Majorana fermions in quasi-one-dimensional and higher-dimensional ultracold optical lattices

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We study Majorana fermions (MFs) in quasi-one dimensional (quasi-1D) and higher-dimensional fermionic optical lattices with a strictly 1D spin-orbit coupling, which has already been realized in cold atom experiments. We show that when the superfluid order parameters are homogeneous and are enforced to be identical along different chains, there are multiple MFs at each end with or without an experimentally tunable in-plane Zeeman field $V_z$. For $V_z = 0$ the multiple MFs are topologically protected by a chiral symmetry; however, for $V_z \neq 0$ the existence of multiple MFs is related to the peculiar spectrum properties of the system despite the broken chiral symmetry. In the generalization to higher dimensions, the multiple MFs form a zero-energy flat band. Furthermore, when the superfluid order parameters are solved self-consistently, the multiple MFs are usually destroyed because of the inhomogeneous order parameters of either Bardeen-Cooper-Schrieffer ($V_z = 0$) type or Fulde-Ferrell ($V_z \neq 0$) type. Our results are useful to guide the experimentalists on searching for MFs in ultracold spin-orbit coupled fermionic superfluids.

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I. INTRODUCTION

Majorana fermions (MFs), quantum particles which are their own antiparticles, have attracted a lot of attention because of their topological properties and the potential applications in fault-tolerant topological quantum computation [1–3]. Many solid state materials have been predicted to be candidates for the realization of MFs [4–16]. Even though experimental progress in the solid state systems has been made in the past two years and possible signatures of MFs have been observed [17–25], a “smoking gun” signature of MFs is still lacking due to many factors influencing the measurement results in solid state materials [26–30]. On the other hand, ultracold atoms provide an ideal playground for the quantum simulations of many condensed matter systems because they are clean and highly controllable in the system parameters. The recent realization of spin-orbit coupling (SOC) in Bose-Einstein condensate (BEC) [31–34] and Fermi gases [35,36] paves a way for the observation of MFs in cold atoms [37–41]. In this context, many schemes for the creation and observation of MFs in a one-dimensional (1D) cold atom quantum wire have been studied [42–45].

The realistic experiments in ultracold atoms are not on strictly 1D systems, which motivates our present study of the existence of MFs in quasi-1D and higher dimensional ultracold atom systems [46]. The necessity of studying the physics beyond 1D systems also arises from the failure of mean field theory in one dimension where there is no long-range ordering due to the Mermin-Wagner theorem. The inclusion of a weak tunneling in the transverse directions in a quasi-1D system could effectively suppress the quantum fluctuations and stabilize the long-range superfluid order, which is essential for MFs [47]. However, the presence of such transverse tunneling terms, even if treated as a perturbation, may pairwise couple the MFs and create a gap in the low-energy spectrum. It follows that, unless the number of chains in the transverse
reality, the finite momentum $Q_x$ superfluid phase which also supports MFs [57–61]. In parameter regime, the system could be driven to a topological lattices with a finite number $\rho_x$ and $d$. For simplicity, in the following analysis we first assume proximity-induced superconductivity in solid state materials.

For a single chain, the presence of the in-plane Zeeman field $V_x$, and SOC breaks the spatial inversion symmetry of the Fermi surface, leading to an FF superfluid with a finite momentum for the Cooper pairing $\Delta_1 = \Delta_0 e^{i\beta_n}$ [55,56]. In an appropriate parameter regime, the system could be driven to a topological FF superfluid phase which also supports MFs [57–61]. In reality, the finite momentum $Q_x$ and the order parameter $\Delta_0$ is usually determined self-consistently [62]. However, homogeneous superfluid order parameters can also be induced by loading ultracold fermionic atoms in a 3D molecular BEC cloud with Feshbach resonance [43], similar to the proximity-induced superconductivity in solid state materials. For simplicity, in the following analysis we first assume $\Delta_1 = \Delta_0$ and then consider the self-consistent solutions in Sec. IV.

III. HOMOGENEOUS ORDER PARAMETERS

To illustrate the basic physical picture of MFs in 2D and 3D optical lattices, we first consider the quasi-1D optical lattices with a finite number $N_y$ of chains in the transverse $\hat{y}$ direction. After the Fourier transformation, the multichain Bogoliubov-de Gennes (BdG) equation in momentum space can be written as

$$H_{\text{BdG}}(k_x) = h_0(k_x)\tau_z - V_y\sigma_y - \Delta_0\sigma_x\tau_y - t_y\tau_x\rho_x,$$

where $h_0(k_x) = -2t\cos(k_xd) - \mu - V_x\sigma_z + \alpha\sin(k_xd)\sigma_y$ and $d$ is the lattice spacing. The Pauli matrices $\sigma_j$, $\tau_j$ act on the spin and particle-hole spaces, respectively. The $N_x \times N_y$ matrix $\rho_x$ acts on the chain space, and it is defined as $(\rho_x)_{jk} = 1$ for $|j - k| = 1$ and 0 otherwise. The above BdG Hamiltonian preserves a particle-hole symmetry $\Sigma H(k_x)\Sigma^{-1} = -H(-k_x)$, where $\Sigma = \tau_x\hat{K}$ and $\hat{K}$ is the complex conjugate.

A. Chiral symmetry protected MFs for $V_y = 0$

When $V_y = 0$, Eq. (1) can be written as $H = H_x\tau_z + i\Delta\tau_y$, which preserves an additional chiral symmetry $S \equiv H(k_x)S^{-1} = -H(-k_x)$, where $H_x = h_0(k_x) - t_y\rho_x$, $\Delta = i\Delta\sigma_y$, and $S = \tau_z$. With an auxiliary pseudotime reversal symmetry operator defined as $\Theta = \hat{Z}$ such that $\Theta \cdot \Delta = \Delta \cdot \Theta$, the system belongs to the BDI topological class characterized by an integer $Z$ topological invariant [63,64]. The presence of the chiral symmetry $S$ allows the definition of a winding number $W$, which is equal to the number of MFs in a quasi-1D system [48,49]:

$$W = -\frac{i}{\pi} \int_{k_x = 0}^{k_x = \pi/\Delta_1} \frac{dz(k_x)}{z(k_x)} = -\frac{i}{\pi} \left[ \ln[z(\pi)] - \ln[z(0)] \right],$$

where $z(k_x) = \det[A(k_x)]/|\det[A(k_x)]|$ and $A(k_x) = H_x + \Delta$. As long as $W$ is nonzero, the multiple MFs at the ends of the chains, even if coupled by the transverse coupling, are topologically protected by the chiral symmetry $S$. Such a chiral symmetry cannot be broken by disorder (either site or bond disorder), nearest- or next-nearest-neighbor hopping [which influences only $h_0$ in Eq. (1)], and Zeeman fields (or magnetic impurities) in the $\hat{x}$ or $\hat{z}$ directions.

As a concrete example, we consider a two-chain system with weak transverse tunneling $t_y$, which is the simplest quasi-1D system. The winding number is shown in Fig. 1, which agrees very well with the band structure of the BdG Hamiltonian. We have chosen the chemical potential to lie in the middle of the Zeeman splitting of the two uncoupled chains $\mu = -2t$. Thus, for uncoupled chains ($t_y = 0$) both lattices are in the topological phase when $V_x > \Delta_0$, supporting a total of two pairs of MFs. Increasing the transverse tunneling $t_y$, we see that the winding number changes from $W = 2$ to $W = 0$ at some critical tunneling $t_y^c = \sqrt{V_y^2 - \Delta_0^2} = 0.6245t$ where the band gap closes [Fig. 1(b)]. The band gap closes at $k_x = 0$ at $t_y = t_y^c$ signaling a topological phase transition and the disappearance of the MFs. In Fig. 1(e) we show the phase diagram of a two-chain system indicating the number of MFs for different parameters. The number of MFs could be any value no more than the number of chains in the transverse
direction \( N_x \). As increasing \( t_y \), \( W \) can change from \( 2 \rightarrow 1 \rightarrow 0 \) for \( \mu \neq 2t \). We emphasize that this result is quite general for a quasi-1D system: the number of MFs can be controlled by the interchain coupling.

### B. Effect of a transverse SOC

To compare with the spin-independent interchain coupling, we here consider instead a weak SOC between the chains in the transverse direction, \( H_{\text{so}} = -\alpha_y/2 \sum_x (i c^\dagger_{x+y} c_x - i c^\dagger_{x+y} c_{x+1}) + \text{H.c.} \), which forms essentially a 2D Rashba SOC but with a difference in the tunneling magnitudes between the longitudinal and the transverse directions. We find that the effect of \( \alpha_y \) is dramatically different from the effect of \( t_y \) in the above analysis. The chiral symmetry is no longer preserved for each transformed chain, and thus the original multiple MFs for \( \alpha_y = 0 \) disappear because of the finite transverse SOC. An effect of \( \alpha_y \) is dramatically different from the effect of \( t_y \) above analysis. The chiral symmetry is no longer preserved for each transformed chain, and thus the original multiple MFs for \( \alpha_y = 0 \) disappear because of the finite transverse SOC. An effect of \( \alpha_y \) is dramatically different from the effect of \( t_y \) above analysis.

For a nonzero in-plane Zeeman field \( V_y \), we see that the pseudo-time-reversal symmetry \( \Theta = K \) is broken and it is no longer possible to find a chiral symmetry operator to be anticommuting with the full BdG Hamiltonian [see Eq. (1)]. As a result, the system no longer belongs to the BDI class [46,48,49]. However, we find that there are still multiple MFs even for \( V_y \neq 0 \) in the weakly coupled multichain system when the order parameters along different chains are assumed to be identical. We plot the lowest four quasiparticle excitation energies of the BdG equation for \( N_y = 2 \) and \( N_y = 3 \) in Fig. 3. We find that there are two and three zero-energy modes, respectively, and the system enters a gapless topologically trivial region only for \( V_y > \Delta_0 \).

To understand this surprising result, we note that the multichain system is now of the form \( H_{\text{BdG}}(k_x) = H(V_y)\rho_0 - \alpha_y \sigma_x \rho_y \) where we have assumed that there is no transverse tunneling \( t_y \). Here \( \rho_i \) is an \( N_y \times N_y \) matrix which acts on the chain space. It is defined as \((\rho_i)_{jk} = -i \) for \( k = j = 1 \), \((\rho_i)_{jk} = i \) for \( k = j = -1 \), and 0 otherwise. We note that the eigenvalues of \( \rho_i \) are of the form \((\pm \lambda_1, \pm \lambda_2, \pm \lambda_3, \ldots)\) for \( N_y = \text{even} \) and \((0, \pm \lambda_1, \pm \lambda_2, \pm \lambda_3, \ldots)\) for \( N_y = \text{odd} \), which form the diagonal matrix \( \rho_i \). So the above BdG Hamiltonian [Eq. (1)] can be rotated with a unitary transformation in the chain space to

\[
U H_{\text{BdG}}(k_x) U^\dagger = H(V_y)\rho_0 - \alpha_y \sigma_x \rho_y,
\]

where \( U \rho_i U^{-1} = \rho_i \).

Explicitly, for a system with a number of chains \( N_y \) in the \( y \) direction, the Hamiltonian after the rotation is of the form

\[
H_{\text{BdG}} = \begin{bmatrix}
H - \alpha_y (\rho_0)_{11} \sigma_x & 0 & \cdots & 0 \\
0 & H - \alpha_y (\rho_0)_{22} \sigma_x & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots & H - \alpha_y (\rho_0)_{N_y N_y} \sigma_x
\end{bmatrix}.
\]

For the whole system, the particle-hole symmetry preserves with the presence of the transverse SOC. However, after the rotation, the transverse SOC term is now \( H_{\text{so}} = -\alpha_y (\rho_0)_{jk} \sigma_x \) for each transformed chain. We find that \( H_{\text{so}} \) does not have a unitary transformation in the chain space to \( \rho_0 \). Thus the particle-hole \( Z_2 \) symmetry is broken for each transformed chain, and thus the original multiple MFs for \( \alpha_y = 0 \) disappear because of the finite transverse SOC. An exception occurs for an odd number of chains where the chain spin matrix \( \rho_y \) has a \( \lambda = 0 \) eigenvalue, i.e., \((\rho_i)_{N_y N_y} = 0 \) if the diagonal elements are arranged in an ascending order. For this specific transformed chain, the particle-hole symmetry is intact, and thus it still has a \( Z_2 \) symmetry which supports one MF at each end [46].

To compare the different effects of weak transverse tunneling \( t_y \) and \( \alpha_y \), we plot the edge states of a 2D strip (confined in the \( x \) direction and infinite in the \( y \) direction) in these cases. With only a weak SOC in the transverse direction \( \alpha_y = 0.2t \), there exist chiral MFs, with the edge state energy spectrum plotted in Fig. 2(b), in contrast to the energy spectrum with only a weak transverse tunneling \( t_y \) in Fig. 2(a). We see \( \alpha_y \) induces a spin-dependent splitting, and its effect vanishes at \( k_x = 0, \pm \pi \), while for a nonzero \( t_y \), the zero energies preserve the spin degeneracies and thus form a flat band in the full parameter regime of \( k_x \) as long as \( t_y \) is small.

### C. Multiple MFs without chiral symmetry for \( V_y \neq 0 \)

For a nonzero in-plane Zeeman field \( V_y \), we see that the pseudo-time-reversal symmetry \( \Theta = K \) is broken and it is no longer possible to find a chiral symmetry operator to be phase, and for an odd number of chains, it is in the nontrivial \( Z_2 \) phase with one MF at each end. This can also be understood from the following analysis.

The multichain system is of the form \( H_{\text{BdG}}(k_x) = H(V_y)\rho_0 - \alpha_y \sigma_x \rho_y \) where we have assumed that there is no transverse tunneling \( t_y \). Here \( \rho_i \) is an \( N_y \times N_y \) matrix which acts on the chain space. It is defined as \((\rho_i)_{jk} = -i \) for \( k = j = 1 \), \((\rho_i)_{jk} = i \) for \( k = j = -1 \), and 0 otherwise. We note that the eigenvalues of \( \rho_i \) are of the form \((\pm \lambda_1, \pm \lambda_2, \pm \lambda_3, \ldots)\) for \( N_y = \text{even} \) and \((0, \pm \lambda_1, \pm \lambda_2, \pm \lambda_3, \ldots)\) for \( N_y = \text{odd} \), which form the diagonal matrix \( \rho_i \). So the above BdG Hamiltonian [Eq. (1)] can be rotated with a unitary transformation in the chain space to

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As a result, the system no longer belongs to the BDI class [46,48,49]. However, we find that there are still multiple MFs even for \( V_y \neq 0 \) in the weakly coupled multichain system when the order parameters along different chains are assumed to be identical. We plot the lowest four quasiparticle excitation energies of the BdG equation for \( N_y = 2 \) and \( N_y = 3 \) in Fig. 3.

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We find that there are two and three zero-energy modes, respectively, and the system enters a gapless topologically trivial region only for \( V_y > \Delta_0 \).
As long as the transverse tunneling induced effective chemical potentials are small, the weakly coupled multichain system will thus have the same number of MFs as that with chemical potentials zero. Since the transformed “effective” chains are independent of each other, such a system belongs to the topological class $\mathbb{Z}_2 \otimes \mathbb{Z}_2 \cdots \otimes \mathbb{Z}_2 = \mathbb{Z}_2^{\otimes N_y}$ for weak transverse tunneling.

### D. Majorana flat band

We now study the crossover of the Majorana fermion physics from a quasi-1D to a real 3D system for $V_y = 0$. Assume that the 3D lattices with a strictly 1D SOC are confined in the $\hat{x}$ direction. With periodic boundary conditions along the transverse directions, $k_x$ and $k_z$ are good quantum numbers. Such 3D lattices are equivalent to a quasi-1D system with a number of chains equal to the discrete values of $k_{y,z}$, and $-2t_y \cos(k_y,d) - 2t_z \cos(k_z,d)$ can be treated as a chemical potential which does not break the symmetry of the system compared to 1D. The chemical potential $\mu$ is assumed to occupy the middle of the lower bands when the transverse tunneling $t_z$ is zero. We also take a Zeeman field large enough to drive the system to the topological regime for each value of $k_x$ and $k_z$. Thus, the lowest quasiparticle excitations of the uncoupled 3D lattices show a MF’s flat band [65,66].

The zero-energy MFs flat band persists for a small transverse tunneling $t_z$ [Fig. 4(a)]. With increasing $t_z$, the zero energy MFs disappear first at the Brillouin zone (BZ) edges while the BZ center is still a zero-energy flat band [Fig. 4(b)]. Further increasing $t_z$, we see that the MFs flat band is enclosed by the bulk quasiparticle excitations, showing a configuration of the Majorana flat plate. When the transverse coupling is strong enough, MFs disappear from the entire BZ, transforming the system to a trivial superconductor. Note that the bulk excitation gap at the center of BZ also decreases. These demonstrate that MFs exist at the confined surface of a 3D system and the zero-energy flat band is topologically protected by an energy gap from the bulk excitations.

### IV. EFFECT OF INHOMOGENEOUS ORDER PARAMETER

In the above discussions, we have assumed a uniform order parameter $\Delta_0$. In practice, when the superfluid order parameter originates from the intrinsic atomic scattering interaction, the order parameter of the superfluid needs to be obtained from the self-consistent calculations of the BdG equation, which is naturally inhomogeneous due to the hard wall boundary. Without an in-plane Zeeman field $V_y$, the order parameters for the topological BCS superfluid are still identical on different chains as shown in Fig. 5(a) if the initial random order parameter is chosen to be real in the self-consistent calculation. The chiral symmetry guarantees that the $\tilde{Z}$ invariant and multiple MFs are found at each end in a quasi-1D system [here $N_y = 2$, $N_x = 2$].
FIG. 5. (Color online) Effects of inhomogeneous order parameters from the self-consistent calculation. The order parameters $\Delta$ (in units of $t$) along different chains and quasiparticle excitation energies $E_n$ (in unit of $t$) are plotted for a two-chain system ($N_y = 2$) for (a, c) $V_y = 0.0$ and (b, d) $V_y = 0.5t$. Only the real parts of the order parameters for the two chains are plotted in (b). (d) Inset: Quasiparticle excitation energies for a three-chain system ($N_y = 3$), indicating one MF at each end, where the order parameter structures are similar as in (b). Other parameters are $\alpha = 2.0t$, $U = 4.5t$, $V_z = 1.2t$, $\mu = -2.25t$.

see Fig. 5(c)] after a self-consistent calculation. However, inhomogeneous order parameters will appear spontaneously on the system boundaries in the self-consistent calculation if a complex initial random input order parameter is used [67]. In this case, the zero-energy degeneracy of MFs are slightly lifted in the presence of a weak transverse tunneling [67] due to the interaction between MFs.

With a nonzero $V_y$, the FF superfluid order parameters of the system are identical along different chains for periodic boundary conditions [62]. However, for open boundary conditions, the order parameters are not identical on the edges for different chains due to the interplay of the finite $Q_y$ and the boundary, or the presence of edge states. As shown in Fig. 5(b), we see that the order parameters for the two parallel chains are identical in the bulk but different on the boundaries. From the quasiparticle excitation spectrum [Fig. 5(d)], the multiple MFs are gapped out because of the inhomogeneity of the order parameters on the boundaries. However, for an odd number of chains ($N_y = 3$), even though the order parameters are still inhomogeneous on the boundaries, one pair of MFs remains as shown in the inset of Fig. 5(d). More numerical results show that one pair of MFs survives in self-consistent calculations only when $N_y$ and $N_z$ are both odd for systems with a nonzero $V_y$. Similar results can also arise in a realistic system with an external trapping potential.

V. CONCLUSION

In summary, we have studied MFs in quasi-1D, 2D, and 3D optical lattices in the presence of weak transverse tunnelings between the chains. The realistic experimentally realized SOC is strictly 1D, leading to new intriguing results comparing to systems with a 2D Rashba SOC. We find that, topologically robust MFs exist even in a coupled multichain system as long as the transverse couplings are weak. We have studied the robustness of the MFs to in-plane Zeeman fields (that break the chiral symmetry) and to spatially inhomogeneous order parameters resulting from the self-consistent calculations. For the 3D optical lattices confined in the SOC direction, a zero-energy MFs flat band may exist even in the presence of a weak transverse tunneling. The existence of MFs in cold atom systems can be probed using radio-frequency spectroscopy [68]. Spin-orbit-coupled fermionic optical lattices have been experimentally realized. Because of the lack of disorder and the precisely controllable experiment parameters, it provides a feasible platform to search for MFs in context of cold atoms.

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