Majorana Landau Level Spectroscopy – a proposal for observing pseudo magnetic fields in strained thin films of α-RuCl$_3$

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abstract

I. INTRODUCTION

Lattice strain can induce effective magnetic fields without actually breaking time reversal symmetry. An out of plane (along the z-axis) magnetic field can be induced by strain fields of the form $B = \beta\left[2\partial_x u_{xy} - \partial_y(u_{xx} - u_{yy})\right]$. Here, in addition to our numerical evaluations we try to obtain a more microscopic understanding of the influence of such a pseudo magnetic field on a Majorana fermion system and how the expected Landau level degeneracy is manifest in the Raman response function.

Via minimal coupling of the vector potential we use the canonical momenta $\mathbf{\Pi} = \mathbf{p} - \frac{e}{c}\mathbf{A}$ and work in the Landau gauge $\mathbf{A} = B(0, x)$. We study the low energy behaviour of our Majorana fermion systems in the flux free low temperature sector by expanding the Majorana field operators $\hat{\Psi} = (\Psi_A(\mathbf{r})\Psi_B(\mathbf{r}))^T$ around the two Dirac points (labeled by $\nu = \pm 1$)

$$H_\nu \approx i\int \mathrm{d}^2\mathbf{r}\hat{\Psi}^\dagger \begin{pmatrix} 0 & \nu p_x - i(p_y - \nu Bx) \\ -\nu p_x - i(p_y - \nu Bx) & 0 \end{pmatrix} \hat{\Psi}.$$

Note that B has opposite sign at the two Dirac points leaving TRS intact, which however prevents the usual trick of combining the two Majorana cones into a single cone of complex fermions. Nevertheless, we can concentrate on only one of the cones because there is no coupling between the two.

We introduce the ladder operator $a = \frac{l}{2\hbar}(\Pi_x - i\Pi_y)$ with $l^2 = \frac{c\hbar}{e|B|}$. Then we expand the field operators in terms of the standard Landau Level wave functions $\Psi_A(\mathbf{r}) = \sum_{n,p}\Phi_{n-1,p}(\mathbf{r})f_{Anp}$ and $\Psi_B(\mathbf{r}) = \sum_{n,p}\Phi_{n,p}(\mathbf{r})f_{Bnp}$ with Majorana operators $f_{A/Bnp}$ obeying the Majorana commutation relations (but note the sign change of momenta from conjugation $\Psi_B^\dagger(\mathbf{r}) = \sum_{n,p}\Phi^*_{n,p}(\mathbf{r})f_{Bn-p}$). Using the ladder operator properties $a\Phi_n = \sqrt{n}\Phi_{n-1}$ and $a^\dagger\Phi_n = \sqrt{n+1}\Phi_{n+1}$ we obtain the Hamiltonain

$$H_+ \approx \begin{pmatrix} f_{An-p} & f_{Bn-p} \end{pmatrix} \begin{pmatrix} 0 & i\frac{2\hbar}{l}\sqrt{n} \\ -i\frac{2\hbar}{l}\sqrt{n} & 0 \end{pmatrix} \begin{pmatrix} f_{Anp} \\ f_{Bnp} \end{pmatrix} \quad (1)$$

It is diagonalized by introducing the complex fermions a_{np} with $f_{Bnp} = a_{np} + a^\dagger_{n-p}$ and $f_{Anp} = i\left(a_{np} - a^\dagger_{n-p}\right)$ such that

$$H_+ \approx \sum_{np} E(n)\left[a^\dagger_{np}a_{np} - \frac{1}{2}\right] \quad (2)$$

with the energies $E(n) = 4\frac{\sqrt{2\hbar}}{l}\sqrt{n}$ obeying the well known $\propto \sqrt{n}$ scaling of Dirac fermions.

Next, we look at the low energy behaviour of the Raman response $I(\omega) = \int_{-\infty}^{\infty}\mathrm{d}te^{i\omega t}\langle R(t)R(0)\rangle$. The main difference between the non-resonant and resonant Raman vertices is that the former couples both sublattices whereas the latter does not

$$\begin{aligned} R_{\text{non-res}} &\propto i\int \mathrm{d}^2\mathbf{r}\Psi^\dagger_A(\mathbf{r})(t)\Psi_B(\mathbf{r}) \\ &\propto \sum_{np}\left[a_{n-p}(t) - a^\dagger_{np}(t)\right]\left[a_{n-1p} + a^\dagger_{n-1-p}\right] \\ R_{\text{res}} &\propto i\int \mathrm{d}^2\mathbf{r}\left[\Psi^\dagger_A(\mathbf{r})(t)\Psi_B(\mathbf{r}+\delta) - \Psi^\dagger_A(\mathbf{r})(t)\Psi_B(\mathbf{r}-\delta)\right] \\ &\propto \sum_{np}\sin(p\delta)\left[a_{n-p}(t) - a^\dagger_{np}(t)\right]\left[a_{np} + a^\dagger_{n-p}\right]. \end{aligned} \quad (3)$$

The form of both vertices is very similar but only the non-resonant vertex mixes states which differ by one LL index. From the time dependence $a_{np}(t) = a_{np}e^{-itE(n)}$ and $a_{np}|0\rangle = 0$ we can directly calculate the low energy Raman responses

$$\begin{aligned} I_{\text{non-res}} &\propto \sum_{np}\delta\left[\omega - E(n) - E(n+1)\right] \\ I_{\text{res}} &\propto \sum_{np}\delta\left[\omega - 2E(n)\right]. \end{aligned} \quad (4)$$

In agreement with the numerical observation we find different scaling of the resonant and non-resonant intensities which originates from the sub-lattice selectivity of the vertices and the special structure of LL wave functions in Dirac systems which mix adjacent LL indices.

II. FINITE TEMPERATURE FORMALISM

By the simple form of the canonical ensemble we can write

$$I(\omega) \propto \sum_{\text{flux sectors } M} e^{-\beta E_0^M} I^M(\omega) \quad (5)$$

where E_0^M is the energy of the lowest-energy state in the flux-configuration M. Within each flux sector the Hamiltonian can be written in the Kitaev fermionization as

$$\mathcal{H} = \frac{1}{2}\sum_{\langle rr'\rangle} J^\alpha u^\alpha_{\langle rr'\rangle} i c_r c_{r'} \equiv \frac{1}{2}\sum_{r,r'} H_{rr'}c_r c_{r'}, \quad (6)$$

where $u^\alpha_{\langle rr'\rangle} = ib^\alpha_r b^\alpha_{r'} = \pm 1$. In terms of these Majorans H has a chiral symmetry S that flips sign of c_r on one of two sublattices (so that $\{S,H\}=0$). In the basis where S is diagonal H takes the block-off-diagonal form

$$H = i\begin{pmatrix} 0 & G \\ -G^\dagger & 0 \end{pmatrix}. \tag{7}$$

In this case the a diagonalization of H can be obtained from the singular value decomposition of G. Given unitary u and v such that $u^\dagger G v = \epsilon/4$, then

$$U = \frac{1}{\sqrt{2}}\begin{pmatrix} u & u \\ -iv & iv \end{pmatrix}. \tag{8}$$

Now

$$U^\dagger H U = \Omega = \begin{bmatrix} \mathrm{diag}(\vec{\epsilon}) & 0 \\ 0 & -\mathrm{diag}(\vec{\epsilon}) \end{bmatrix}, \tag{9}$$

with $\epsilon^\mu \geq 0$. We can define operators $a_\lambda = U^\dagger_{\lambda\lambda'} c_\lambda$ for $\lambda = 1, ..., n/2$ to get the set of $n/2$ fermionic quasiparticles $\{a^\dagger_\lambda, a_{\lambda'}\} = \delta_{\lambda,\lambda'}$ so the Hamiltonian becomes

$$\mathcal{H} = \frac{1}{2}\sum_\lambda \epsilon^\mu \left[2a^\dagger_\lambda a_\lambda - 1\right]. \tag{10}$$

Therefore the excitation created by $(a^\dagger)^\mu$ has energy ϵ^μ.

We can view the quasiparticles formed by u and v as n Majorana fermions, while the formation of U from u and v corresponds to the usual Dirac-fermionization of a pair of Majoranas.

Following 1602.05277 the Raman operator for the Kitaev model is given by

$$\begin{aligned}
\mathcal{R} &= \sum_{\alpha=x,y,z}\sum_{\langle ij\rangle_\alpha} (\boldsymbol{\epsilon}_{\mathrm{in}}\cdot\mathbf{d}^\alpha)(\boldsymbol{\epsilon}_{\mathrm{out}}\cdot\mathbf{d}^\alpha) J^\alpha S^\alpha S^\alpha && (11)\\
&= \sum_{\langle rr'\rangle} (\boldsymbol{\epsilon}_{\mathrm{in}}\cdot\mathbf{d}^\alpha)(\boldsymbol{\epsilon}_{\mathrm{out}}\cdot\mathbf{d}^\alpha) H_{rr'} c_r c_{r'} && (12)\\
&= \frac{1}{2}\begin{pmatrix} \mathbf{c}_A \\ \mathbf{c}_B \end{pmatrix}^T i \begin{pmatrix} A & B \\ -B^\dagger & A' \end{pmatrix}\begin{pmatrix} \mathbf{c}_A \\ \mathbf{c}_B \end{pmatrix} && (13)\\
&= \frac{1}{2}\begin{pmatrix} \mathbf{a} \\ (\mathbf{a}^\dagger)^T \end{pmatrix}^\dagger \begin{pmatrix} C & D \\ D^\dagger & -C \end{pmatrix}\begin{pmatrix} \mathbf{a}_{\lambda'} \\ (\mathbf{a}^\dagger_{\lambda'})^T \end{pmatrix}. && (14)
\end{aligned}$$

Here $C = u^\dagger B v + v^\dagger B^\dagger u$ and $D = -u^\dagger B v + v^\dagger B^\dagger u$ for a Raman operator that is symmetric w.r.t. swapping in and out polarizations and $C = u^\dagger A u + v^\dagger A' v$ and $D = u^\dagger A u - v^\dagger A' v$ for an antisymmetric channel. Then finally,

$$\begin{aligned}
I^M(\omega) \propto \sum_{\lambda\lambda'} & \left[2|C_{\lambda\lambda'}|^2 f(\varepsilon_\lambda)[1-f(\varepsilon_{\lambda'})]\delta(\omega+\varepsilon_\lambda-\varepsilon_{\lambda'})\right. \\
& \left. +|D_{\lambda\lambda'}|^2[1-f(\varepsilon_\lambda)][1-f(\varepsilon_{\lambda'})]\delta(\omega-\varepsilon_\lambda-\varepsilon_{\lambda'})\right],
\end{aligned} \tag{15}$$

where B and therefore C and D depend on the gauge chosen for each flux configuration M.

We evaluate the sum (5) using a classical Monte-Carlo approach following the VEGAS algorithm where we sample the entire two-particle spinon spectrum of pseudorandomly-chosen flux configurations until the expected error in the total $I(\omega)$ is sufficiently low. This is made slightly faster by treating the summand as a different random function for each flux sector of p total fluxes, independent of their placement.

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