

Coherent hole propagation in an exactly solvable gapless spin liquid

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We examine the dynamics of a single hole in the gapless phase of the Kitaev honeycomb model, focusing on the slow-hole regime where the bare hopping amplitude t is much less than the Kitaev exchange energy J . In this regime, the hole does not generate gapped flux excitations and is dressed only by the gapless fermion excitations. Investigating the single-hole spectral function, we find that the hole propagates coherently with a quasiparticle weight that is finite but approaches zero as $t/J \rightarrow 0$. This conclusion follows from two approximate treatments, which capture the same physics in complementary ways. Both treatments use the stationary limit as an exactly solvable starting point to study the spectral function approximately (i) by employing a variational approach in terms of a trial state that interpolates between the limits of a stationary hole and an infinitely fast hole and (ii) by considering a special point in the gapless phase that corresponds to a simplified one-dimensional problem.

I. INTRODUCTION

The physics of a doped Mott insulator is a central problem in the field of strongly correlated electrons,¹ being motivated in part by high-temperature superconductivity in the cuprates.² One main question is whether the charge carriers (electrons or holes) form a Fermi liquid or a non-Fermi liquid in a lightly doped Mott insulator.³ In a Fermi liquid, charge carriers propagate as coherent quasiparticles, which is indicated by a corresponding delta-function peak in the single-particle spectral function. Conversely, non-Fermi liquids are characterized by a completely incoherent propagation of charge carriers.⁴ Due to their different spectral functions, one can distinguish these two possibilities by using angle-resolved photoemission spectroscopy.⁵ Moreover, Fermi liquids and non-Fermi liquids exhibit different thermodynamic and transport properties at low temperatures.⁶

Since the ground state of a stereotypical Mott insulator is antiferromagnetically (AFM) ordered, the standard description of a lightly doped Mott insulator is in terms of an appropriate t - J model with AFM Heisenberg interactions.⁷ It has been established that, in two dimensions, a single hole propagates coherently in such an AFM ordered state.⁸ However, it is also known that the ground state of a Mott insulator does not have to be AFM ordered or even magnetically ordered at all.⁹ In particular, Anderson suggested¹⁰ that the parent state of a high-temperature superconductor is a quantum spin liquid,¹¹ an exotic strongly-correlated state exhibiting long-range entanglement,¹² fractional excitations,¹³ and a topological ground-state degeneracy.¹⁴ The melting of the AFM order into such a spin-liquid state is particularly favored by doping as the holes can then propagate more freely without scrambling an underlying magnetic order.^{15,16} Nevertheless, it is far from obvious whether a single hole in a spin liquid propagates as a coherent quasiparticle.

In this work, we address this challenging question for the Kitaev honeycomb model, an exactly solvable yet realistic spin model with a spin-liquid ground state.¹⁷ This model consists of $S = 1/2$ spins at the sites of a honeycomb lattice, which are coupled via different spin components along the

three bonds connected to any given site. The Hamiltonian is

$$H_K = -J_x \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle_x} \sigma_{\mathbf{r}}^x \sigma_{\mathbf{r}'}^x - J_y \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle_y} \sigma_{\mathbf{r}}^y \sigma_{\mathbf{r}'}^y - J_z \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle_z} \sigma_{\mathbf{r}}^z \sigma_{\mathbf{r}'}^z, \quad (1)$$

where $J_{x,y,z}$ are the coupling constants for the three types of bonds x , y , and z (see Fig. 1). Depending on these coupling constants, the ground state is either a gapped or a gapless spin liquid. In an earlier work,¹⁸ we provided a systematic study of slow-hole dynamics in the gapped phase of the model, discussing the single-particle properties (e.g., particle statistics) of individual holes and describing two different (fractional) Fermi-liquid ground states at finite doping. Due to the absence of low-energy excitations, slow holes in the gapped phase are necessarily coherent quasiparticles. In the present work, we focus on the gapless phase and investigate whether a single hole propagates coherently. The answer to this question is one step towards understanding whether the holes form a Fermi liquid at a small but finite density.

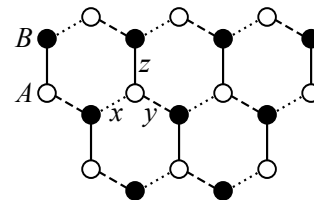


FIG. 1: Illustration of the honeycomb lattice. Sites in sublattices A and B are marked by white and black circles, while x , y , and z bonds are marked by dotted, dashed, and solid lines, respectively.

This work complements several papers in the existing literature. First, the lightly doped Kitaev honeycomb model has been studied extensively in the framework of slave-particle mean-field theories.^{19–21} Although this approach provides a full classification of spin-liquid ground states consistent with a given set of symmetries,²² it is not immediately clear which one of these ground states is actually realized for a particular Hamiltonian. Indeed, the conclusions of Refs. 20 and 21 disagree as the former predicts a Fermi-liquid state and the latter predicts a non-Fermi-liquid state at small doping. Second, a single hole in the Kitaev honeycomb model has been studied in Ref. 23 via exact diagonalization of small systems.

Within the limits of their calculation, the authors find that a fast hole with hopping amplitude $t \gtrsim J_{x,y,z}$ propagates incoherently. Our study is complementary to theirs in two ways as we consider a slow hole with hopping amplitude $t \ll J_{x,y,z}$ and employ the exact solution of the model to obtain analytic results that are applicable in the thermodynamic limit.

The main result of this paper is that a slow hole in the gapless phase of the Kitaev honeycomb model propagates as a coherent quasiparticle. Indeed, the single-hole spectral function is found to have a low-energy delta-function peak. The quasiparticle weight, the coefficient of this delta-function peak, is finite for any hopping amplitude $t > 0$ but vanishes in the stationary limit $t \rightarrow 0$. Since the model is no longer exactly solvable in the presence of a mobile hole, we deal with the problem approximately by using two complementary directions. First, we employ a variational approach in terms of a single-parameter trial state that interpolates smoothly between the extreme limits of a stationary hole and an infinitely fast hole. Second, we consider a simplified one-dimensional problem that captures the low-energy physics at a special point in the gapless phase. The results from these two directions are fully consistent with each other and strongly corroborate our claims on coherent propagation.

The paper is structured as follows. In Sec. II, we introduce the problem in a convenient formalism that is used throughout the rest of the paper. In Sec. III, we consider the exactly solvable limit of a stationary hole as a starting point of our investigation. In Secs. IV and V, we discuss the two complementary directions for treating a mobile hole, the variational approach and the simplified one-dimensional problem, respectively. In Sec. VI, we compare the results from these two directions and also those from previous works. Finally, in Sec. VII, we conclude the paper with suggestions for future research.

II. GENERAL FORMULATION

In the most general case, the lightly doped Kitaev honeycomb model is described by a modified t - J model⁷ where the usual Heisenberg interactions are substituted with the Kitaev couplings in Eq. (1). The Hamiltonian of this model reads

$$H = H_K - t \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} \sum_{\sigma} \left(\mathcal{P} a_{\mathbf{r}, \sigma}^{\dagger} a_{\mathbf{r}', \sigma} \mathcal{P} + \text{H.c.} \right), \quad (2)$$

where $a_{\mathbf{r}, \sigma}^{\dagger}$ creates an electron with spin σ at site \mathbf{r} , and \mathcal{P} projects out states with double occupancy. Formally, the spin operators in H_K are expressed as $\sigma_{\mathbf{r}}^{\alpha} = a_{\mathbf{r}, \sigma_1}^{\dagger} \tau_{\sigma_1, \sigma_2}^{\alpha} a_{\mathbf{r}, \sigma_2}$ in terms of the electron operators, where τ^{α} are the Pauli matrices with $\alpha = \{x, y, z\}$. Our main quantity of interest, the single-hole spectral function, is then given by

$$\mathcal{A}(\varepsilon, \mathbf{K}) = \sum_{\lambda} \sum_{\sigma} \left| \langle \tilde{\Phi}_{\lambda} | \hat{a}_{-\mathbf{K}, \sigma} | \Omega \rangle \right|^2 \delta[\varepsilon - \tilde{E}_{\lambda}], \quad (3)$$

where $|\Omega\rangle$ is the ground state of the model without any holes (undoped model), $|\tilde{\Phi}_{\lambda}\rangle$ are the eigenstates of the model with a single hole (doped model), and $\hat{a}_{-\mathbf{K}, \sigma} \propto \sum_{\mathbf{r}} e^{i\mathbf{K}\cdot\mathbf{r}} a_{\mathbf{r}, \sigma}$ creates a hole with momentum \mathbf{K} . Since \tilde{E}_{λ} is the energy of the

eigenstate $|\tilde{\Phi}_{\lambda}\rangle$, the spectral function $\mathcal{A}(\varepsilon, \mathbf{K})$ is the energy distribution of the single-hole state $\hat{a}_{-\mathbf{K}, \sigma} |\Omega\rangle$. Note that we consistently use a tilde to distinguish quantities of the doped model from those of the undoped model.

Restricting our attention to a single hole in the model, we do not consider the general Hamiltonian in Eq. (2) but describe the mobile hole in first quantization instead. The Hamiltonian of the undoped model is simply $H_{\sigma} \equiv H_K$ in terms of the spin degrees of freedom, while the doped model contains an additional degree of freedom specifying the hole position in the lattice (i.e., the hole site). Furthermore, we account for the presence of the hole via the hole-spin picture used in Ref. 18. Instead of actually removing the spin from the hole site, we switch off its couplings to all the other spins. To avoid introducing an unphysical degeneracy, we may demand that this hole spin is always in the spin-up state. In terms of the hole hopping amplitude t , the block of the doped Hamiltonian connecting hole sites \mathbf{r}_1 and \mathbf{r}_2 is then

$$\tilde{H}_{\sigma}(\mathbf{r}_1, \mathbf{r}_2) = \left[H_{\sigma} + \sum_{\alpha} J_{\alpha} \sigma_{\mathbf{r}_1}^{\alpha} \sigma_{\mathbf{r}_1 \pm \hat{\mathbf{r}}_{\alpha}}^{\alpha} \right] \delta_{\mathbf{r}_1, \mathbf{r}_2} - \frac{t}{2} [1 + \boldsymbol{\sigma}_{\mathbf{r}_1} \cdot \boldsymbol{\sigma}_{\mathbf{r}_2}] \sum_{\alpha} \delta_{\mathbf{r}_1 \pm \hat{\mathbf{r}}_{\alpha}, \mathbf{r}_2}, \quad (4)$$

where $\hat{\mathbf{r}}_{\alpha}$ is the vector along an α bond from a site in sublattice A to a neighboring site in sublattice B (see Fig. 1), and the upper (lower) sign in front of $\hat{\mathbf{r}}_{\alpha}$ corresponds to $\mathbf{r}_1 \in A$ ($\mathbf{r}_1 \in B$). The terms $J_{\alpha} \sigma_{\mathbf{r}_1}^{\alpha} \sigma_{\mathbf{r}_1 \pm \hat{\mathbf{r}}_{\alpha}}^{\alpha}$ in the diagonal blocks describe the switched-off couplings around the hole site, while the operators $[1 + \boldsymbol{\sigma}_{\mathbf{r}_1} \cdot \boldsymbol{\sigma}_{\mathbf{r}_2}]/2$ in the off-diagonal blocks exchange the hole spin with one of its neighbors.

In its gapless phase, the elementary excitations of the Kitaev model are gapless fermions and gapped fluxes. Since we are interested in the low-energy physics for a small hopping amplitude $t \ll J_{\alpha}$ and vanishing hole density, we neglect the flux excitations and consider the interplay between the mobile hole and the fermion excitations only. Employing the exact solution of the model in the standard way,¹⁷ and restricting our attention to the low-energy sector with no flux excitations, we end up with one Majorana fermion $\hat{c}_{\mathbf{r}}$ at each site \mathbf{r} , and an effective Hamiltonian in terms of these Majorana fermions. The details of this procedure are explained in Appendix A. For the undoped model, the effective low-energy Hamiltonian is

$$H_c = \sum_{\alpha} \sum_{\mathbf{r} \in A} i J_{\alpha} \hat{c}_{\mathbf{r}} \hat{c}_{\mathbf{r} + \hat{\mathbf{r}}_{\alpha}}, \quad (5)$$

while for the doped model, its respective blocks are

$$\tilde{H}_c(\mathbf{r}_1, \mathbf{r}_2) = \left[H_c \mp \sum_{\alpha} i J_{\alpha} \hat{c}_{\mathbf{r}_1} \hat{c}_{\mathbf{r}_1 \pm \hat{\mathbf{r}}_{\alpha}} \right] \delta_{\mathbf{r}_1, \mathbf{r}_2} - \frac{t}{2} [1 \mp i \hat{c}_{\mathbf{r}_1} \hat{c}_{\mathbf{r}_2}] \sum_{\alpha} \delta_{\mathbf{r}_1 \pm \hat{\mathbf{r}}_{\alpha}, \mathbf{r}_2}, \quad (6)$$

where the upper (lower) sign again corresponds to $\mathbf{r}_1 \in A$ ($\mathbf{r}_1 \in B$). The undoped Hamiltonian consists of quadratic coupling terms between neighboring Majorana fermions. In

the diagonal blocks of the doped Hamiltonian, these coupling terms are switched off around the hole site.

Since the low-energy fermions are perturbed by the presence of the hole in the doped model, it is useful to relabel the Majorana fermions \hat{c}_r by their relative positions with respect to the hole site \mathbf{r}_0 . Taking a reference site $\mathbf{0} \in A$, the Majorana fermions are consistently relabeled as

$$\begin{aligned}\hat{c}_r &\rightarrow c_{r-r_0} & (\mathbf{r}_0 \in A), \\ \hat{c}_r &\rightarrow c_{r_0-r} & (\mathbf{r}_0 \in B, \mathbf{r} \in A), \\ \hat{c}_r &\rightarrow -c_{r_0-r} & (\mathbf{r}_0 \in B, \mathbf{r} \in B).\end{aligned}\quad (7)$$

In the case of $\mathbf{r}_0 \in A$, this relabeling corresponds to a translation, while in the case of $\mathbf{r}_0 \in B$, it corresponds to an inversion exchanging the two sublattices.

In terms of the relabeled Majorana fermions c_r , the undoped Hamiltonian in Eq. (5) is then

$$H_c = \sum_{\alpha} \sum_{\mathbf{r} \in A} iJ_{\alpha} c_{\mathbf{r}} c_{\mathbf{r}+\hat{\mathbf{r}}_{\alpha}}, \quad (8)$$

while the blocks of the doped Hamiltonian in Eq. (6) are

$$\begin{aligned}\tilde{H}_c(\mathbf{r}_1, \mathbf{r}_2) &= \left[H_c - \sum_{\alpha} iJ_{\alpha} c_0 c_{\hat{\mathbf{r}}_{\alpha}} \right] \delta_{\mathbf{r}_1, \mathbf{r}_2} \\ &\quad - \frac{t}{2} \sum_{\alpha} \left[\hat{R}_{\alpha} - ic_0 \hat{R}_{\alpha} c_0 \right] \delta_{\mathbf{r}_1 \pm \hat{\mathbf{r}}_{\alpha}, \mathbf{r}_2}.\end{aligned}\quad (9)$$

In each off-diagonal block of the doped Hamiltonian, the two relabeling conventions for the two neighboring hole sites must be related by an appropriate operator \hat{R}_{α} that corresponds to an inversion R_{α} around the center of the α bond connecting the two sites. We express this inversion operator \hat{R}_{α} via the fermions that diagonalize the undoped Hamiltonian in Eq. (8). Since these fermions are labeled by their momenta \mathbf{k} due to translation symmetry, and those with momenta $\pm\mathbf{k}$ are degenerate due to inversion symmetry, we can define appropriate even (η) and odd (μ) complex fermions

$$\begin{aligned}\psi_{\mathbf{k},\eta}(\alpha) &= \frac{1}{2} [\gamma_{\mathbf{k},\eta,A}(\alpha) + i\gamma_{\mathbf{k},\eta,B}(\alpha)], \\ \psi_{\mathbf{k},\mu}(\alpha) &= \frac{1}{2} [\gamma_{\mathbf{k},\mu,A}(\alpha) + i\gamma_{\mathbf{k},\mu,B}(\alpha)]\end{aligned}\quad (10)$$

such that their Majorana fermion components

$$\begin{aligned}\gamma_{\mathbf{k},\eta,\Xi}(\alpha) &\propto \sum_{\mathbf{r} \in \Xi} \cos[\mathbf{k} \cdot (\mathbf{r} - \hat{\mathbf{r}}_{\alpha}/2)] c_{\mathbf{r}}, \\ \gamma_{\mathbf{k},\mu,\Xi}(\alpha) &\propto \sum_{\mathbf{r} \in \Xi} \sin[\mathbf{k} \cdot (\mathbf{r} - \hat{\mathbf{r}}_{\alpha}/2)] c_{\mathbf{r}}\end{aligned}\quad (11)$$

corresponding to the two sublattices $\Xi = A, B$ have even (η) and odd (μ) envelope functions with respect to the center of the α bond. Under the inversion R_{α} , these Majorana fermion components transform as

$$\begin{aligned}\hat{R}_{\alpha} [\gamma_{\mathbf{k},\eta,A}(\alpha)] &= \gamma_{\mathbf{k},\eta,B}(\alpha), \\ \hat{R}_{\alpha} [\gamma_{\mathbf{k},\eta,B}(\alpha)] &= -\gamma_{\mathbf{k},\eta,A}(\alpha), \\ \hat{R}_{\alpha} [\gamma_{\mathbf{k},\mu,A}(\alpha)] &= -\gamma_{\mathbf{k},\mu,B}(\alpha), \\ \hat{R}_{\alpha} [\gamma_{\mathbf{k},\mu,B}(\alpha)] &= \gamma_{\mathbf{k},\mu,A}(\alpha),\end{aligned}\quad (12)$$

and therefore the complex fermions transform as

$$\begin{aligned}\hat{R}_{\alpha} [\psi_{\mathbf{k},\eta}(\alpha)] &= -i\psi_{\mathbf{k},\eta}(\alpha), \\ \hat{R}_{\alpha} [\psi_{\mathbf{k},\mu}(\alpha)] &= i\psi_{\mathbf{k},\mu}(\alpha).\end{aligned}\quad (13)$$

Since the vacuum state $|\omega\rangle$ of these fermions [i.e., the ground state of the undoped Hamiltonian in Eq. (8)] is invariant under R_{α} , the inversion operator is then given by

$$\begin{aligned}\hat{R}_{\alpha} &= \exp \left\{ \frac{i\pi}{2} \sum_{\pm\mathbf{k}} \left[\psi_{\mathbf{k},\eta}^{\dagger}(\alpha) \psi_{\mathbf{k},\eta}(\alpha) - \psi_{\mathbf{k},\mu}^{\dagger}(\alpha) \psi_{\mathbf{k},\mu}(\alpha) \right] \right\} \\ &= \prod_{\pm\mathbf{k}} \left\{ \left[1 - (1-i) \psi_{\mathbf{k},\eta}^{\dagger}(\alpha) \psi_{\mathbf{k},\eta}(\alpha) \right] \right. \\ &\quad \left. \times \left[1 - (1+i) \psi_{\mathbf{k},\mu}^{\dagger}(\alpha) \psi_{\mathbf{k},\mu}(\alpha) \right] \right\},\end{aligned}\quad (14)$$

where $\pm\mathbf{k}$ corresponds to pairs of momenta. Since the unitary operator \hat{R}_{α} is Hermitian for even fermion number and anti-Hermitian for odd fermion number, it is effectively Hermitian because the fermion number is always even for physical states in the zero-flux sector of the Kitaev model.¹⁷

While the eigenstates of the undoped Hamiltonian in Eq. (8) belong to fermion space only, those of the doped Hamiltonian in Eq. (9) belong to the product of fermion space and hole position space. If we assume that they do not break translation or inversion symmetry, these eigenstates can be written as

$$|\tilde{\theta}_{\mathbf{K}}\rangle \propto \left[\sum_{\mathbf{r} \in A} e^{i\mathbf{K} \cdot \mathbf{r}} |\mathbf{r}\rangle + \sum_{\mathbf{r} \in B} e^{i\mathbf{K} \cdot \mathbf{r} + i\tilde{\vartheta}_{\mathbf{K}}} |\mathbf{r}\rangle \right] \otimes |\tilde{\chi}_{\mathbf{K}}\rangle, \quad (15)$$

where $|\tilde{\chi}_{\mathbf{K}}\rangle$ is a state in fermion space, and $|\mathbf{r}\rangle$ is a state in hole position space corresponding to hole site \mathbf{r} . Translation symmetry gives rise to a hole momentum \mathbf{K} , while inversion symmetry gives rise to a phase difference $\tilde{\vartheta}_{\mathbf{K}}$ between the two sublattices. Substituting Eq. (15) into Eq. (9), we obtain that $|\tilde{\chi}_{\mathbf{K}}\rangle$ are eigenstates of the effective Hamiltonian

$$\begin{aligned}\tilde{H}_c(\mathbf{K}) &= H_c - \sum_{\alpha} iJ_{\alpha} c_0 c_{\hat{\mathbf{r}}_{\alpha}} \\ &\quad - \frac{t}{2} \sum_{\alpha} \left[\hat{R}_{\alpha} - ic_0 \hat{R}_{\alpha} c_0 \right] \cos[\mathbf{K} \cdot \hat{\mathbf{r}}_{\alpha} + \tilde{\vartheta}_{\mathbf{K}}],\end{aligned}\quad (16)$$

where the phase difference $\tilde{\vartheta}_{\mathbf{K}}$ is in general determined self-consistently for each eigenstate by

$$\sum_{\alpha} \sin[\mathbf{K} \cdot \hat{\mathbf{r}}_{\alpha} + \tilde{\vartheta}_{\mathbf{K}}] \langle \tilde{\chi}_{\mathbf{K}} | \left[\hat{R}_{\alpha} - ic_0 \hat{R}_{\alpha} c_0 \right] | \tilde{\chi}_{\mathbf{K}} \rangle = 0. \quad (17)$$

In the special case of zero hole momentum $\mathbf{K} = \mathbf{0}$, it is either $\tilde{\vartheta}_{\mathbf{0}} = 0$ or $\tilde{\vartheta}_{\mathbf{0}} = \pi$ for all eigenstates $|\tilde{\chi}_{\mathbf{0}}\rangle$. The main advantage of Eq. (16) with respect to Eq. (9) is that its eigenstates $|\tilde{\chi}_{\mathbf{K}}\rangle$ belong to fermion space only and are therefore directly comparable to the eigenstates $|\chi\rangle$ of the undoped Hamiltonian in Eq. (8). In particular, the single-hole spectral function can

be expressed in terms of these eigenstates as

$$\mathcal{A}(\varepsilon, \mathbf{K}) = \frac{1}{2} \sum_{\lambda_{\mathbf{K}}} \left(1 + \cos \tilde{\vartheta}_{\mathbf{K}, \lambda_{\mathbf{K}}} \right) \left| \langle \tilde{\chi}_{\mathbf{K}, \lambda_{\mathbf{K}}} | \omega \rangle \right|^2 \times \delta \left[\varepsilon - \tilde{E}_{\mathbf{K}, \lambda_{\mathbf{K}}} \right], \quad (18)$$

where $\tilde{E}_{\mathbf{K}, \lambda_{\mathbf{K}}}$ is the energy of the eigenstate $|\tilde{\chi}_{\mathbf{K}, \lambda_{\mathbf{K}}}\rangle$, and $\lambda_{\mathbf{K}}$ is an additional label to distinguish eigenstates that correspond to the same hole momentum \mathbf{K} . We provide a detailed derivation of this result in Appendix B.

III. STATIONARY LIMIT

As a starting point of our investigation, we first consider the stationary limit ($t = 0$) when the undoped Hamiltonian H_c in Eq. (8) and the doped Hamiltonian $\tilde{H}_c \equiv \tilde{H}_c(\mathbf{K})$ in Eq. (16) are both quadratic and hence exactly solvable.²⁴ For simplicity, we also restrict our attention to the spatially isotropic point of the model, at which $J_{x,y,z} = J_0$. Since we are interested in the presence (or absence) of a delta-function peak in the spectral function $\mathcal{A}(\varepsilon) \equiv \mathcal{A}(\varepsilon, \mathbf{K})$, we aim to calculate the overlap $\langle \tilde{\omega} | \omega \rangle$ between the undoped ground state $|\omega\rangle$ and the doped ground state $|\tilde{\omega}\rangle$. If this ground-state overlap is finite in the thermodynamic limit, there is a delta-function peak in the spectral function with a corresponding hole quasiparticle weight $Z = |\langle \tilde{\omega} | \omega \rangle|^2 > 0$. Conversely, if the ground-state overlap vanishes in the thermodynamic limit, the presence of the hole leads to an orthogonality catastrophe,²⁵ and the spectral function has no delta-function peak ($Z = 0$).

To set up our calculation in a more standard formulation, we employ a fermion doubling procedure, which turns our quadratic Majorana fermion problems into quadratic number-conserving complex fermion problems. We introduce Majorana fermion copies c'_r of the original Majorana fermions c_r , and define corresponding complex fermions as

$$f_{\mathbf{r} \in A} = \frac{1}{2} (c_{\mathbf{r}} + i c'_{\mathbf{r}}), \quad f_{\mathbf{r} \in B} = \frac{i}{2} (c_{\mathbf{r}} + i c'_{\mathbf{r}}). \quad (19)$$

For the undoped model, the doubled Hamiltonian is then

$$\begin{aligned} H_c + H'_c &= J_0 \sum_{\alpha} \sum_{\mathbf{r} \in A} (i c_{\mathbf{r}} c_{\mathbf{r} + \hat{\mathbf{r}}_{\alpha}} + i c'_{\mathbf{r}} c'_{\mathbf{r} + \hat{\mathbf{r}}_{\alpha}}) \\ &= 2J_0 \sum_{\alpha} \sum_{\mathbf{r} \in A} (f_{\mathbf{r}}^{\dagger} f_{\mathbf{r} + \hat{\mathbf{r}}_{\alpha}} + f_{\mathbf{r} + \hat{\mathbf{r}}_{\alpha}}^{\dagger} f_{\mathbf{r}}) \\ &\equiv \sum_{\mathbf{r}, \mathbf{r}'} \mathcal{H}_{\mathbf{r}, \mathbf{r}'} f_{\mathbf{r}}^{\dagger} f_{\mathbf{r}'} \equiv f^{\dagger} \cdot \mathcal{H} \cdot f, \end{aligned} \quad (20)$$

while for the doped model, it takes the form

$$\begin{aligned} \tilde{H}_c + \tilde{H}'_c &= 2J_0 \sum_{\alpha} \sum_{\mathbf{r} \in A} (f_{\mathbf{r}}^{\dagger} f_{\mathbf{r} + \hat{\mathbf{r}}_{\alpha}} + f_{\mathbf{r} + \hat{\mathbf{r}}_{\alpha}}^{\dagger} f_{\mathbf{r}}) \\ &\quad - 2J_0 \sum_{\alpha} (f_{\mathbf{0}}^{\dagger} f_{\hat{\mathbf{r}}_{\alpha}} + f_{\hat{\mathbf{r}}_{\alpha}}^{\dagger} f_{\mathbf{0}}) \\ &\equiv \sum_{\mathbf{r}, \mathbf{r}'} \tilde{\mathcal{H}}_{\mathbf{r}, \mathbf{r}'} f_{\mathbf{r}}^{\dagger} f_{\mathbf{r}'} \equiv f^{\dagger} \cdot \tilde{\mathcal{H}} \cdot f. \end{aligned} \quad (21)$$

The doubled Hamiltonian of the undoped model is identical to that of graphene, and the additional term for the doped model corresponds to an infinite potential introduced at site $\mathbf{0}$. Each doubled Hamiltonian is particle-hole symmetric by construction and is diagonalized by fermions that come in pairs with opposite (i.e., positive and negative) energies. In particular, the undoped model has doubled fermions $\phi_{m, \pm}$ with energies $\epsilon_{m, \pm} = \pm \epsilon_{m, +}$, and the doped model has doubled fermions $\tilde{\phi}_{m, \pm}$ with energies $\tilde{\epsilon}_{m, \pm} = \pm \tilde{\epsilon}_{m, +}$. The doubled ground state in each case is then the state in which all of the negative-energy fermions and none of the positive-energy fermions are excited. Mathematically, these ground states read

$$\begin{aligned} |\Omega'\rangle &= |\omega\rangle \otimes |\omega'\rangle = \prod_m \phi_{m, -}^{\dagger} |0\rangle, \\ |\tilde{\Omega}'\rangle &= |\tilde{\omega}\rangle \otimes |\tilde{\omega}'\rangle = \prod_m \tilde{\phi}_{m, -}^{\dagger} |0\rangle, \end{aligned} \quad (22)$$

where $|0\rangle$ is the vacuum state of both the doubled fermions $\phi_{m, \pm}$ and the doubled fermions $\tilde{\phi}_{m, \pm}$. In the graphene language, the Fermi energy is at zero energy in both cases, and all negative-energy levels are filled with particles. However, the levels are perturbed by the infinite potential and, in particular, there is mixing between the positive-energy and the negative-energy levels. The perturbed ground state $|\tilde{\Omega}'\rangle$ is therefore different from the unperturbed one $|\Omega'\rangle$.

Using the doubled formulation, the quasiparticle weight is given by $Z = |\langle \tilde{\omega} | \omega \rangle|^2 = \sqrt{|\langle \tilde{\Omega}' | \Omega' \rangle|^2}$. If we define a unitary matrix \tilde{W} that transforms the perturbed fermions $\tilde{\phi}_{m, \pm}$ into the unperturbed fermions $\phi_{m, \pm}$ with the block structure

$$\begin{pmatrix} \phi_{+} \\ \phi_{-} \end{pmatrix} = \begin{pmatrix} \tilde{W}_{+,+} & \tilde{W}_{+,-} \\ \tilde{W}_{-,+} & \tilde{W}_{-,-} \end{pmatrix} \cdot \begin{pmatrix} \tilde{\phi}_{+} \\ \tilde{\phi}_{-} \end{pmatrix}, \quad (23)$$

the square of the quasiparticle weight becomes

$$\begin{aligned} Z^2 &= |\langle \tilde{\Omega}' | \Omega' \rangle|^2 = \left| \det \tilde{W}_{-,-} \right|^2 \\ &= \det \{ \tilde{W}_{-,-} \cdot \tilde{W}_{-,-}^{\dagger} \}. \end{aligned} \quad (24)$$

Introducing $G = I - \tilde{W}_{-,-} \cdot \tilde{W}_{-,-}^{\dagger}$, where I is the identity matrix, this determinant can then be written as

$$Z^2 = \exp[\text{tr} \{ \log [I - G] \}] = \exp \left[- \sum_{r=1}^{\infty} \frac{T_r}{r} \right], \quad (25)$$

$$T_r = \text{tr} \{ G^r \} = \sum_{m_1, \dots, m_r} G_{m_1, m_2} G_{m_2, m_3} \cdots G_{m_r, m_1}.$$

Importantly, since the matrix \tilde{W} is unitary, a generic matrix element of G takes the form

$$\begin{aligned} G_{m, m'} &= \delta_{m, m'} - \sum_n \tilde{W}_{m, -, n, -} \tilde{W}_{m', -, n, -}^* \\ &= \sum_n \tilde{W}_{m, -, n, +} \tilde{W}_{m', -, n, +}^*. \end{aligned} \quad (26)$$

Furthermore, the (real) eigenvalues of G are all non-negative because $\tilde{W} \cdot \tilde{W}^{\dagger} = I$, and each expansion term T_r in Eq. (25) is therefore generically non-negative.

To calculate the expansion terms in Eq. (25), we must determine the matrix elements of \tilde{W} . Writing $\phi_m^\dagger = \sum_{\mathbf{r}} \varphi_{m,\mathbf{r}} f_{\mathbf{r}}^\dagger$ and $\tilde{\phi}_m^\dagger = \sum_{\mathbf{r}} \tilde{\varphi}_{m,\mathbf{r}} f_{\mathbf{r}}^\dagger$ with the label m now running over both positive-energy and negative-energy levels, the single-particle wavefunctions $\varphi_{m,\mathbf{r}}$ and $\tilde{\varphi}_{m,\mathbf{r}}$ are related by

$$\tilde{\varphi}_{n,\mathbf{r}} = \sum_m \tilde{W}_{m,n} \varphi_{m,\mathbf{r}}, \quad (27)$$

and they respectively satisfy

$$\sum_{\mathbf{r}'} \mathcal{H}_{\mathbf{r},\mathbf{r}'} \varphi_{m,\mathbf{r}'} = \epsilon_m \varphi_{m,\mathbf{r}}, \quad (28)$$

$$\sum_{\mathbf{r}'} \tilde{\mathcal{H}}_{\mathbf{r},\mathbf{r}'} \tilde{\varphi}_{n,\mathbf{r}'} = \tilde{\epsilon}_n \tilde{\varphi}_{n,\mathbf{r}}, \quad (29)$$

where the single-particle Hamiltonians can be written as

$$\mathcal{H}_{\mathbf{r},\mathbf{r}'} = 2J_0 \sum_{\alpha} \delta_{\mathbf{r} \pm \hat{\alpha}, \mathbf{r}'}, \quad (30)$$

$$\tilde{\mathcal{H}}_{\mathbf{r},\mathbf{r}'} = \mathcal{H}_{\mathbf{r},\mathbf{r}'} + \tilde{\mathcal{V}}_{\mathbf{r},\mathbf{r}'}, \quad \tilde{\mathcal{V}}_{\mathbf{r},\mathbf{r}'} = \lim_{V \rightarrow \infty} \{V \delta_{\mathbf{r},\mathbf{0}} \delta_{\mathbf{r}',\mathbf{0}}\}.$$

Note that the particle-hole symmetry of the perturbed Hamiltonian is broken by the finite potential V but is restored in the limit of infinite potential $V \rightarrow \infty$. Substituting Eq. (27) into Eq. (29), and using Eq. (28) gives

$$\sum_m \tilde{W}_{m,n} \epsilon_m \varphi_{m,\mathbf{r}} + \sum_{\mathbf{r}'} \tilde{\mathcal{V}}_{\mathbf{r},\mathbf{r}'} \tilde{\varphi}_{n,\mathbf{r}'} = \tilde{\epsilon}_n \sum_m \tilde{W}_{m,n} \varphi_{m,\mathbf{r}}. \quad (31)$$

The matrix element $\tilde{W}_{m,n}$ can then be expressed as

$$\begin{aligned} \tilde{W}_{m,n} &= (\tilde{\epsilon}_n - \epsilon_m)^{-1} \sum_{\mathbf{r},\mathbf{r}'} \tilde{\mathcal{V}}_{\mathbf{r},\mathbf{r}'} \varphi_{m,\mathbf{r}}^* \tilde{\varphi}_{n,\mathbf{r}'} \\ &= \frac{V \varphi_{m,\mathbf{0}}^* \tilde{\varphi}_{n,\mathbf{0}}}{\tilde{\epsilon}_n - \epsilon_m}. \end{aligned} \quad (32)$$

This result for $\tilde{W}_{m,n}$ is not final because we do not know the perturbed energies $\tilde{\epsilon}_n$ or even the perturbed wavefunction $\tilde{\varphi}_{n,\mathbf{0}}$ at site $\mathbf{0}$. However, since the matrix \tilde{W} is unitary, its matrix elements satisfy the normalization condition

$$\sum_m |\tilde{W}_{m,n}|^2 = \tilde{\mathcal{N}}_n \sum_m (\tilde{\epsilon}_n - \epsilon_m)^{-2} = 1, \quad (33)$$

where $\tilde{\mathcal{N}}_n = V^2 |\tilde{\varphi}_{n,\mathbf{0}}|^2 / N$ is a normalization constant, and N is the system size. Note that $|\varphi_{m,\mathbf{0}}|^2 = 1/N$ for all m due to the translation symmetry of the unperturbed system. Furthermore, substituting Eq. (32) into Eq. (27), and setting $\mathbf{r} = \mathbf{0}$ results in the self-consistency condition

$$\frac{1}{N} \sum_m (\tilde{\epsilon}_n - \epsilon_m)^{-1} = \frac{1}{V} \rightarrow 0. \quad (34)$$

Note that the opposite limit $V = 0$ corresponds to the unperturbed system and gives $\tilde{\epsilon}_n = \epsilon_n$ for all levels.

We use Eqs. (33) and (34) to determine the matrix elements $\tilde{W}_{m,n}$ via the normalization constant $\tilde{\mathcal{N}}_n$ and the perturbed

energies $\tilde{\epsilon}_n$. Since the perturbation $\tilde{\mathcal{V}}_{\mathbf{r},\mathbf{r}'}$ is represented by a rank-1 matrix, it couples to only one (suitably chosen) level within any set of degenerate levels, and the unperturbed energies ϵ_m in Eq. (34) are therefore effectively non-degenerate. Each perturbed energy $\tilde{\epsilon}_n$ satisfies $\epsilon_n \leq \tilde{\epsilon}_n \leq \epsilon_{n+1}$, and the sum in m can be turned into a (non-divergent) integral for $m \neq \{n, n+1\}$. However, since $\tilde{\epsilon}_n$ can be arbitrarily close to either ϵ_n or ϵ_{n+1} , the corresponding two terms must be treated separately. Setting the overall energy scale to $J_0 = 1$ for simplicity, the schematic form of Eq. (34) is then

$$\mathbb{P} \int_{-1}^1 \frac{d\epsilon g(\epsilon)}{\tilde{\epsilon}_n - \epsilon} + \frac{1}{N} \left(\frac{1}{\tilde{\epsilon}_n - \epsilon_n} + \frac{1}{\tilde{\epsilon}_n - \epsilon_{n+1}} \right) = 0, \quad (35)$$

where $g(\epsilon) \sim |\epsilon|$ is the density of states around a Dirac point in two dimensions. Close to the Fermi energy, when $|\tilde{\epsilon}_n| \ll 1$, the integral in Eq. (35) is approximately

$$\mathbb{P} \int_{-1}^1 \frac{d\epsilon |\epsilon|}{\tilde{\epsilon}_n - \epsilon} \sim -\tilde{\epsilon}_n \log(1/|\tilde{\epsilon}_n|). \quad (36)$$

Just above (below) the Fermi energy, when $\tilde{\epsilon}_n > 0$ ($\tilde{\epsilon}_n < 0$), this integral is negative (positive), and the perturbed energy $\tilde{\epsilon}_n$ is therefore closest to ϵ_n (ϵ_{n+1}) among the unperturbed energies ϵ_m . In either case, the corresponding minimal energy difference is $\min_m |\tilde{\epsilon}_n - \epsilon_m| \sim [N|\tilde{\epsilon}_n| \log(1/|\tilde{\epsilon}_n|)]^{-1}$, which is parametrically smaller than the mean level spacing $[Ng(\tilde{\epsilon}_n)]^{-1} \sim [N|\tilde{\epsilon}_n|]^{-1}$ at the given energy. The sum in Eq. (33) is then dominated by this minimal energy difference, and the normalization constant becomes

$$\tilde{\mathcal{N}}_n \sim \min_m (\tilde{\epsilon}_n - \epsilon_m)^2 \sim [N\tilde{\epsilon}_n \log(1/|\tilde{\epsilon}_n|)]^{-2}. \quad (37)$$

Substituting Eq. (37) into Eq. (32), the absolute value of the matrix element $\tilde{W}_{m,n}$ takes the form

$$|\tilde{W}_{m,n}| \sim \frac{[N|\tilde{\epsilon}_n| \log(1/|\tilde{\epsilon}_n|)]^{-1}}{|\tilde{\epsilon}_n - \epsilon_m|}. \quad (38)$$

The matrix element itself could in principle have a complex phase factor, but it is not necessary as $\varphi_{m,\mathbf{0}}$ and $\tilde{\varphi}_{n,\mathbf{0}}$ can all be set real simultaneously.

We are now ready to calculate the quasiparticle weight via the expansion terms T_r in Eq. (25). In particular, by using Eq. (26), the first expansion term becomes

$$\begin{aligned} T_1 &= \sum_m G_{m,m} = \sum_{m,n} \left| \tilde{W}_{m,-,n,+} \right|^2 \\ &\sim \sum_{\tilde{\epsilon}_n > 0} \sum_{\epsilon_m < 0} \frac{[N\tilde{\epsilon}_n \log(1/|\tilde{\epsilon}_n|)]^{-2}}{(\tilde{\epsilon}_n - \epsilon_m)^2}. \end{aligned} \quad (39)$$

Turning the sums into integrals and using $g(\epsilon) \sim |\epsilon|$, this expansion term takes the schematic low-energy form

$$\begin{aligned} T_1 &\sim \int_0^1 d\tilde{\epsilon} \int_0^1 d\epsilon \frac{g(\tilde{\epsilon})g(\epsilon)}{(\tilde{\epsilon} + \epsilon)^2 [\tilde{\epsilon} \log(1/\tilde{\epsilon})]^2} \\ &\sim \int_0^1 \frac{d\tilde{\epsilon}}{\tilde{\epsilon} \log(1/\tilde{\epsilon})}. \end{aligned} \quad (40)$$

The infrared divergence at $\tilde{\epsilon} = 0$ can be regularized by a cutoff at $\tilde{\epsilon} \sim 1/N$ for any finite system size N . The first expansion term is then $T_1 \sim \log \log N$. Since the remaining expansion terms T_r are all non-negative, the square of the quasiparticle weight can be bounded from above as

$$Z^2 \leq \exp[-T_1] \sim \exp[-\kappa \log \log N] \sim [\log N]^{-\kappa}, \quad (41)$$

where κ is an unknown positive exponent. Regardless of its precise value, the quasiparticle weight Z vanishes in the limit of $N \rightarrow \infty$. We therefore conclude that there is an orthogonality catastrophe in the stationary limit. Note that this orthogonality catastrophe is weaker than in the standard case because the ground-state overlap decays with a logarithm and not with a power law of the system size.²⁵ This difference is explained by the smaller density of states around the Fermi energy, which is linear in our case and not constant as in the standard case. In fact, for a finite potential V in Eq. (30), there would no longer be an orthogonality catastrophe.²⁶

IV. VARIATIONAL APPROACH

If the hole is mobile ($t > 0$), the doped Hamiltonian $\tilde{H}_c(\mathbf{K})$ in Eq. (16) is no longer quadratic, and therefore the ground state of the doped model is not exactly known. Furthermore, unlike in the gapped phase of the model,¹⁸ there is no well-controlled perturbative approach around the stationary limit because there are infinitely many low-energy eigenstates arbitrarily close to the stationary ground state. To obtain an approximate ground state for a slow hole ($t \ll J_0$), we employ a variational approach in terms of a single-parameter trial state that interpolates smoothly between the ground state for a stationary hole and that for an infinitely fast hole.

In the limit of a stationary hole ($t = 0$), the doped ground state is known exactly (see Sec. III). In the doped Hamiltonian, the fermion coupling terms of the undoped Hamiltonian are fully switched off around the hole site [see Eq. (16)]. In the limit of an infinitely fast hole ($t \rightarrow \infty$), we expect that the doped ground state is close to the undoped ground state because the hole can hop most freely in its translation-symmetric fermion configuration. In particular, the expectation value of the inversion operator \hat{R}_α is maximized in Eq. (16) by the undoped ground state as $\langle \omega | \hat{R}_\alpha | \omega \rangle = +1$. For the trial state at $t \ll J_0$, it is then natural to choose the ground state $|\hat{\omega}\rangle$ of the Hamiltonian $\hat{H}_c(\varrho) = (1 - \varrho)\tilde{H}_c + \varrho H_c$, which interpolates smoothly between the stationary doped Hamiltonian \tilde{H}_c and the undoped Hamiltonian H_c as a function of a variational parameter $0 \leq \varrho \leq 1$. In this Hamiltonian, the fermion coupling terms of the undoped Hamiltonian are partially switched off around the instantaneous hole site (see Fig. 2).

Note that our intuition for the infinitely fast hole appears to be in contradiction with Nagaoka's theorem²⁷ which predicts a spin-polarized ground state for $t \rightarrow \infty$. The reason for this apparent contradiction is that the flux excitations are not negligible for $t \gg J_0$. From the point of view of such a high-energy hole, the spins are not fractionalized into fluxes and fermions. In this regime, the translation-symmetric spin

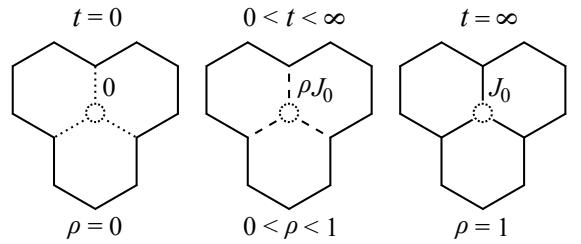


FIG. 2: Fermion coupling strengths around the instantaneous hole site (dotted circle) for the quadratic variational Hamiltonian $\hat{H}_c(\varrho)$ at $t = 0$ (left), finite t (middle), and $t \rightarrow \infty$ (right). Default couplings J_0 are marked by solid lines, partially switched-off couplings ϱJ_0 are marked by dashed lines (where $0 < \varrho < 1$), and fully switched-off couplings 0 are marked by dotted lines.

configuration of Nagaoka's ground state minimizes the kinetic energy of the hole by maximizing its effective hopping amplitude between neighboring hole positions. However, it is possible to imagine a scenario in which $E_{\text{fermion}}^{\text{max}} \ll t \ll E_{\text{flux}}^{\text{min}}$ and the spins are fractionalized into (high-energy) fluxes and (low-energy) fermions from the point of view of the hole. In this regime, the translation-symmetric fermion configuration of the undoped ground state minimizes the kinetic energy within the zero-flux sector. In some sense, it is the natural generalization of Nagaoka's ground state for this fractionalized scenario. Although there is no such intermediate regime for the Kitaev model due to $E_{\text{fermion}}^{\text{max}} \sim E_{\text{flux}}^{\text{min}} \sim J_0$, the fluxes are nevertheless negligible for $t \ll J_0$, and it is therefore reasonable to choose a trial state that interpolates between the stationary doped and the undoped ground states.

Since the Hamiltonian $\hat{H}_c(\varrho)$ is quadratic, the quasiparticle weight $Z = |\langle \hat{\omega} | \omega \rangle|^2$ in terms of the trial state $|\hat{\omega}\rangle$ can be calculated in exactly the same way as in Sec. III. Using the doubled formulation, the perturbed fermions $\hat{\phi}_m$ and the unperturbed fermions ϕ_m are related to each other by Eq. (23), but via a different unitary matrix \hat{W} . The corresponding single-particle wavefunctions are then related by

$$\hat{\varphi}_{n,\mathbf{r}} = \sum_m \hat{W}_{m,n} \varphi_{m,\mathbf{r}}, \quad (42)$$

and the perturbed wavefunction satisfies

$$\sum_{\mathbf{r}'} \hat{\mathcal{H}}_{\mathbf{r},\mathbf{r}'} \hat{\varphi}_{n,\mathbf{r}'} = \hat{\epsilon}_n \hat{\varphi}_{n,\mathbf{r}}, \quad (43)$$

where the appropriate single-particle Hamiltonian is

$$\begin{aligned} \hat{\mathcal{H}}_{\mathbf{r},\mathbf{r}'} &= \mathcal{H}_{\mathbf{r},\mathbf{r}'} + \hat{\mathcal{V}}_{\mathbf{r},\mathbf{r}'}, \\ \hat{\mathcal{V}}_{\mathbf{r},\mathbf{r}'} &= -(1 - \varrho) \mathcal{H}_{\mathbf{r},\mathbf{r}'} (\delta_{\mathbf{r},\mathbf{0}} + \delta_{\mathbf{r}',\mathbf{0}}). \end{aligned} \quad (44)$$

Using Eq. (32), the matrix element $\hat{W}_{m,n}$ is then given by

$$\begin{aligned} \hat{W}_{m,n} &= (\hat{\epsilon}_n - \epsilon_m)^{-1} \sum_{\mathbf{r},\mathbf{r}'} \hat{\mathcal{V}}_{\mathbf{r},\mathbf{r}'} \varphi_{m,\mathbf{r}}^* \hat{\varphi}_{n,\mathbf{r}'} \\ &= -(1 - \varrho) \frac{\epsilon_m \varphi_{m,\mathbf{0}}^* \hat{\varphi}_{n,\mathbf{0}} + \varphi_{m,\mathbf{0}}^* \hat{\varphi}'_{n,\mathbf{0}}}{\hat{\epsilon}_n - \epsilon_m}, \end{aligned} \quad (45)$$

where $\hat{\varphi}'_{n,\mathbf{0}} \equiv \sum_{\mathbf{r}} \mathcal{H}_{\mathbf{0},\mathbf{r}} \hat{\varphi}_{n,\mathbf{r}}$. Since the matrix \hat{W} is unitary, its matrix elements satisfy the normalization condition

$$\sum_m |\hat{W}_{m,n}|^2 = \hat{\mathcal{N}}_n \sum_m \left| \hat{\xi}_n + \epsilon_m \right|^2 (\hat{\epsilon}_n - \epsilon_m)^{-2} = 1, \quad (46)$$

where $\hat{\mathcal{N}}_n = (1 - \varrho)^2 |\hat{\varphi}_{n,\mathbf{0}}|^2 / N$ is a normalization constant, and $\hat{\xi}_n \equiv \hat{\varphi}'_{n,\mathbf{0}} / \hat{\varphi}_{n,\mathbf{0}}$ is a wavefunction ratio. Note again that $|\varphi_{m,\mathbf{0}}|^2 = 1/N$ for all m due to the translation symmetry of the unperturbed system. Using Eqs. (28), (42), and (45), we also obtain two independent self-consistency conditions

$$\begin{aligned} \hat{\varphi}_{n,\mathbf{0}} &= \sum_m \hat{W}_{m,n} \varphi_{m,\mathbf{0}} = -\frac{1-\varrho}{N} \sum_m \frac{\epsilon_m \hat{\varphi}_{n,\mathbf{0}} + \hat{\varphi}'_{n,\mathbf{0}}}{\hat{\epsilon}_n - \epsilon_m}, \\ \hat{\varphi}'_{n,\mathbf{0}} &= \sum_m \hat{W}_{m,n} \sum_{\mathbf{r}} \mathcal{H}_{\mathbf{0},\mathbf{r}} \varphi_{m,\mathbf{r}} = \sum_m \hat{W}_{m,n} \epsilon_m \varphi_{m,\mathbf{0}} \\ &= -\frac{1-\varrho}{N} \sum_m \frac{\epsilon_m^2 \hat{\varphi}_{n,\mathbf{0}} + \epsilon_m \hat{\varphi}'_{n,\mathbf{0}}}{\hat{\epsilon}_n - \epsilon_m}. \end{aligned} \quad (47)$$

Demanding non-trivial solutions for $\hat{\varphi}_{n,\mathbf{0}}$ and $\hat{\varphi}'_{n,\mathbf{0}}$ leads to the combined self-consistency condition

$$\begin{vmatrix} 1 + (1-\varrho)\Sigma'_n & (1-\varrho)\Sigma_n \\ (1-\varrho)\Sigma''_n & 1 + (1-\varrho)\Sigma'_n \end{vmatrix} = 0, \quad (48)$$

where the sums Σ_n , Σ'_n , and Σ''_n are given by

$$\begin{aligned} \Sigma_n &= \frac{1}{N} \sum_m (\hat{\epsilon}_n - \epsilon_m)^{-1}, \\ \Sigma'_n &= \frac{1}{N} \sum_m \epsilon_m (\hat{\epsilon}_n - \epsilon_m)^{-1} = \hat{\epsilon}_n \Sigma_n - 1, \\ \Sigma''_n &= \frac{1}{N} \sum_m \epsilon_m^2 (\hat{\epsilon}_n - \epsilon_m)^{-1} = \hat{\epsilon}_n^2 \Sigma_n - \hat{\epsilon}_n. \end{aligned} \quad (49)$$

Note that $\sum_m 1 = N$ counts the number of energy levels and that $\sum_m \epsilon_m = 0$ due to particle-hole symmetry. Substituting Eq. (49) into Eq. (48), the self-consistency condition becomes

$$\Sigma_n = \frac{1}{N} \sum_m (\hat{\epsilon}_n - \epsilon_m)^{-1} = -\frac{\varrho^2}{(1-\varrho^2)\hat{\epsilon}_n}. \quad (50)$$

This result reduces to the $V \rightarrow \infty$ limit of Eq. (34) for $\varrho = 0$ and the $V = 0$ limit of Eq. (34) for $\varrho = 1$. However, Eq. (50) is particle-hole symmetric for all values of $0 \leq \varrho \leq 1$ as it is invariant under $\epsilon_m \rightarrow -\epsilon_m$ and $\hat{\epsilon}_n \rightarrow -\hat{\epsilon}_n$.

We use Eqs. (46), (47), and (50) to determine the matrix elements $\hat{W}_{m,n}$ via the normalization constant $\hat{\mathcal{N}}_n$, the wavefunction ratio $\hat{\xi}_n$, and the perturbed energies $\hat{\epsilon}_n$. Although the perturbation $\hat{V}_{\mathbf{r},\mathbf{r}'}$ is represented by a rank-2 matrix, it only couples to levels that have finite wavefunctions at site $\mathbf{0}$. Since there is only one such (suitably chosen) level within any set of degenerate levels, the unperturbed energies ϵ_m in Eq. (50) are still effectively non-degenerate. Turning the sum in m into an integral, but treating the terms with $m = \{n, n+1\}$ separately, the schematic form of Eq. (50) is

$$\frac{1}{N} \left(\frac{1}{\hat{\epsilon}_n - \epsilon_n} + \frac{1}{\hat{\epsilon}_n - \epsilon_{n+1}} \right) = -\frac{\varrho^2}{(1-\varrho^2)\hat{\epsilon}_n}, \quad (51)$$

where the integral is immediately neglected because its value $\sim \hat{\epsilon}_n \log(1/|\hat{\epsilon}_n|)$ [see Eq. (36)] is much smaller than the term $\sim 1/\hat{\epsilon}_n$ for any $\varrho > 0$ and $|\hat{\epsilon}_n| \ll 1$. For both $\hat{\epsilon}_n > 0$ and $\hat{\epsilon}_n < 0$, the sum in Eq. (46) is then dominated by the minimal energy difference $\min_m |\hat{\epsilon}_n - \epsilon_m| \sim (1 - \varrho^2)|\hat{\epsilon}_n|/(N\varrho^2)$. Since Eqs. (47) and (50) give $\hat{\xi}_n = \hat{\epsilon}_n/\varrho$ for the wavefunction ratio, the normalization constant becomes

$$\begin{aligned} \hat{\mathcal{N}}_n &\sim \min_m \left[\left| \hat{\xi}_n + \epsilon_m \right|^{-2} (\hat{\epsilon}_n - \epsilon_m)^2 \right] \\ &\sim \frac{(1-\varrho^2)^2 \hat{\epsilon}_n^2}{N^2 \varrho^4 |\hat{\xi}_n + \hat{\epsilon}_n|^2} \sim \frac{(1-\varrho)^2}{N^2 \varrho^2}. \end{aligned} \quad (52)$$

Substituting Eq. (52) into Eq. (45), the absolute value of the matrix element $\hat{W}_{m,n}$ takes the form

$$|\hat{W}_{m,n}| \sim \frac{(1-\varrho)|\hat{\epsilon}_n + \varrho\epsilon_m|}{N\varrho^2|\hat{\epsilon}_n - \epsilon_m|}. \quad (53)$$

The matrix elements again do not need to have complex phase factors as $\varphi_{m,\mathbf{0}}$ and $\hat{\varphi}_{n,\mathbf{0}}$ can all be set real simultaneously.

We finally calculate the quasiparticle weight via the expansion terms T_r in Eq. (25). The first expansion term reads

$$\begin{aligned} T_1 &= \sum_m G_{m,m} = \sum_{m,n} \left| \hat{W}_{m,-,n,+} \right|^2 \\ &\sim \sum_{\hat{\epsilon}_n > 0} \sum_{\epsilon_m < 0} \frac{(1-\varrho)^2 (\hat{\epsilon}_n + \varrho\epsilon_m)^2}{N^2 \varrho^4 (\hat{\epsilon}_n - \epsilon_m)^2}. \end{aligned} \quad (54)$$

Turning the sums into integrals and using $g(\epsilon) \sim |\epsilon|$, this expansion term takes the schematic low-energy form

$$T_1 \sim \frac{(1-\varrho)^2}{\varrho^4} \int_0^1 d\hat{\epsilon} \int_0^1 d\epsilon \frac{\hat{\epsilon} \epsilon [\hat{\epsilon} - \varrho\epsilon]^2}{(\hat{\epsilon} + \epsilon)^2}. \quad (55)$$

By counting the powers of ϵ and $\hat{\epsilon}$, we deduce that this integral has no infrared divergence. Furthermore, the same power-counting argument reveals that the integrals for the remaining expansion terms T_r are also finite. We conclude that there is no orthogonality catastrophe for any $\varrho > 0$ within the variational framework and that the quasiparticle weight Z remains finite in the thermodynamic limit.

To relate the variational results to our original formulation, we would in principle need to perform a variational optimization that determines the best possible trial state $|\hat{\omega}\rangle$ for a given hopping amplitude t . Such a calculation would give the best variational parameter $\varrho(t)$ as a function of t , which could then be substituted directly into our variational results. However, it would require a more accurate calculation of the quasiparticle weight Z and is beyond the scope of this work.²⁸ Nevertheless, we would necessarily find $\varrho > 0$ and hence $Z > 0$ for any $t > 0$. According to Eq. (16), a small hole momentum \mathbf{K} does not matter either because it only renormalizes the hopping amplitude along an α bond as $t \rightarrow t \cos[\mathbf{K} \cdot \hat{\mathbf{r}}_\alpha + \hat{\vartheta}_{\mathbf{K}}]$. We therefore anticipate that the hole propagates as a coherent quasiparticle for any hopping amplitude $t > 0$ and any hole momentum $|\mathbf{K}| \ll |\hat{\mathbf{r}}_\alpha|^{-1}$. The quasiparticle weight is then finite for $t > 0$ but vanishes in the limit of $t \rightarrow 0$.

V. ONE-DIMENSIONAL LIMIT

As a complementary direction to the variational approach, we consider a spatially anisotropic special point in the gapless phase characterized by $J_{x,y} = J_0$ and $J_z = 0$, where the Kitaev model breaks down into non-interacting one-dimensional (1D) chains along the x and y bonds. Exploiting the relative simplicity of this 1D limit, and studying a modified problem that is asymptotically (i.e., for the lowest-energy fermions) equivalent to the original one, we can then determine if there is an orthogonality catastrophe for a mobile hole ($t > 0$) without resorting to a variational framework.

For a single 1D chain of length $2N$, the sites are labeled by $\ell = \{1, 2, \dots, 2N \equiv 0\}$, and the instantaneous hole site $\mathbf{0} \in A$ is labeled by $\ell = 0$ (see Fig. 3). The hole momentum is $K = \mathbf{K} \cdot \delta\mathbf{R}$, and the fermion momenta are $k = \mathbf{k} \cdot \delta\mathbf{R}$, where $\delta\mathbf{R} = \hat{\mathbf{r}}_y - \hat{\mathbf{r}}_x$ is the lattice constant. Since the even (η) and odd (μ) fermions $\psi_{k,\eta}(\alpha)$ and $\psi_{k,\mu}(\alpha)$ that diagonalize the inversion operator \hat{R}_α in Eq. (14) are defined for pairs of momenta $\pm k$ [see Eq. (10)], we restrict our attention to non-negative momenta $k = \{0, \delta k, 2\delta k, \dots, \pi\}$, where $\delta k = 2\pi/N$ is the momentum spacing. The total number of complex fermions is then N because there are two fermions $\psi_{k,\eta}(\alpha)$ and $\psi_{k,\mu}(\alpha)$ for each $0 < k < \pi$ and there is one fermion $\psi_{k,\eta}(\alpha)$ for each of $k = 0$ and $k = \pi$.

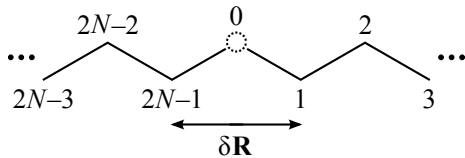


FIG. 3: Illustration of the one-dimensional (1D) chain with the lattice constant $\delta\mathbf{R}$ and the site labeling convention around the instantaneous hole site $\ell = 0$ (dotted circle).

Since the distinction between the two sublattices is entirely artificial in the 1D chain, the phase difference $\vartheta_{\mathbf{K}}$ in Eq. (16) vanishes for any hole momentum K . Using the 1D notation, the undoped Hamiltonian in Eq. (8) is then

$$H_c = J_0 \sum_{\ell \in A} (ic_\ell c_{\ell+1} + ic_\ell c_{\ell-1}), \quad (56)$$

while the doped Hamiltonian in Eq. (16) takes the form

$$\begin{aligned} \tilde{H}_c(K) &= H_c - J_0 (ic_0 c_1 + ic_0 c_{2N-1}) \\ &\quad - \frac{t}{2} \cos \frac{K}{2} \sum_{\alpha=x,y} \left[\hat{R}_\alpha - ic_0 \hat{R}_\alpha c_0 \right]. \end{aligned} \quad (57)$$

The inversion operators $\hat{R}_{x,y}$ are diagonalized by the fermions $\psi_{k,\eta}(x, y)$ and $\psi_{k,\mu}(x, y)$. In the 1D notation, the Majorana fermion components of these fermions in Eq. (11) are

$$\begin{aligned} \gamma_{k,\eta,\Xi}(x, y) &\propto \sum_{\ell \in \Xi} \cos \left[\frac{k\ell}{2} \pm \frac{k}{4} \right] c_\ell, \\ \bar{\gamma}_{k,\mu,\Xi}(x, y) &\propto \sum_{\ell \in \Xi} \sin \left[\frac{k\ell}{2} \pm \frac{k}{4} \right] c_\ell. \end{aligned} \quad (58)$$

The fermions corresponding to \hat{R}_x and \hat{R}_y also each diagonalize the undoped Hamiltonian H_c with degenerate energies $\epsilon_{k,\eta} = \epsilon_{k,\mu} = 4J_0 \cos(k/2)$.

In the limit of the lowest energies at $k \rightarrow \pi$, the Majorana fermion components in Eq. (58) are related to each other by $\gamma_{k,\eta,\Xi}(y) = \gamma_{k,\mu,\Xi}(x)$ and $\gamma_{k,\mu,\Xi}(y) = -\gamma_{k,\eta,\Xi}(x)$. The inversion operators \hat{R}_x and \hat{R}_y are therefore diagonalized by the same fermions at the lowest energies. This property motivates us to define modified operators \bar{R}_x and \bar{R}_y that are diagonalized by the same fermions at all energies and reduce to the inversion operators \hat{R}_x and \hat{R}_y at the lowest energies. These modified operators are given by Eq. (14) but in terms of modified fermions $\bar{\psi}_{k,\eta}(x, y)$ and $\bar{\psi}_{k,\mu}(x, y)$ that have modified Majorana fermion components

$$\begin{aligned} \bar{\gamma}_{k,\eta,\Xi}(x, y) &\propto \sum_{\ell \in \Xi} \cos \left[\frac{k\ell}{2} \pm \frac{\pi}{4} \right] c_\ell, \\ \bar{\gamma}_{k,\mu,\Xi}(x, y) &\propto \sum_{\ell \in \Xi} \sin \left[\frac{k\ell}{2} \pm \frac{\pi}{4} \right] c_\ell. \end{aligned} \quad (59)$$

Indeed, $\bar{\gamma}_{k,\eta,\Xi}(x, y)$ and $\bar{\gamma}_{k,\mu,\Xi}(x, y)$ reduce to $\gamma_{k,\eta,\Xi}(x, y)$ and $\gamma_{k,\mu,\Xi}(x, y)$ in the limit of $k \rightarrow \pi$, and they also satisfy

$$\begin{aligned} \bar{\gamma}_{k,\eta,\Xi} &\equiv \bar{\gamma}_{k,\eta,\Xi}(x) = -\bar{\gamma}_{k,\mu,\Xi}(y), \\ \bar{\gamma}_{k,\mu,\Xi} &\equiv \bar{\gamma}_{k,\mu,\Xi}(x) = \bar{\gamma}_{k,\eta,\Xi}(y) \end{aligned} \quad (60)$$

for all $0 \leq k \leq \pi$. Furthermore, the modified fermions $\bar{\psi}_{k,\eta} \equiv \bar{\psi}_{k,\eta}(x) = -\bar{\psi}_{k,\mu}(y)$ and $\bar{\psi}_{k,\mu} \equiv \bar{\psi}_{k,\mu}(x) = \bar{\psi}_{k,\eta}(y)$ still diagonalize the undoped Hamiltonian H_c with energies $\epsilon_k = \epsilon_{k,\eta} = \epsilon_{k,\mu} = 4J_0 \cos(k/2)$.

For the corresponding modified problem, the inversion operators \hat{R}_x and \hat{R}_y in Eq. (57) are replaced by the modified operators \bar{R}_x and \bar{R}_y . On the one hand, since the orthogonality catastrophe is determined by the lowest-energy fermions, the modified problem must have the same kind of orthogonality catastrophe as the original one. On the other hand, the doped Hamiltonian in the modified problem is simplified considerably with respect to Eq. (57). In particular, \bar{R}_x and \bar{R}_y are diagonalized by the same fermions, but each excited fermion multiplies them by opposite factors $\pm i$. They therefore take identical values for even fermion number and opposite values for odd fermion number. Since the fermion number is even for physical states, and the fermion parity is flipped by c_0 , several terms in Eq. (57) can be related to each other as

$$\begin{aligned} \bar{R} &\equiv \bar{R}_x = \bar{R}_y, \\ ic_0 \bar{R} c_0 &= ic_0 \bar{R}_x c_0 = -ic_0 \bar{R}_y c_0. \end{aligned} \quad (61)$$

In terms of the modified Majorana fermion components $\bar{\gamma}_{k,\eta,\Xi}$ and $\bar{\gamma}_{k,\mu,\Xi}$, the undoped Hamiltonian in Eq. (56) is then

$$\begin{aligned} H_c &= \frac{i}{2} \sum_k \epsilon_k (\bar{\gamma}_{k,\eta,A} \bar{\gamma}_{k,\eta,B} + \bar{\gamma}_{k,\mu,A} \bar{\gamma}_{k,\mu,B}) \\ &= \sum_k \epsilon_k \left(\bar{\psi}_{k,\eta}^\dagger \bar{\psi}_{k,\eta} + \bar{\psi}_{k,\mu}^\dagger \bar{\psi}_{k,\mu} - 1 \right), \end{aligned} \quad (62)$$

while the doped Hamiltonian in Eq. (57) takes the form

$$\begin{aligned} \bar{H}_c(K) = H_c - \frac{i}{2N} \sum_{k,k'} \left[\epsilon_{k'} (\bar{\gamma}_{k,\eta,A} + \bar{\gamma}_{k,\mu,A}) \right. \\ \left. \times (\bar{\gamma}_{k',\eta,B} + \bar{\gamma}_{k',\mu,B}) \right] - t_K \bar{R}. \end{aligned} \quad (63)$$

Note that this Hamiltonian only depends on the hopping amplitude t and the hole momentum K via the renormalized hopping amplitude $t_K = t \cos(K/2)$.

The modified problem characterized by Eqs. (62) and (63) has two important properties. First, like the original problem in Eqs. (56) and (57), it has a single energy scale t_K at energies much less than J_0 . The corresponding spectral function therefore must take the universal functional form

$$A(\varepsilon, K) = \mathcal{N} [\varepsilon - \bar{E}_{K,0}]^{-\zeta} F\left(\frac{\varepsilon - \bar{E}_{K,0}}{t_K}\right) \quad (64)$$

in the energy range $0 < \varepsilon - \bar{E}_{K,0} \ll J_0$, where $\bar{E}_{K,0}$ is the ground-state energy of $\bar{H}_c(K)$. The function F and the exponent ζ are universal but unknown, while the normalization constant \mathcal{N} and the ground-state energy $\bar{E}_{K,0}$ depend on both t_K and J_0 . Nevertheless, the spectral function has the same low-energy functional form for all $t_K > 0$, up to a rescaling with t_K , a renormalization, and a constant shift in ε , while its low-energy functional form is a fully self-similar power law for $t_K = 0$. Second, the Hamiltonian $\bar{H}_c(K)$ is effectively quadratic for both $t_K = 0$ and $t_K \rightarrow \infty$, and its ground state $|\bar{\omega}_K\rangle$ is therefore known exactly in both of these limits. Since the Hamiltonian H_c is also quadratic, the quasiparticle weight $Z = |\langle \bar{\omega}_K | \omega \rangle|^2$ can then be calculated exactly.

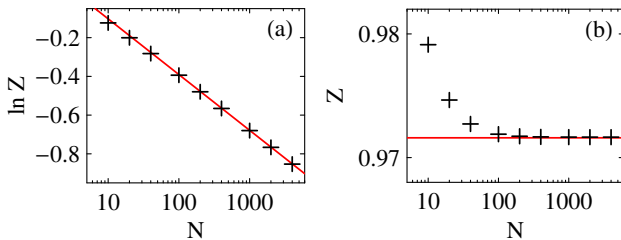


FIG. 4: Quasiparticle weight Z as a function of the system size N for $t_K = 0$ (a) and for $t_K \rightarrow \infty$ (b). Numerical data points are marked by black crosses, while asymptotic fits of the form $Z \propto N^{-0.125}$ (a) and $Z \approx 0.9716$ (b) are marked by red lines.

For both $t_K = 0$ and $t_K \rightarrow \infty$, we calculate the quasiparticle weight numerically for up to $N = 4000$, and study its behavior in the range $10 \leq N \leq 4000$ (see Fig. 4). For $t_K = 0$, Eq. (63) is obviously quadratic, and the quasiparticle weight is found to decay with a power law $Z \propto N^{-\nu}$, where the exponent is $\nu = 0.125 \pm 0.001$. This result indicates that there is a standard orthogonality catastrophe in the stationary limit.²⁵ For $t_K \rightarrow \infty$, the dominant term in Eq. (63) is $-t_K \bar{R}$. Since the operator \bar{R} is both unitary and Hermitian, its eigenvalues are ± 1 , and the low-energy subspace for $t_K \rightarrow \infty$ is the one with $\bar{R} = +1$. Projecting the remaining terms of $\bar{H}_c(K)$ onto

this subspace with the appropriate operator $(1 + \bar{R})/2$, we obtain the quadratic low-energy Hamiltonian

$$\begin{aligned} \bar{H}_c(K) \rightarrow H_c - \frac{i}{4N} \sum_{k,k'} \left[\epsilon_{k'} (\bar{\gamma}_{k,\eta,A} + \bar{\gamma}_{k,\mu,A}) \right. \\ \left. \times (\bar{\gamma}_{k',\eta,B} + \bar{\gamma}_{k',\mu,B}) - \epsilon_{k'} (\bar{\gamma}_{k,\eta,B} - \bar{\gamma}_{k,\mu,B}) \right. \\ \left. \times (\bar{\gamma}_{k',\eta,A} - \bar{\gamma}_{k',\mu,A}) \right] - t_K. \end{aligned} \quad (65)$$

The quasiparticle weight is then found to converge to a large finite value $Z = |\langle \bar{\omega}_K | \omega \rangle|^2 \approx 0.97$. This result corroborates our intuition that the doped ground state is close to the undoped ground state for $t_K \rightarrow \infty$. In fact, we believe that the ground-state overlap is only different from 1 because the modified problem is equivalent to the original one in terms of the lowest-energy fermions only. Furthermore, since there is a low-energy delta-function peak with $Z \sim 1$ in the spectral function for $t_K \rightarrow \infty$, and the spectral function has the same low-energy functional form for all $t_K > 0$, we deduce that there is a delta-function peak with a finite quasiparticle weight $Z > 0$ for all hopping amplitudes $t > 0$ and all hole momenta $K \ll 1$. The quasiparticle weight only vanishes in the stationary limit when the low-energy functional form of the spectral function becomes a power law.

VI. DISCUSSION

In the previous two sections, we investigated two complementary directions to determine whether a mobile hole in the gapless phase of the Kitaev honeycomb model propagates as a coherent quasiparticle. In Sec. IV, we described a variational approach for the spatially isotropic point ($J_{x,y,z} = J_0$), where the model is fully two dimensional (2D). The results apply for a generic point of the gapless phase because they are robust against perturbations in $J_{x,y,z}$, and they are valid for both ferromagnetic and antiferromagnetic couplings because they are invariant under the transformation $J_{x,y,z} \rightarrow -J_{x,y,z}$. However, the variational approach is somewhat uncontrolled as it is not immediately clear how close our trial state is to the actual ground state of the model. In Sec. V, we considered a spatially anisotropic special point ($J_{x,y} = J_0$ and $J_z = 0$), where the model becomes effectively one dimensional. In this 1D limit, we used an asymptotically exact calculation to make definite statements about the actual ground state. However, the different dimensionality might correspond to different physics, and it is not immediately clear if the results are applicable for a generic point of the gapless phase.

To make a connection between the two complementary directions, it is useful to check what the variational approach gives in the 1D limit. First, by repeating the steps of Sec. III with the density of states $g(\varepsilon) \sim 1$ around a Dirac point in one dimension, we find that the quasiparticle weight can be bounded from above as $Z \leq \exp[-T_1] \sim N^{-\nu_1}$ in the stationary limit, where $\nu_1 > 0$ is an unknown exponent. Next, by repeating the steps of Sec. IV, we find that Z remains finite in the thermodynamic limit for any finite variational parameter $\rho > 0$. Due to the relative simplicity of the 1D limit, it

is also possible to make these results more quantitative by determining that $Z \sim N^{-1/8}$ for $\varrho = 0$ and that $Z \sim \varrho^{1/4}$ for $\varrho > 0$. The result for $\varrho = 0$ is in agreement with the numerical exponent $\nu \approx 1/8$ found in Sec. V. Furthermore, the variational optimization can be performed explicitly, and it can be verified that the best variational parameter is $\varrho \sim (t/J_0)^{4/7}$ in the limit of $t \ll J_0$ (modulo logarithmic corrections). The details of this procedure are reported elsewhere.²⁸

We conclude that the variational approach gives the same results in the 1D limit as our asymptotically exact calculation in Sec. V. The standard orthogonality catastrophe in the stationary limit is straightforward to understand as the density of states is constant around the Fermi energy.²⁵ However, it might be surprising that there is no orthogonality catastrophe for a mobile hole as a standard orthogonality catastrophe is typically found for both stationary and mobile holes in 1D quantum liquids.²⁹ This difference with respect to previous studies is explained by the particle-hole symmetric nature of the Kitaev spin liquid. As a result of particle-hole symmetry, the phase shift is an odd function of energy, and therefore it vanishes at zero energy (i.e., at the Fermi energy).

In fact, this difference between the standard case and the particle-hole-symmetric case is immediately manifest in the variational approach if we compare Eqs. (34) and (50). In the standard case, a generic perturbation takes the form of a finite potential V appearing in Eq. (34). The corresponding form in Eq. (50) for the particle-hole-symmetric case can then be interpreted as a potential whose strength is linearly proportional to the fermion energy and therefore vanishes for the lowest-energy fermions. Also, the same feature appears in the asymptotically exact calculation, where the factor $\epsilon_{k'}$ in the second term of Eq. (63) indicates that the lower-energy fermions are perturbed less by the presence of the hole. Despite their different formulations, the two complementary directions seem to capture the same essential physics.

Since the variational approach is in full agreement with the asymptotically exact calculation for the 1D limit, we expect that our variational results for the 2D case in Sec. IV are also valid for the actual ground state at $t > 0$. Furthermore, our intuition suggests that the hole propagates more coherently in the 2D case than in the 1D limit because the fermions have a smaller density of states around the Fermi energy. This intuition is corroborated by the respective orthogonality catastrophes found in the stationary limit. For the 1D limit, we find a standard orthogonality catastrophe with a power-law decay, while for the 2D case, we find a weaker orthogonality catastrophe with a logarithmic decay. Since we know from Sec. V that a mobile hole propagates coherently in the 1D limit, we also anticipate coherent propagation in the 2D case corresponding to a generic point of the gapless phase.

We finally address the validity of our results for a generic Kitaev spin liquid, where H_K in Eq. (1) may be perturbed by generic time-reversal-invariant terms. The low-energy physics is still captured by a single mode of (dressed) Dirac fermions, but any local disturbance must be represented by a sum of all local fermion terms allowed by symmetry.³⁰ In this case, the disturbance due to the hole might not couple to a set of non-degenerate levels (see Secs. III and IV), and therefore the

orthogonality catastrophe might not be governed by a single (vanishing) phase shift at the Fermi energy. Nevertheless, in the 1D limit, the levels generically split into independent even and odd sectors with respect to the mirror-reflection symmetry around the hole site [see Fig. 3 and Eq. (57)]. Since the levels are non-degenerate within each sector, our earlier arguments apply and indicate that there is no orthogonality catastrophe in either sector. Furthermore, there is generically no orthogonality catastrophe in the 2D case.²⁶ For a finite phase shift at the Fermi energy, the integrand in Eq. (55) has two fewer powers of energy, but the integral is nevertheless finite. We therefore expect that our claims on coherent propagation remain applicable for a generic Kitaev spin liquid.

VII. OUTLOOK

In this work, we demonstrated that a single hole propagates as a coherent quasiparticle in the gapless phase of the Kitaev honeycomb model. In particular, it was found that the quasiparticle weight Z is finite for any small hopping amplitude $t \ll J_0$ but vanishes in the stationary limit $t \rightarrow 0$. It is then natural to ask how the quasiparticle weight scales with the hopping amplitude for $t \ll J_0$. In the 1D limit, this question is addressed elsewhere,²⁸ and it is found that $Z \sim (t/J_0)^{1/7}$, modulo logarithmic corrections. Assuming that Eq. (41) is a tight upper bound for Z^2 , with perhaps a renormalized exponent κ , we expect by analogy that the leading-order quasiparticle weight is $Z \sim [\log(J_0/t)]^{-\hat{\kappa}}$ in the 2D case, where $\hat{\kappa}$ is an unknown positive exponent. Nevertheless, it would be instructive to verify this expectation with a rigorous calculation and determine the exponents κ and $\hat{\kappa}$ in doing so.

The coherent propagation of a single hole suggests that the holes might form a Fermi liquid at finite doping.²⁰ However, it is far from obvious whether such a Fermi-liquid state would actually be stable as hole interactions could be relevant in the gapless phase and turn the Fermi liquid into some more exotic state. It would therefore be interesting to develop a controlled approach for describing the interactions between the holes and discussing the multi-hole ground state at a small but finite hole density. As a first step towards achieving this goal, it could be useful to consider the interactions between two holes in the gapless phase.¹⁶ Looking at the various interaction channels, one could then confirm the Fermi-liquid hypothesis²⁰ or even find unconventional superconductivity.²¹

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APPENDIX A: LOW-ENERGY SECTOR OF THE KITAEV HONEYCOMB MODEL

The standard solution of the Kitaev honeycomb model¹⁷ introduces four Majorana fermions at each site \mathbf{r} and represents the three spin components as $\sigma_{\mathbf{r}}^{\alpha} = i\hat{b}_{\mathbf{r}}^{\alpha}\hat{c}_{\mathbf{r}}$ in terms of these four Majorana fermions $\hat{b}_{\mathbf{r}}^x, \hat{b}_{\mathbf{r}}^y, \hat{b}_{\mathbf{r}}^z,$ and $\hat{c}_{\mathbf{r}}$. The undoped spin Hamiltonian in Eq. (1) then becomes

$$H_{\sigma} = \sum_{\alpha} \sum_{\mathbf{r} \in A} J_{\alpha} (i\hat{b}_{\mathbf{r}}^{\alpha}\hat{b}_{\mathbf{r}+\hat{\mathbf{r}}_{\alpha}}) (i\hat{c}_{\mathbf{r}}\hat{c}_{\mathbf{r}+\hat{\mathbf{r}}_{\alpha}}). \quad (\text{A1})$$

Since there is a conserved quantity $\hat{u}_{\mathbf{r},\mathbf{r}+\hat{\mathbf{r}}_{\alpha}} \equiv i\hat{b}_{\mathbf{r}}^{\alpha}\hat{b}_{\mathbf{r}+\hat{\mathbf{r}}_{\alpha}}$ for each bond and these conserved quantities all commute with one another, the model splits into independent bond sectors characterized by $\hat{u}_{\mathbf{r},\mathbf{r}+\hat{\mathbf{r}}_{\alpha}} = \pm 1$. Within each bond sector, the Hamiltonian in Eq. (A1) is quadratic and hence exactly solvable. However, there is some subtlety as the Majorana fermion representation increases the local Hilbert-space dimension from 2 to 4 at each site \mathbf{r} . All physical states then satisfy a corresponding local constraint $D_{\mathbf{r}} \equiv \hat{b}_{\mathbf{r}}^x\hat{b}_{\mathbf{r}}^y\hat{b}_{\mathbf{r}}^z\hat{c}_{\mathbf{r}} = 1$ in the Majorana fermion representation, which acts as a local gauge transformation $\hat{u}_{\mathbf{r},\mathbf{r}+\hat{\mathbf{r}}_{\alpha}} \rightarrow -\hat{u}_{\mathbf{r},\mathbf{r}+\hat{\mathbf{r}}_{\alpha}}$ at the three bonds around the site \mathbf{r} . Importantly, unlike the bond operators $\hat{u}_{\mathbf{r},\mathbf{r}+\hat{\mathbf{r}}_{\alpha}}$ themselves, their product $W_C = \prod_C \hat{u}_{\mathbf{r},\mathbf{r}+\hat{\mathbf{r}}_{\alpha}}$ is gauge invariant around any closed loop C of the lattice, and the flux operators W_C are then identified as corresponding to gapped flux excitations. Indeed, it can be shown^{17,31} that the ground state of the model is in the zero-flux sector characterized by $W_C = +1$ for all C and that any flux excitation $W_C = -1$ costs a finite energy $\Delta \sim J_{x,y,z}$.

For a small enough hopping amplitude $t \ll \Delta$, we can restrict our attention to the low-energy sector with no flux excitations and represent this zero-flux sector with the trivial bond sector characterized by $\hat{u}_{\mathbf{r},\mathbf{r}+\hat{\mathbf{r}}_{\alpha}} = +1$ for all bonds. The undoped spin Hamiltonian in Eq. (A1) then immediately reduces to the corresponding fermion Hamiltonian in Eq. (5). Furthermore, in the Majorana fermion representation, the diagonal blocks of the doped spin Hamiltonian in Eq. (4) are

$$\tilde{H}_{\sigma}(\mathbf{r}, \mathbf{r}) = \left[H_{\sigma} - \sum_{\alpha} J_{\alpha} (i\hat{b}_{\mathbf{r}}^{\alpha}\hat{b}_{\mathbf{r}+\hat{\mathbf{r}}_{\alpha}}) (i\hat{c}_{\mathbf{r}}\hat{c}_{\mathbf{r}+\hat{\mathbf{r}}_{\alpha}}) \right], \quad (\text{A2})$$

while its non-vanishing off-diagonal blocks are

$$\tilde{H}_{\sigma}(\mathbf{r}, \mathbf{r} \pm \hat{\mathbf{r}}_{\alpha}) = -\frac{t}{2} \left[1 - \sum_{\alpha'} (i\hat{b}_{\mathbf{r}}^{\alpha'}\hat{b}_{\mathbf{r} \pm \hat{\mathbf{r}}_{\alpha}}^{\alpha'}) (i\hat{c}_{\mathbf{r}}\hat{c}_{\mathbf{r} \pm \hat{\mathbf{r}}_{\alpha}}) \right], \quad (\text{A3})$$

where the upper (lower) sign in front of $\hat{\mathbf{r}}_{\alpha}$ corresponds to $\mathbf{r} \in A$ ($\mathbf{r} \in B$). Since the terms with $\alpha' \neq \alpha$ in Eq. (A3) create flux excitations, they have vanishing matrix elements within the zero-flux sector.¹⁸ Neglecting these terms, and using $i\hat{b}_{\mathbf{r}}^{\alpha}\hat{b}_{\mathbf{r}-\hat{\mathbf{r}}_{\alpha}}^{\alpha} = -i\hat{b}_{\mathbf{r}-\hat{\mathbf{r}}_{\alpha}}^{\alpha}\hat{b}_{\mathbf{r}}^{\alpha}$ in the case of $\mathbf{r} \in B$, the blocks of the fermion Hamiltonian in Eq. (6) are then recovered.

APPENDIX B: FERMION-ONLY REPRESENTATION OF THE SPECTRAL FUNCTION

In terms of the position-space electron operators $a_{\mathbf{r},\sigma}^{\dagger}$, the single-hole spectral function in Eq. (3) is

$$\mathcal{A}(\varepsilon, \mathbf{K}) = \frac{1}{2N} \sum_{\lambda} \sum_{\sigma} \sum_{\mathbf{r}, \mathbf{r}'} \langle \Omega | a_{\mathbf{r},\sigma}^{\dagger} | \tilde{\Phi}_{\lambda} \rangle \langle \tilde{\Phi}_{\lambda} | a_{\mathbf{r}',\sigma} | \Omega \rangle \times \delta[\varepsilon - \tilde{E}_{\lambda}] e^{-i\mathbf{K} \cdot (\mathbf{r} - \mathbf{r}')}. \quad (\text{B1})$$

The ground state of the undoped model reads $|\Omega\rangle = \mathcal{D}|\omega\rangle$ in the Majorana fermion representation, where $|\omega\rangle$ is the fermion vacuum state, and $\mathcal{D} \propto \prod_{\mathbf{r}} (1 + D_{\mathbf{r}})$ is a projection onto the physical subspace with $D_{\mathbf{r}} = 1$ for all \mathbf{r} . Using the hole-spin picture, the single-hole states $a_{\mathbf{r},\sigma}|\Omega\rangle$ are then

$$\begin{aligned} a_{\mathbf{r},\uparrow}|\Omega\rangle &= |\mathbf{r}\rangle \otimes \left[\frac{1}{2} (1 + \sigma_{\mathbf{r}}^z) |\Omega\rangle \right] \\ &= |\mathbf{r}\rangle \otimes \left[\frac{\mathcal{D}}{2} (1 + i b_{\mathbf{0}}^z c_{\mathbf{0}}) |\omega\rangle \right], \\ a_{\mathbf{r},\downarrow}|\Omega\rangle &= |\mathbf{r}\rangle \otimes \left[\frac{1}{2} \sigma_{\mathbf{r}}^x (1 - \sigma_{\mathbf{r}}^z) |\Omega\rangle \right] \\ &= |\mathbf{r}\rangle \otimes \left[\frac{\mathcal{D}}{2} (i b_{\mathbf{0}}^x c_{\mathbf{0}}) (1 - i b_{\mathbf{0}}^z c_{\mathbf{0}}) |\omega\rangle \right]. \end{aligned} \quad (\text{B2})$$

After projecting onto the subspaces with $\sigma_{\mathbf{r}}^z = \pm 1$ in the two cases, respectively, the spin rotation $\sigma_{\mathbf{r}}^x$ in the second case ensures that the hole spin is in the $\sigma_{\mathbf{r}}^z = +1$ state. Note that the Majorana fermions in Eq. (B2) are relabeled by their relative positions with respect to the hole site \mathbf{r} [see Eq. (7)].

Due to the overall translation symmetry, the eigenstates $|\tilde{\Phi}_{\lambda}\rangle \equiv |\tilde{\Phi}_{\mathbf{K},\lambda_{\mathbf{K}}}\rangle$ of the doped model are generically labeled by the hole momentum \mathbf{K} and an additional label $\lambda_{\mathbf{K}}$. Also, eigenstates with hole momentum $\mathbf{K}' \neq \mathbf{K}$ do not contribute to the spectral function $\mathcal{A}(\varepsilon, \mathbf{K})$. Using the hole-spin picture, and projecting the hole spin into the $\sigma_{\mathbf{r}}^z = +1$ state in the Majorana fermion representation, the contributing eigenstates with hole momentum \mathbf{K} take the forms [see Eq. (15)]

$$\begin{aligned} |\tilde{\Phi}_{\mathbf{K},\lambda_{\mathbf{K}}}^{p=0}\rangle &= \frac{1}{\sqrt{N}} \left[\sum_{\mathbf{r} \in A} e^{i\mathbf{K} \cdot \mathbf{r}} |\mathbf{r}\rangle + \sum_{\mathbf{r} \in B} e^{i\mathbf{K} \cdot \mathbf{r} + i\tilde{\vartheta}_{\mathbf{K},\lambda_{\mathbf{K}}}(\mathbf{r})} |\mathbf{r}\rangle \right] \\ &\otimes \left[\frac{\mathcal{D}}{2} (1 + i b_{\mathbf{0}}^z c_{\mathbf{0}}) |\tilde{\chi}_{\mathbf{K},\lambda_{\mathbf{K}}}\rangle \right], \\ |\tilde{\Phi}_{\mathbf{K},\lambda_{\mathbf{K}}}^{p=1}\rangle &= \frac{1}{\sqrt{N}} \left[\sum_{\mathbf{r} \in A} e^{i\mathbf{K} \cdot \mathbf{r}} |\mathbf{r}\rangle + \sum_{\mathbf{r} \in B} e^{i\mathbf{K} \cdot \mathbf{r} + i\tilde{\vartheta}_{\mathbf{K},\lambda_{\mathbf{K}}}(\mathbf{r})} |\mathbf{r}\rangle \right] \\ &\otimes \left[\frac{\mathcal{D}}{2} (1 + i b_{\mathbf{0}}^z c_{\mathbf{0}}) (i b_{\mathbf{0}}^x c_{\mathbf{0}}) |\tilde{\chi}_{\mathbf{K},\lambda_{\mathbf{K}}}\rangle \right]. \end{aligned} \quad (\text{B3})$$

There are two degenerate eigenstates $|\tilde{\Phi}_{\mathbf{K},\lambda_{\mathbf{K}}}^{p=0}\rangle$ and $|\tilde{\Phi}_{\mathbf{K},\lambda_{\mathbf{K}}}^{p=1}\rangle$ for each fermion state $|\tilde{\chi}_{\mathbf{K},\lambda_{\mathbf{K}}}\rangle$, which respectively correspond to hole quantum numbers $p = 0$ and $p = 1$ in the language of Ref. 18. The remaining two quantum numbers are $h = 0$ and $q = 0$ for all eigenstates in Eq. (B3), even

though eigenstates with $h = 1$ might have lower energies because flux binding is energetically favorable.^{18,24} Nevertheless, eigenstates with $h \neq 0$ or $q \neq 0$ have fractional excitations (i.e., fluxes and/or fermions) bound to the hole and therefore do not contribute to the spectral function. Using Eqs. (B2) and (B3), the matrix elements in Eq. (B1) are given by

$$\begin{aligned} \langle \tilde{\Phi}_{\mathbf{K},\lambda_{\mathbf{K}}}^{p=0} | a_{\mathbf{r} \in A, \uparrow} | \Omega \rangle &= \langle \tilde{\Phi}_{\mathbf{K},\lambda_{\mathbf{K}}}^{p=1} | a_{\mathbf{r} \in A, \downarrow} | \Omega \rangle \\ &= \frac{1}{2\sqrt{N}} \langle \tilde{\chi}_{\mathbf{K},\lambda_{\mathbf{K}}} | \omega \rangle e^{-i\mathbf{K} \cdot \mathbf{r}}, \end{aligned}$$

$$\begin{aligned} \langle \tilde{\Phi}_{\mathbf{K},\lambda_{\mathbf{K}}}^{p=0} | a_{\mathbf{r} \in B, \uparrow} | \Omega \rangle &= \langle \tilde{\Phi}_{\mathbf{K},\lambda_{\mathbf{K}}}^{p=1} | a_{\mathbf{r} \in B, \downarrow} | \Omega \rangle \\ &= \frac{1}{2\sqrt{N}} \langle \tilde{\chi}_{\mathbf{K},\lambda_{\mathbf{K}}} | \omega \rangle e^{-i\mathbf{K} \cdot \mathbf{r} - i\tilde{\theta}_{\mathbf{K},\lambda_{\mathbf{K}}}}, \\ \langle \tilde{\Phi}_{\mathbf{K},\lambda_{\mathbf{K}}}^{p=0} | a_{\mathbf{r}, \downarrow} | \Omega \rangle &= \langle \tilde{\Phi}_{\mathbf{K},\lambda_{\mathbf{K}}}^{p=1} | a_{\mathbf{r}, \uparrow} | \Omega \rangle = 0. \end{aligned} \quad (\text{B4})$$

Substituting Eq. (B4) into Eq. (B1), and summing over p , the single-hole spectral function in Eq. (18) is then recovered.

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