{S}^{xx}(\mathbf{q},\omega) + \mathcal{S}^{yy}(\mathbf{q},\omega) + \mathcal{S}^{zz}(\mathbf{q},\omega)$$

Results: $\mathcal{S}(\mathbf{q},\omega)$ @ $\kappa = 0.0$

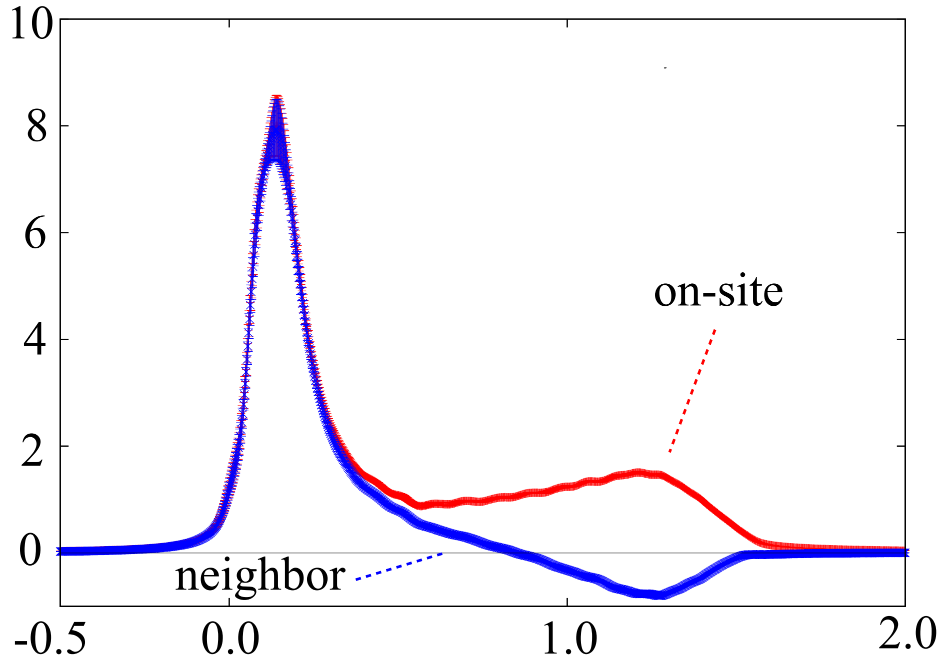
$\Gamma : \mathbf{q} = (0,0)$



K: $\mathbf{q} = (\frac{4}{3}\pi, 0)$



– Local correlation @ $T = 0.01$



– Almost single peak evolution

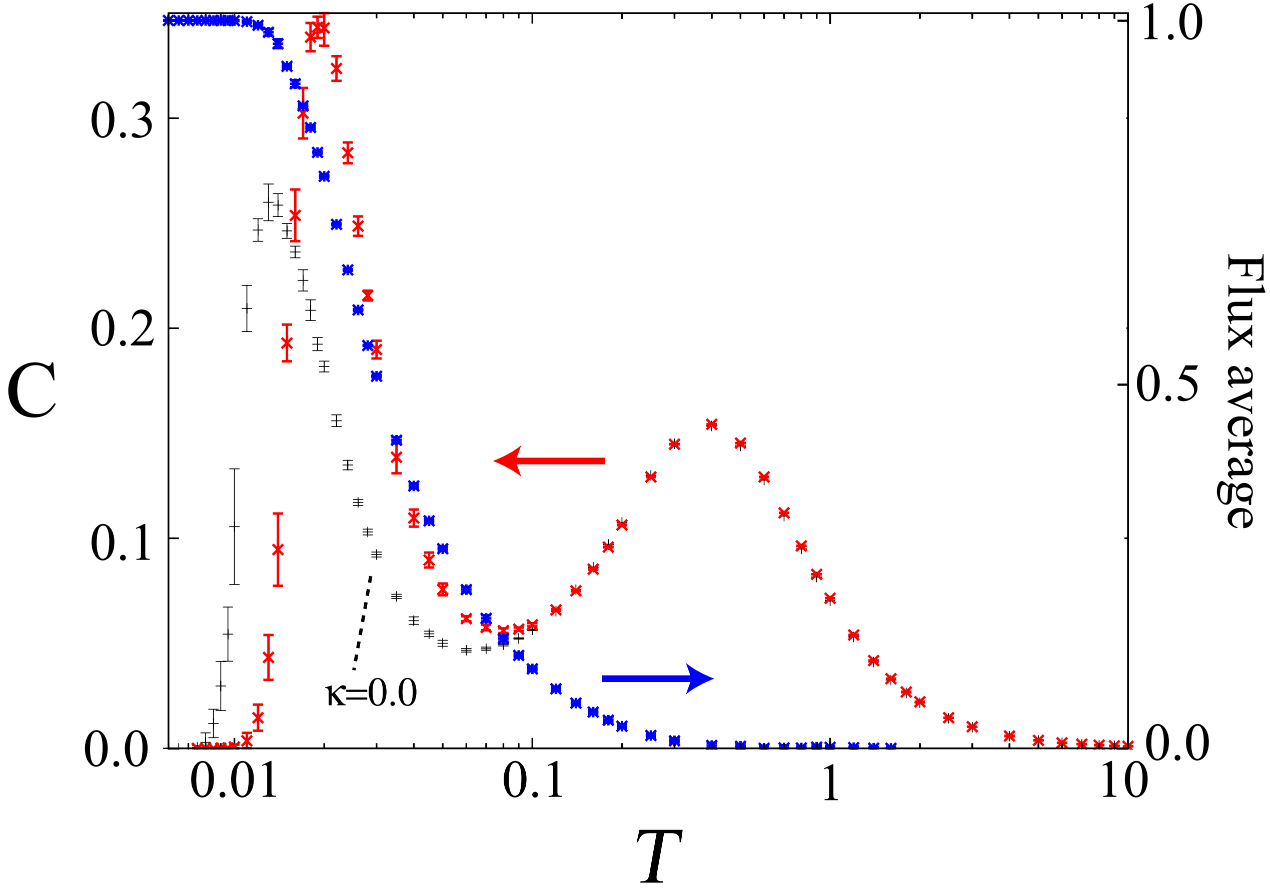
– $\mathbf{q}$ dep. determined by $\mathcal{S}_{i,i}$ and $\mathcal{S}_{i,i+\delta}$

$$\mathcal{S}(\mathbf{q},\omega) \propto 3\mathcal{S}_{i,i} + \mathcal{S}_{i,i+\delta}(\cos\mathbf{q}\cdot\boldsymbol{\delta}_x + \cos\mathbf{q}\cdot\boldsymbol{\delta}_y + \cos\mathbf{q}\cdot\boldsymbol{\delta}_z)$$

– Consistent with previous studies

J. Knolle et al. ($T = 0$), J. Yoshitake et al. (finite T)

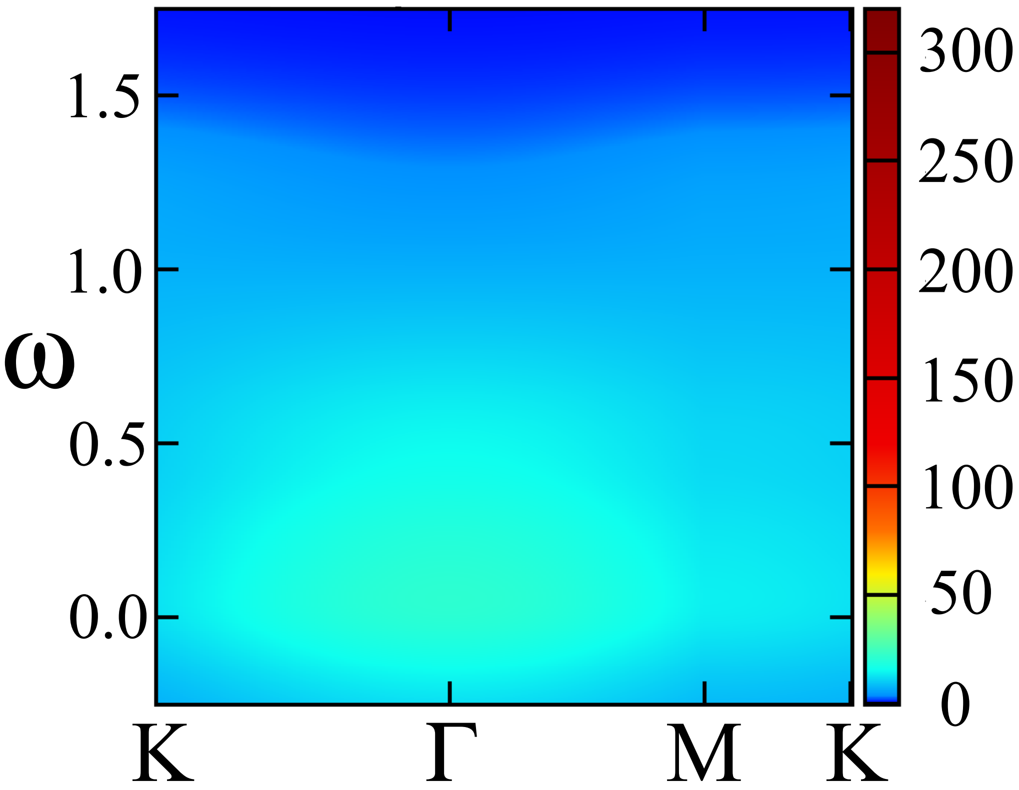
Results: $\mathcal{S}(\mathbf{q}, \omega)$ @ $\kappa = 0.1$

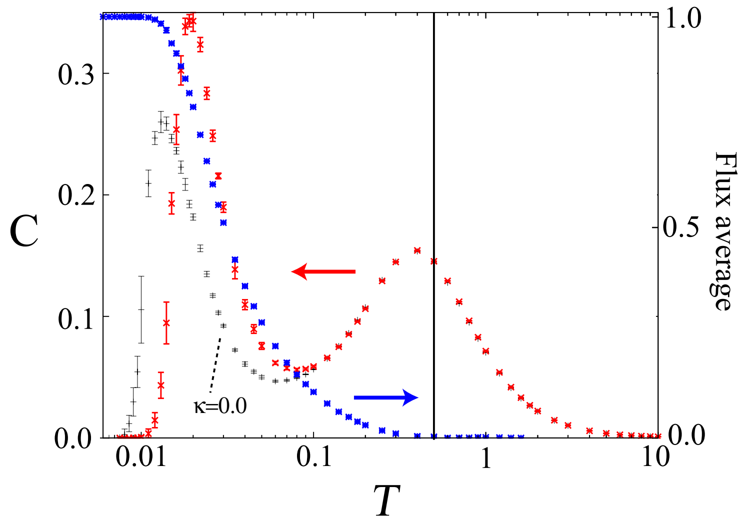


– The Vison peak shifts to higher energy by magnetic field

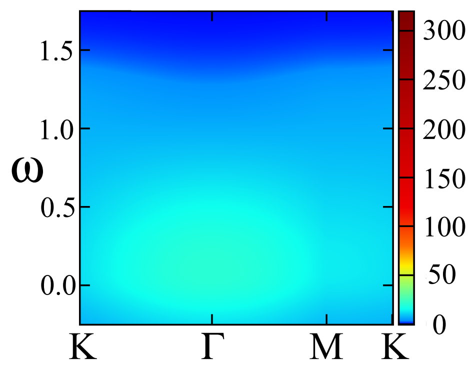
Results: $\mathcal{S}(\mathbf{q},\omega)$ @ $\kappa = 0.1$

$T = 0.5$



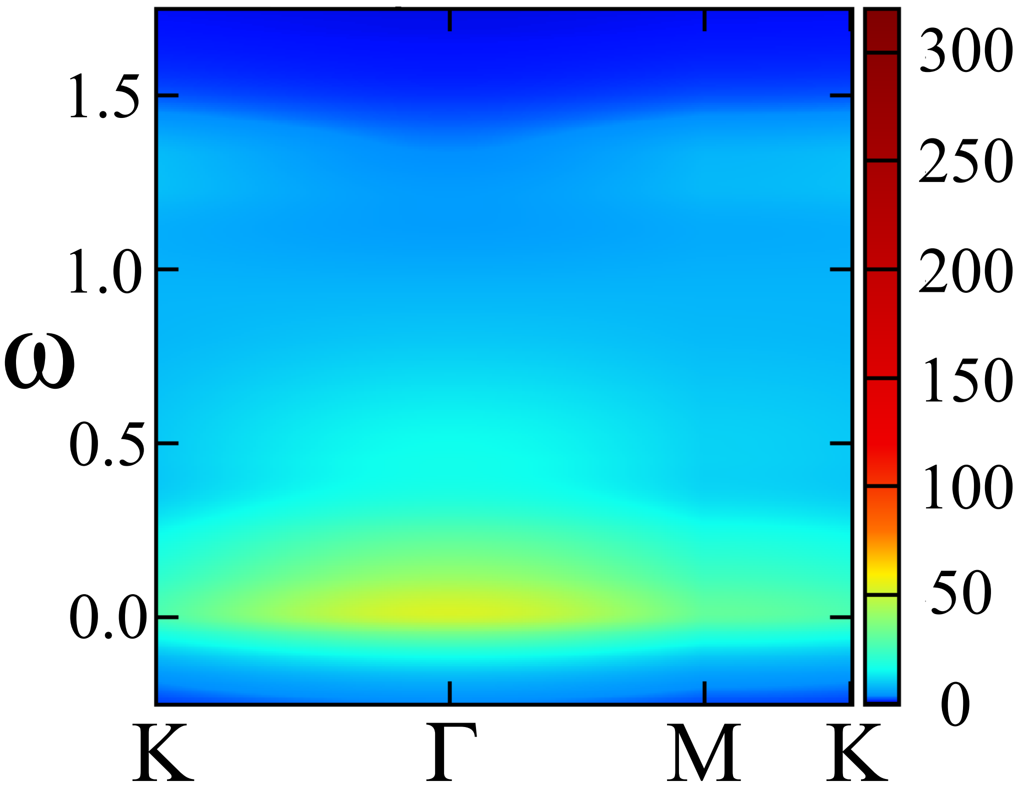


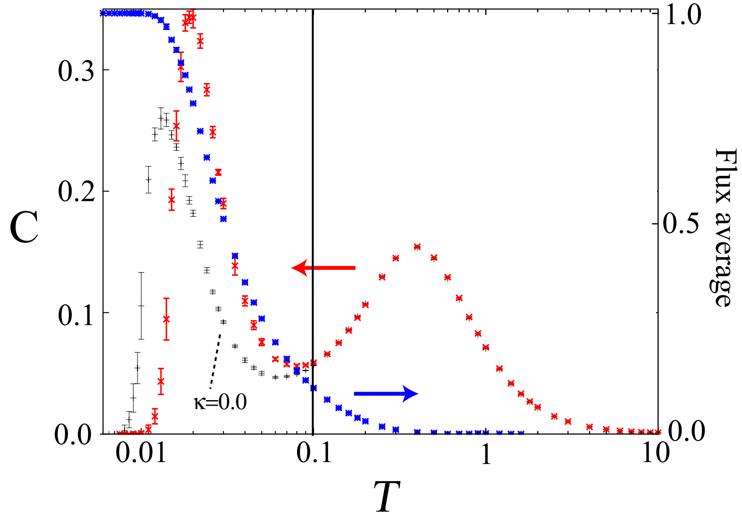
$\kappa = 0.0$



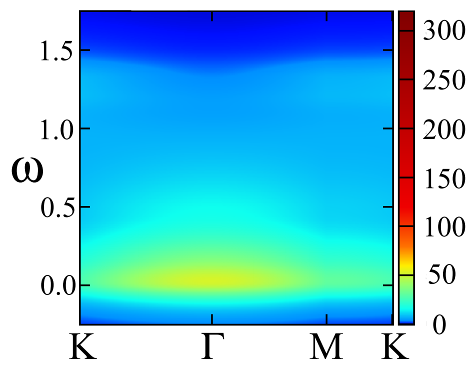
Results: $\mathcal{S}(\mathbf{q},\omega)$ @ $\kappa = 0.1$

$T = 0.1$



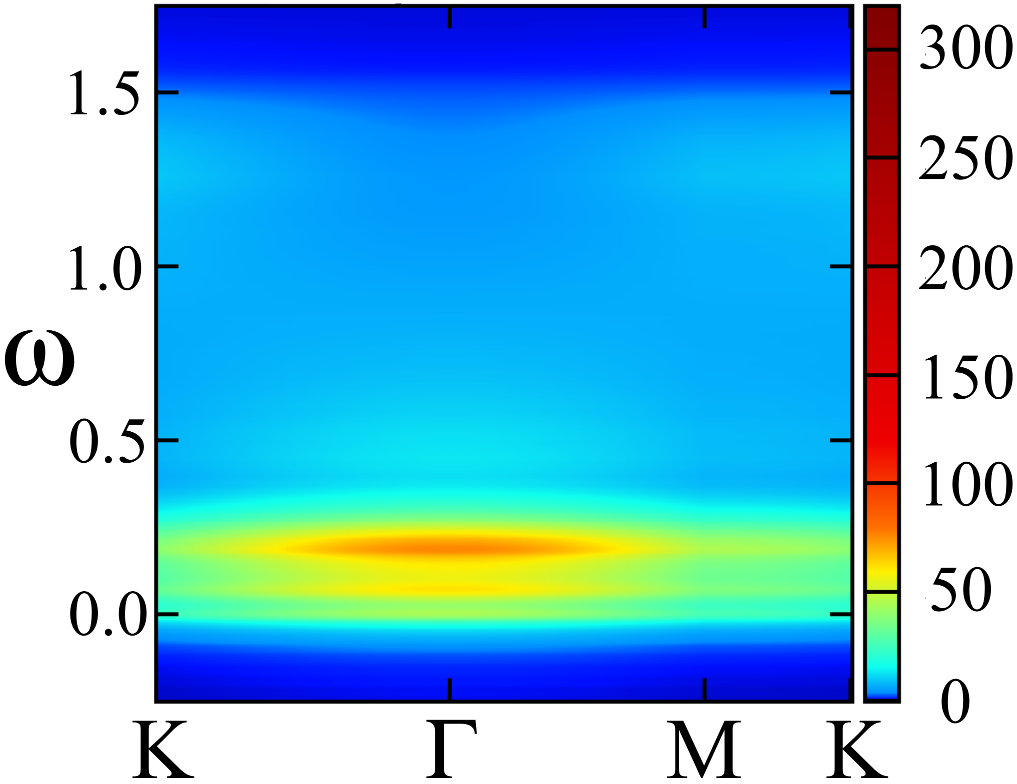


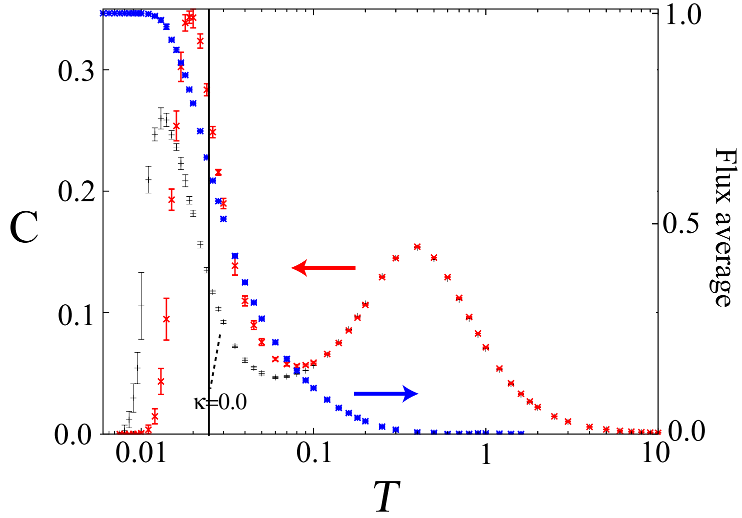
$\kappa = 0.0$



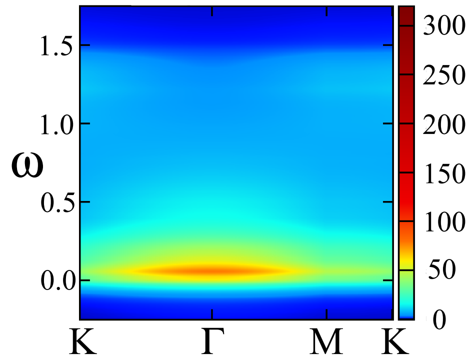
Results: $\mathcal{S}(\mathbf{q},\omega)$ @ $\kappa = 0.1$

$T = 0.025$



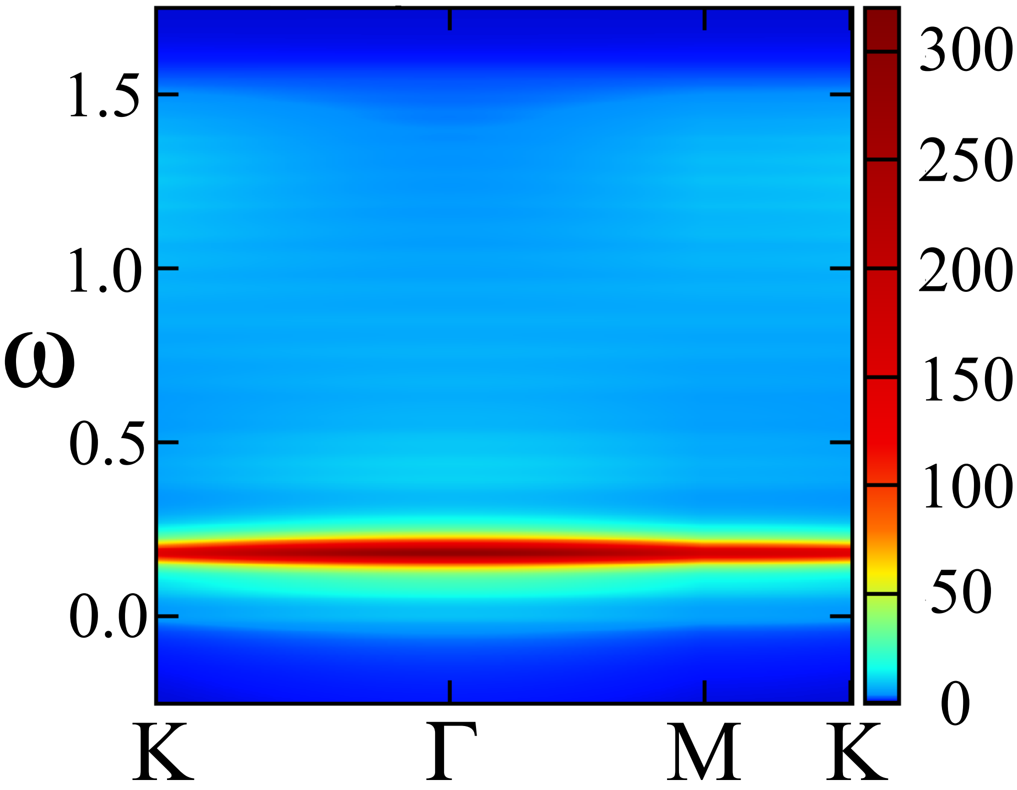


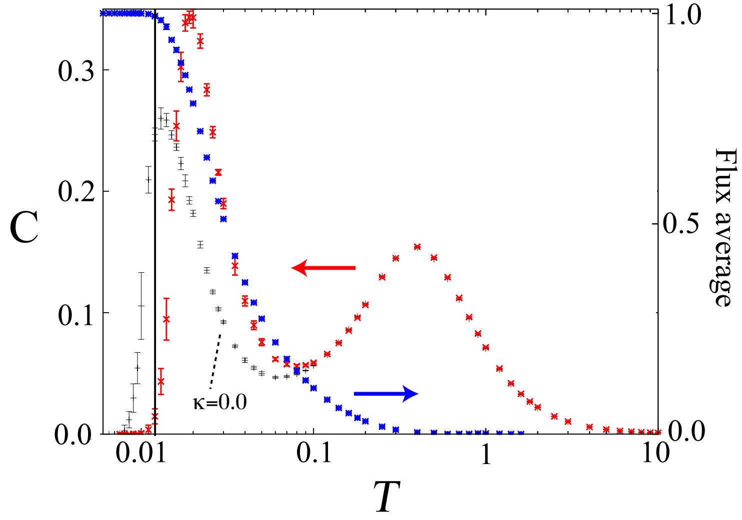
$\kappa = 0.0$



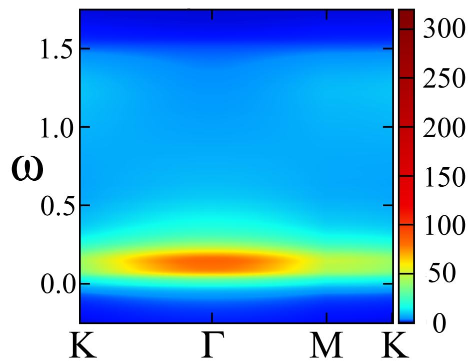
Results: $\mathcal{S}(\mathbf{q},\omega)$ @ $\kappa = 0.1$

$T = 0.012$



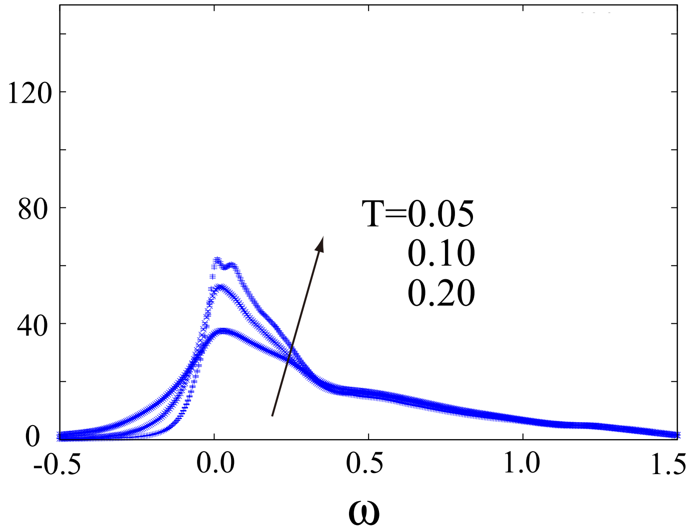


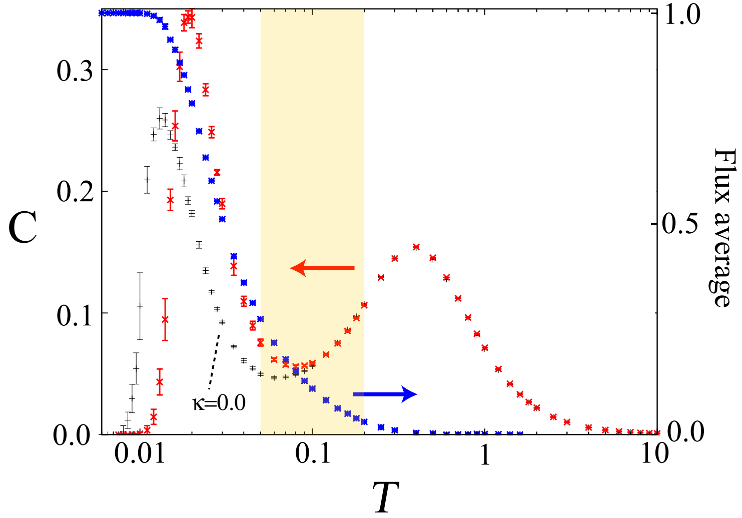
$\kappa = 0.0$



Results: @ $\kappa = 0.1$

– Incoherent region



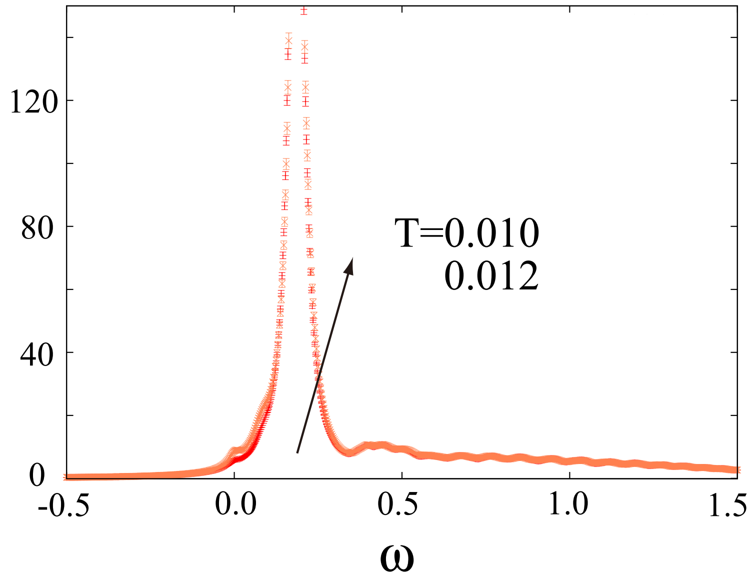


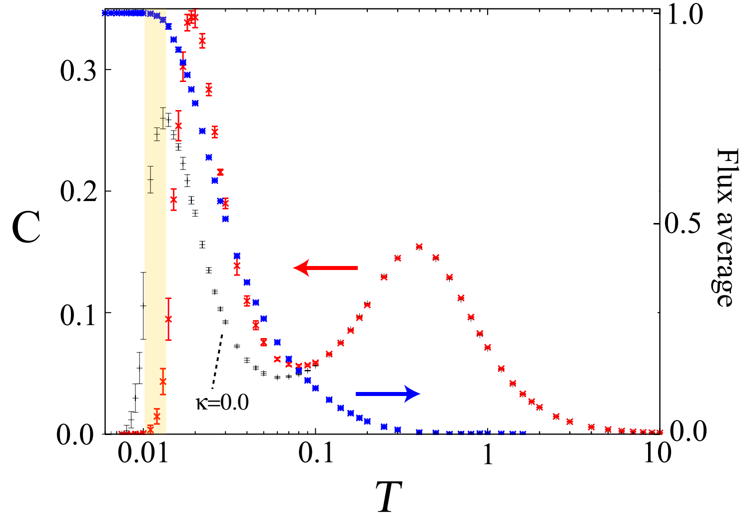
Gradual growth of zero-energy weight

– Basically same as zero magnetic field

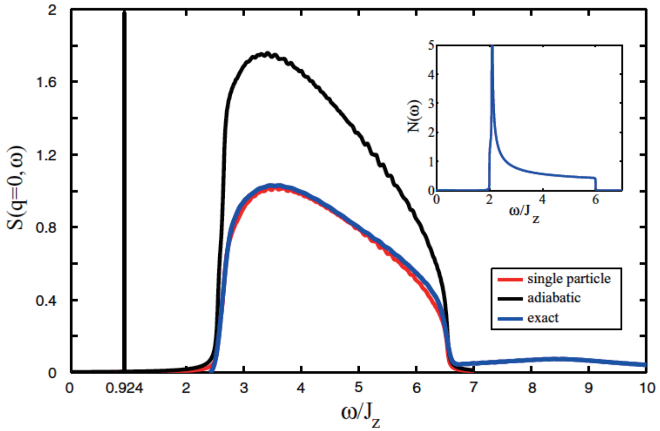
Results: @ $\kappa = 0.1$

– Chiral spin liquid phase





c.f. Resonance peak @ $T = 0$



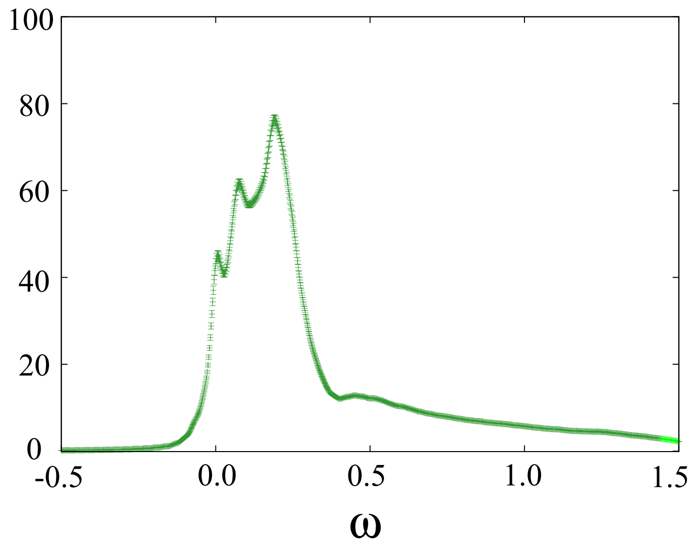
– low-energy resonance peak

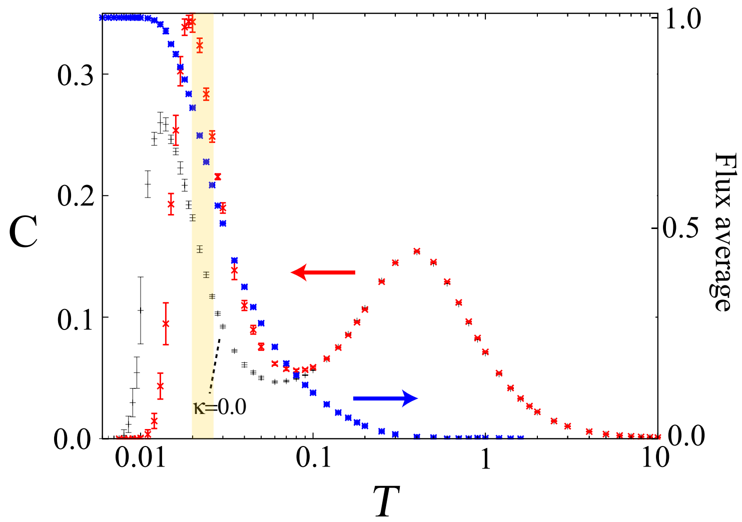
– Vison pair creation

J. Knolle, D. L. Kovrizhin, J. Chalker and R. Moessner (2015)

Results: $\mathcal{S}(\Gamma, \omega)$ @ $\kappa = 0.1$

– Crossover region





– Excitation of Vison and fermion at the same time

$$\mathcal{S}_{ij}^{\alpha}(\omega) = \frac{i}{4}\frac{1}{Z}\sum_{n,m}\frac{\langle n|c_i b_i^{\alpha}|m\rangle\langle m|b_j^{\alpha}c_j|n\rangle}{\omega - (E_m - E_n) + i\delta}.$$

– $\mathcal{H} = \sum_{m>0} \varepsilon_m (2\gamma_m^{\dagger}\gamma_m - 1)$

$\varepsilon_m(> 0)$ depends on flux configuration

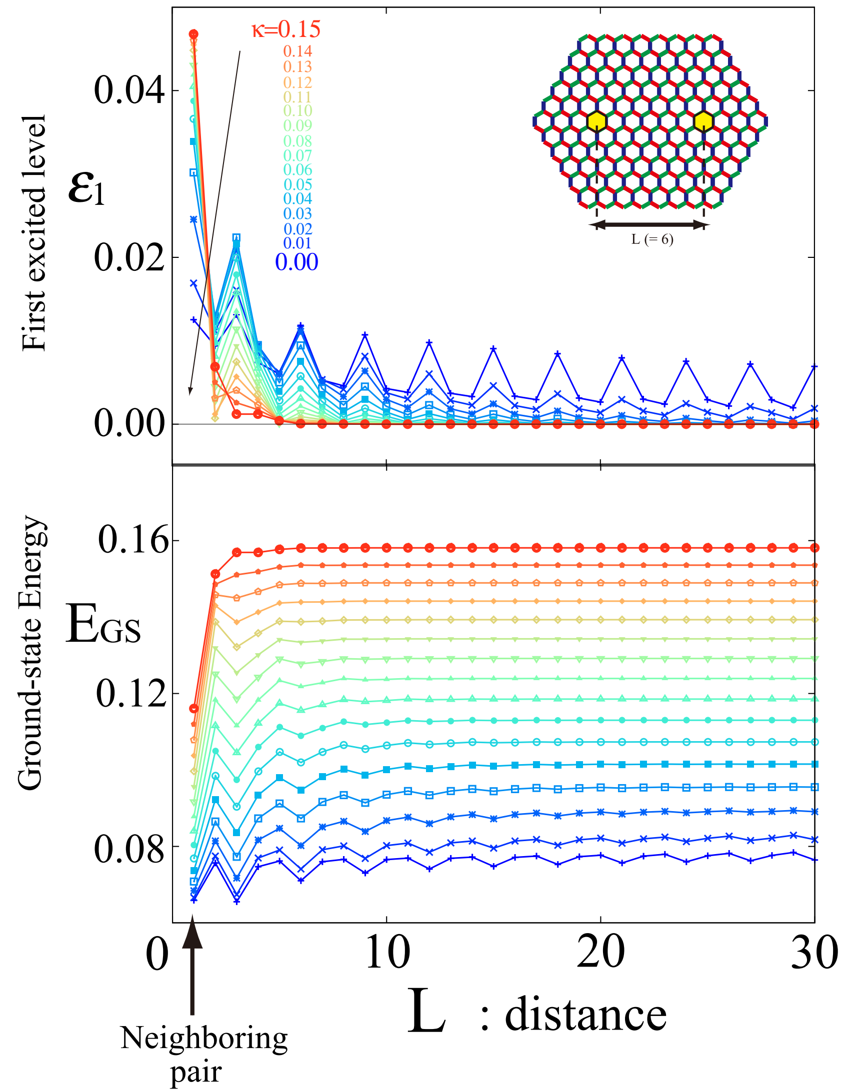
$E_0 = -\sum_{m>0}\varepsilon_m$: Ground-state energy

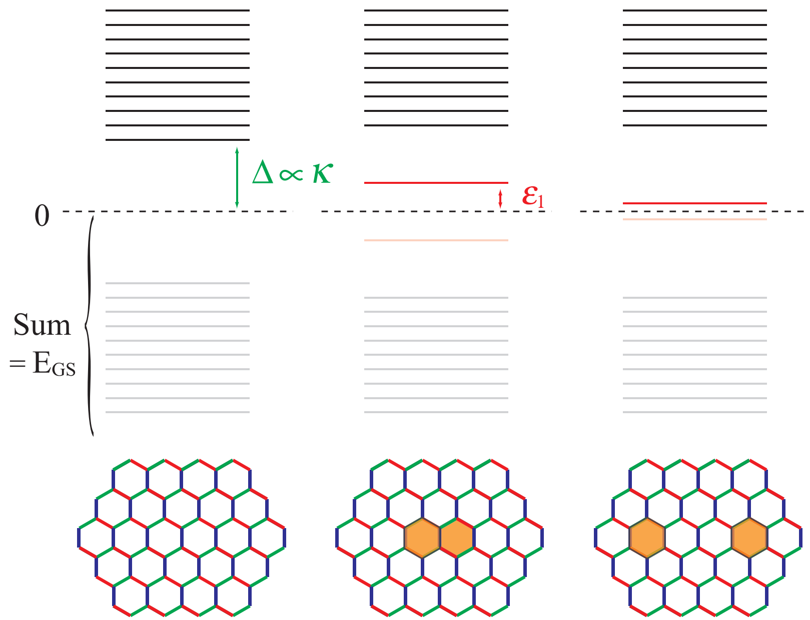
(Vison energy)

Peak of $\mathcal{S}(\mathbf{q}, \omega)$

$\omega = 2\varepsilon_m^{(f)} + (E_0^{(f)} - E_0^{(i)})$

Results: Energy level – a pair of Visons (Size: $64 \times 64 \times 2$)





- $L \to \infty$: zero mode
- Bonding orbital (ε_1)

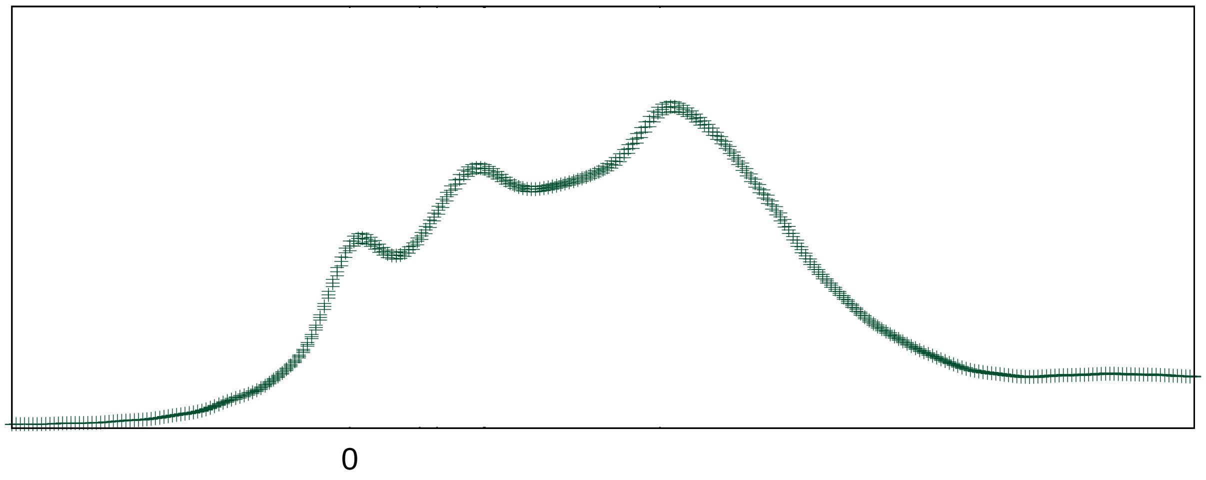
  Visons comfortable next to each other

Reciprocal relation:

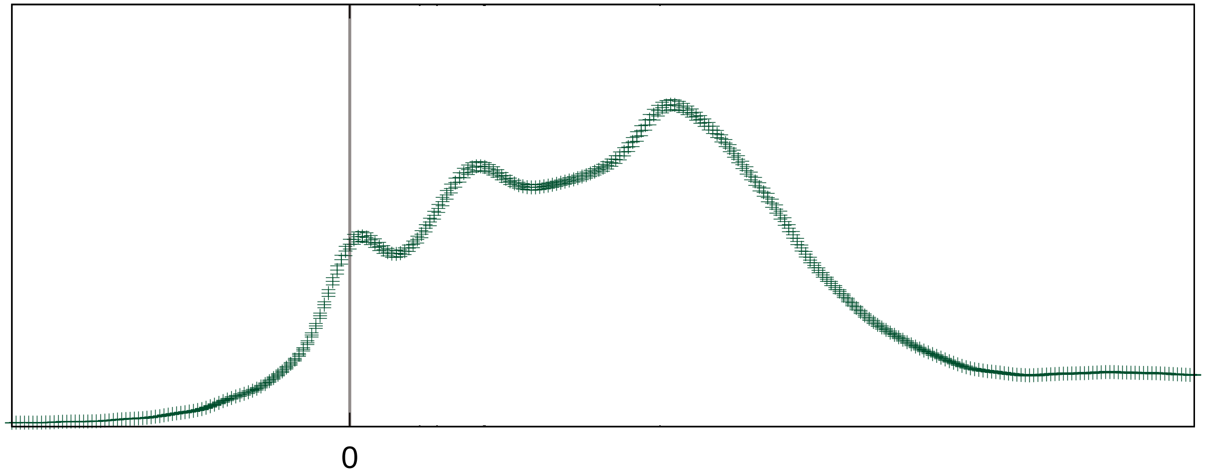
$$2\varepsilon_1^{(f)} + (E_{GS}^{(f)} - E_{GS}^{(i)}) = 2\varepsilon_1^{(i)} + (E_{GS}^{(i)} - E_{GS}^{(f)})$$

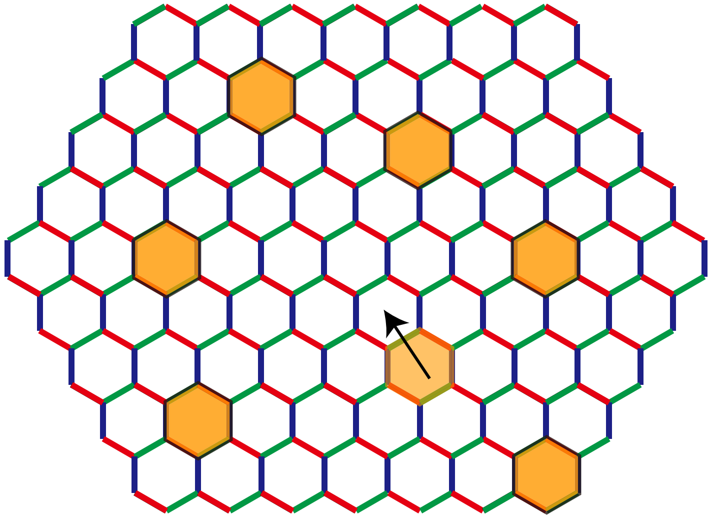
Inverse process has the same resonant energy

Results: Origin of the peaks

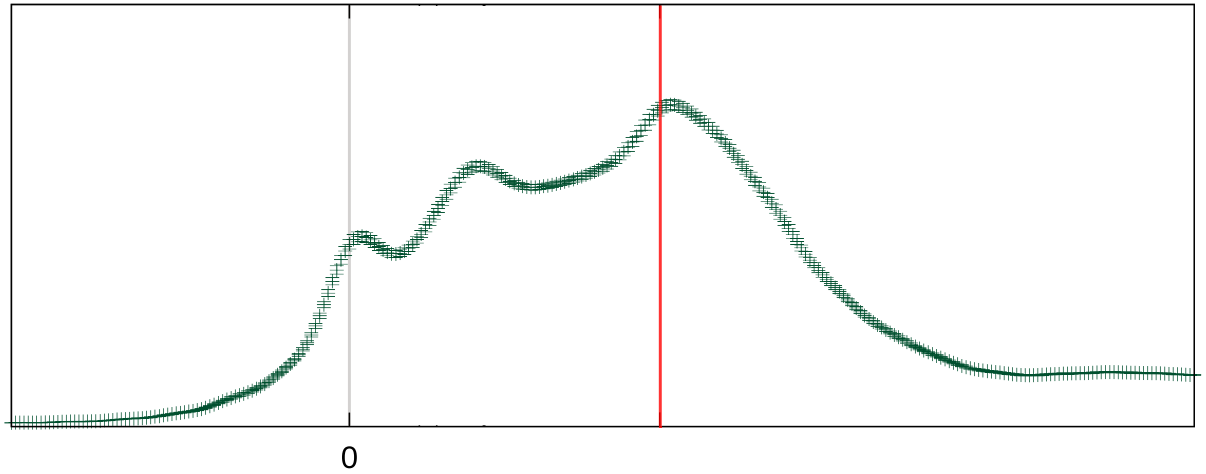


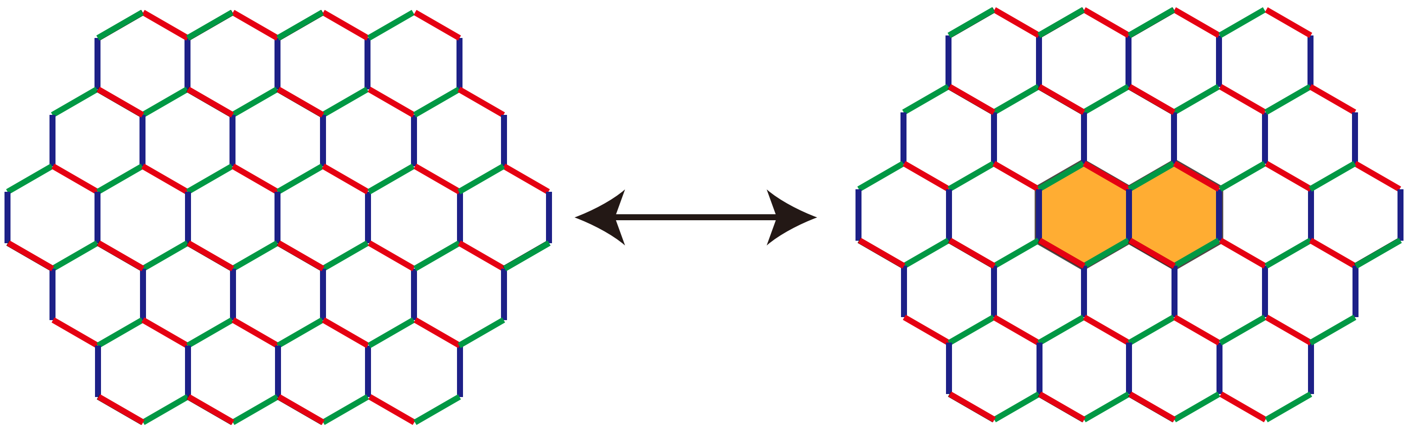
Results: Origin of the peaks





Results: Origin of the peaks

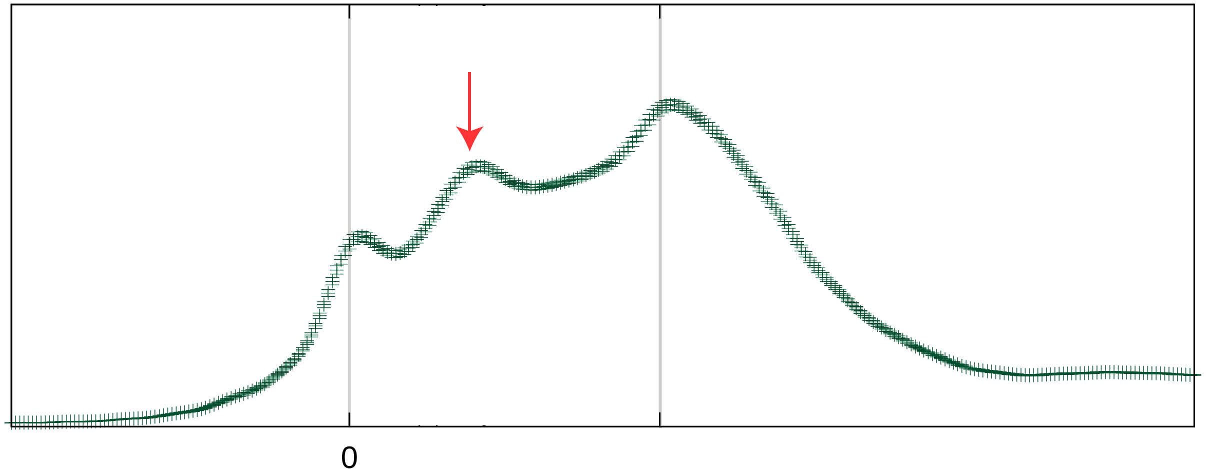




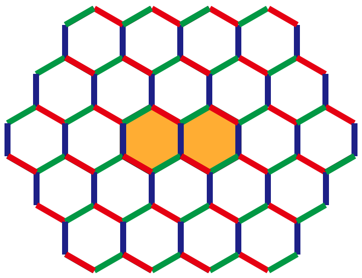
$E_{GS} = 0.095654$

$\varepsilon_1 = 0.043986$

Results: Origin of the peaks

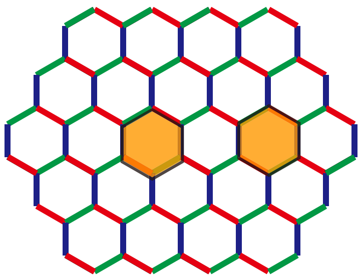


A



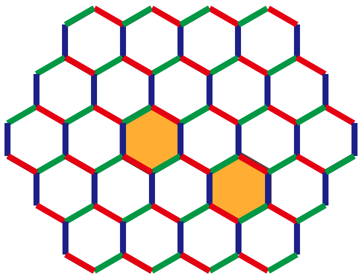
$E_{GS} = 0.095654$
$\varepsilon_1 = 0.043986$

B



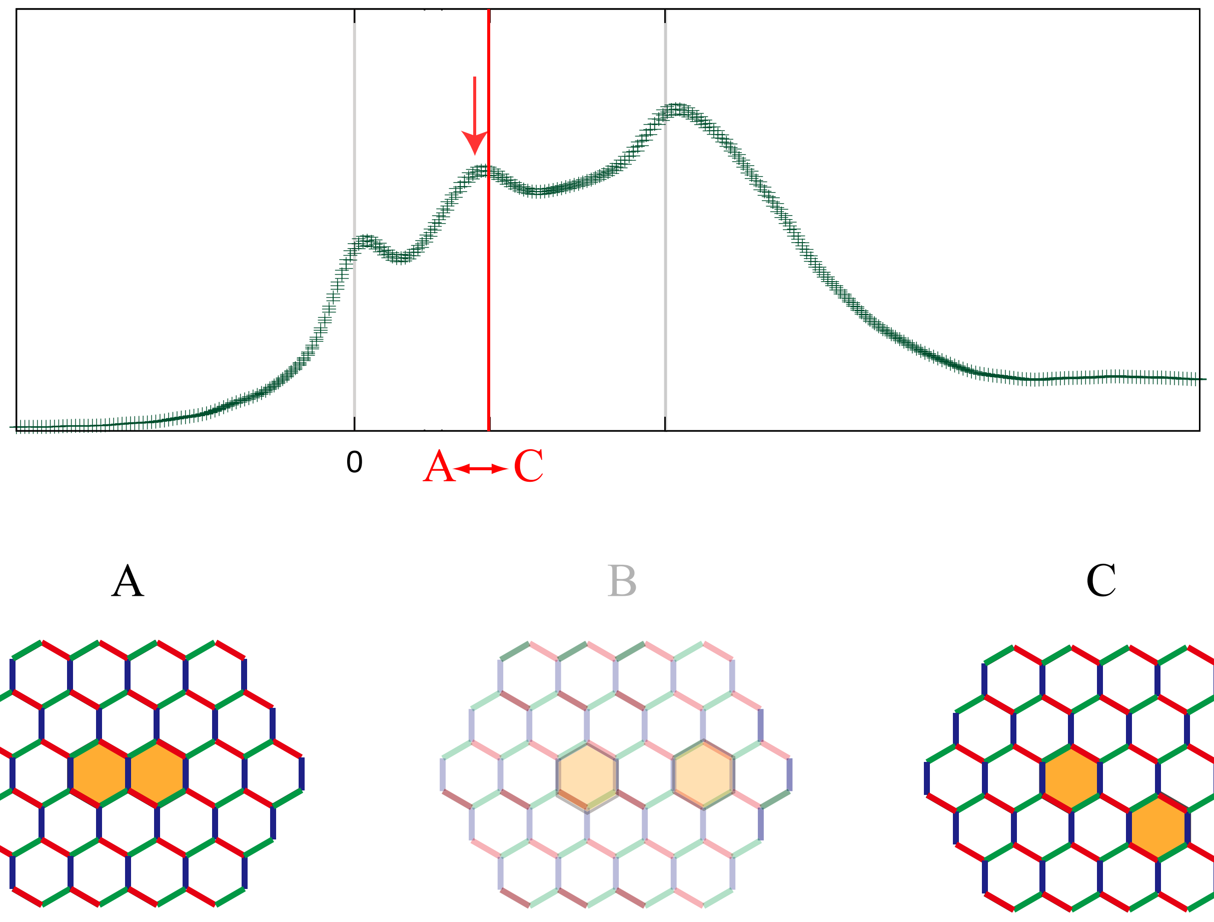
$E_{GS} = 0.131979$
$\varepsilon_1 = 0.0025683$

C



$E_{GS} = 0.103475$
$\varepsilon_1 = 0.035740$

Results: Origin of the peaks

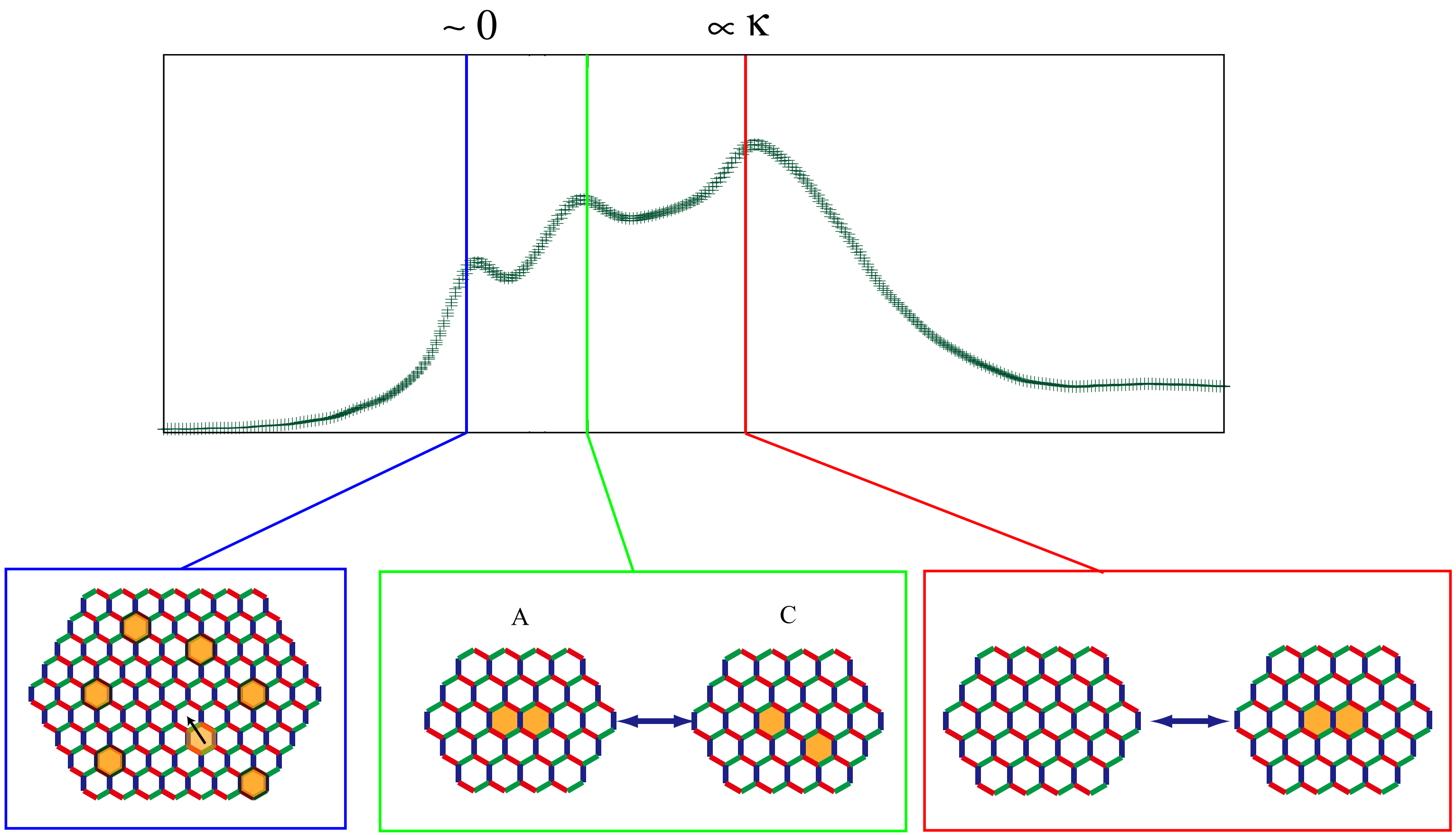


$E_{GS} = 0.095654$
$\varepsilon_1 = 0.043986$

$E_{GS} = 0.131979$
$\varepsilon_1 = 0.0025683$

$E_{GS} = 0.103475$
$\varepsilon_1 = 0.035740$

Results: Summary of the peaks



– The pair creation peak sensitive to magnetic field $\propto \kappa$

– Thermal anyon liquid state

c.f. Disorder-induced Majorana metal, Chris R. Laumann et al., Phys. Rev. B 85, 161301(R) (2012)

Results

– Charge response of Kitaev's spin liquid –

Results: Charge response of Kitaev QSL

– Charge in Kitaev QSL

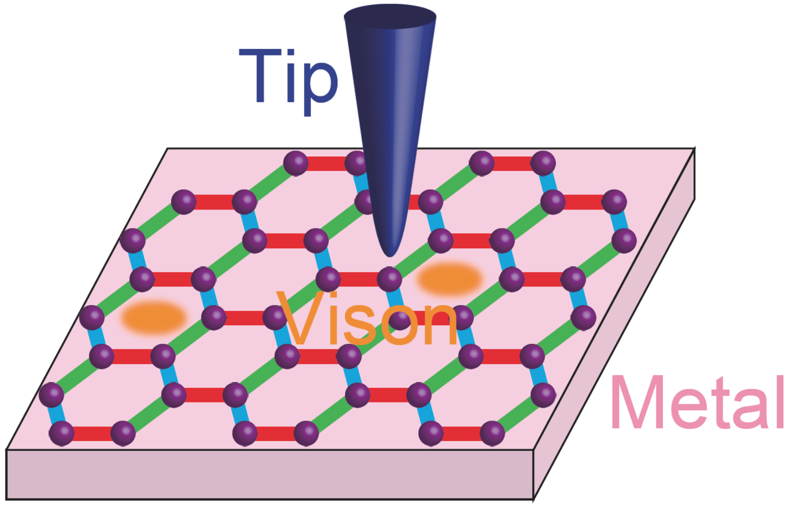
Optical response

L. J. Sandilands et al., PRB 94, 195156 (2016)

Proximity to Graphene

S. Biswas et al., arXiv:1908.04793

STM ?



$$I(eV) = \frac{2\pi e}{\hbar} \int d\omega \rho_{\rm tip}(\omega - eV)\rho_K(\omega)[f(\omega - eV) - f(\omega)]$$

M. Maltseva, M. Dzero and P. Coleman, Phys. Rev. Lett. **103**, 206402 (2009)

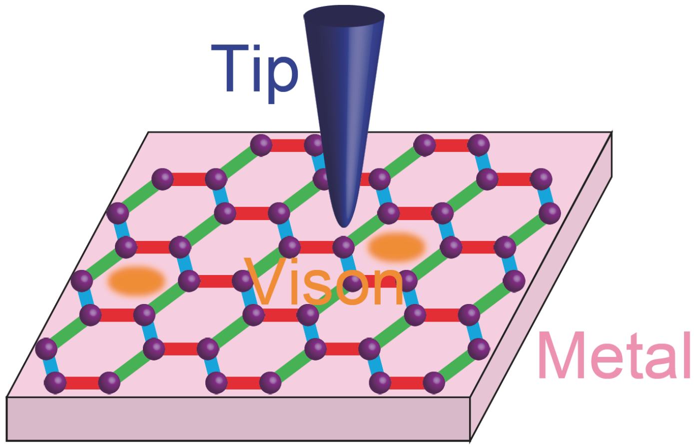
– Analytical solution of Hole Green's function $\rightarrow \rho_K(\omega)$

$$g_{js}(t) = -i\langle f^\dagger_{js}(t) f_{js}\rangle - \frac{i}{2}\frac{1}{Z}\sum_{\{W_p\}} Z(\{W_p\})\sqrt{\det\Big(\frac{1 + e^{-(\beta - it)iA}e^{-itiA_j}}{1 + e^{-\beta iA}}\Big)}$$

Results: Hole Green's function: $\kappa = 0.0$

Results: Hole Green's function – magnetic field dependence

Results: Control of Visons

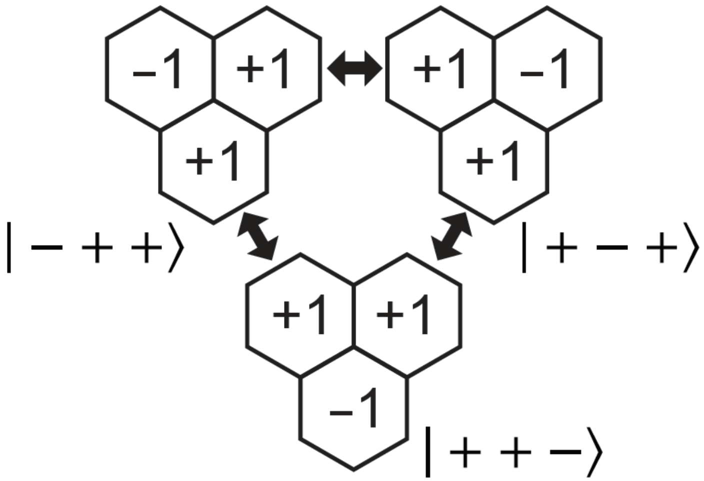


– Quantum coherency between tip and system
  c.f. Quantum dot, adsorbed magnetic ions...

– s-d coupling Hamiltonian

$$\mathcal{H} = \mathcal{H}_{\mathrm{Kitaev}} + \mathcal{H}_{\mathrm{tip}} + J_{\mathrm{sd}} c_{\alpha}^{\dagger} \boldsymbol{\sigma}_{\alpha\beta} c_{\beta} \cdot \mathbf{S}_{\mathrm{K}}$$

– Vison acquires dynamics



– Low-energy model:
  Effective $L = 1$ Kondo model

$$\mathcal{H} = \mathcal{H}_{\mathrm{tip}} + J_{\mathrm{sd}} c_{\alpha}^{\dagger} \boldsymbol{\sigma}_{\alpha\beta} c_{\beta} \cdot \mathbf{L}$$

$\rightarrow$ Stabilization of odd Vison config.

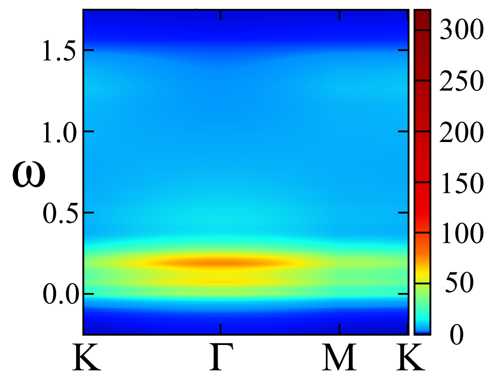
Results: Vison twizzer

Summary

– Finite-T spin dynamics of Kitaev's CSL

  Identification of peaks

  Thermal anyon liquid at intermediate T



– Charge response of Kitaev's spin liquid

  Vison signatures at low energy

  Possibility of control