Optical phonons coupled to a Kitaev spin liquid

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Introduction. – There is an ongoing pursuit of the signatures of the elusive quantum spin-liquid (QSL) state of matter [7–9]. The difficulty to identify such states is due to the fact that they do not break any symmetries and lack conventional local order parameters of magnetic or related nature down to zero temperature. Recently, QSLs with a $\mathbb{Z}_2$ gauge structure may have actually come close to material realization, motivated by the exact solution of the famous Kitaev spin model (KSM) with compass-exchange on the two-dimensional (2D) honeycomb lattice [10]. In this model, spins fractionalize into static $\mathbb{Z}_2$ gauge fluxes and itinerant Majorana fermions, with a gapless QSL ground state. In external magnetic fields the KSM opens a gap and displays chiral Majorana edge-modes. Variants and generalizations of the KSM in 1D [11–17], 2D [18], and 3D [19–21], as well as for spins larger than 1/2 [22–24] have been considered.

Mott-insulators with strong spin-orbit coupling (SOC) are promising materials to realize the KSM [25–28]. However, residual non-Kitaev exchange interactions remain an issue, with all current systems under consideration eventually displaying magnetic order at low temperatures. From a present perspective [9, 29–32], $\alpha$-RuCl$_3$, either above its ordering temperature, or with magnetic order suppressed by external magnetic fields, is one of the prime candidates under scrutiny for $\mathbb{Z}_2$ QSL physics. Recent thermal Hall effect measurements in $\alpha$-RuCl$_3$, suggest half-integer quantization plateaus [33] which are consistent with Majorana edge states, including a field-angular variation of the topological Chern number identical to that of the Kitaev QSL [34], and a bulk-boundary correspondence claimed in specific heat measurements [35]. In addition to edge transport, a multitude of bulk spectroscopic probes have been invoked, aiming to identify continua characteristic of the fractional Majorana excitations. This pertains to inelastic neutron scattering [36–41] and local resonance techniques [42, 43], as well as to magnetic Raman scattering [44–46].

An interesting open question is whether the coupling of Majorana fermions of the putative KSM to other degrees of freedom can be used to provide signatures of their existence. Coupling to phonons [47–50] can induce characteristic renormalizations, examples of which seem to have been observed recently for acoustic phonons [51]. Regarding optical phonons, Raman scattering [1–6] has provided early on evidence for Raman active phonons with Fano line-shapes, overlapping with the magnetic Raman continuum [44, 45]. This has been speculated to be a signature of renormalization of optical phonons by Majorana fermions but up to now a microscopic description was missing.

Here, we provide a theory of optical phonons and coupled to a KSM. We describe the microscopic details of the coupling and evaluate the phonon self-energy. The phonon renormalization versus energy and temperature is studied, the relative importance of Majorana and flux excitations is discussed, and the implications for Raman scattering are clarified. We find convincing qualitative agreement with experimental data, which points to an intriguing interpretation of a Majorana scattering induced optical phonon renormalization in the candidate material $\alpha$-RuCl$_3$.

Optical-phonon Majorana mixing. – Here, we consider phonons of a 2D Honeycomb lattice coupled magnetoelectrically to the Kitaev QSL. The total Hamiltonian of the system reads $H = H_P + H_K + H_{KP}$ where $H_P$ stands for the quadratic free phonon contribution $H_P = \sum_{\mathbf{q}m} (\omega_m + \frac{1}{2}) b_{\mathbf{q}m}^\dagger b_{\mathbf{q}m}$ with $b_{\mathbf{q}m}^\dagger$, $b_{\mathbf{q}m}$ being bosonic creation annihilation operators, respectively, at momentum $\mathbf{q}$ for the mode $m$, and $\omega_m$ the corresponding energy.

The magnetic degrees of freedom are described by
the Kitaev spin Hamiltonian $H_K = \sum_{r,\delta} J_{\delta} S_{r}^{d4} S_{r-\delta}^{d4}$, [10] (see also Fig. 1). $r = l_1 a_1 + l_2 a_2$, with $l_{1,2} = 0,1,\ldots,L - 1$, refers to a triangular Bravais lattice of linear dimension $L$, and $\delta$ sets the location of the basis of the honeycomb lattice, with $N = 2L^2$ sites. The components $d_\delta$ of the spin-1/2 operators $S$ assume the values $d_\delta = x, y, z$ depending on the $\delta$-vector, while $J_{\delta}$ are the Kitaev interactions. We consider the isotropic case $J_\delta = J$ and set $\hbar, k_B = 1.$

Following the literature [10, 12], we map the spin model onto one for two species of Majorana fermions $c$ and $\bar{c}$, with $\{c_i, c_i^\dagger\} = 2 \delta_{ij} = \{c_i, c_i\}$ and $\{c_i, c_j\} = 0$. This mapping renders Majorana fermions of, e.g., $c$-type itinerant, while the other type pairs into a static $Z_2$ gauge fields $\eta = \pm 1$ along, e.g., the $\delta_3$ direction. The gauge field generates a conserved flux, equivalent to a macroscopic number of conserved local operators in the spin language [10, 52]. In the Majorana representation, $H_K$ reads

$$H_K = J \sum_{r,\delta} h_\delta(r), \quad h_\delta(r) = -\frac{i}{4} \eta_\delta(r) c_r c_{r-\delta},$$

where the gauge field $\eta_\delta$ acquires the values $\eta_\delta(r) = \eta_\delta(r) = 1$, and $\eta_\delta(r) = \pm 1$. Primed Majorana fermions reside on the basis sites. The ground state resides within the uniform gauge sector, which is separated from other sectors by a gap $\Delta \approx 0.065 J$. At finite temperature $T$ fluxes become thermally excited and proliferate in a narrow range near a very low $T^* \approx 0.012 J$. For several observables the emergent disorder introduced by the visons has been shown to be of physical significance [14, 49, 53, 54]. For the present case of interest, i.e., optical phonons, we show that gauge excitations imply only negligible quantitative modifications.

We focus on magnetoelastic coupling between spins and lattice degrees of freedom, i.e., on the leading order variation $J(\mathbf{u}_r - \mathbf{u}_r - \delta) \approx J + \nabla J \cdot (\mathbf{u}_r - \mathbf{u}_r - \delta)$ of the exchange with respect to lattice deforma-

$$H_{KP} = \sum_{m,q} B_{mq} \mathcal{H}_{m,-q}, \quad \mathcal{H}_{m,q} = \sum_{\delta} \Delta_{mq}^\delta h_{\delta,q},$$

where the form factor of the coupling is encoded in $\Delta_{mq}^\delta$.

While Eq. (2) applies to acoustic, as well as to optical phonons, we focus on the $E_{g1}$ and $E_{g2}$ optical modes, observed in Raman experiments. These are of particular interest, since allegedly, they overlap with the Majorana continuum. For Raman scattering it is safe to consider $q \to 0$ only and we drop all $q$-labels hereafter. In the supplemental material we treat also $q \neq 0$ (and moreover weak magnetic fields) [55]. The phonon energies are $\omega_1 = \omega_q \approx 116 cm^{-1} \approx 1.9 J$ and $\omega_2 = \omega_q \approx 165 cm^{-1} \approx 2.6 J$, where we assume a Kitaev coupling of $J \approx 90 K$.

The vibrational pattern of the two modes [2] is shown in Fig. 1. In terms of Eq. (2) the lattice modulations imply $\Lambda_m = \Lambda_m[1,-1^m,\lambda_m]$, with $m = 1,2$, and $\lambda_m$ denotes a possible anisotropy between the $\delta_{1,2}$ and $\delta_3$ directions. The magnitude of $\Lambda_m$ can be assumed to be in the perturbative regime [49]. Note, a detailed microscopic derivation of the spin-phonon coupling including the effect of spin-orbit effects beyond the pure Kitaev model is given in the supplementary material [55], see also Refs. [56-58].

The coupling of the phonons to the fractionalized magnetic excitations, Eq. (2), leads to a renormalization of the bare phonon propagators, $D^0_m(z) = \omega_m^2 / (z^2 - \omega_m^2)$, with $z = \omega + i0^+$, the frequency dependence. The dressed phonon propagators can then be determined by the $2 \times 2$ self-energy matrix $\Sigma(z)$ and the corresponding Dyson’s equation,

$$D(z) \approx [D_0^{-1}(z) - \Sigma(z)]^{-1}, \quad \Sigma_{mm'} = \langle \langle H_m; H_{m'}^\dagger \rangle \rangle,$$
acquires a uniform gauge configuration, $\eta g = 1$, allowing for the analytical calculation of the phonon self-energy. First, the Kitaev terms in Eq. (1) can be brought to a diagonal form by going to reciprocal space $k = k_1 G_1 + k_2 G_2$, where $G_1 = \frac{1}{3x}(\sqrt{3} e_x - e_y)$ and $G_2 = \frac{2}{3x} e_y$ are the reciprocal lattice vectors, i.e., $a_i \cdot G_1 = \delta_{i,j}$ for $i(j) = 1, 2$. The coefficients $k_{1,2}$ are set to antiperiodic boundary conditions $k_j = 2\pi i (j + \frac{1}{2})/L$, to allow all Majoranas to pair into complex fermions. The Fourier transform of the Majoranas reads $c_k = \sum_r e^{-i k r} c_{r,k}/\sqrt{2N}$ such that $(c_k, c_k^\dagger) = \delta_{k, -k}$, and similarly for the $c'$ operators.

In the diagonal complex fermion basis, $\Psi_k^\dagger = (d_{1,k}^\dagger, d_{2,k}^\dagger)$, $H_K$ and $H_m$ of Eq. (1) and (2) read $H_K = \frac{1}{2} \sum_k \Psi_k^\dagger E_k \Psi_k$ and $H_m = \frac{1}{2} \sum_k \Psi_k^\dagger V_{m,k} \Psi_k$ with

$$E_k = \begin{pmatrix} \epsilon_k & 0 \\ 0 & -\epsilon_k \end{pmatrix}, \quad V_{m,k} = \begin{pmatrix} g_{m,k}^g & ig_{m,k}^g \\ -ig_{m,k}^g & -g_{m,k}^g \end{pmatrix}.$$ (4)

The energy eigenvalues are given by $\epsilon_k = |f_k| = \frac{1}{2} \sqrt{3 + 2 \cos k_1 + 2 \cos k_2 + 2 \cos (k_1 - k_2)}/2$, with $f_k = (\sum \delta_\delta k_\delta k_\delta, \text{ and } \delta_k^j = -\frac{1}{2} e^{-ik j} \delta_k$. The real ($g'$) and imaginary part ($g''$) of the function $g$ of the scattering matrix $V$ are given by $g_{m,k} = (f_k^\ast \sum_k \Lambda_{m,k} \delta_k^j)/\sqrt{N}$.

The evaluation of the self-energy using (3) and (4) is straightforward. In that process and due to $c_k^\dagger = c_{-k}$, anomalous commutators $\{d_{1,k}, d_{2,k}\} = \delta_{k,-k}$ and their corresponding contractions arise, implying also a time evolution $d_{j,k}(t) = d_{j,k} e^{i\epsilon_k t}$ for $j = 1, 2$, respectively. Thus, the self-energy exhibits particle-hole (ph) and particle-particle (pp) absorption channels, the amplitudes of which are determined via the diagonal and off-diagonal matrix elements of the matrix $V$. In the $q = 0$ limit, considered here, the pp-channel vanishes. The pp-scattering-amplitudes acquire simple forms, and all diagonal and off-diagonal self-energies are described by a single function

$$\Sigma(z) = \begin{pmatrix} a_1 & b \\ b & a_2 \end{pmatrix} \Sigma(z), \quad \Sigma(z) = \frac{1}{N} \sum_{k, \pm} A_k^2 \frac{1 - 2f_k}{2e_k + \pm},$$ (5)

with the matrix elements $a_1 = \Lambda_1 (3 + \lambda_1^2)/\Lambda_1$, $a_2 = \Lambda_2 (1 - \lambda_2^2)/\Lambda_1$, and $b = \lambda_1 (1 - \lambda_2)$, the scattering amplitude $A_k = \Lambda_1 \Lambda_2 \cos(k_2 a/2) \sin(\sqrt{3} k_2 a/2)/(2\epsilon_k)$, and the Fermi-Dirac distribution $f_k = 1/(e^{\epsilon_k/T} + 1)$. Two special cases arise. For $\lambda_2 = 1$ the $E_{g_2}$ spin phonon Hamiltonian satisfies $H_2 \propto \epsilon_k$, leading to no scattering for that mode. For $\lambda_1 = 0$, symmetry prevents mixing of the $E_{g_1}$ and $E_{g_2}$ modes.

**Phonon self-energy: random gauge.** For temperatures $T \gtrsim 0.1 \ldots 0.2 J \gg T^*$, thermal gauge excitations need to be taken into account. For that, a random averaging over maximally disordered configurations of $\eta_g(r)$ is sufficient to describe the fermionic system’s properties. As this breaks translational invariance, we resort to a numerical real-space evaluation of the defect-averaged self-energy $\Sigma(z)$. This approach has been detailed in Refs. [49, 53] and is recapitulated in [55].

**Phonon self-energy: results.** In Fig. 2, we present results for the self-energy $\Sigma$ versus frequency and temperature, for both homogeneous as well as random gauge states. In Fig. 2(a), we plot $\Sigma(\omega)$ obtained from the analytical approach for two temperatures, $T = 0.005 J < T^*$ and $T = 0.030 J \gtrsim T^*$ (curves overlap). Calculations are performed on lattices with $L = 200$. For $\omega < 0$, analyticity requires $-\Sigma(\omega) = \Sigma(\omega)$ for the real/imaginary part [left(right) y-axis of panel [a(b)]].

Both, $\Sigma'$ and $\Sigma''$, contribute to the renormalization of the $E_{g_1}$ and $E_{g_2}$ phonons, the energy of which is marked with a blue and purple dotted line, respectively. Since $\Sigma'(\omega_r, T) < 0$ at both anticipated phonon energies $\omega_r$, a downward renormalization will occur. Most importantly however, regarding their life time, both phonons reside in a range of negative slope of $\Sigma''$ versus $\omega$. Therefore the life time will be dispersive, with phonon spectral functions that display asymmetric line shapes with enhanced left-broadening.

Regarding the gauge excitations, Fig. 2(b) shows $\Sigma$ from the numerical approach for $T \gg T^*$ on lattices of $L = 30$, averaging over $N_R = 200$ maximally disordered
gauge field configurations. First, the overall shape of \( \Sigma \) displays no qualitative change compared to Fig. 2(a), with only some additional fine structure arising from the gauge-field excitations. Second however, there is a reduction of the bandwidth to \( \omega \ll 1 \), where the mixing is weak and can be ignored. Fig. 3(a) depicts the individual (off)diagonal phonon spectra \( D_{mm}''(\omega) \) for intermediate \( \Lambda_1(\Lambda_2) = 0.3 J(0.9 J) \), \( \lambda_{1,2} = 2 \) and for \( T = 0.005 J \). First, both diagonal elements of \( D \) exhibit the anticipated downward renormalization with respect to \( \omega_m \), largest for \( E_{g2} \). In accordance with Fig. 2(c), the modes’ peaks will shift upwards to \( \omega_m \) as the temperature is increased. Second, the frequency dependence of \( \Sigma''(\omega) \) leads to slightly asymmetric phonon line shapes. We emphasize, that this asymmetry is not related to the Fano effect [59], commonly cited in such cases. The width of the phonon mode is expected to shrink as the temperature is increased, Fig. 2(d). I.e., in contrast to most conventional excitations in many-body systems, their life-time grows with temperature. Third, the phonon mixing is rather weak, i.e., \( D_{12} \ll D_{11}(22) \) and \( D_{mm} \approx D_m \), essentially rendering the two phonon modes decoupled.

**Raman response and Fano-lineshape.**– Finally, we speculate on the Raman cross section \( I(z) \). Light scatters from both, the lattice and the magnetic degrees of freedom. This forces the Fano effect to occur [59] and renders the Raman cross section a coupled three-channel problem, with Raman vertices \( F \) and \( R_{m=1,2} \), encoding the couplings of incoming(outgoing) light fields to the fermions and the two phonon modes, respectively. Presently, only the Loudon-Fleury vertex \( F \) is known microscopically [44, 45, 60]. Therefore, obtaining \( I(z) \) from first principles is infeasible. To make progress, we resort to phenomenological simplifications. These are detailed in the supplemental material [55], but essentially amount to: (i) We replace the Raman vertices \( F \) and \( R_{m=1,2} \) by mere constants, dependent on the scattering geometry, (ii) We approximate all fermionic two-particle Greens functions of the three-channel problem beyond \( \Sigma(\omega) \) by the latter. Contrasting Figs. 2(a,b) against the known magnetic Raman response [44, 45] this is acceptable. (iii) We ignore phonon-mixing. This leads to [55]

\[
I(z) \approx \Pi(z) + \sum_{m=1,2} \left[ r_m + C_m \Pi(z) \right]^2 D_{mm}(z),
\]

where \( \Pi(z) = \Sigma(z) J/(\Lambda_1 \Lambda_2) \) and \( I(z) \) is here normalized to \( F \), i.e., \( I(z) \rightarrow I(z)/F^2 \), leaving four free parameters, namely \( r_m = R_m/F \) and the coupling constants \( C_m \), which allows to adjust the strength of the Fano effect. \( I(z) \) is a retarded propagator and maps to the cross section by the fluctuation-dissipation prefactor.

In Fig. 3(b), we plot \( I''(\omega) \), for empirically chosen \( r_m = 0.3 \), \( C_m = -0.8 J \), together with \( \Pi''(\omega) \), as well as the rescaled diagonal intensity \( \sum_m D_{mm}(\omega) \) from Fig. 3(a). The spectrum is remarkably similar to the experimental findings in Refs. [1–5]. A broad continuum due to the fractionalized magnetic excitations is visible, on top of which two asymmetric phonon line-shapes ride, with a characteristic sharp, almost vertical, drop-off only on the high frequency side of the mode. The overall shape of

![Diagram](image-url)
the Raman response $I''(\omega)$ is distinctly different from the diagonal phonon intensity, $\propto \sum_m D_{mm}''(\omega)$, green dashed line in Fig. 3(b), which would approximately describe the response, if only the Majorana-Phonon scattering was taken into account but not the Fano effect.

Conclusion.– We have provided a microscopic theory of optical phonons coupled to a KSL. Our analysis strongly supports the origin of the Fano line-shapes observed in Raman experiments on Kitaev candidate materials to be due to the fractionalized magnetic excitations. Moreover, the line-shape asymmetry is twofold, namely due to the fractionalized magnetic excitations. Moreover, direct comparison between Fig. 3(a) and (b) shows that the origin of the line-shape asymmetry is twofold, namely stemming from the Majorana-phonon scattering itself, as well as from the Fano effect.

In the future, it would be desirable to obtain the spin-phonon coupling constants from ab-initio calculations [61] for a quantitative description and to extend the analysis to other QSL candidate materials. We also expect that a better understanding spin-phonon coupling is crucial for understanding the thermal transport behavior of $\alpha$-RuCl$_3$.

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