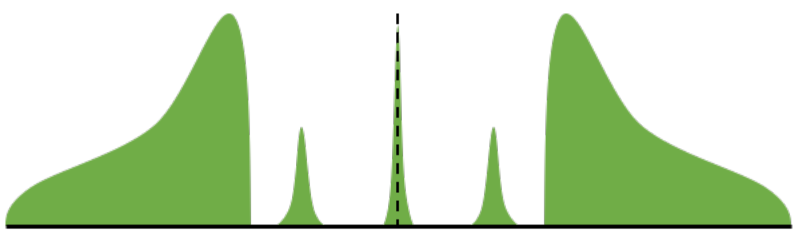
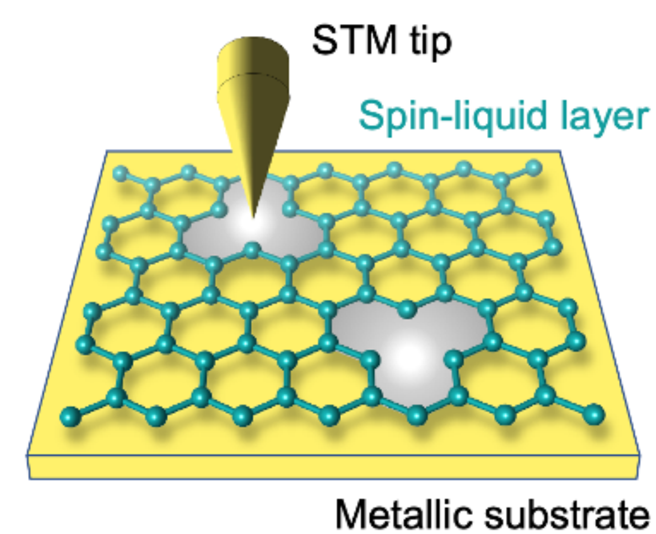
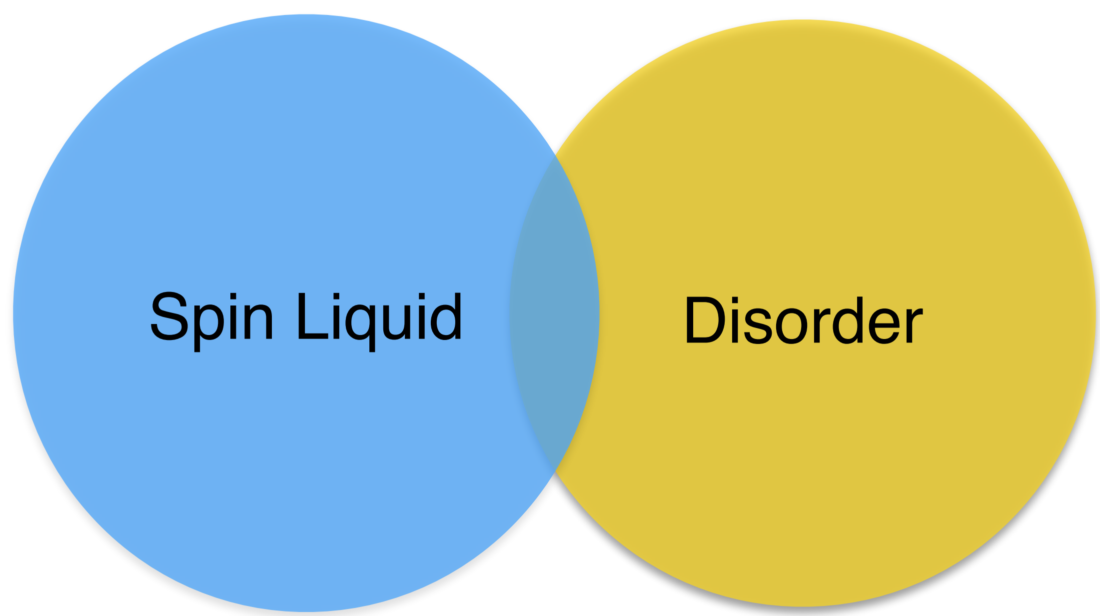
Dynamics of vacancy-induced modes in the non-Abelian Kitaev spin liquid



Natalia Perkins
University of Minnesota





ICTP/Conference on Fractionalization and Emergent Gauge Fields in Quantum Matter (2023)

Wen-Han Kao
University of Minnesota

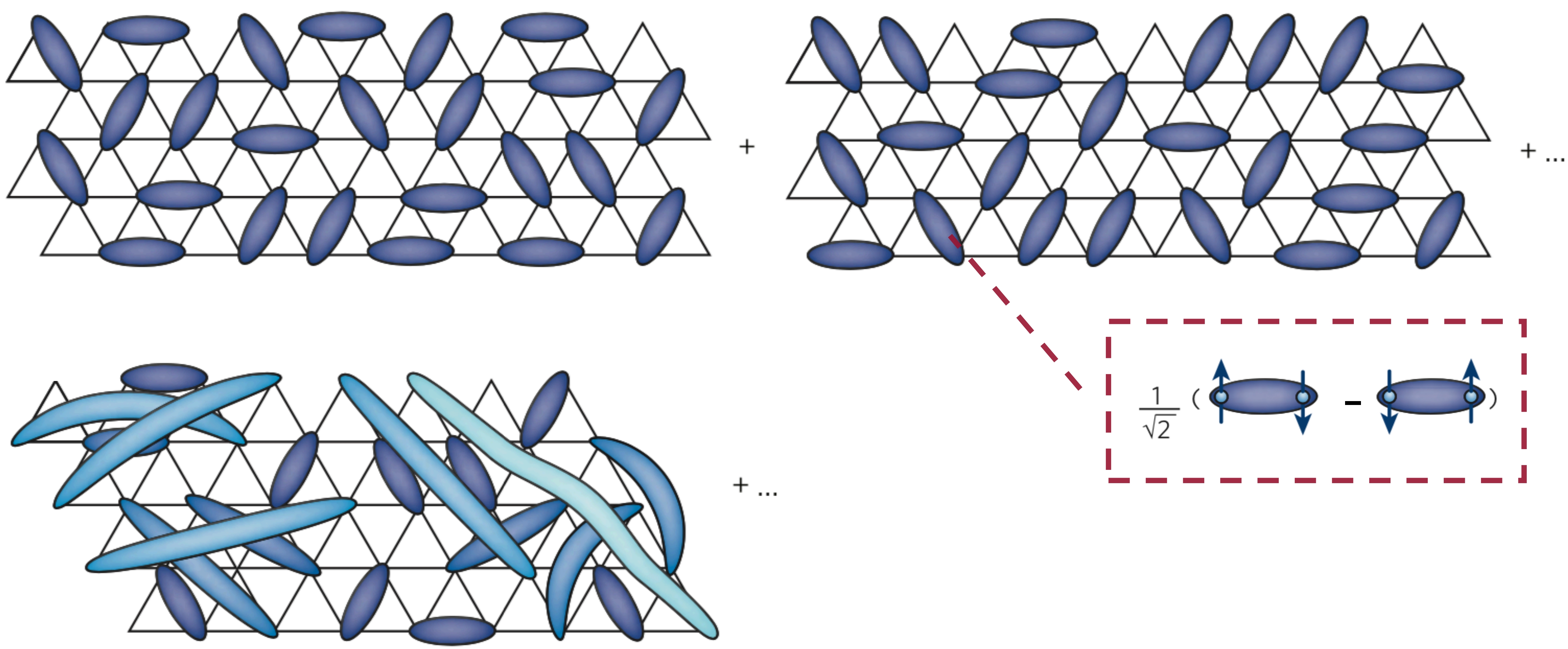
Gabor Halasz
ORNL,Oak Ridge

Wen-Han Kao, Gábor B. Halász, Natalia B. Perkins,
Dynamics of vacancy-induced modes in the non-Abelian Kitaev spin liquid
arXiv:2310.06891

Wen-Han Kao, Natalia B. Perkins, Gábor B. Halász,
Vacancy spectroscopy of non-Abelian Kitaev spin liquids
arXiv:2307.10376

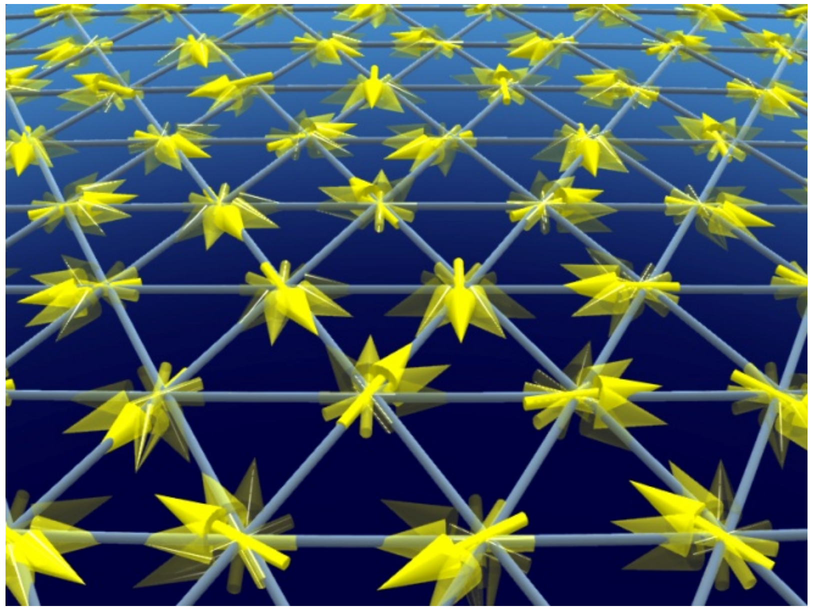
Quantum spin liquid

Resonating Valence Bond
(RVB)



P. Anderson,Mater. Res. Bull.,8, 153 (1973).
L. Balents, Nature 464, 199–208 (2010)

Quantum spin liquid



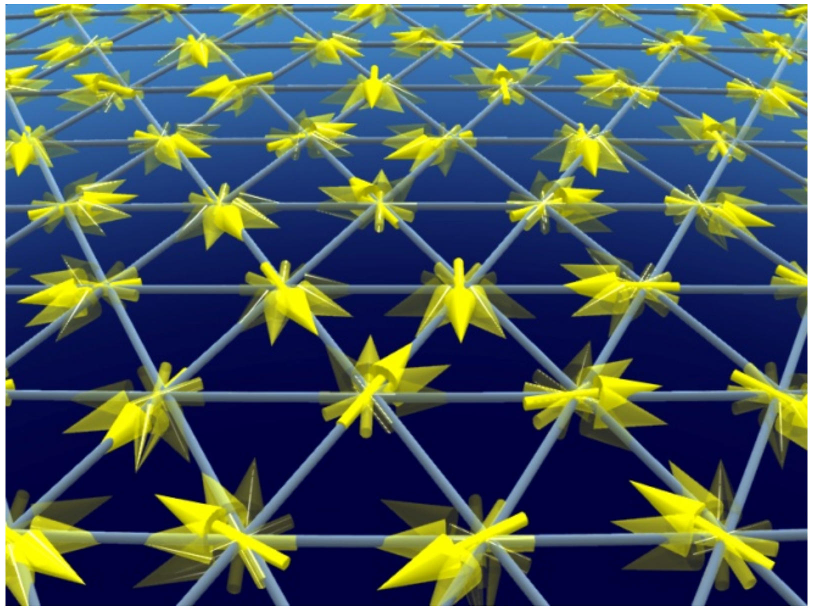
QSL is a state of interacting spins that breaks no rotational or translational symmetry.

QSLs are characterized by **topological order**, **long range entanglement**, and **fractionalized non-local excitations**.

Signatures of **fractionalization** in dynamical probes:

- Inelastic neutron scattering (INS)
- Raman scattering with visible light
- Resonant inelastic X-ray scattering (RIXS)
- Ultrafast spectroscopy
- Phonon dynamics
- …
-

Quantum spin liquids



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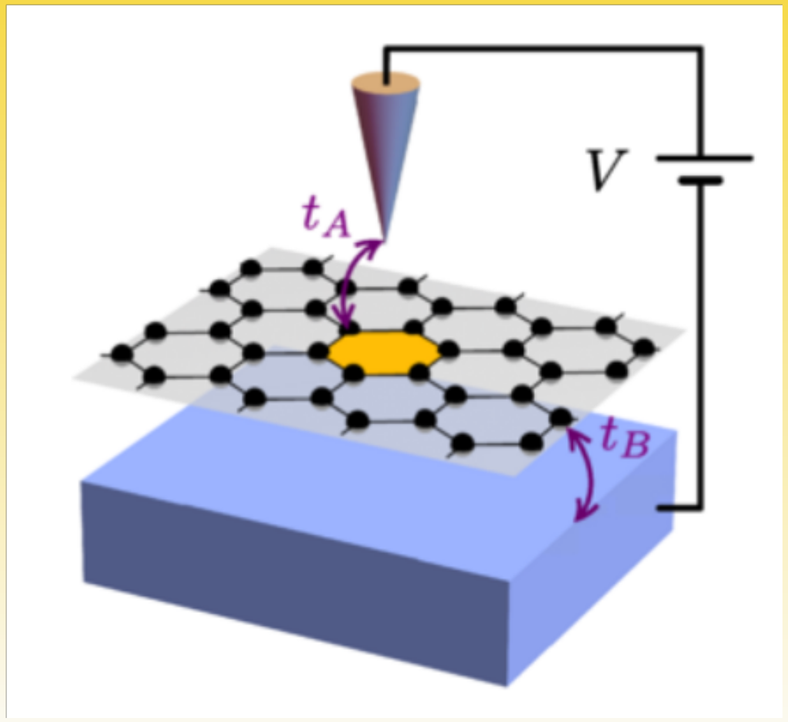
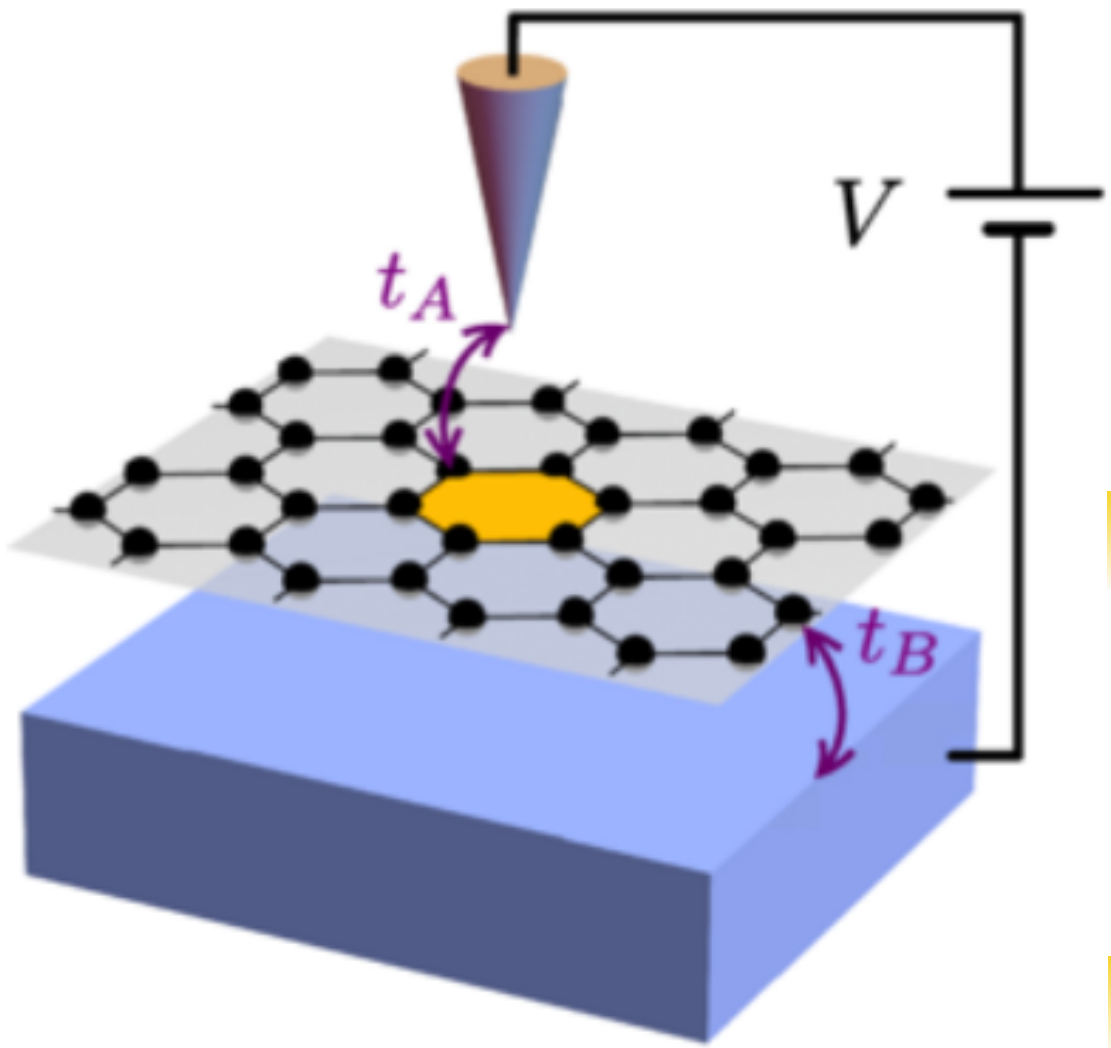
- …
- **Scanning tunneling spectroscopy**



Tunnel conductance is determined by dynamical spin correlations!

Local probe of 2D quantum magnets



Electron tunnels through (not into) material.

Bauer *et al.*, PRB2023

Feldmeier *et al.*, PRB2020

König *et al.*, PRL2020

General idea: Derivative of tunneling conductance in voltage

$$\frac{d^2 I}{dV^2} \propto \sum_{\mathbf{r},\mathbf{r}'} \sum_{\alpha,\beta} C^{\alpha\beta}_{\mathbf{r},\mathbf{r}'} \, S^{\alpha\beta}_{\mathbf{r},\mathbf{r}'}(eV)$$

is proportional to dynamical spin correlation function

$$S^{\alpha\beta}_{\mathbf{r},\mathbf{r}'}(\omega) = \int dt \, e^{i\omega t} \left\langle \sigma^{\alpha}_{\mathbf{r}}(t) \sigma^{\beta}_{\mathbf{r}'}(0) \right\rangle$$

If tip is very sharp, and points directly on the cite ***R***

$$C^{\alpha\beta}_{\mathbf{r},\mathbf{r}'} \approx \delta_{\mathbf{r},\mathbf{R}} \, \delta_{\mathbf{r}',\mathbf{R}} \, \delta_{\alpha,\beta}$$

$$\frac{d^2 I}{dV^2} \propto \sum_{\alpha} S^{\alpha\alpha}_{\mathbf{R},\mathbf{R}}(eV)$$

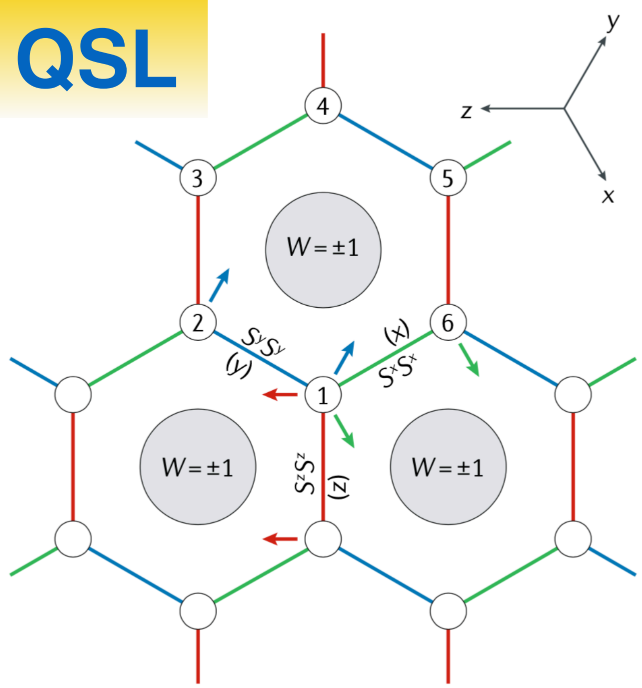
Single-site structure factor

Kitaev spin liquid

$$H = -\sum_{x-bonds} J_x \sigma_j^x \sigma_k^x - \sum_{y-bonds} J_y \sigma_j^y \sigma_k^y - \sum_{z-bonds} J_z \sigma_j^z \sigma_k^z$$

A. Kitaev, Annals of Physics **321**, 2 (2006)

exact QSL



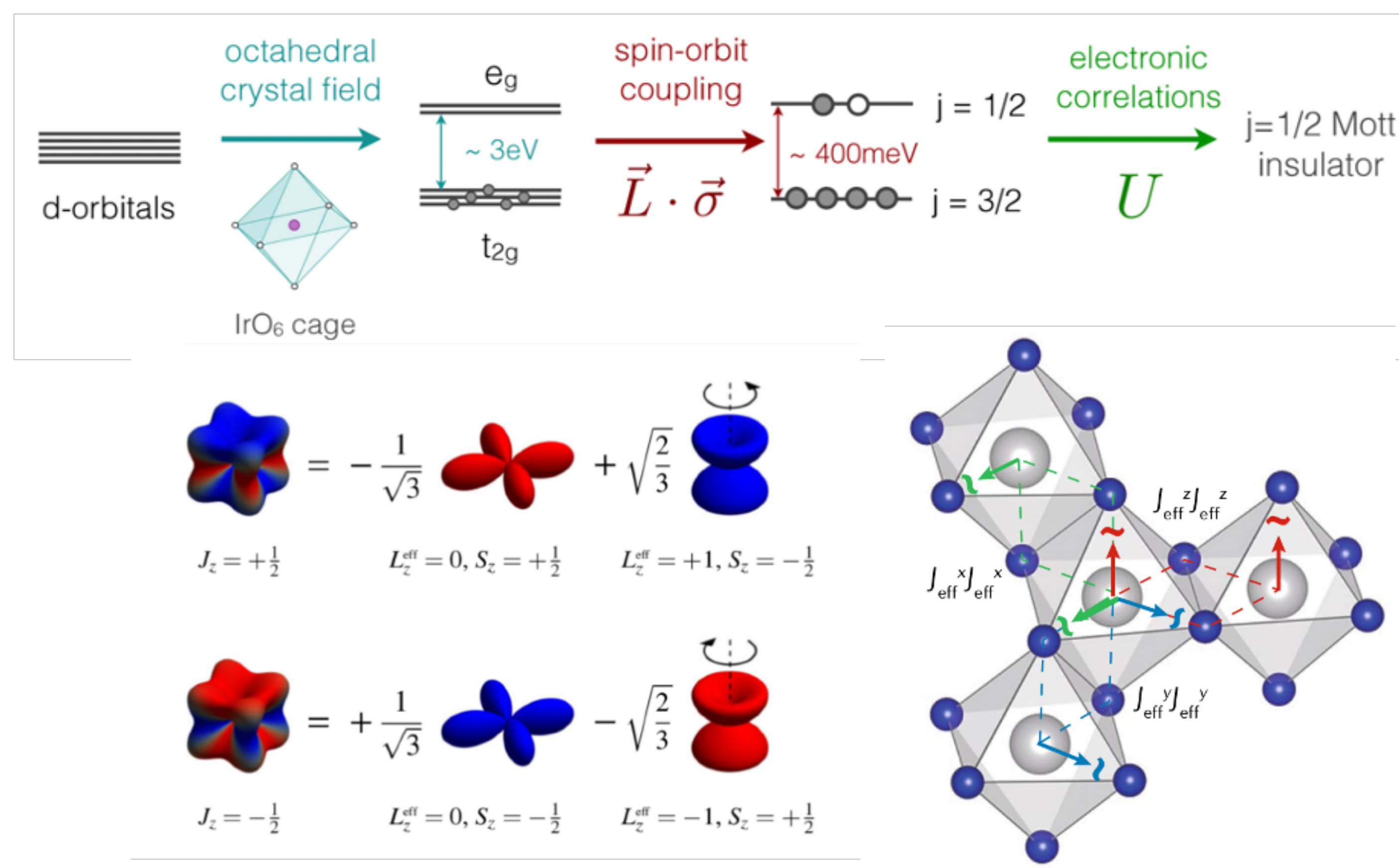
$$\tilde{W}_p = \hat{\sigma}_1^x \hat{\sigma}_2^y \hat{\sigma}_3^z \hat{\sigma}_4^x \hat{\sigma}_5^y \hat{\sigma}_6^z$$

$$[\tilde{W}_p, \hat{H}] = 0$$

$$W_p = \pm 1$$

H. Takagi *et al.*, Nature Reviews Physics **1**, 264 (2019)

Kitaev Materials



G. Jackeli and G. Khaliullin, PRL (2009)

S. Trebst and C. Hickey, Phys. Rep. (2022)

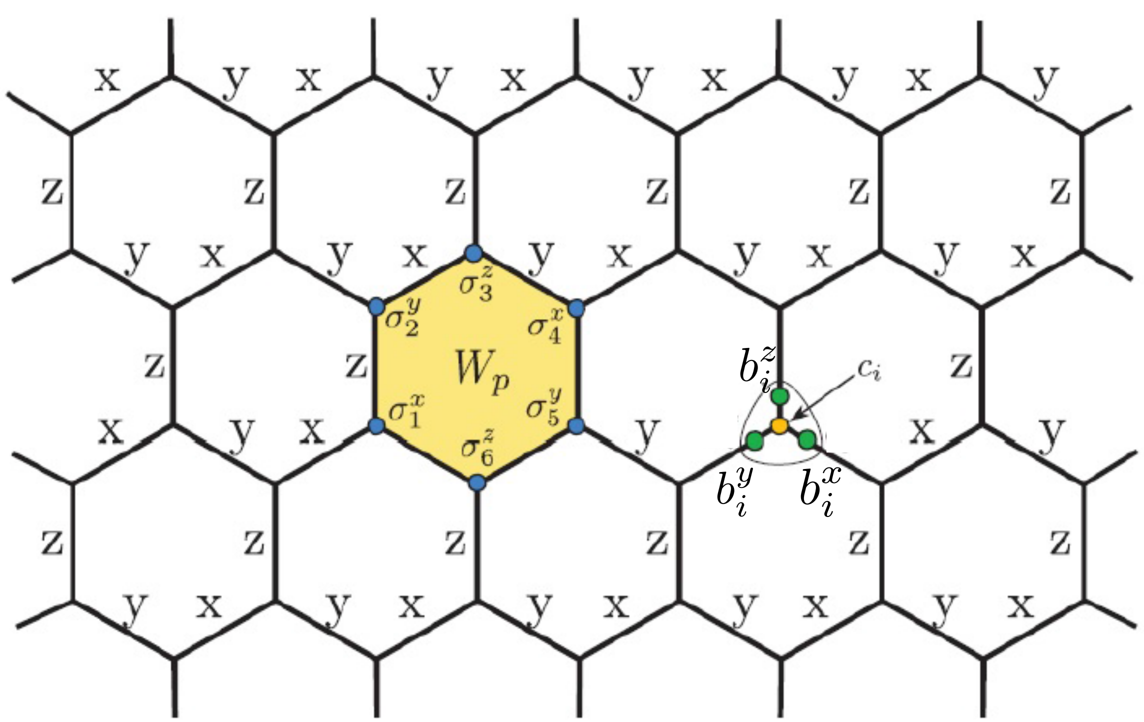
Fractionalization in the Kitaev spin liquid

Physical spins: $\sigma_i^\alpha = i c_i b_i^\alpha, \qquad \alpha = x, y, z$

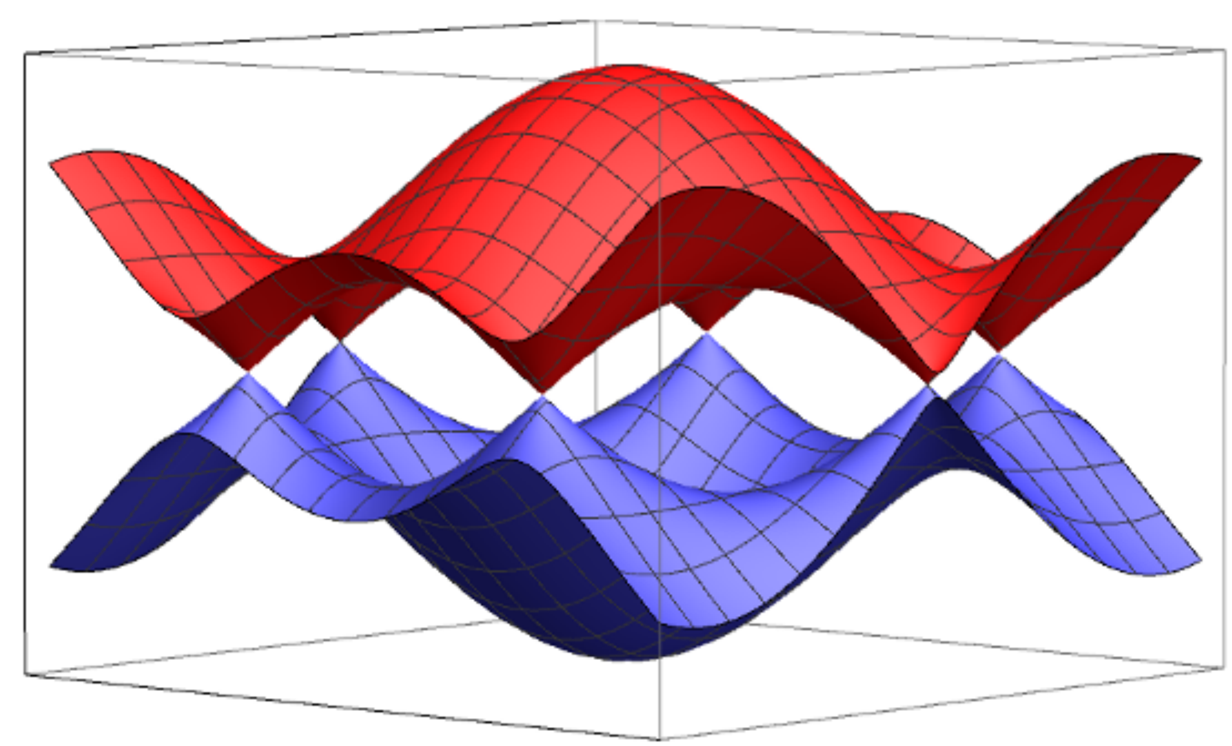
$$\mathcal{H} = \sum_{\alpha=x,y,z} J_\alpha \sum_{\langle ij \rangle_\alpha} i c_i \hat{u}_{\langle ij \rangle_\alpha} c_j$$

Bond fermions (Flux pairs)

$$\hat{u}_{\langle ij \rangle_\alpha} \equiv i b_i^\alpha b_j^\alpha$$



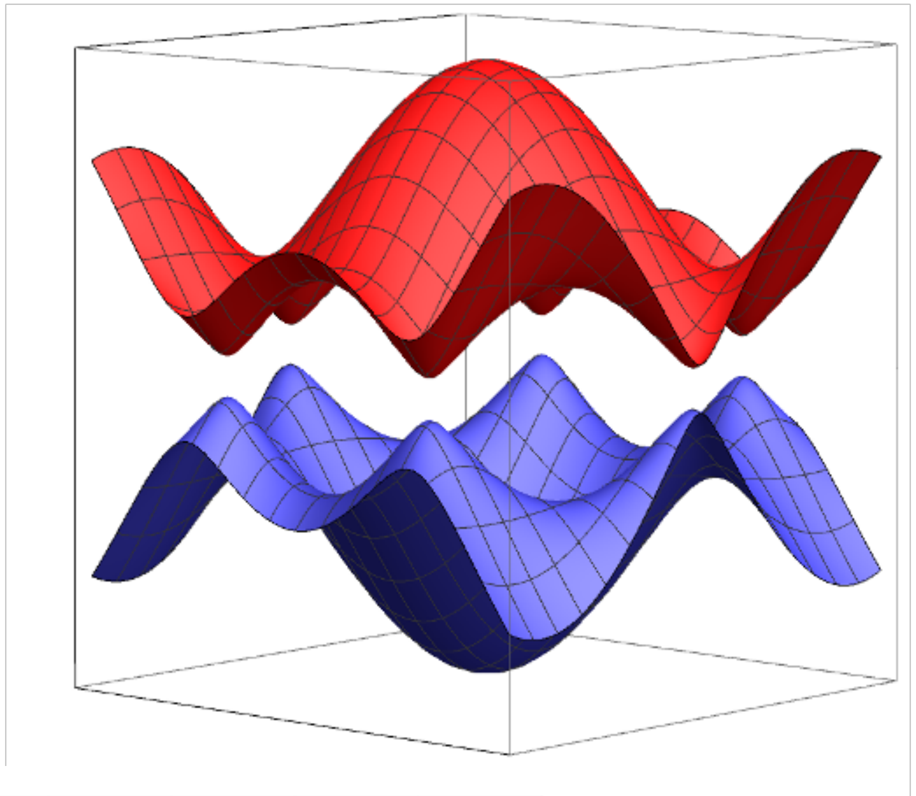
Matter fermions (Majorana fermions)



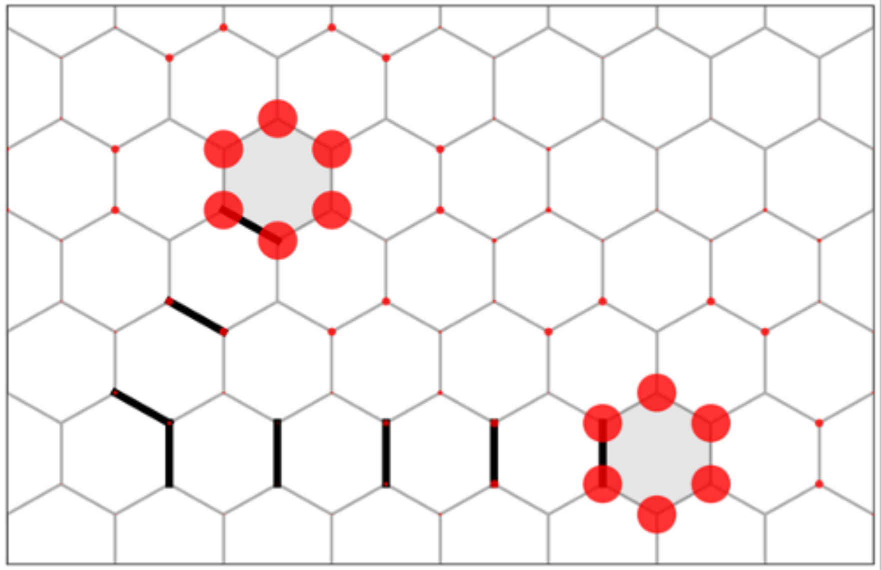
Fractionalization in the Kitaev spin liquid

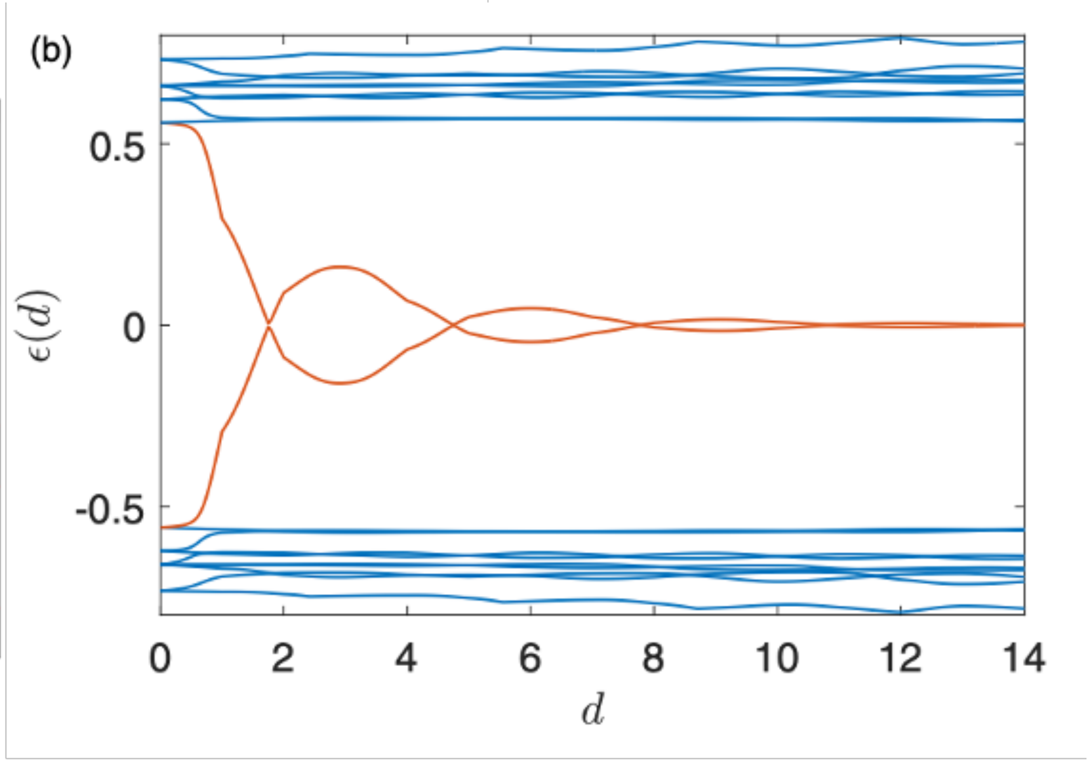
Majorana fermions are gapped

$$\kappa \sim \frac{h_x h_y h_z}{\Delta_f^2}, \quad \Delta_\kappa = 6\sqrt{3}\,\kappa$$



Gapped gauge fluxes becomes non-Abelian Ising anyone





Fusion rule

$$\sigma \times \sigma = 1 + \psi$$

Two fluxes with f-modes

Fluxes annihilate with one QP

Separated fluxes induce in-gap modes (**f-mode**)

Two f-modes **hybridize** when close in proximity

Scanning tunneling spectroscopy of Kitaev QSL

- Total Hamiltonian: $H = H_t + H_s + H_K + H_T$

$$H_t + H_s = \sum_{\mathbf{p}\sigma} \varepsilon_{\mathbf{p}} p^\dagger_{\mathbf{p}\sigma} p_{\mathbf{p}\sigma} + \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}$$

$$H_K = \sum_{\langle ij\rangle_\alpha} J^\alpha S^\alpha_i S^\alpha_j + \kappa \sum_{\langle ij\rangle_\alpha, \langle jk\rangle_\gamma} S^\alpha_i S^\beta_j S^\gamma_k$$

$$H_T = \sum_{\mathbf{pk}\sigma\sigma'} \hat{T}^{\sigma\sigma'}_{\mathbf{r}}\, p^\dagger_{\mathbf{p}\sigma}\, c_{\mathbf{k}\sigma'}\, e^{i(\mathbf{k}\cdot\mathbf{r}+eVt)} + \mathrm{h.\,c.}$$

- Co-tunneling matrix element:

$$\hat{T}^{\sigma\sigma'}_{\mathbf{r}} = t_0\, \delta_{\sigma\sigma'} + \sum_i t_1(\mathbf{r}-\mathbf{r}_i)\, \vec{\sigma}_{\sigma\sigma'} \cdot \vec{S}_i$$

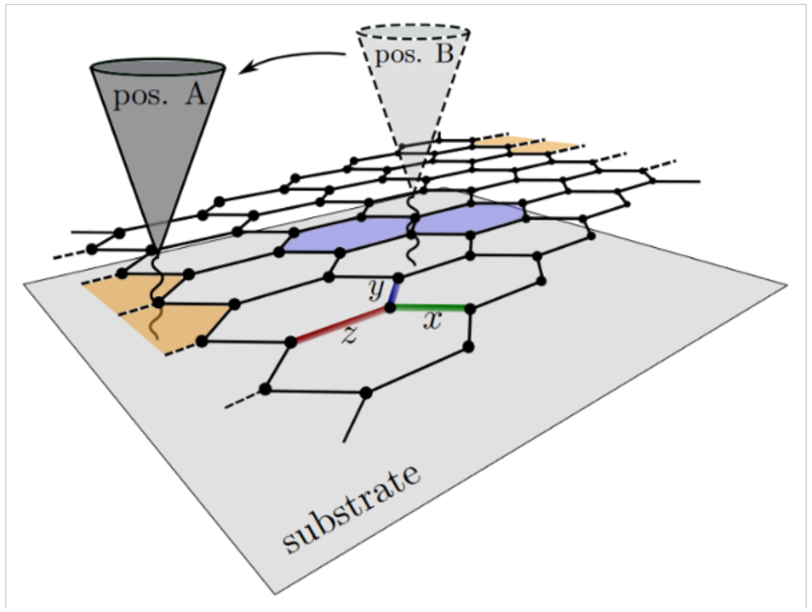
$$t_1(\mathbf{r}-\mathbf{r}_i) \sim e^{-d/d_0} e^{-|\mathbf{r}-\mathbf{r}_i|/\lambda}$$

- Tunneling conductance:

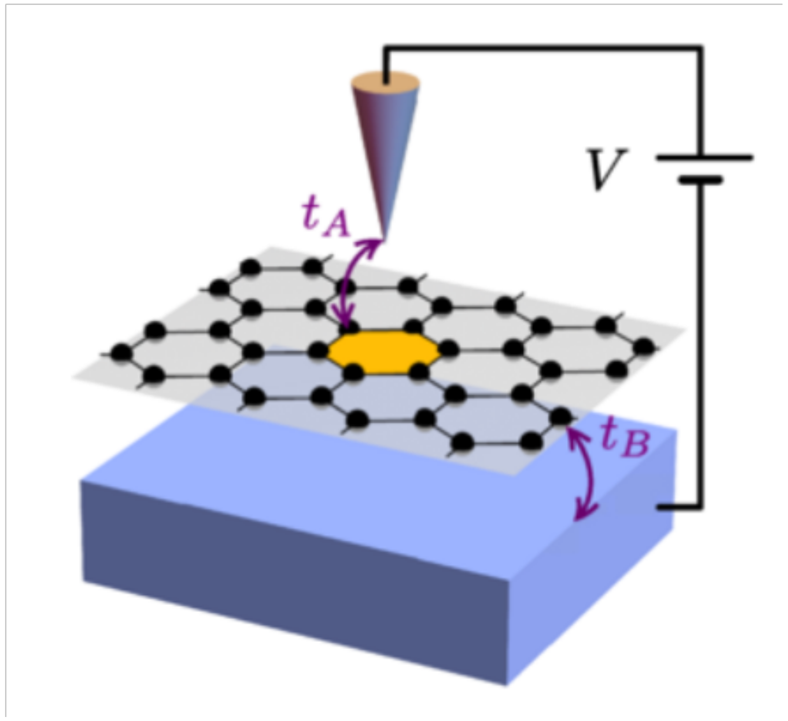
$$\frac{\partial I}{\partial V} = \frac{2\pi e^2}{\hbar} \sum_{\alpha\beta} \sum_{ij} t_1(\mathbf{r}-\mathbf{r}_i)\, t_1(\mathbf{r}-\mathbf{r}_j)\, C_{\alpha\beta} \int_0^{eV} \mathrm{d}\omega\, S^{\alpha\beta}_{ij}(\omega)$$

J. Feldmeier, W. Natori, M. Knap, and J. Knolle, Phys. Rev. B 102, 134423 (2020)
T. Bauer, L. R. D. Freitas, R. G. Pereira, and R. Egger, Phys. Rev. B 107, 054432 (2023)

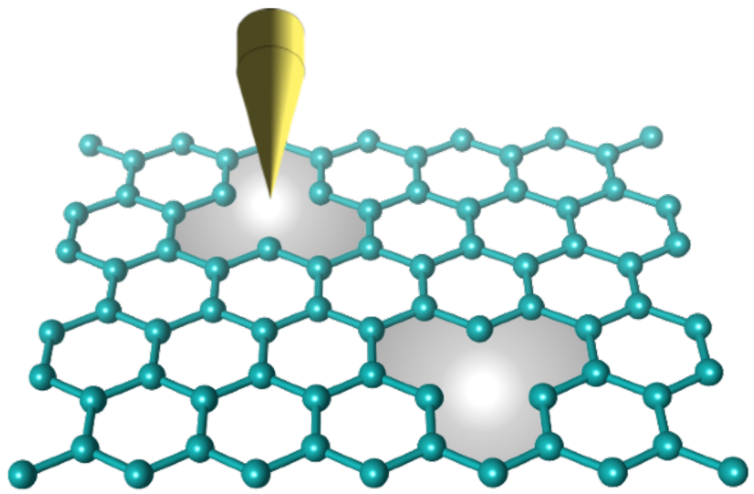
Scanning tunneling spectroscopy of Kitaev QSL



Feldmeier *et al.*, PRB2020
König *et al.*, PRL2020

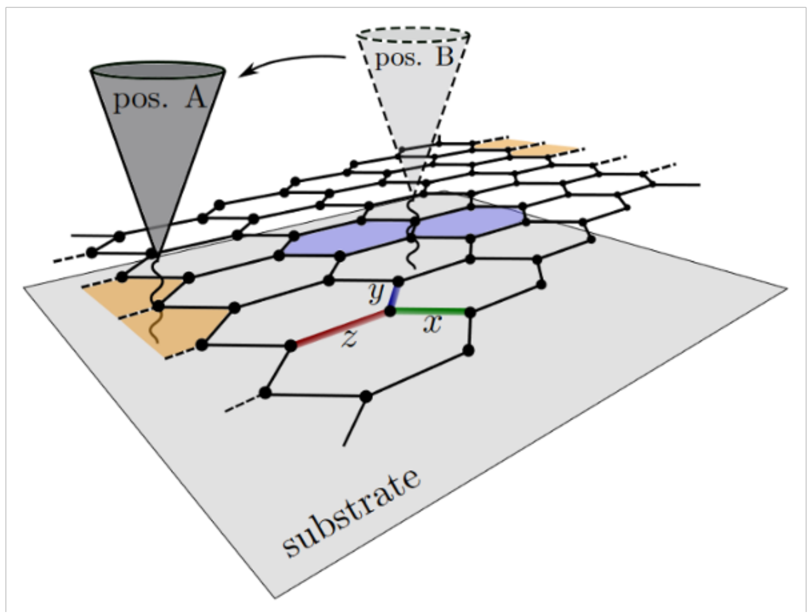


Bauer *et al.*, PRB2023
Udagawa *et al.*, PRL2021

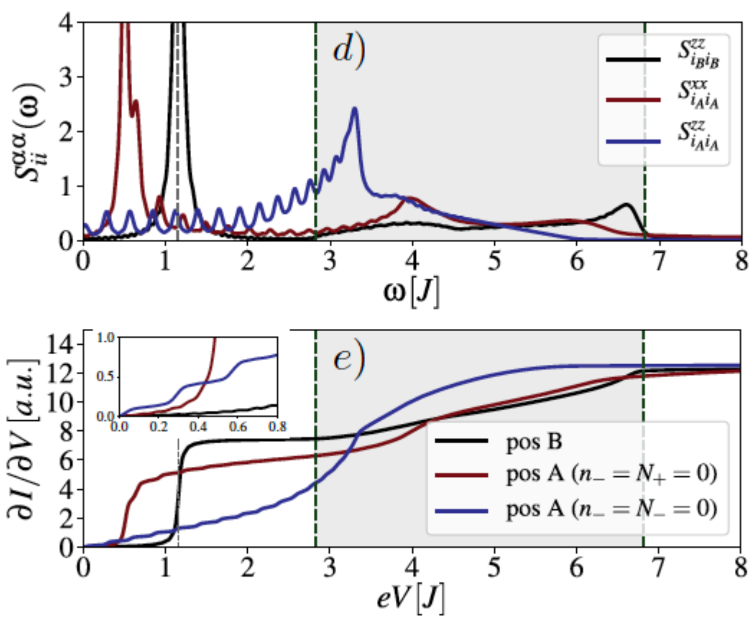


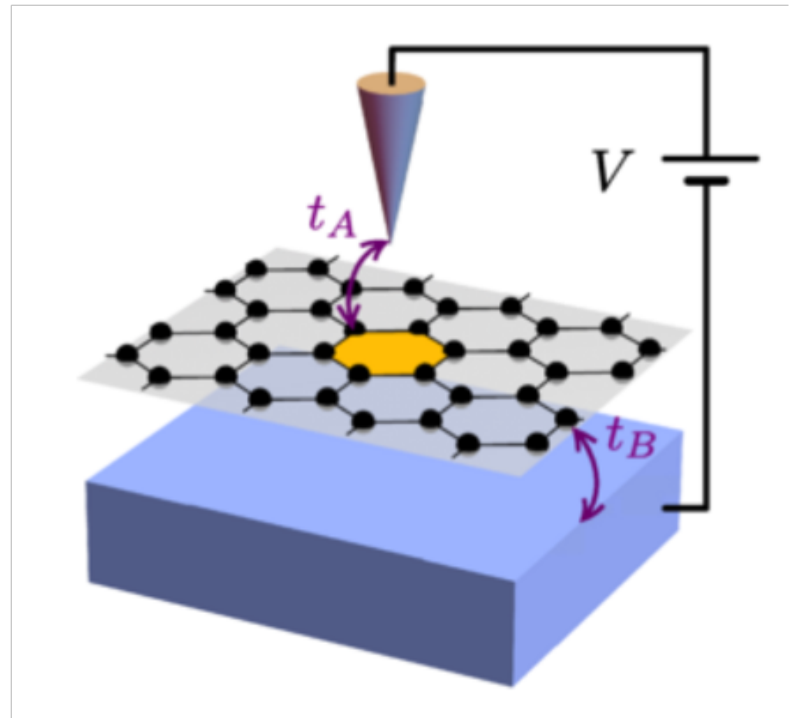
Kao *et al.*,arxiv:2307.10376
Kao *et al.*, arxiv:2310.06891
Takahashi *et al.*, arxiv:2211.13884

Scanning tunneling spectroscopy of Kitaev QSL

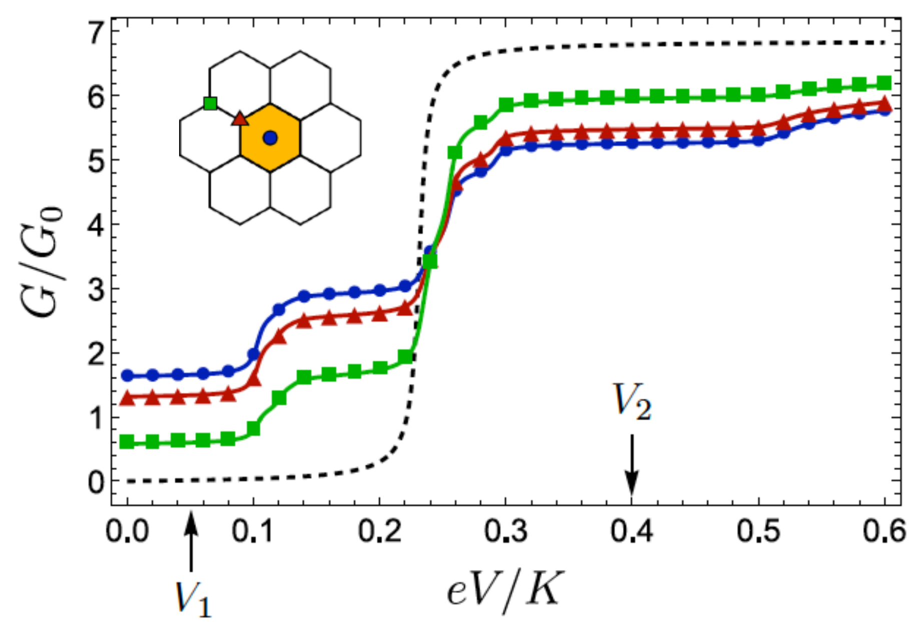


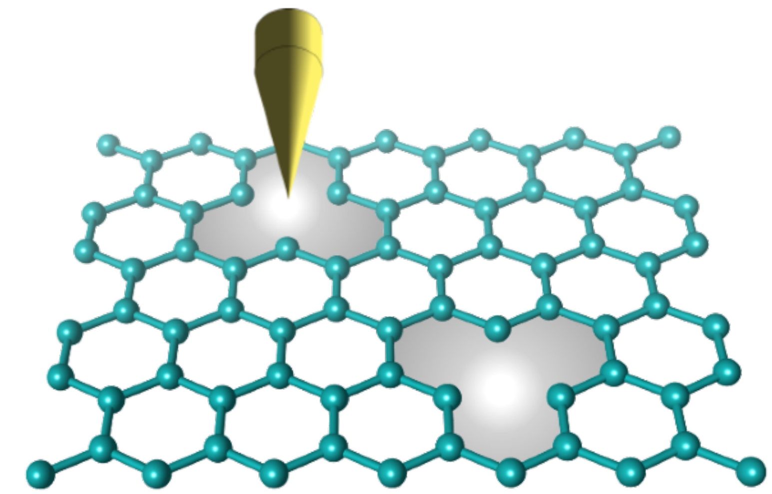
Feldmeier *et al.*, PRB2020
König *et al.*, PRL2020



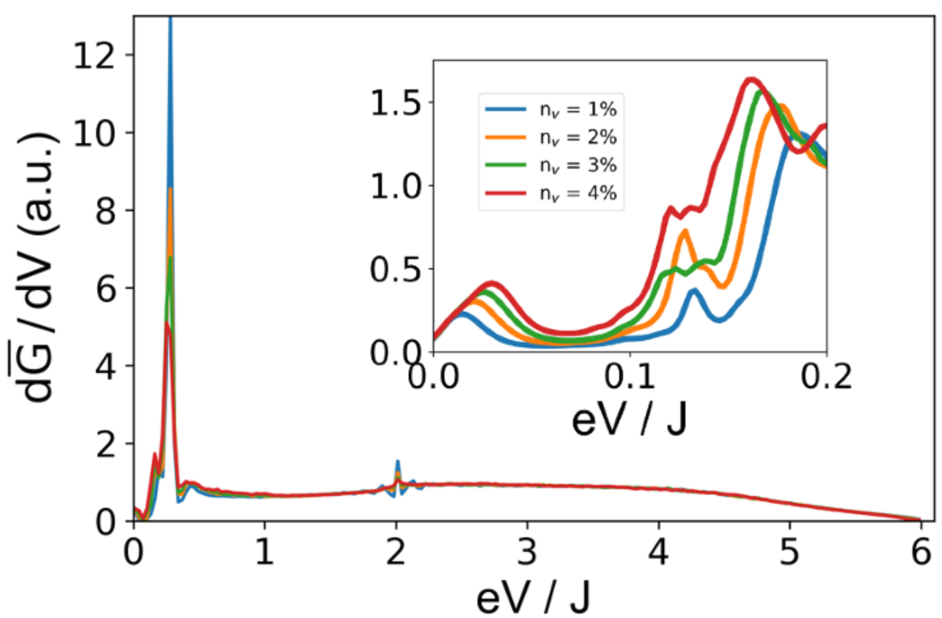


Bauer *et al.*, PRB2023
Udagawa *et al.*, PRL2021



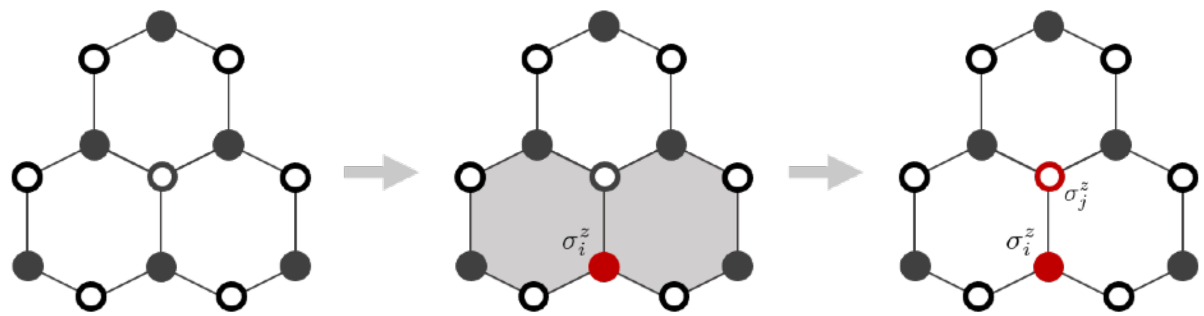


Kao *et al.*,arxiv:2307.10376
Kao *et al.*, arxiv:2310.06891
Takahashi *et al.*, arxiv:2211.13884



Different tip position => different correlation functions

Dynamical Correlation Function (bulk)



G. Baskaran, S. Mandal, R. Shankar, PRL **98**, 247201 (2007)
J. Knolle *et al*., Phys. Rev. Lett. **112**, 207203 (2014)
J. Knolle *et al*., Phys. Rev. B **92**, 115127 (2015)

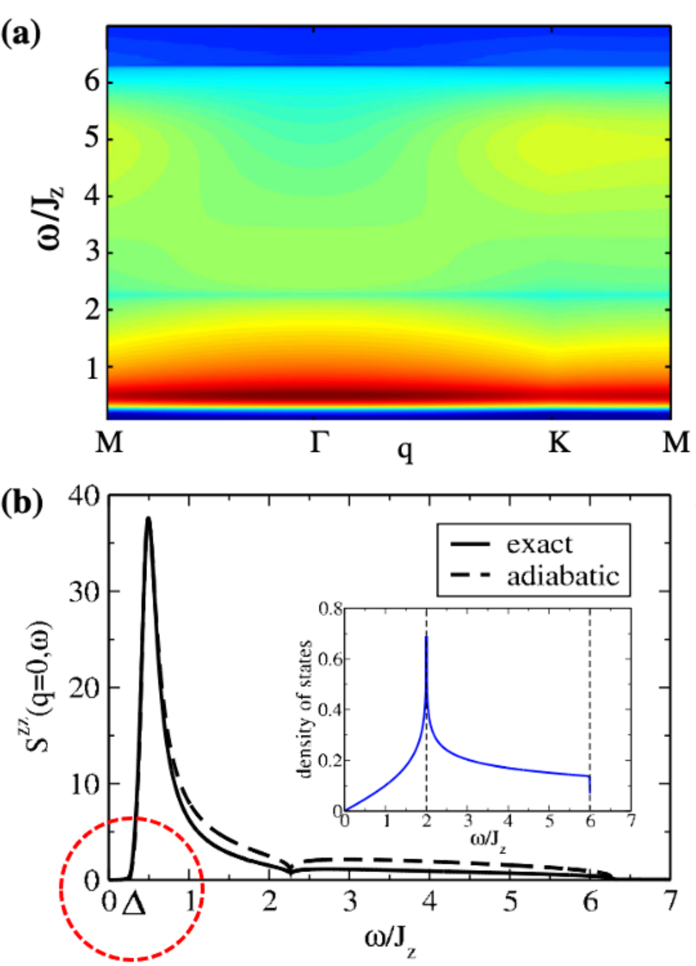
$$S_{ij}^{\alpha\beta}(\omega) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}t\, e^{i\omega t}\, \langle 0|\, \sigma_i^\alpha(t)\sigma_j^\beta(0)\, |0\rangle$$

$$= \sum_{\lambda_F} \langle M_0|\, c_i\, |\lambda_F\rangle\, \langle \lambda_F|\, c_j\, |M_0\rangle\, \delta[\omega - (E_\lambda^F - E_0)].$$

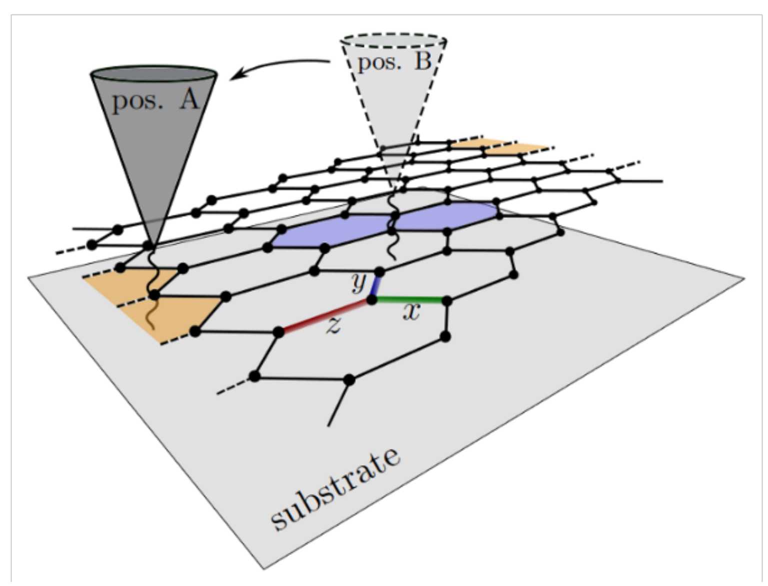
Bulk spin correlation function
- On-site correlation
- Nearest-neighbor correlation

one-particle contribution

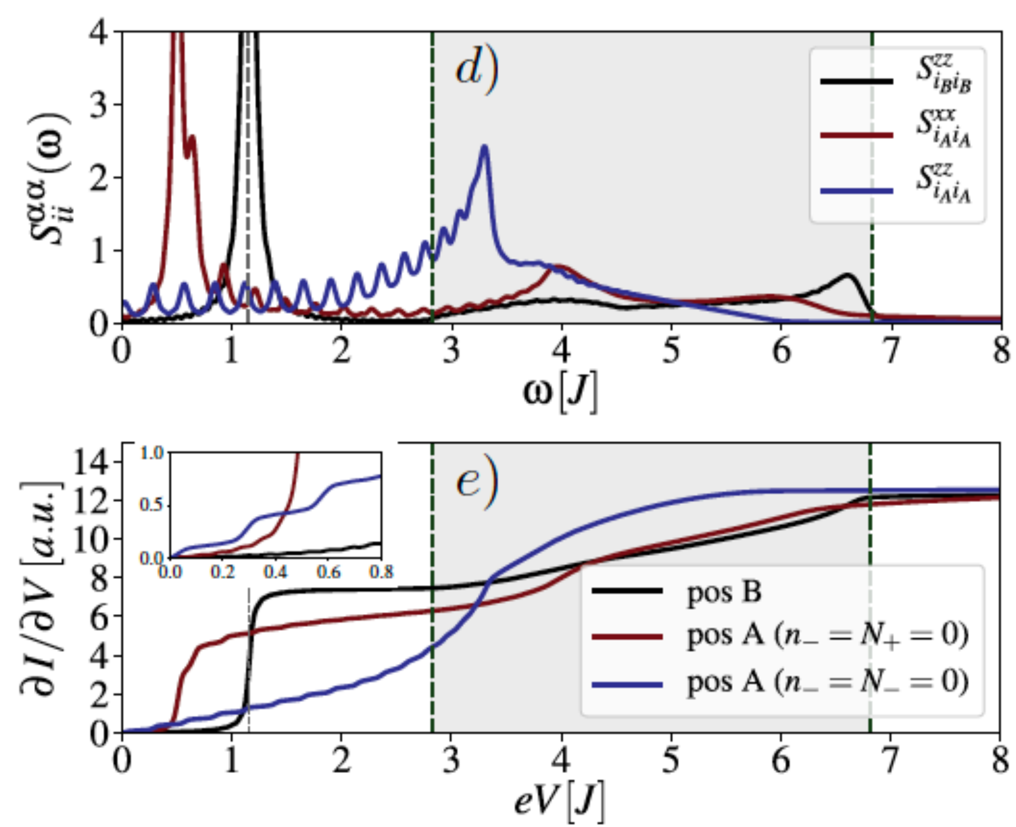
$$\langle M_0|c_i|\lambda_F\rangle \sim \langle M_0|c_i\, (a_\lambda^F)^\dagger|M_F\rangle \sim \langle M_F|c_i\, (a_\lambda^F)^\dagger|M_F\rangle$$



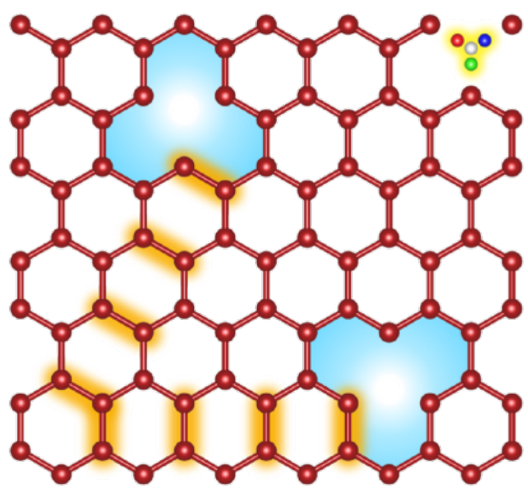
No intensity below 2-flux gap



Feldmeier *et al.*, PRB2020

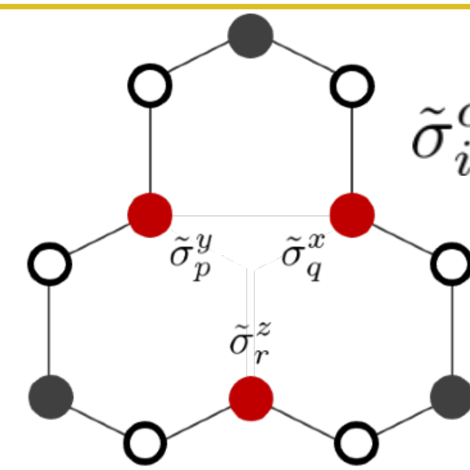


Kitaev spin liquid with vacancies



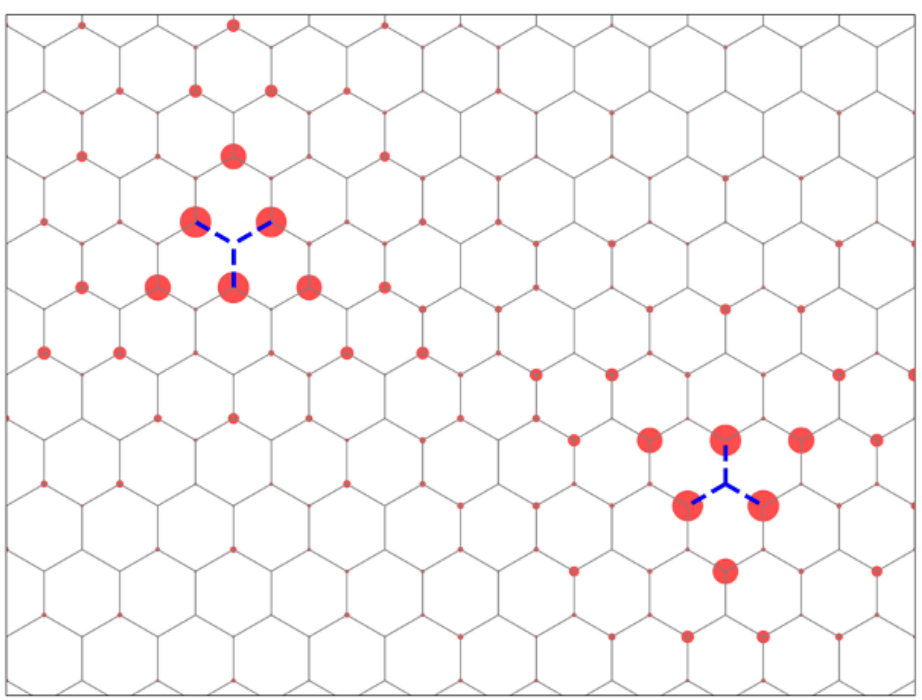
A. Willans *et al.*, Phys. Rev. Lett. **104**, 237203 (2010)
A. Willans *et al.*, Phys. Rev. B **84**, 115146 (2011)
F. Zschocke *et al.*, Phys. Rev. B **92**, 014403 (2015)
W.-H. Kao *et al.*, Phys. Rev. X **11**, 011034 (2021)

$$\mathcal{H} = -J \sum_{\langle ij \rangle_\alpha} \sigma_i^\alpha \sigma_j^\alpha$$



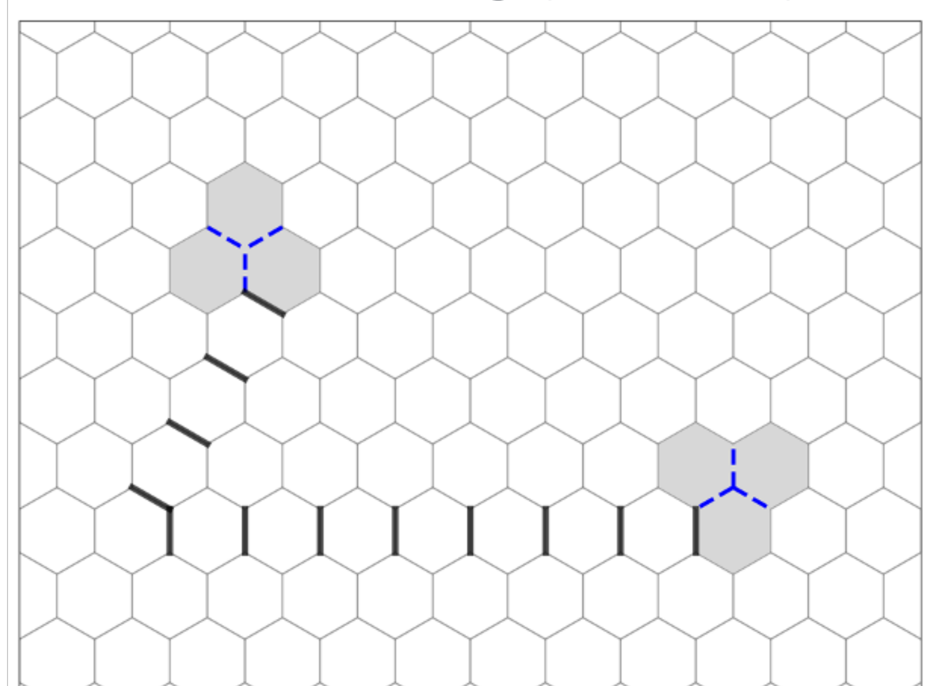
$$\tilde{\sigma}_i^\alpha = i\, \tilde{b}_i^\alpha c_i$$

Peripheral Modes (p-mode)



- Quasi-localized and E ~ 0
- The same as in graphene

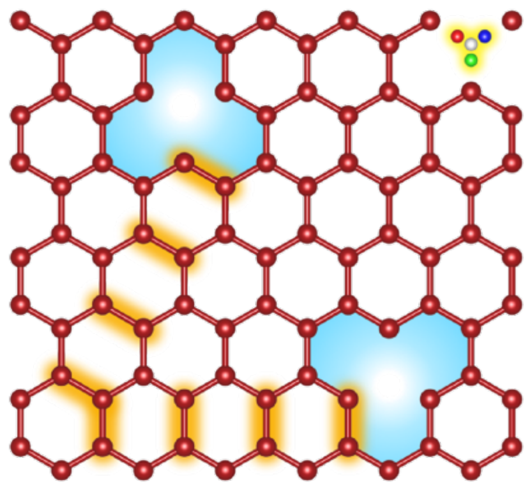
Flux Binding (f-mode)

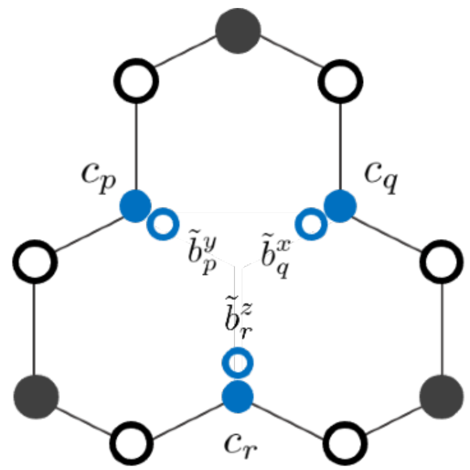


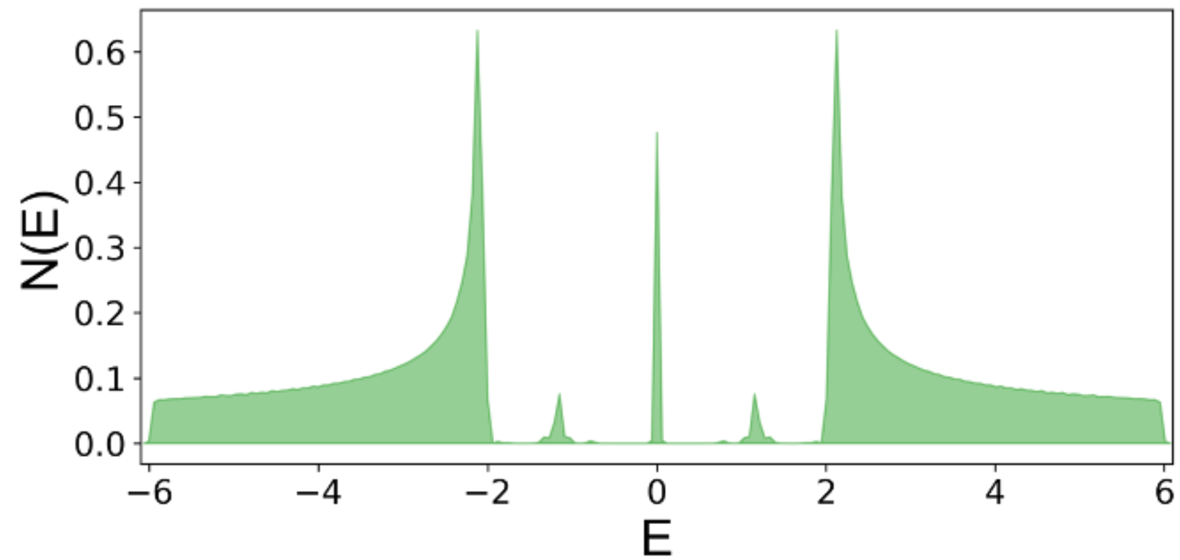
- Flux introduced in pairs
- Ground-state flux sector

Vacancy-induced in-gap Majorana modes

$$\mathcal{H} = -J \sum_{\langle ij \rangle_\alpha} \sigma_i^\alpha \sigma_j^\alpha - \kappa \sum_{\langle ijk \rangle} \sigma_i^\alpha \sigma_j^\gamma \sigma_k^\beta - h \sum_{i \in \mathbb{D}_\alpha} \tilde{\sigma}_i^\alpha$$

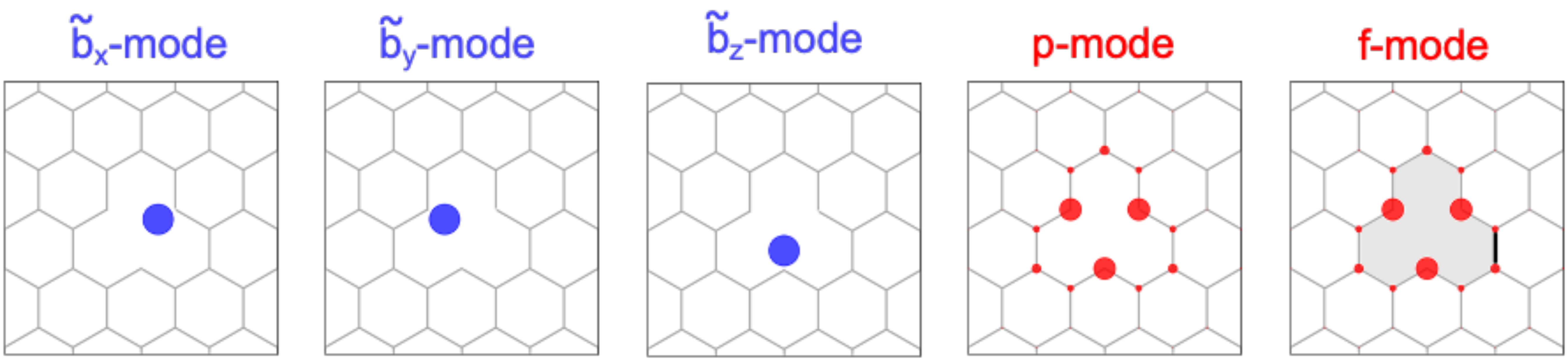






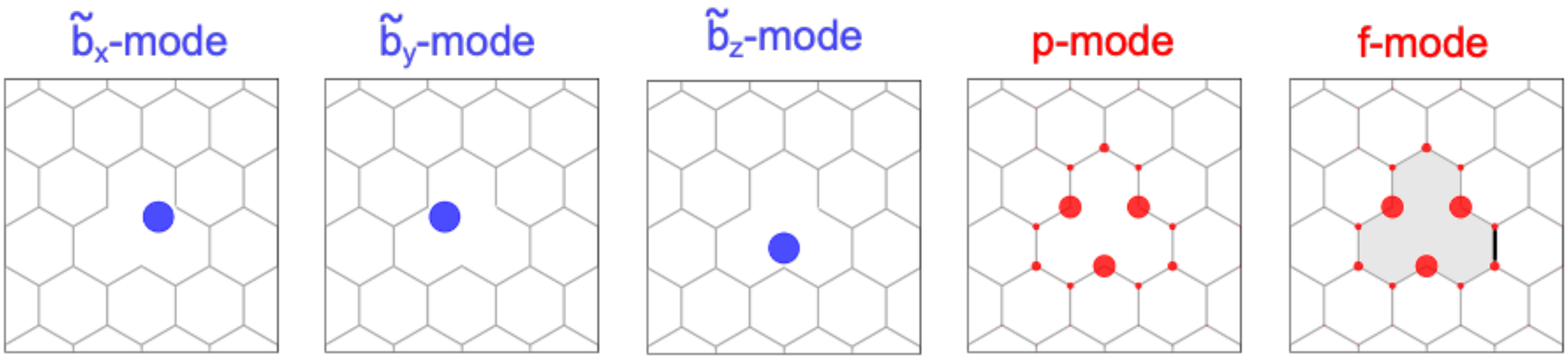
A. Willans *et al.*, Phys. Rev. Lett. **104**, 237203 (2010)
A. Willans *et al.*, Phys. Rev. B **84**, 115146 (2011)
F. Zschocke *et al.*, Phys. Rev. B **92**, 014403 (2015)
W.-H. Kao *et al.*, Phys. Rev. X **11**, 011034 (2021)

$$\mathcal{H}_i^{\text{Zeeman}} = -ih\, \tilde{b}_i^\alpha c_i$$



Dangling Majorana fermions (b-modes)

Majorana modes hybridization



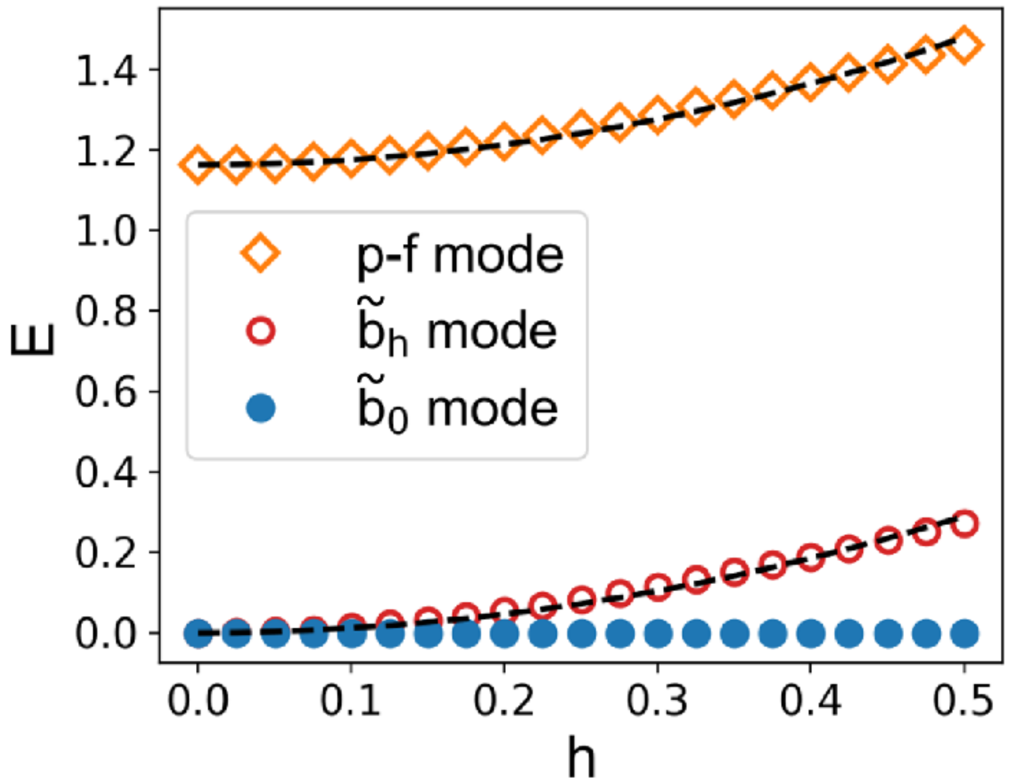
Toy model:

$$i\begin{pmatrix} 0 & \gamma_b h^2 & -\gamma_b h^2 & \gamma_p h & \gamma_f h \\ -\gamma_b h^2 & 0 & \gamma_b h^2 & \gamma_p h & \gamma_f h \\ \gamma_b h^2 & -\gamma_b h^2 & 0 & \gamma_p h & \gamma_f h \\ -\gamma_p h & -\gamma_p h & -\gamma_p h & 0 & f(J,\kappa) \\ -\gamma_f h & -\gamma_f h & -\gamma_f h & -f(J,\kappa) & 0 \end{pmatrix}$$

Energy of the Majorana eigenmodes:

$$\epsilon \approx 0,\ \pm\sqrt{3}\gamma_b h^2,\ \pm\left[f(J,\kappa) + \frac{3(\gamma_p^2+\gamma_f^2)}{2f(J,\kappa)}h^2\right]$$

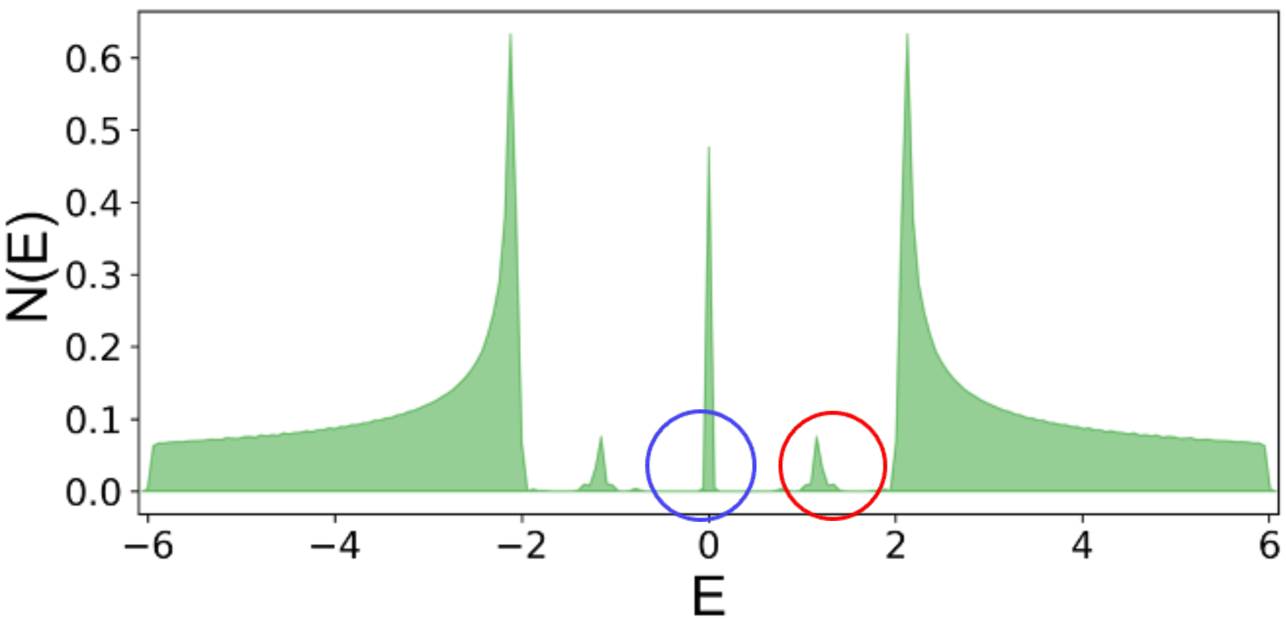
Full calculation from the site-diluted KSL model:



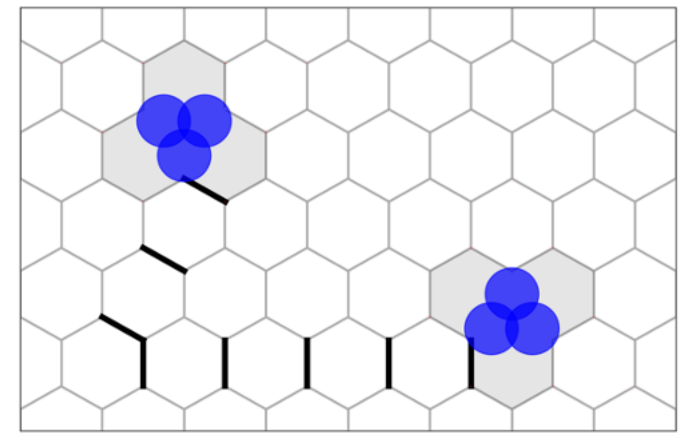
Protected Majorana zero mode!
(with pure b-Majorana character)

Density of States and in-gap modes

h = 0.1



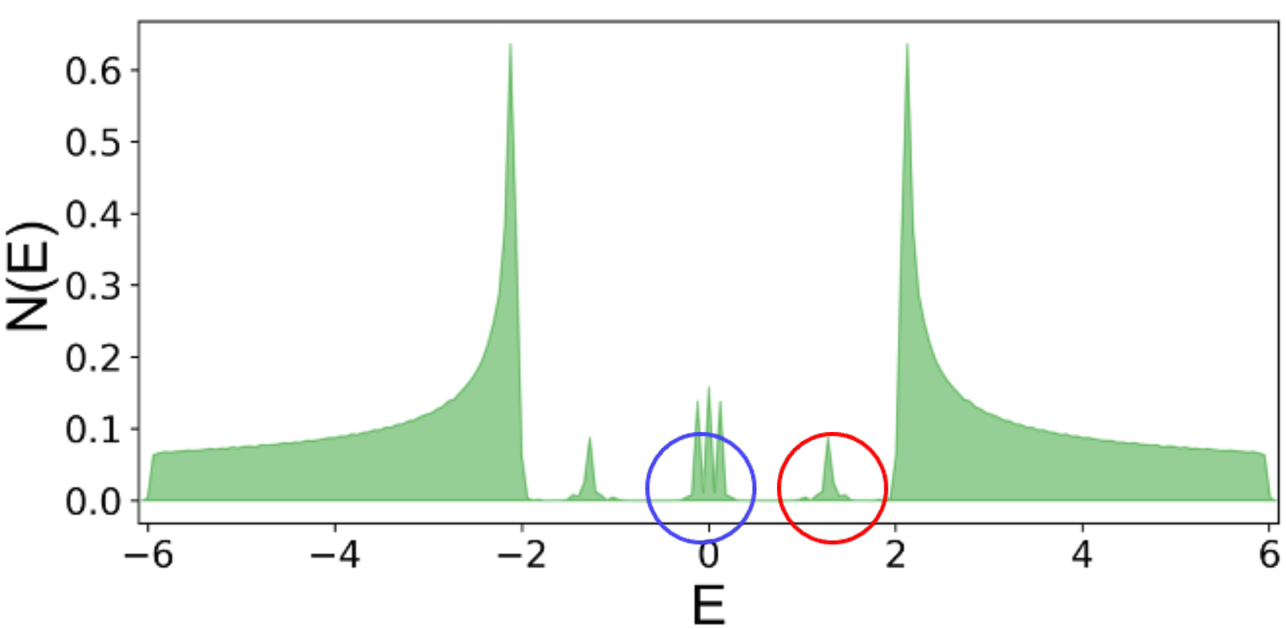
Dangling b-modes



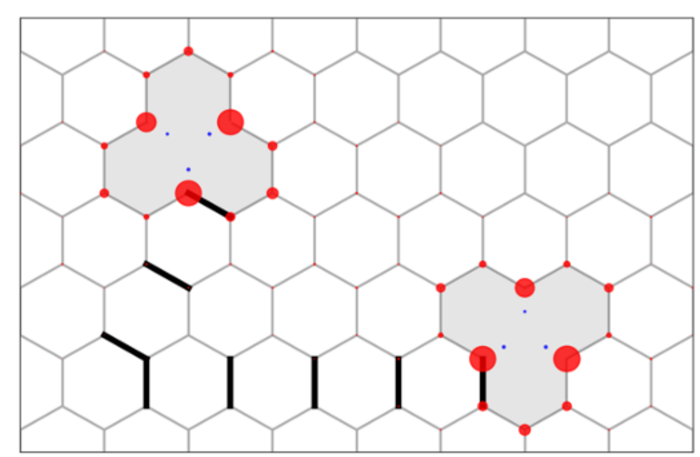
$$\epsilon \sim 0, \;\; \pm\sqrt{3}\gamma_b h^2$$

Open the bulk gap first ($\kappa = 0.2$), then Zeeman field $\boldsymbol{h}$ can split peak 1 but not peak 2

h = 0.3

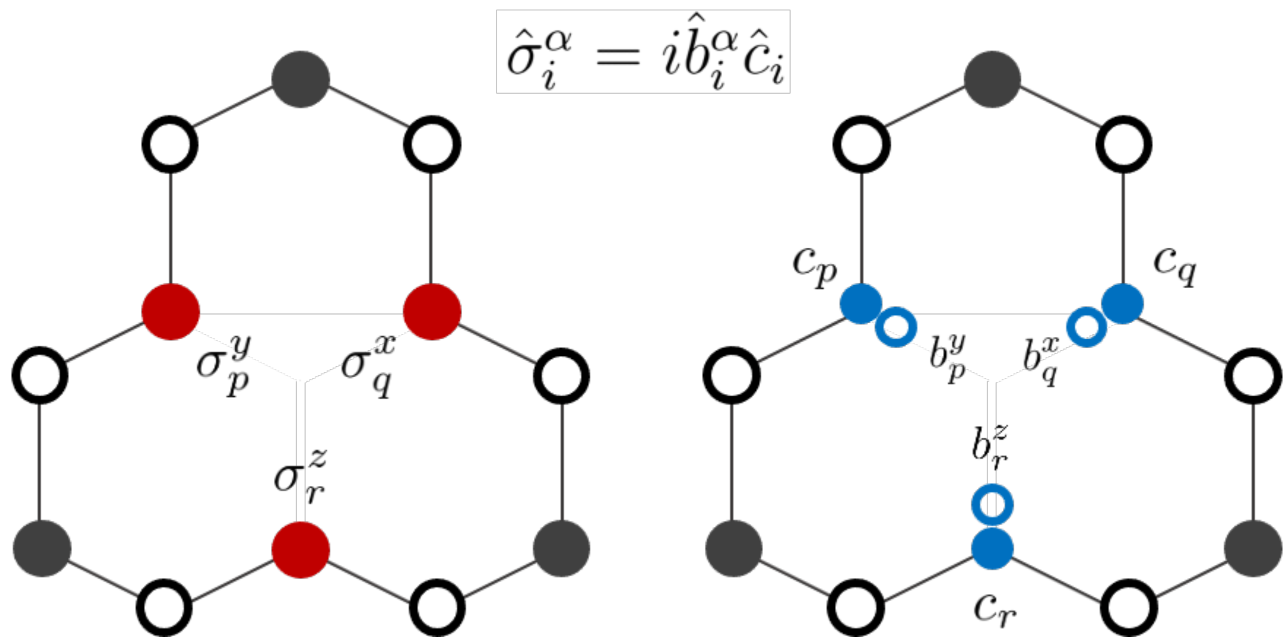


Hybridized p-f modes



$$\epsilon \sim \pm\left[f(J,\kappa) + \frac{3(\gamma_p^2 + \gamma_f^2)}{2f(J,\kappa)} h^2 \right]$$

Dynamical Correlation Function (dangling MF)



Dangling spins preserve the flux sector:

- On-site dangling correlation
- Off-diagonal dangling correlation
- Non-local dangling correlation

$$\tilde{S}_{pq}^{\alpha\beta}(\omega) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}t\, e^{i\omega t} \langle 0| \tilde{\sigma}_i^\alpha(t)\tilde{\sigma}_j^\beta(0) |0\rangle = -\sum_{\lambda_0} \langle M_0| \tilde{b}_p^\alpha c_p |\lambda_0\rangle \langle \lambda_0| \tilde{b}_q^\beta c_q |M_0\rangle\, \delta[\omega - (E_\lambda - E_0)].$$

No flux gap involved

No restriction on range or components!

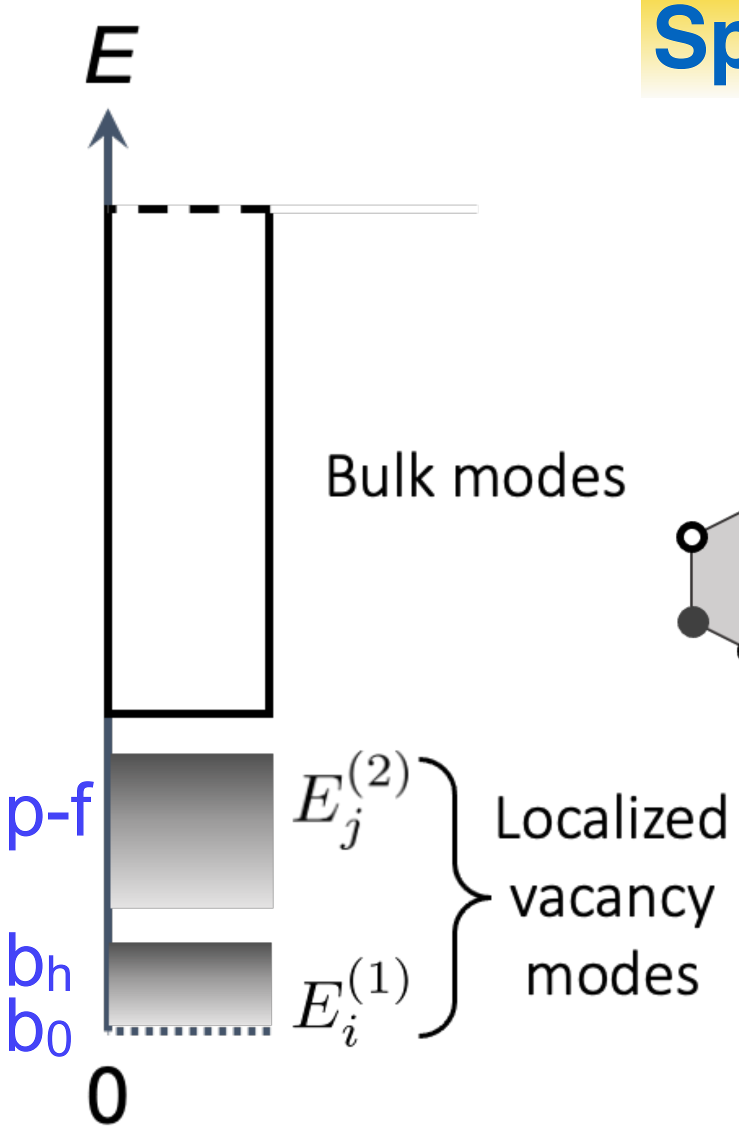
$$\langle M_0|\tilde{b}_p^\alpha\, c_p|\lambda_0\rangle \sim \langle M_0|\tilde{b}_p^\alpha\, c_p\, a_{\lambda_1}^\dagger a_{\lambda_2}^\dagger|M_0\rangle\,, \quad E_\lambda = E_0 + \epsilon_{\lambda_1} + \epsilon_{\lambda_2}$$

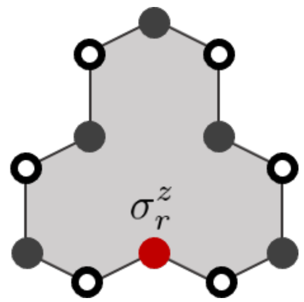
two-particle contribution

M. O. Takahashi *et al.*, arXiv:2211.13884 (2022)
W.-H. Kao, N. B. Perkins , G. B. Halász, arXiv:2307.10376 (2023)
W.-H. Kao, G. B. Halász, N. B. Perkins, arXiv:2310.06891 (2023)

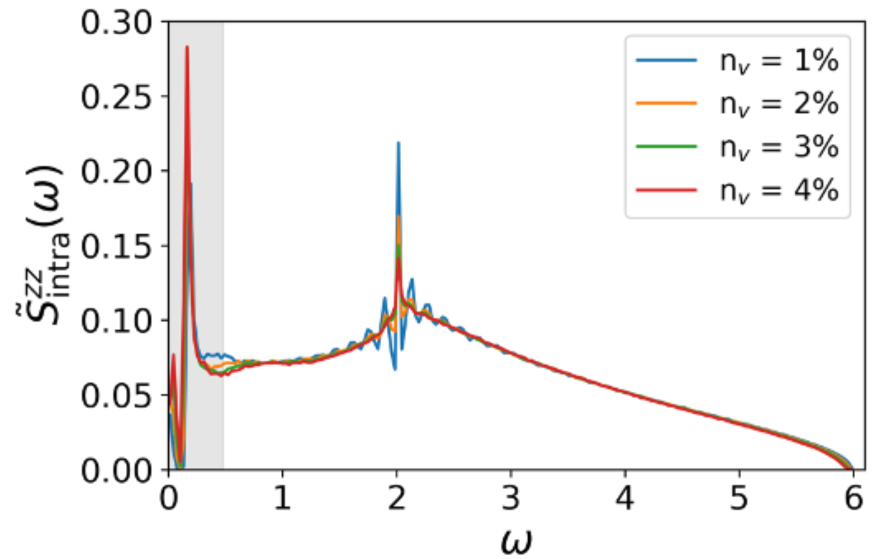
Spin-polarized tunneling conductance

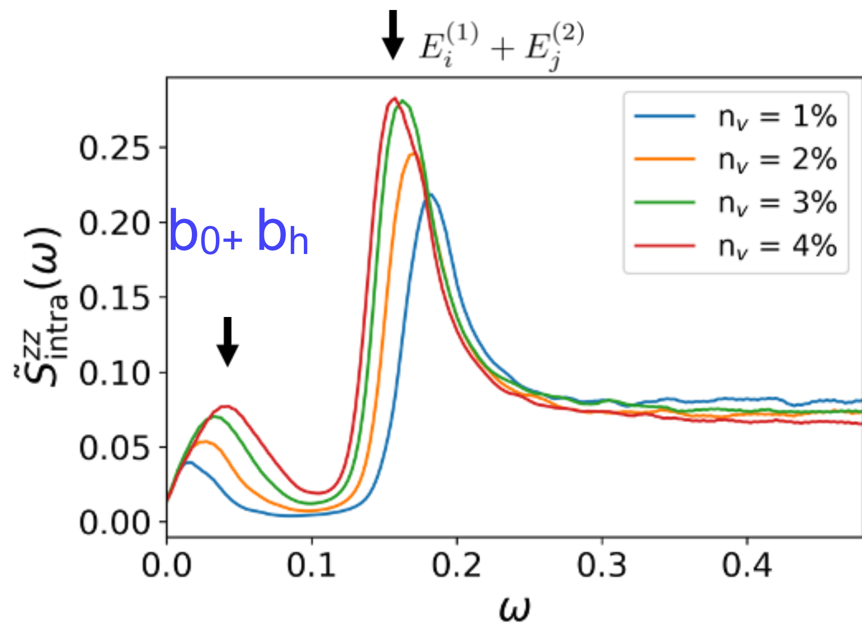
$$G_{\text{polarized}} \sim \int_0^{eV} \mathrm{d}\omega\, \rho^t_\uparrow \rho^s_\uparrow \left(S^{zz}_{pp} + S^{zz}_{qq} + S^{zz}_{rr}\right)$$





Bound-flux

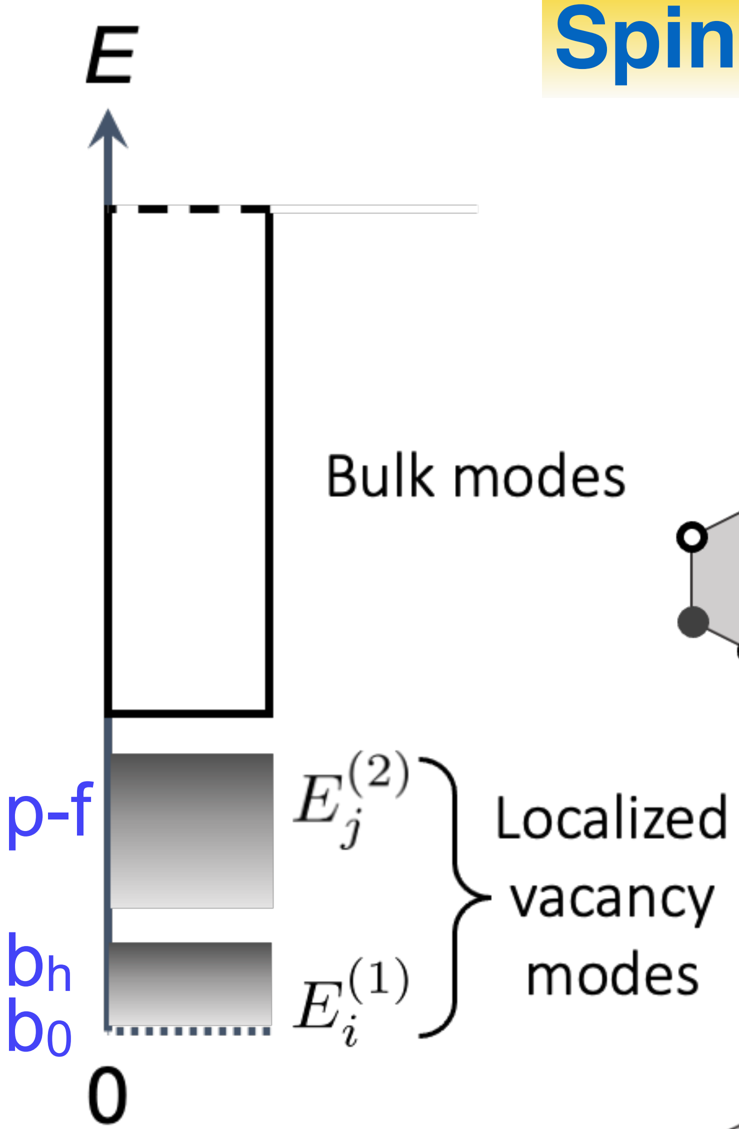


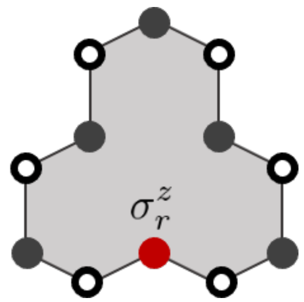


Quasi-zero-frequency response

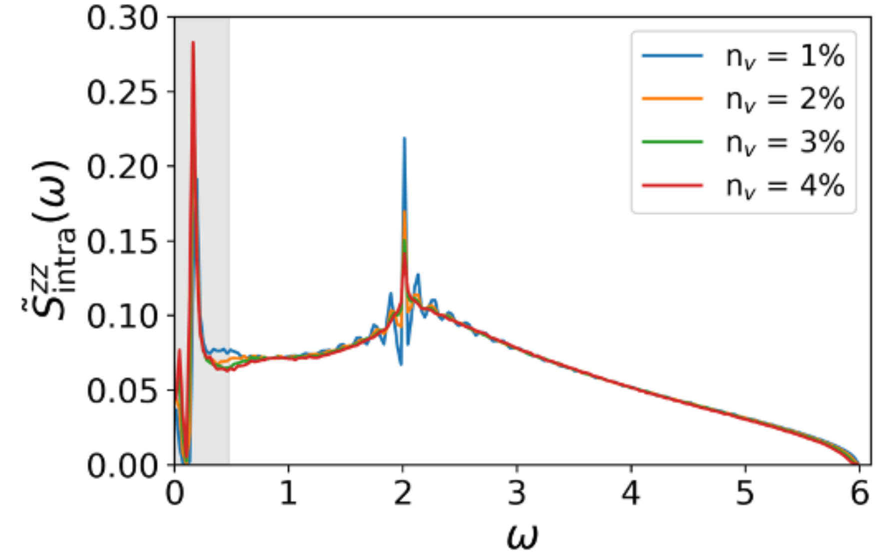
Spin-polarized tunneling conductance:

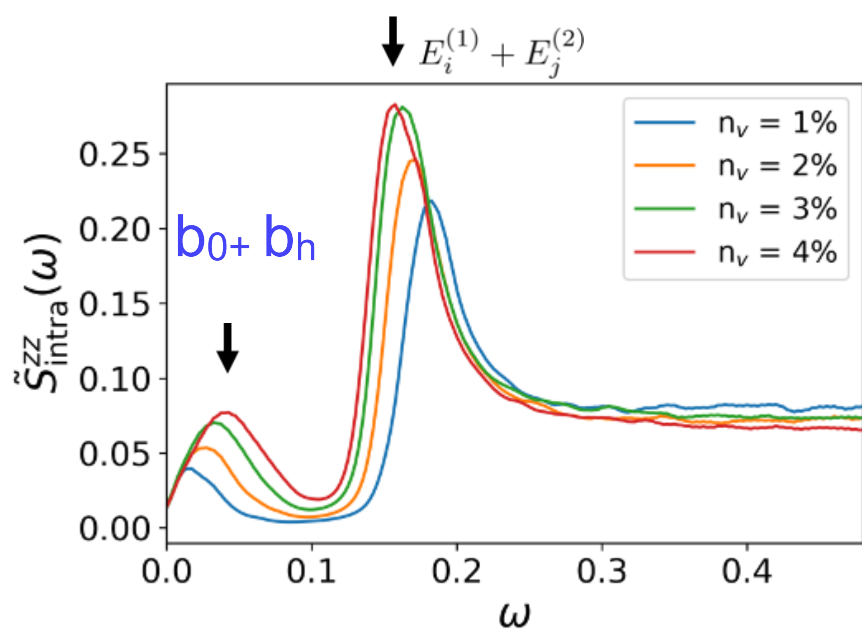
$$G_{\text{polarized}} \sim \int_0^{eV} \mathrm{d}\omega\, \rho^t_\uparrow \rho^s_\uparrow \left(S^{zz}_{pp} + S^{zz}_{qq} + S^{zz}_{rr}\right)$$

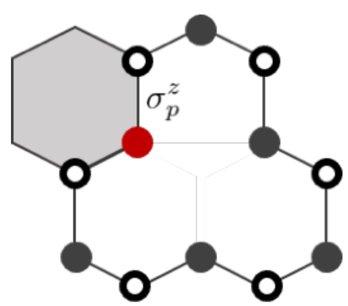




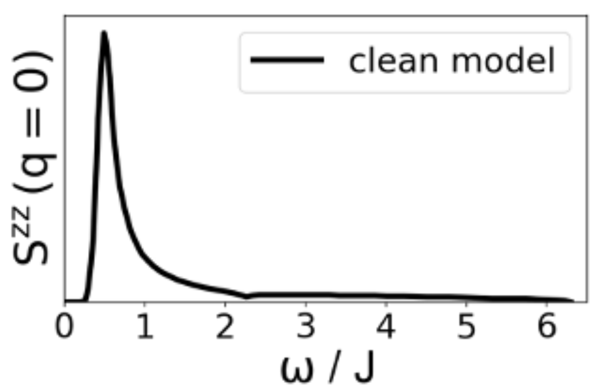
Bound-flux

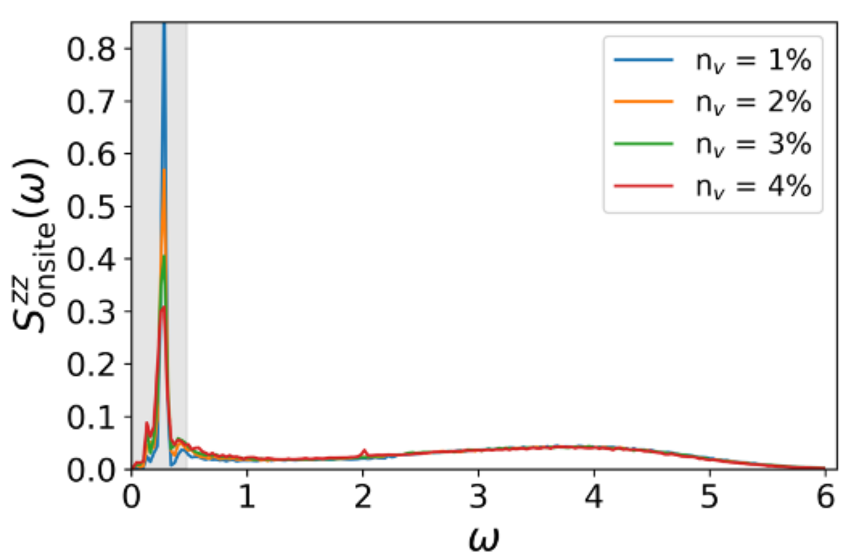


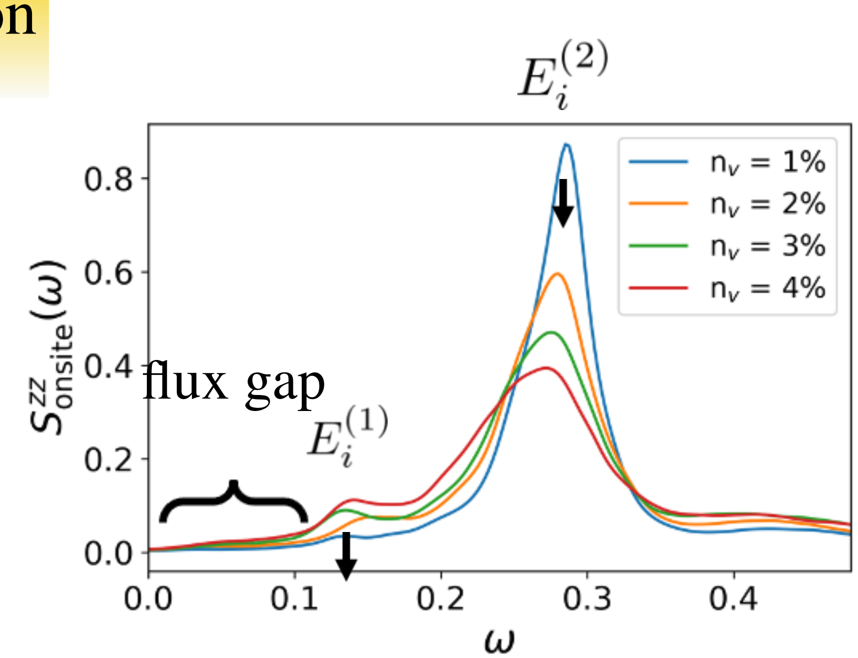




Two-flux Excitation



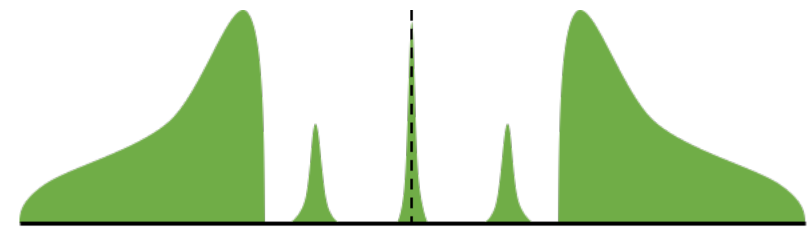


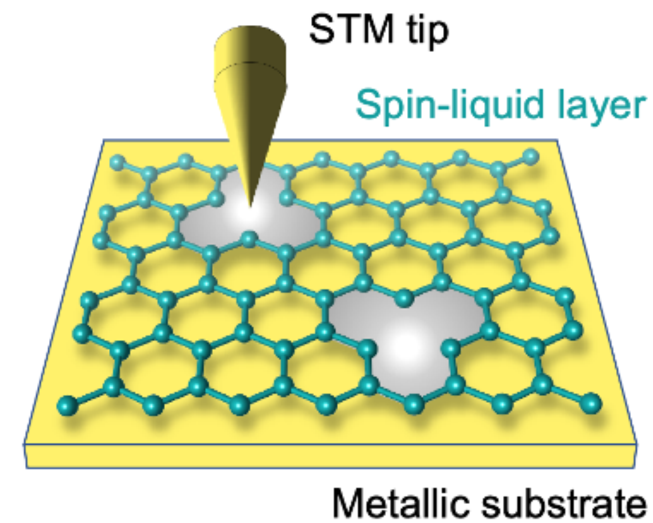


STM summary

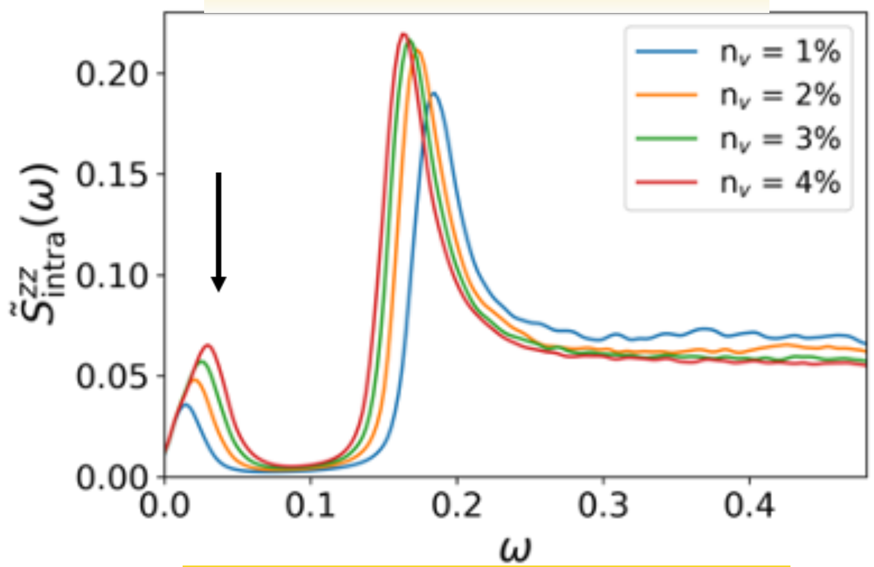
Derivative of tunneling conductance

$$\frac{\mathrm{d}\overline{G}(V)}{\mathrm{d}V} \propto \sum_{\alpha}\sum_{j=1}^{3}\overline{S_{jj}^{\alpha\alpha}}(eV) = 6\,\overline{S}_{\mathrm{bulk}}(eV) + 3\,\overline{S}_{\mathrm{dangling}}(eV)$$

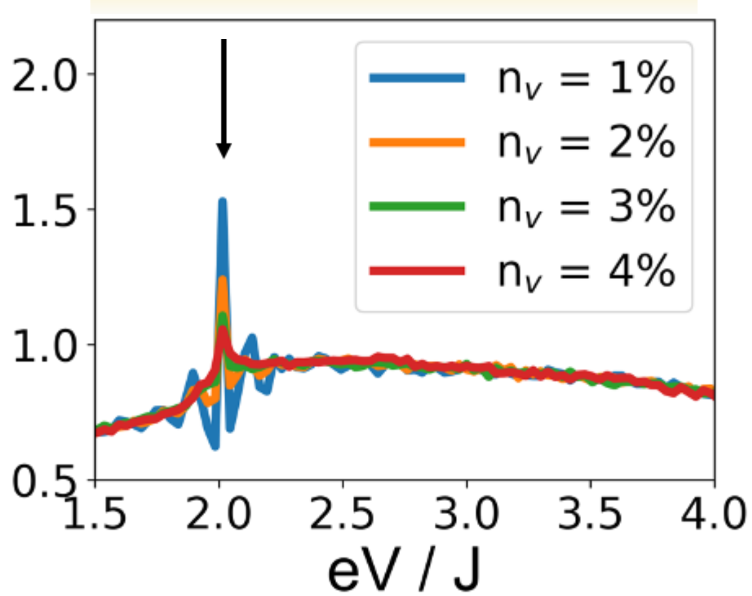


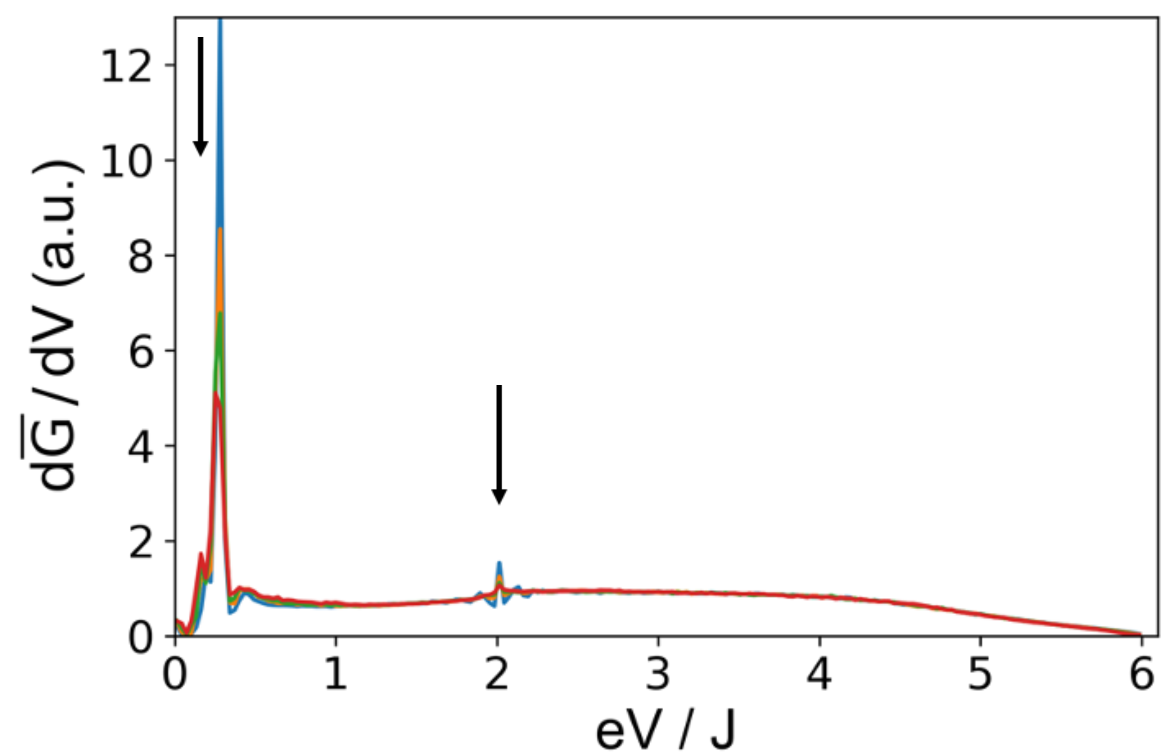


Quasi-zero-bias peak



van Hove singularity





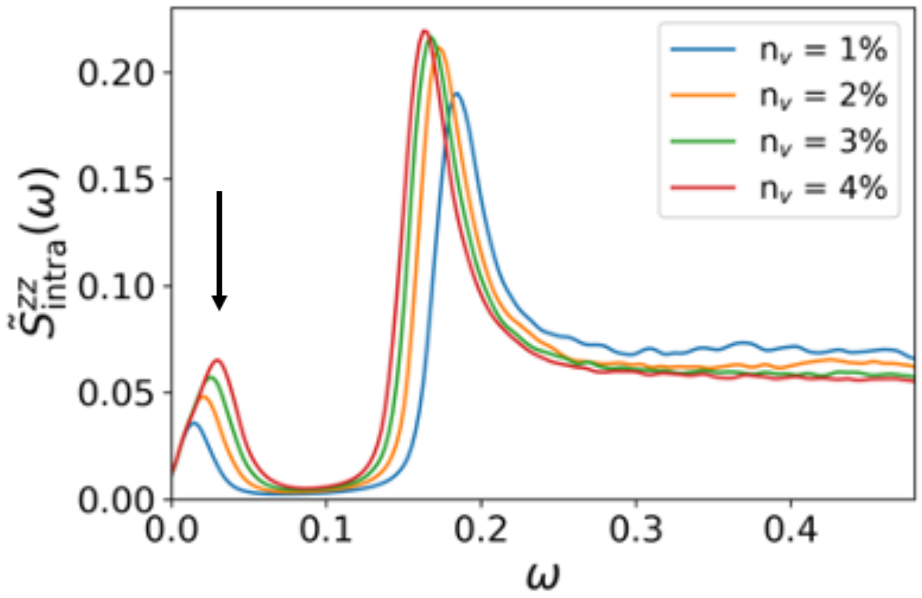
Conclusions

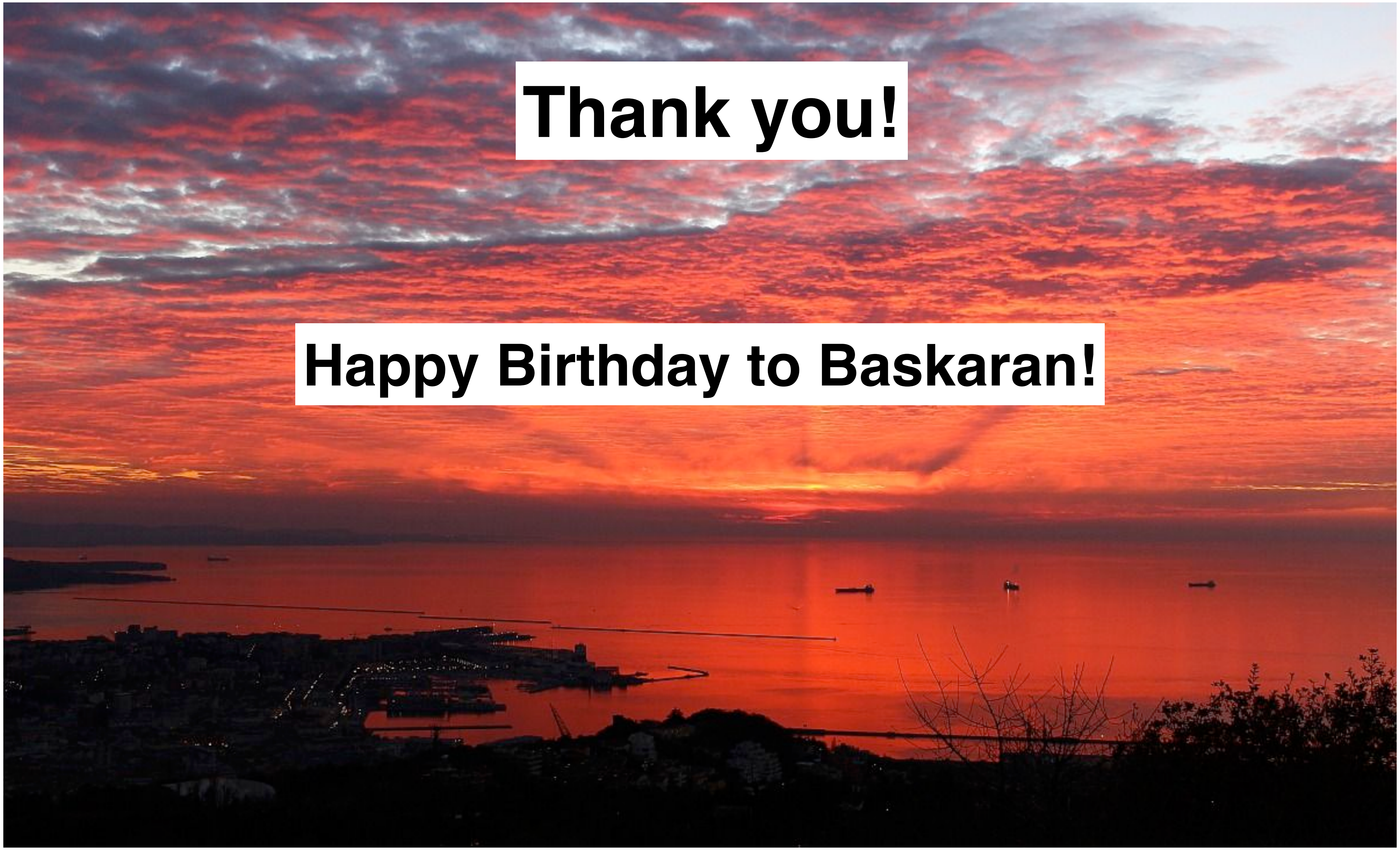
Site-diluted Kitaev Spin Liquid

- Bound-flux sector as the ground state
- Dangling b modes and hybridized p-f modes

Inelastic STM response on KSL

- Flux gap for bulk correlations
- Quasi-zero-bias peak for dangling correlations
- Dependence on vacancy concentration




Thank you!
Happy Birthday to Baskaran!