2D spectroscopy of a Kitaev spin liquid

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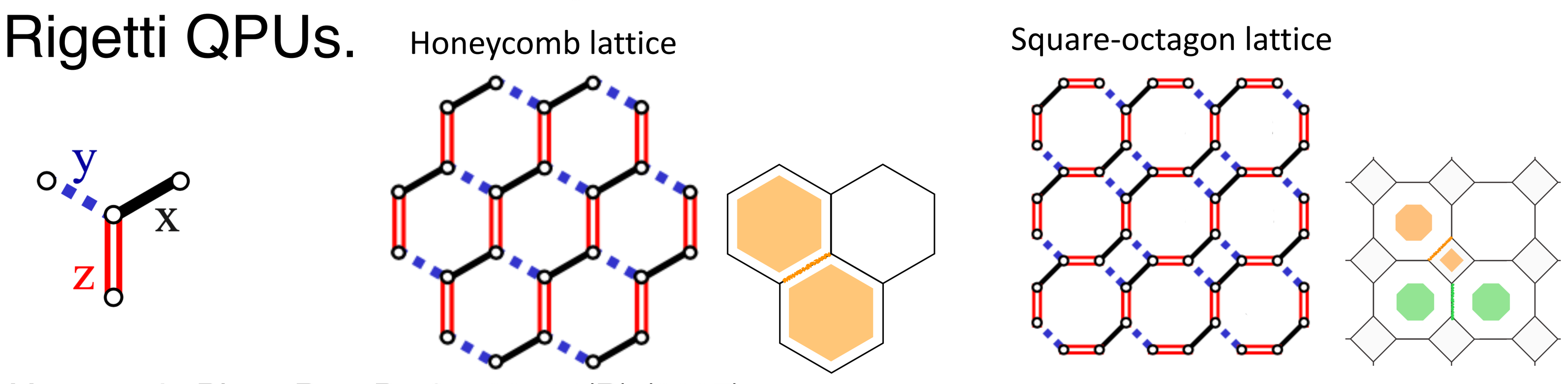
Introduction

Quantum computing promises to significantly accelerate research in materials discovery, characterization, and understanding. Simulations of correlated quantum spin systems and their dynamics are a primary application since such simulations are difficult on classical computers. Here, we focus on the computation of nonlinear correlation functions in frustrated quantum spin systems and perform a purely classical first benchmarking calculation in the Kitaev model on the honeycomb and square-octagon lattice.

Kitaev spin model

Hamiltonian $H = -J_x \sum_{\text{x-link}} \sigma_i^x \sigma_j^x - J_y \sum_{\text{y-link}} \sigma_i^y \sigma_j^y - J_z \sum_{\text{z-link}} \sigma_i^z \sigma_j^z$

Model can be studied on various mosaic lattices [1]. This includes the square-octagon lattice which is the layout of qubits on Rigetti QPUs.



[1] S. Yang et al., Phys. Rev. B **76**, 180404(R) (2007).

- Mapping of spins to Majorana fermions

$$\sigma_j^\alpha = i b_j^\alpha c_j \qquad \{b_i^\alpha, b_j^\beta\} = 2\delta_{ij}\delta_{a,\beta}, \quad \{c_i, c_j\} = 2\delta_{ij}.$$

- Action of spin operator on a state

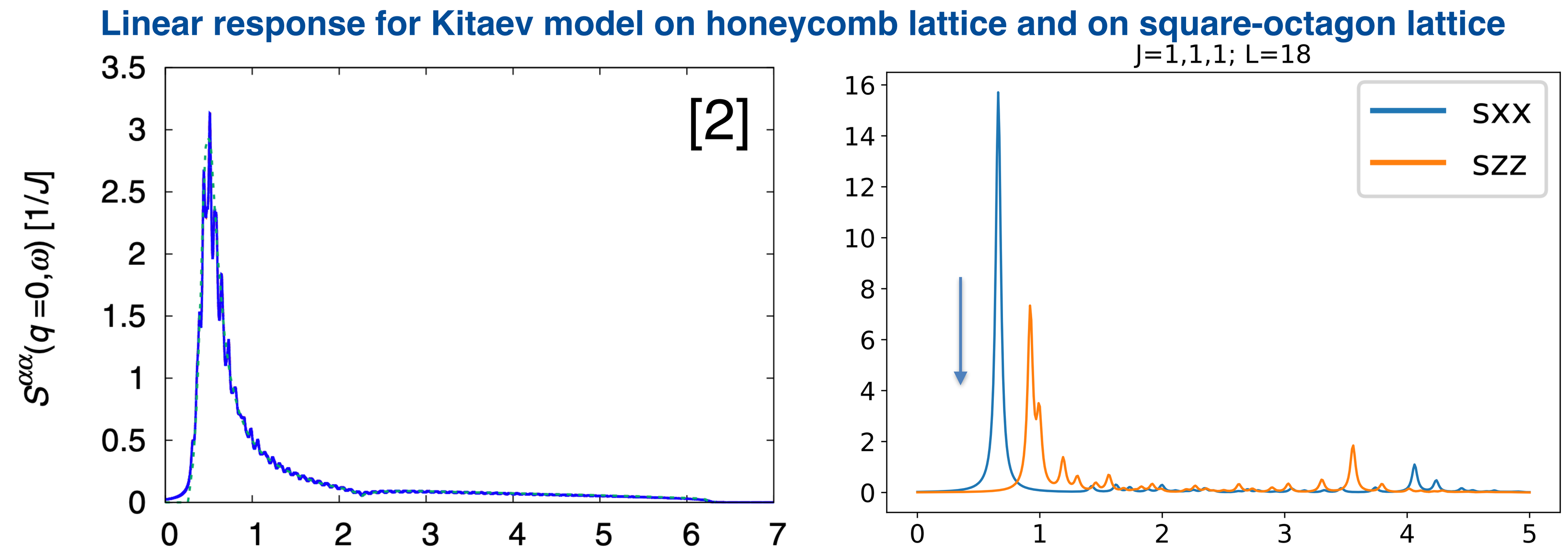
$$\hat{u}_{jk} \equiv i b_j^\alpha b_k^\alpha = 2\chi_{ij}^\dagger \chi_{ij} - 1 \qquad \sigma_i^\alpha = i\left(\chi_{ij} + \chi_{ij}^\dagger\right) c_i$$

Linear response

$$S_{ij}^{\alpha\beta}(t) = \langle 0|\hat{\sigma}_i^\alpha(t)\hat{\sigma}_j^\beta(0)|0\rangle \qquad |0\rangle = |M_0\rangle\,|F_0\rangle$$

$$S_{ij}^{\alpha\beta}(\omega) = -i\sum_\lambda \langle M_0|\hat{c}_i|\lambda\rangle\langle\lambda|\hat{c}_j|M_0\rangle\,\delta\left[\omega - (E_\lambda - E_0)\right]\delta_{\langle ij\rangle_\alpha}\delta_{\alpha\beta}$$

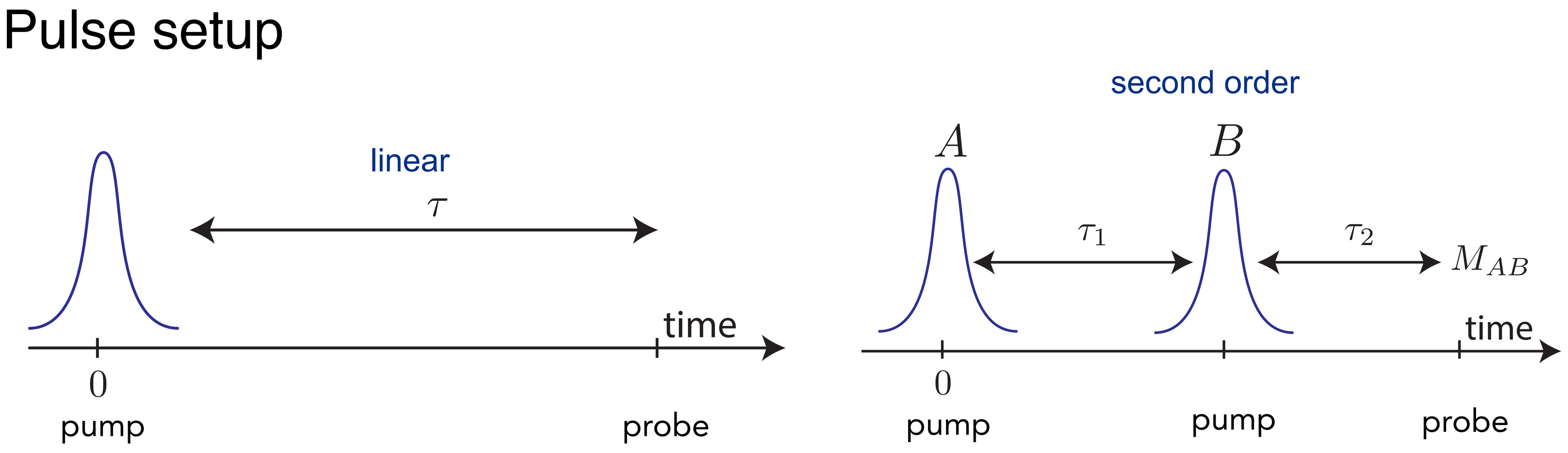
Linear response for Kitaev model on honeycomb lattice and on square-octagon lattice



[2] F. Zschocke et al., Phys. Rev. B **92**, 014403 (2015).

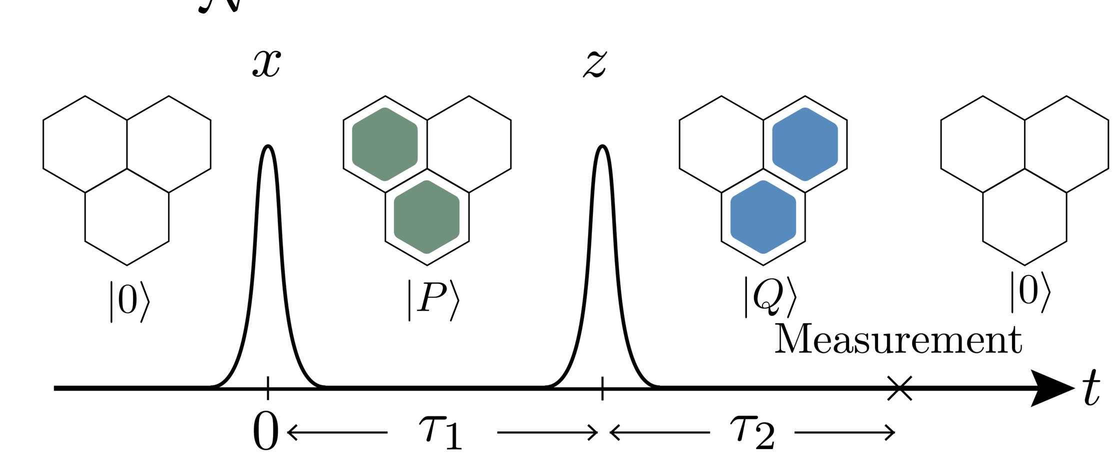
Nonlinear response

- Pulse setup

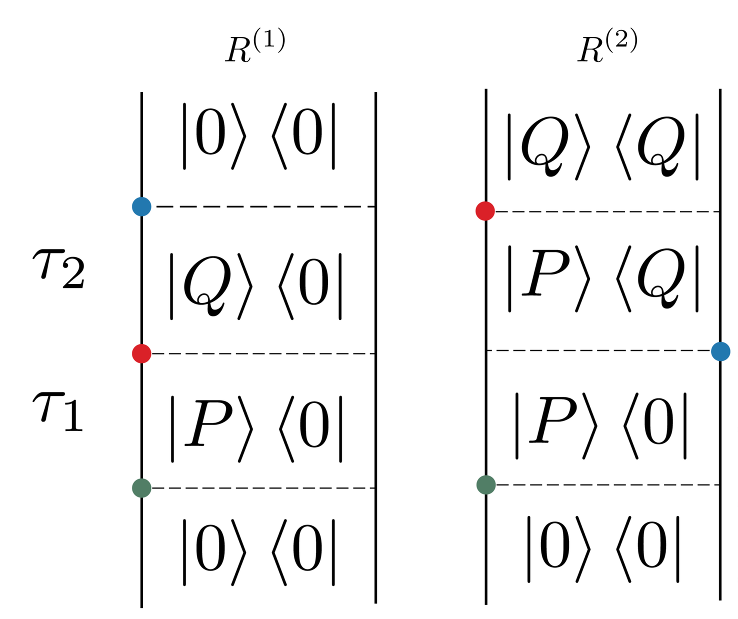


- y, z, x component (and its permutations) are finite

$$\chi^{y,z,x}(\tau_1,\tau_2) = \frac{i^2}{\mathcal{N}}\theta(\tau_1)\theta(\tau_2)\langle[[M^y(\tau_1+\tau_2), M^z(\tau_1)], M^x(0)]\rangle$$



Liouville pathways



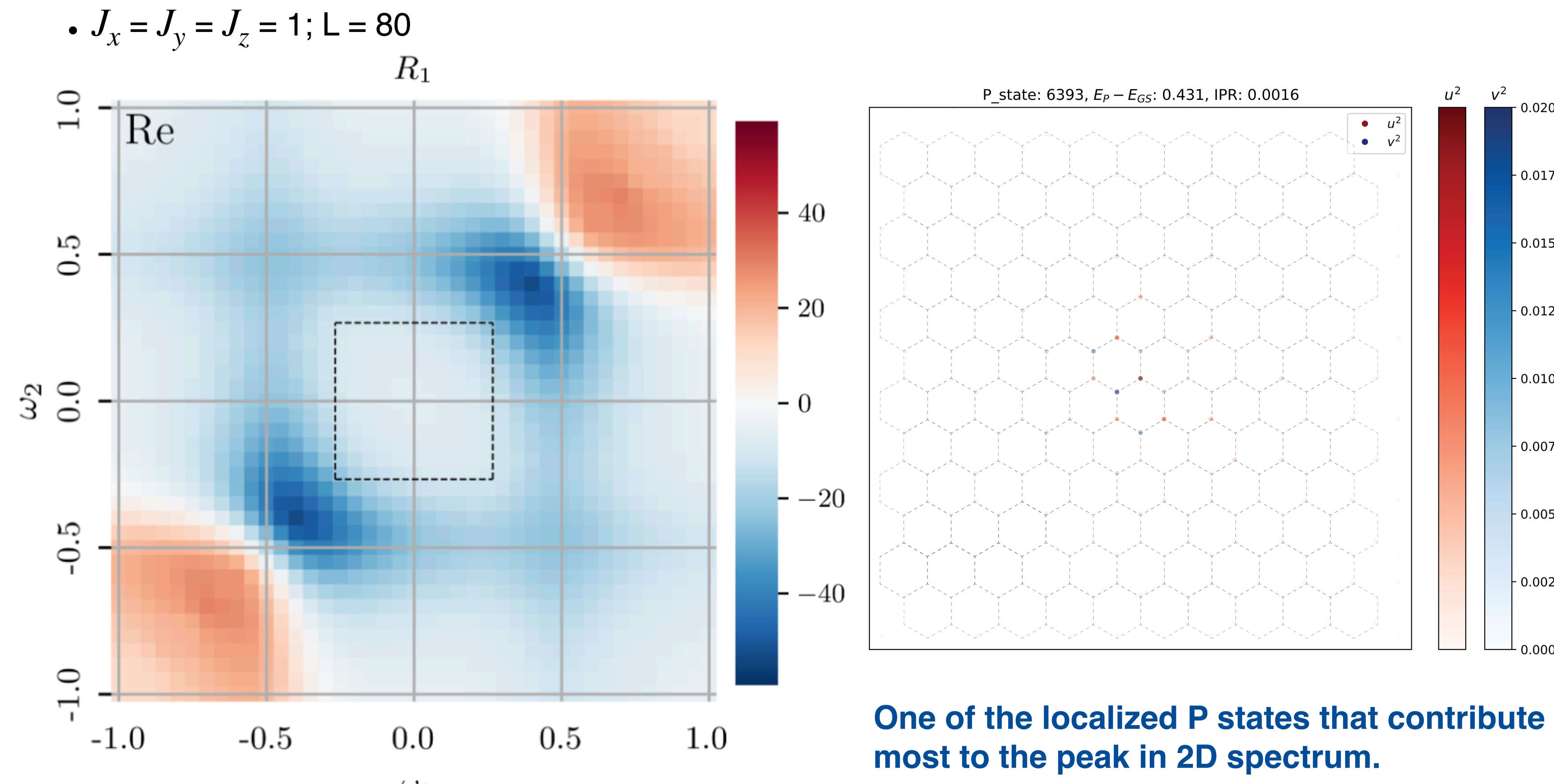
$\langle 0|\,\sigma_k^y\,|Q\rangle\,\langle Q|\,\sigma_j^z\,|P\rangle\,\langle P|\,\sigma_i^x\,|0\rangle$

Quantum pathways representation for the two processes involved in the second-order response.

- System initialized in ground state
- P and Q are eigenstates of the Hamiltonian
- Time evolves from bottom to top
- Dots represent operations on density matrix

Two-dimensional coherent spectroscopy

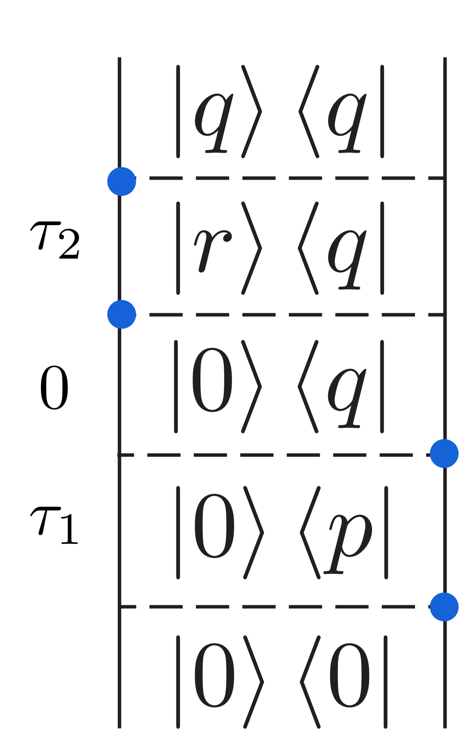
- For honeycomb model: y, z, x component
  - $J_x = J_y = J_z = 1$; L = 80



One of the localized P states that contribute most to the peak in 2D spectrum.

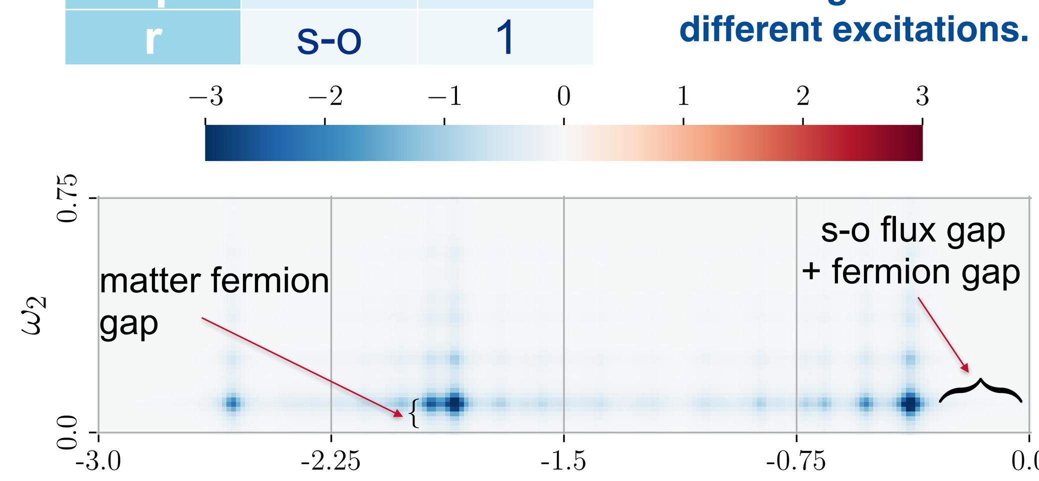
2DCS of second-order response for Kitaev honeycomb model. Real part of response function due to R1 process. Two frequencies are conjugate to the two independent time delay. Dashed black box indicates the flux gap in thermal dynamic limit.

- For square-octagon model: $\langle\sigma_j^y(0)\sigma_k^z(\tau_1)\sigma_l^z(\tau_1+\tau_2)\sigma_m^y(\tau_1)\rangle$
  - $J_x = J_y = 0.8$, $J_z = 1$; L = 18; second quadrant



	Flux	Matter
GS	0	0
p	s-o	1
q	s-o	0
r	s-o	1

2DCS of third-order response for Kitaev model on square-octagon model. It disentangles different excitations.



Information contained in the nonlinear response functions allows distinguishing between different types of fractionalized excitations in the system, which we identify as a suitable benchmark for future calculations using quantum computers.

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