Projective symmetry group analysis of inelastic light scattering in Kitaev spin liquids

Shoji Yamamoto (山本 昌司) *Hokkaido University*

The Kitaev Hamiltonian reads

$$\mathscr{H} = -\sum_{\lambda=x,y,z}\sum_{<m,n>_\lambda} J_\lambda \sigma_m^\lambda \sigma_n^\lambda = iJ\sum_{\lambda=x,y,z}\sum_{<m,n>_\lambda} \hat{u}_{<m,n>_\lambda} c_m c_n, \tag{1}$$

where $<m,n>_\lambda$ $(\lambda = x,y,z)$ each run over a different set of $L/2$ nearest-neighbor bonds between the λ components of the Pauli matrices $(\sigma_l^x, \sigma_l^y, \sigma_l^z)$ $(l = 1,\cdots,L)$, which can be expressed in terms of four Majorana fermions, $\sigma_l^\lambda = i\eta_l^\lambda c_l$, to introduce bond operators, $\hat{u}_{<m,n>_\lambda} \equiv i\eta_m^\lambda \eta_n^\lambda$. Since $[\hat{u}_{<m,n>_\lambda}, \mathscr{H}] = 0$ and $\hat{u}^2_{<m,n>_\lambda} = 1$, $\hat{u}_{<m,n>_\lambda}$ reads a $\mathbb{Z}_2$ classical variable. The eigenspectrum of (1) depends on $\{u_{<m,n>_\lambda} = \pm 1\}$ only through $\{W_p = \pm 1\}$ with the flux operator defined as

$$\hat{W}_p \equiv e^{i\hat{\Phi}_p} = \prod_{<m,n>_\lambda \in \partial p} \sigma_m^\lambda \sigma_n^\lambda = (-i)^{N_p} \prod_{<m,n>_\lambda \in \partial p} \hat{u}_{<m,n>_\lambda}. \tag{2}$$

We set this model in various polyhedral (Fig. 1) and planar (Fig. 2) geometries and describe its Raman responses in terms of projective symmetry groups intending to identify the Majorana spinons singly. Parton single excitations in Kitaev spin polyhedra are characterized by double-valued irreducible representations of their belonging projective symmetry groups $\widetilde{\mathbf{P}}$, whereas parton geminate excitations relevant to Raman scattering are decomposed into single-valued irreducible representations of the corresponding point symmetry groups $\mathbf{P}$ (Table I). We combine a standard point-symmetry-group analysis of the Loudon-Fleury vertices and an elabo-

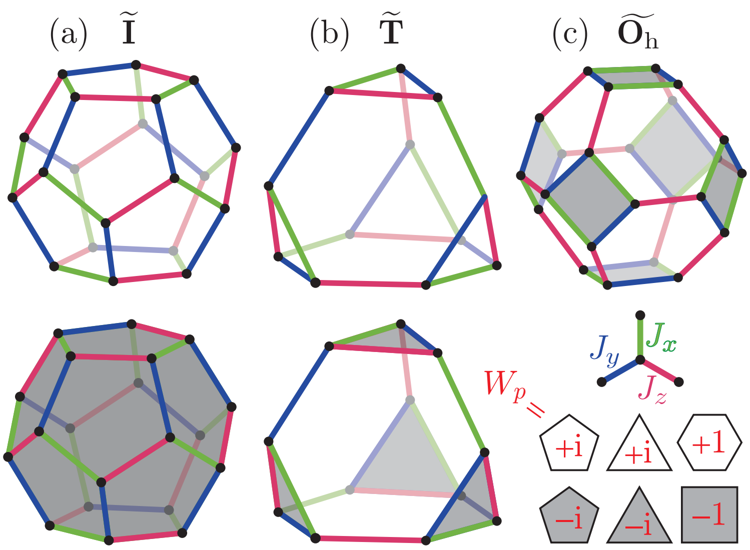

FIG. 1. Kitaev spin balls consisting of dodecahedral (a), truncated tetrahedral (b), and truncated octahedral (c) lattices in their ground flux configurations. The ground state of the truncated octahedron (c) is unique, whereas those of the dodecahedron (a) and the truncated tetrahedron (b) are both degenerate [1] with their constituent pentagons arrangeable into either $\{W_p = +i;\, p = 1,\cdots,12\}$ or $\{W_p = -i;\, p = 1,\cdots,12\}$ and triangles arrangeable into either $\{W_p = +i;\, p = 1,\cdots,4\}$ or $\{W_p = -i;\, p = 1,\cdots,4\}$.

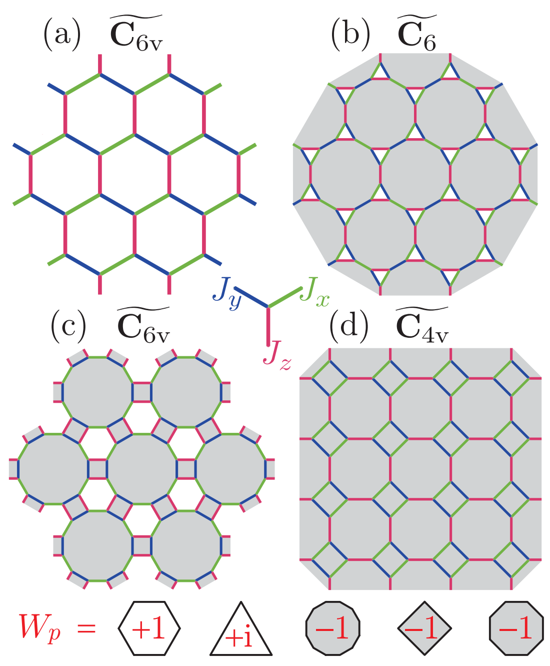

FIG. 2. Kitaev models consisting of the pure (a)-, triangle (b)-, square-hexagon (c)-honeycomb and diamond-square (d) lattices in their ground flux configurations. The ground state of (b) is degenerate [1] with its constituent triangles arrangeable into either $\{W_p = +i;\, p = 1,\cdots,\frac{L}{3}\}$ or $\{W_p = -i;\, p = 1,\cdots,\frac{L}{3}\}$.

TABLE I. Spinon-geminate-excitation-relevant direct-product representations made of double-valued irreducible representations $\widetilde{\mathit{\Xi}}_i \otimes \widetilde{\mathit{\Xi}}_j$ and their decompositions into single-valued irreducible representations $\widetilde{\mathit{\Xi}}_k$, which are doubly or singly underlined when they are relevant to inelastic (Raman) or elastic (Rayleigh) scatterings, for various double groups $\widetilde{\mathbf{P}}$. Note that $\widetilde{\mathit{\Xi}}_k$ of $\widetilde{\mathbf{P}}$ is nothing but $\mathit{\Xi}_k$ of $\mathbf{P}$.

$\widetilde{\mathbf{P}}$	$\widetilde{\mathit{\Xi}}_i \otimes \widetilde{\mathit{\Xi}}_j$	$\bigoplus_k \widetilde{\mathit{\Xi}}_k = \bigoplus_k \mathit{\Xi}_k$	$\widetilde{\mathbf{P}}$	$\widetilde{\mathit{\Xi}}_i \otimes \widetilde{\mathit{\Xi}}_j$	$\bigoplus_k \widetilde{\mathit{\Xi}}_k = \bigoplus_k \mathit{\Xi}_k$
$\widetilde{\mathbf{I}}$	$\{\mathrm{I}_{\frac{5}{2}} \otimes \mathrm{I}_{\frac{5}{2}}\}$	$\{\underline{\mathrm{A}}\}\oplus\{\mathrm{G}\}\oplus 2\{\underline{\underline{\mathrm{H}}}\}$	$\widetilde{\mathbf{O}}$	$\{\mathrm{E}_{\frac{1}{2}} \otimes \mathrm{E}_{\frac{1}{2}}\}$	$\{\underline{\mathrm{A}_1}\}$
	$\mathrm{I}_{\frac{5}{2}} \otimes \mathrm{G}_{\frac{3}{2}}$	$\mathrm{T}_1\oplus\mathrm{T}_2\oplus 2\mathrm{G}\oplus 2\underline{\underline{\mathrm{H}}}$		$\mathrm{E}_{\frac{1}{2}} \otimes \mathrm{E}_{\frac{5}{2}}$	$\mathrm{A}_2\oplus\underline{\underline{\mathrm{T}_2}}$
	$\{\mathrm{G}_{\frac{3}{2}} \otimes \mathrm{G}_{\frac{3}{2}}\}$	$\{\underline{\mathrm{A}}\}\oplus\{\underline{\underline{\mathrm{H}}}\}$		$\{\mathrm{E}_{\frac{5}{2}} \otimes \mathrm{E}_{\frac{5}{2}}\}$	$\{\underline{\mathrm{A}_1}\}$
$\widetilde{\mathbf{T}}$	$\{\mathrm{G}^{(2)}_{\frac{3}{2}} \otimes \mathrm{G}^{(2)}_{\frac{3}{2}}\}$	$\{\underline{\underline{\mathrm{E}^{(1)}}}\}$		$\mathrm{G}_{\frac{3}{2}} \otimes \mathrm{E}_{\frac{1}{2}}$	$\underline{\underline{\mathrm{E}}}\oplus\mathrm{T}_1\oplus\underline{\underline{\mathrm{T}_2}}$
	$\mathrm{G}^{(2)}_{\frac{3}{2}} \otimes \mathrm{E}_{\frac{1}{2}}$	$\underline{\underline{\mathrm{E}^{(2)}}}\oplus\underline{\underline{\mathrm{T}}}$		$\mathrm{G}_{\frac{3}{2}} \otimes \mathrm{E}_{\frac{5}{2}}$	$\underline{\underline{\mathrm{E}}}\oplus\mathrm{T}_1\oplus\underline{\underline{\mathrm{T}_2}}$
	$\{\mathrm{E}_{\frac{1}{2}} \otimes \mathrm{E}_{\frac{1}{2}}\}$	$\{\underline{\mathrm{A}}\}$		$\mathrm{G}_{\frac{3}{2}} \otimes \mathrm{G}_{\frac{3}{2}}$	$\{\underline{\mathrm{A}_1}\}\oplus[\mathrm{A}_2]\oplus\{\underline{\underline{\mathrm{E}}}\}\oplus 2[\mathrm{T}_1]\oplus[\underline{\underline{\mathrm{T}_2}}]\oplus\{\underline{\underline{\mathrm{T}_2}}\}$
	$\mathrm{G}^{(1)}_{\frac{3}{2}} \otimes \mathrm{G}^{(2)}_{\frac{3}{2}}$	$\underline{\mathrm{A}}\oplus\underline{\underline{\mathrm{T}}}$	$\widetilde{\mathbf{O}_\mathrm{h}}$	$\{\mathrm{G}_{\frac{1}{2}+\frac{5}{2}} \otimes \mathrm{G}_{\frac{1}{2}+\frac{5}{2}}\}$	$\{\underline{\mathrm{A}_{1\mathrm{g}}}\}\oplus\{\mathrm{A}_{1\mathrm{u}}\}\oplus\{\mathrm{A}_{2\mathrm{u}}\}\oplus\{\underline{\underline{\mathrm{T}_{2\mathrm{g}}}}\}$
	$\mathrm{G}^{(1)}_{\frac{3}{2}} \otimes \mathrm{E}_{\frac{1}{2}}$	$\underline{\underline{\mathrm{E}^{(1)}}}\oplus\underline{\underline{\mathrm{T}}}$		$\mathrm{G}^{\mathrm{g}}_{\frac{3}{2}} \otimes \mathrm{G}_{\frac{1}{2}+\frac{5}{2}}$	$\underline{\underline{\mathrm{E}_\mathrm{g}}}\oplus\mathrm{E}_\mathrm{u}\oplus\mathrm{T}_{1\mathrm{g}}\oplus\mathrm{T}_{1\mathrm{u}}\oplus\underline{\underline{\mathrm{T}_{2\mathrm{g}}}}\oplus\mathrm{T}_{2\mathrm{u}}$
	$\{\mathrm{G}^{(1)}_{\frac{3}{2}} \otimes \mathrm{G}^{(1)}_{\frac{3}{2}}\}$	$\{\underline{\underline{\mathrm{E}^{(2)}}}\}$		$\{\mathrm{G}^{\mathrm{g}}_{\frac{3}{2}} \otimes \mathrm{G}^{\mathrm{g}}_{\frac{3}{2}}\}$	$\{\underline{\mathrm{A}_{1\mathrm{g}}}\}\oplus\{\mathrm{E}_\mathrm{u}\}\oplus\{\underline{\underline{\mathrm{T}_{2\mathrm{g}}}}\}$
				$\mathrm{G}^{\mathrm{u}}_{\frac{3}{2}} \otimes \mathrm{G}_{\frac{1}{2}+\frac{5}{2}}$	$\underline{\underline{\mathrm{E}_\mathrm{g}}}\oplus\mathrm{E}_\mathrm{u}\oplus\mathrm{T}_{1\mathrm{g}}\oplus\mathrm{T}_{1\mathrm{u}}\oplus\underline{\underline{\mathrm{T}_{2\mathrm{g}}}}\oplus\mathrm{T}_{2\mathrm{u}}$
				$\mathrm{G}^{\mathrm{g}}_{\frac{3}{2}} \otimes \mathrm{G}^{\mathrm{u}}_{\frac{3}{2}}$	$\mathrm{A}_{1\mathrm{u}}\oplus\mathrm{A}_{2\mathrm{u}}\oplus\underline{\underline{\mathrm{E}_\mathrm{g}}}\oplus\mathrm{T}_{1\mathrm{g}}\oplus\mathrm{T}_{1\mathrm{u}}\oplus\underline{\underline{\mathrm{T}_{2\mathrm{g}}}}\oplus\mathrm{T}_{2\mathrm{u}}$
				$\{\mathrm{G}^{\mathrm{u}}_{\frac{3}{2}} \otimes \mathrm{G}^{\mathrm{u}}_{\frac{3}{2}}\}$	$\{\underline{\mathrm{A}_{1\mathrm{g}}}\}\oplus\{\mathrm{E}_\mathrm{u}\}\oplus\{\underline{\underline{\mathrm{T}_{2\mathrm{g}}}}\}$

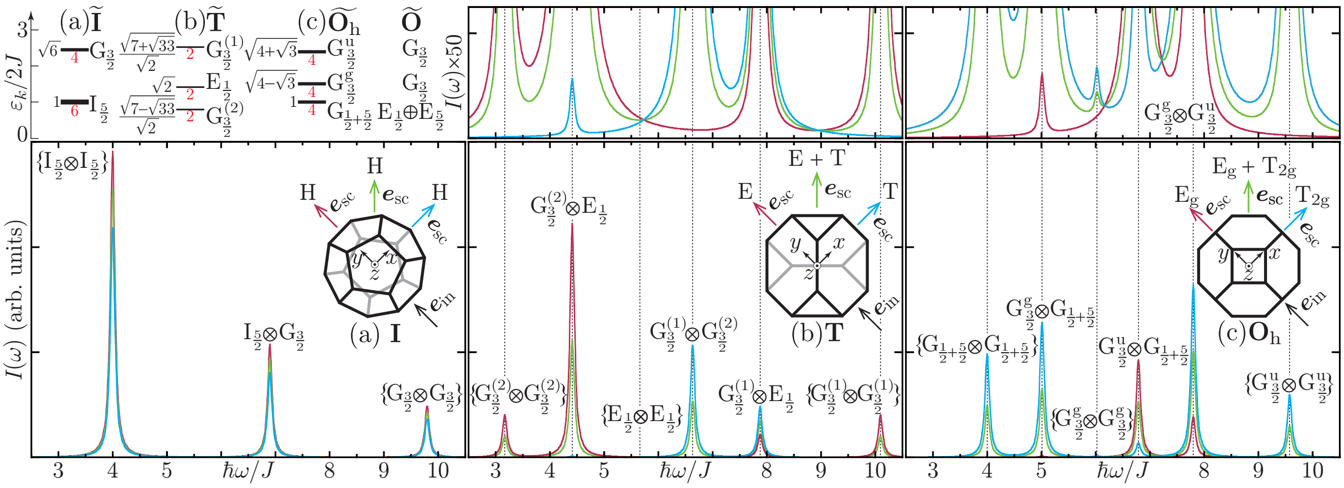

FIG. 3. Spinon excitation energies ε_k and Raman intensities $I(\omega)$ of Kitaev spin balls consisting of dodecahedral (a), truncated-tetrahedral (b), and truncated-octahedral (c) lattices in their ground flux configurations, where δ-function peaks are Lorentzian-broadened by $0.05J$. The eigenenergy, multiplicity, and irreducible representation are specified beside each eigenlevel. For the incident polarization $(\frac{\pi}{2}, \frac{\pi}{2})$, we observe various scattered polarizations $(\frac{\pi}{2}, \frac{l\pi}{4})$ $(l = 0, 1, 2)$, each consisting of peaks attributable to direct-product representations of the projective symmetry groups $\widetilde{\mathbf{I}}$, $\widetilde{\mathbf{T}}$, and $\widetilde{\mathbf{O}_\mathrm{h}}$ ($\widetilde{\mathit{\Xi}}_i \otimes \widetilde{\mathit{\Xi}}_j$ in Table I) on one hand and containing one or more irreducible representations of the point symmetry groups $\mathbf{I}$, $\mathbf{T}$, and $\mathbf{O}_\mathrm{h}$ ($\bigoplus_k \mathit{\Xi}_k$ in Table I) on the other hand.

rate projective-symmetry-group analysis of itinerant spinons against the ground gauge fields to reveal *hidden selection rules* for Raman scattering in $\mathbb{Z}_2$ spin liquids (Fig. 3) [2]. By $\mathbb{Z}_2$-gauging the subgroup $\mathbf{P}'_{\boldsymbol{k}}$ of the $\boldsymbol{k}$-point symmetry group $\mathbf{P}_{\boldsymbol{k}}$ at a high symmetry point $\boldsymbol{k}$ of the reciprocal lattice, which keeps the gauge-ground Majorana Hamiltonian [cf. the rightmost side of Eq. (1)] invariant under the Fourier transformation corresponding to $\boldsymbol{k}$, we can extend the same analysis to planar Kitaev spin models [3].

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[2] T. Kimura and S. Yamamoto, Phys. Rev. B **101**, 214411 (2020).

[3] S. Yamamoto and T. Kimura, J. Phys. Soc. Jpn. **89**, 063701 (2020).