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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 (SOC) 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 $V_y$. For $V_y = 0$ the multiple MFs are topologically protected by a chiral symmetry, however for $V_y \neq 0$ 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 BCS ($V_y = 0$) type or Fulde-Ferrell (FF) ($V_y \neq 0$) 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 anti-particles, have attracted a lot of attention because of their topological properties and the potential applications in fault-tolerant topological quantum computation \cite{1,2}. Many solid state materials have been predicted to be candidates for the realization of MFs \cite{3,4,5,6,7,8,9,10}. 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 \cite{11,12,13,14,15,16,17,18,19,20,21,22,23,24,25,26,27,28,29}, 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) \cite{31,32} and Fermi gases \cite{33,34} paves a way for the observation of MFs in cold atoms \cite{35,36}. In this context, many schemes for the creation and observation of MFs in a 1D cold atom quantum wire have been studied \cite{37,38,39,40,41}.

The realistic experiments in ultracold atoms are not on strictly one dimensional (1D) systems, which motivates our present study on the existence of MFs in quasi-1D and higher dimensional ultracold atom systems \cite{42}. The necessity of studying the physics beyond 1D systems also arise from the failure of mean field theory in 1D where there is no long-range ordering due to 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 \cite{43}. 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 directions is odd (which is difficult to control experimentally), the system of coupled chains may not support any MFs at all. Because of this, whether or not MFs exist in weakly coupled quasi-1D (with finite number of chains), two- and three dimensional (2D, 3D) cold atom systems with artificial SOC and Zeeman fields has remained an important open question both theoretically and experimentally.

In this paper we study the existence of MFs in quasi-1D and higher dimensional optical lattices. In contrast to the previous studies, we have considered here strictly 1D SOC that has been realized in ultracold Fermi gases recently \cite{33,34}. The rest of the paper is organized as follows. In Sec. II we present the model Hamiltonian of the quasi-1D system. In Sec. III we show that when the superfluid order parameters are homogeneous along different chains, there are multiple MFs at each end of the system no matter an experimentally tunable in-plane Zeeman field $V_y$ is present or not. When $V_y = 0$, the multiple MFs are topologically protected by a chiral symmetry \cite{44,45}, while when $V_y \neq 0$ the existence of multiple MFs are related to the peculiar spectrum properties of the system. In the generalization to higher dimensions, the multiple MFs form a zero energy flat band. In Sec. IV we find that when the order parameters are solved self-consistently, the multiple MFs are usually destroyed because of the inhomogeneous order parameters of either BCS ($V_y = 0$) type or Fulde-Ferrell

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II. MODEL HAMILTONIAN

We first consider quasi-1D optical lattices aligned along $\hat{x}$ direction. The tight-binding Hamiltonian in the mean field level can be written as,

$$H^{tb} = -t \sum_{\sigma} (c_{x, \sigma}^\dagger c_{x+\hat{\epsilon}_x, \sigma} + H.c.) - \mu \sum_{\sigma} c_{x, \sigma}^\dagger c_{x, \sigma} + \frac{\alpha}{2} \sum_{x} (c_{x-\hat{\epsilon}_x, \sigma}^\dagger c_{x+\hat{\epsilon}_x, \sigma} - c_{x, \sigma}^\dagger c_{x, \sigma} + H.c.) - V_z \sum_{x} (c_{x}^\dagger c_{x} - c_{x}^\dagger c_{x}),$$

where $t$ is the hopping amplitude along $\hat{x}$ direction (we take $t = 1$ as the energy unit in this paper) with $c_{x, \sigma}^\dagger$ being the fermionic operator creating a particle with spin $\sigma$ in the site $x$, $\mu$ is the chemical potential, $\alpha$ is the 1D SOC strength along $\hat{\epsilon}_x$ direction, and $V_z$ and $V_y$ are the out-of-plane and in-plane Zeeman fields in the $\hat{z}$ and $\hat{y}$ directions, respectively. Here we consider MFs in a bunch of coupled 1D chains, $t_y$ represents the inter-chain coupling strength and $\hat{e}_\perp = \hat{e}_y(z)$ is the transverse unit vector. $\Delta_x = -U(c_{x}^\dagger c_{x})$ is order parameter, with $U > 0$ the corresponding attractive Hubbard interaction strength. The 1D SOC has been realized by the stimulated Raman transitions of two hyperfine states (which can be treated as a spin 1/2 system) of the cold atoms [51, 52, 53], so the above model is readily accessible using state-of-the-art experimental setups. Moreover, the interaction strength $U$ between the atoms could be tuned using a Feshbach resonance, which has been observed in recent experiment for spin-orbit coupled Fermi gases [51, 52].

For a single chain, the presence of the in-plane Zeeman field $V_y$ and SOC breaks the spatial inversion symmetry of the Fermi surface, leading to an FF superfluid with a finite momentum for the Cooper pairing $\Delta = \Delta_0 e^{iQ_x x}$, [51, 52]. In an appropriate parameter regime, the system could be driven to a topological FF superfluid phase which also supports MFs [51, 52]. 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, 44], similar as the proximity-induced superconductivity in solid state materials. For simplicity, in the following analysis we first assume $\Delta_x = \Delta_0$ 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 multi-chain Bogoliubov-de Gennes (BdG) equation in momentum space can be written as

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

where $h_0(k_x) = -2t \cos(k_x d) - \mu - V_z\sigma_z + \alpha \sin(k_x d)\sigma_y$ 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 $p_{k_x}$ act on the chain space and it is defined as $(p_{k_x})_{jk} = 1$ for $|j - k| = 1$ and 0 otherwise. The above BdG Hamiltonian preserves a particle-hole symmetry $\Xi H(k_x)\Xi^{-1} = -H(-k_x)$, where $\Xi = \tau_z K$ and $K$ is the complex conjugate.

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

When $V_y = 0$, Eq. [I] can be written as $H = H_s\tau_z + i\Delta\tau_y$, which preserves an additional chiral symmetry $S H(k_x)S^{-1} = -H(k_x)$, where $H_s = h_0(k_x) - t_y\rho_x$, $\Delta = i\Delta_0\sigma_y$, and $S = \tau_x$. With an auxiliary pseudo-time reversal symmetry operator defined as $\Theta = S$, 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 [18, 49]:

$$W = \frac{i}{\pi} \int_{k_x = 0}^{k_x = \pi/d} dz(k_x) = \frac{i}{\pi} (\ln(z(\pi)) - \ln(z(0))),$$

where $z(k_x) = \det(A(k_x))/|\det(A(k_x))|$ and $A(k_x) = H_s + \Delta$. As along as $W$ is non-zero, 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 only influences $h_0$ in Eq. [I] and Zeeman fields (or magnetic impurities) in $\hat{x}$ or $\hat{z}$ directions.
FIG. 1. (Color online) BdG band structure of two coupled chains with the presence of the transverse SOC. How-
ber of MFs could be any value no more than the number of chains in the transverse direction $N_y$. As increasing $t_y$, $W$ can change from 2 → 1 → 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 inter-chain coupling.

B. Effect of a transverse SOC.

To compare with the spin-independent inter-chain coupling, we here consider instead a weak SOC be-
tween the chains in the transverse direction, $H_{so}^\perp = \alpha_y/2 \sum_{\sigma} (\sigma^\dagger e_x \cdot \hat{\tau} \sigma^x \sigma^\dagger - ic_{\bar{x}} \sigma^y \sigma^\dagger + H.c.$, 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 and the system belongs to the D topological class: for even number of chains, the system is in the topologically non-trivial phase and for odd number of chains it is in the topologically trivial phase with one MF at each end. This can also be understood from the following analysis.

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

$$U H_{BdG}(k_x) U^\dagger = H(V_y)\rho_0 - \alpha_y \sigma_x \rho_z,$$  \hspace{1cm} (3)

where $U \rho_0 U^{-1} = \rho_z$.

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

$$H_{BdG} = \begin{bmatrix}
H - \alpha_y(\rho_z)_{11} \sigma_x & 0 & \cdots & 0 \\
0 & H - \alpha_y(\rho_z)_{22} \sigma_x & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots & H - \alpha_y(\rho_z)_{N_yN_y} \sigma_x
\end{bmatrix}$$

For the whole system, the particle-hole symmetry preserves with the presence of the transverse SOC. How-
ever, after the rotation, the transverse SOC term is now $H_{\alpha_y} = -\alpha_y (\rho_z)_{jj} \sigma_x$ for each transformed chain. We find that $\Xi H_{\alpha_y} \Xi^{-1} \neq -H_{\alpha_y}$, thus the particle-hole $\mathbb{Z}_2$ sym-
metry 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
FIG. 2. (Color online) The BdG quasi-particle excitation energies as a function of \( k_y \) for a 2D strip confined in the \( x \) direction with (a) a weak transverse tunneling \( t_y = 0.1t \) or (b) a weak transverse SOC \( \alpha_y = 0.2t \). Other parameters are: \( \alpha = 1.0t, V_z = 0.8t, \Delta_0 = 0.5t, V_y = 0.0 \).

FIG. 3. (Color online) The lowest three or four quasi-particle excitation energies of weakly coupled chains for (a) \( N_y = 2 \) and (b) \( N_y = 3 \) as a function of the in-plane Zeeman field \( V_y \). The number \( N \) in the shaded box represents the number of zero modes. The other parameters are \( \alpha = 1.0t, t_y = 0.3t, \mu = -2t, \Delta_0 = 0.5t, V_z = 0.8t \).

odd number of chains where the chain spin matrix \( \rho_y \) has a \( \lambda = 0 \) eigenvalue, i.e. \( \langle \rho_z \rangle_{j1} \rho_y = 0 \) 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 \( \mathbb{Z}_2 \) symmetry which supports one MF at each end \([43]\).

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 \( k_y = 0, \pm \pi \). 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 \( k_y \) 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’s no longer possible to find a chiral symmetry operator to be anti-commute with the full BdG Hamiltonian (see Eq. \( 4 \)). 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 multi-chain system when the order parameters along different chains are assumed to be identical. We plot the lowest four quasi-particle 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 multi-chain system is now of the form \( H_{\text{BdG}}(k_x) = H(V_y)\rho_0 - t_y\tau_z\rho_x \) which can be rotated in the chain space to

\[
U H_{\text{BdG}}(k_x) U^\dagger = H(V_y)\rho_0 - t_y\tau_z\rho_z, \tag{4}
\]

where \( U \rho_x U^{-1} = \rho_z \) and \( \rho_z \) is a diagonal matrix consisting of all the eigenvalues of \( \rho_z \) (Eq. \( 1 \)). The second term is nothing but an effective chemical potential \( \bar{\mu} = t_y \langle \rho_z \rangle_{j1} \) for each transformed “effective” chain (which preserves the particle-hole symmetry, breaks the time-reversal symmetry, and thus belongs to topological class \( D \) with a \( \mathbb{Z}_2 \) invariant). After the rotation in the chain space the new transformed “effective” chains are now independent. Explicitly, for a system with a number of chains \( N_y \) in the \( y \) direction

\[
H_{\text{BdG}} = \\
\begin{bmatrix}
H - t_y \langle \rho_z \rangle_{11} \tau_z & 0 & \cdots & 0 \\
0 & H - t_y \langle \rho_z \rangle_{22} \tau_z & \cdots & 0 \\
\vdots & \ddots & \ddots & \ddots \\
0 & 0 & \cdots & H - t_y \langle \rho_z \rangle_{N_yN_y} \tau_z
\end{bmatrix}
\]

As long as the transverse tunneling induced effective chemical potentials are small, the weakly coupled multi-chain system will thus have the same number of MFs as that with \( t_y = 0 \). Since the transformed “effective”
chains are independent of each other, such a system belongs to the topological class $\mathbb{Z}_2 \otimes \mathbb{Z}_2 \cdots \otimes \mathbb{Z}_2 = \mathbb{Z}_2^N$ for weak transverse tunneling.

D. Majorana flat band.

We now study the crossover of the Majorana fermion physics from quasi-1D to a real 3D system for $V_y = 0$. Assume that the 3D lattices with strictly 1D SOC are confined in the $\hat{x}$ direction. With periodic boundary conditions along the transverse directions, $k_y$ 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 $k_y$, and $-2t_\perp \cos(k_y d) - 2t_\perp \cos(k_z d)$ can be treated as a chemical potential which does not break the symmetry of the system comparing to 1D. The chemical potential $\mu$ is assumed to occupy the middle of the lower bands when the transverse tunneling $t_\perp$ is zero. We also take a Zeeman field large enough to drive the system to the topological regime for each value of $k_y$ and $k_z$. Thus, the lowest quasi-particle excitations of the uncoupled 3D lattices shows a MFs flat band $[65, 66]$. The zero energy MFs flat band persists for a small transverse tunneling $t_\perp$ (Fig. 4h). With increasing $t_\perp$, the zero energy MFs disappear first at the Brillouin zone (BZ) edges while the BZ center is still a zero energy flat band (Fig. 4i). Further increasing $t_\perp$, we see that the MFs flat band is enclosed by the bulk quasi-particle excitations, showing a configuration of 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. 4a) if the initial random order parameter is chosen to be real in the self-consistent calculation. The chiral symmetry guarantees the $\mathbb{Z}$ invariant and multiple MFs are found at each end in a quasi-1D system (here $N_y = 2$, see Fig. 5c)) 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 $t_\perp$ 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 $Q_x$ and the boundary, or the presence of edge states. As shown in Fig. 5b), we see that the order parameters for the two parallel chains are identical in the bulk but different on the boundaries. From the quasi-particle excitation spectrum (Fig. 5d), 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. 5d. 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 multi-chain 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 also to spatially inhomogeneous order param-
FIG. 5. (Color online) Effects of inhomogeneous order parameters from the self-consistent calculation. The order parameters $\Delta$ (in unit of $t$) along different chains and quasi-particle excitation energies $E_n$ (in unit of $t$) are plotted for a two-chain system ($N_y = 2$) for (a,c) $V_0 = 0.0$ and (b,d) $V_0 = 0.5t$. Only the real parts of the order parameters for the two chains are plotted in (b). The inset of (d) shows the quasi-particle excitation energies for a three-chain system ($N_y = 3$), indicating one MF at each end, where the order parameter structures are similar as (b). Other parameters are $\alpha = 2.0t$, $U = 4.5t$, $V = 1.2t$, $\mu = -2.5t$.

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