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Topological degeneracy (Majorana zero-mode) and 1+1D fermionic topological order in a magnetic chain on superconductor via spontaneous Z_2^f symmetry breaking

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We study a chain of ferromagnetic sites, ie nano-particles, molecules or atoms, on a substrate of fully gapped superconductors. We find that under quite realistic conditions, the fermion-number-parity symmetry Z_2^f can spontaneously break. In other words, such a chain can realize a 1+1D fermionic *topologically ordered* state and the corresponding two-fold *topological degeneracy* on an open chain. Such a topological degeneracy becomes the so called *Majorana zero mode* in the non-interacting limit.

I. INTRODUCTION

Recently, there has been a strong experimental and theoretical effort to search for the *Majorana zero mode*¹⁻¹⁴ (which is often wrongly and misleadingly referred to as the *Majorana fermion*). However, the Majorana zero mode is actually a feature of systems of non-interacting fermions. So, strictly speaking, the Majorana zero mode does not exist in any realistic systems where electrons interact. In fact, what people are truly interested in is not the Majorana zero mode, but *topological degeneracy*. Topological degeneracy is the ground state degeneracy of a gapped Hamiltonian system in large system size limit, which is robust against any perturbations that can break any symmetry.^{15,16} Topological degeneracy is a sign of *topological order*.^{17,18} So the search for “Majorana fermions”¹⁹ is actually the search for topological degeneracy in topological order.

Topological order is a new kind of order in gapped quantum systems that extends beyond the Landau symmetry breaking description.¹⁵⁻¹⁸ For bosonic systems, topological order can only exist in 2+1-dimensions and higher.²⁰⁻²² Bosonic topological order can lead to topological degeneracy if the system lives on a torus^{15,16} or has several disconnected boundaries.^{23,24} For fermionic systems, fermionic topological order²⁵ can even exist in 1+1D.²⁶ Such 1+1D fermionic topological order can lead to a two-fold topological degeneracy if the system lives on an open line segment.²⁶

Since fermionic systems always have a fermion-number-parity (FNP) symmetry Z_2^f which can never be explicitly broken, the above 1+1D fermionic topological order can be viewed as a spontaneous symmetry breaking order of the FNP symmetry Z_2^f (at least when the systems live on an open line segment).²⁷⁻²⁹ The above mentioned two-fold topological degeneracy is nothing but the two-fold degeneracy of the Z_2^f symmetry breaking. As a result, we can study the 1+1D fermionic topological order and its topological degeneracy on an open line using Landau symmetry breaking theory.

In this paper, we will consider a chain of ferromagnetic nano-particles or ferromagnetic molecule/atoms on

a substrate of superconductor. We find that under quite realistic conditions, the FNP symmetry breaking state can appear (or 1+1D fermionic topologically ordered state can appear), which will lead to an experimental realization of topological degeneracy. Our approach also allows us to understand the relevant energy scales: the energy splitting δE_{eo} between the states of even and odd electrons on a nano-particle, the hopping amplitude t_{ij} between nano-particles, and the Josephson coupling J_i between the superconducting substrate and the nano-particle. We also understand when the topological degeneracy can be observed at higher temperatures: (1) $|t_{ij}| \sim |J_i|$ are large, (2) $|t_{ij}| \gtrsim \delta E_{eo}$, and (3) the phase of $J_i t_{ij}^2 J_j^*$ is not zero.

Chains of magnetic nano-particles on a substrate of fully gapped superconductor have been studied theoretically by mapping the system to an effective free Majorana fermion chain.^{11,12} In this paper, we study a different parameter regime which leads to a different effective theory. Chains of magnetic iron (Fe) atoms on a substrate of superconducting lead (Pb) were recently studied experimentally in Ref. 2, where features of the Majorana zero mode was found.^{13,14}

II. THE MODEL

We will use the following effective Hamiltonian to describe a chain of magnetic dots on a substrate of fully gapped superconductor

$$H = \sum_i [t\hat{c}_{i+1}^\dagger \hat{c}_i + J\hat{c}_i \hat{c}_i + h.c.] + \sum_i \left[U(\hat{n}_i - n_0)^2 + \Delta \frac{(-)^{\hat{n}_i} - 1}{2} \right], \quad (1)$$

where \hat{n}_i is the fermion number operator and \hat{c}_i is the effective (spinless) fermion operator acting on the Hilbert space \mathcal{V}_i on site- i . \mathcal{V}_i is formed by states of n -fermions,

$n = 0, \pm 1, \pm 2$, etc and \hat{n}_i and \hat{c}_i satisfy

$$\begin{aligned} \{\hat{c}_i, \hat{c}_j\} &= \{\hat{c}_i, \hat{c}_j^\dagger\} = [\hat{c}_i, \hat{n}_j] = 0, \quad i \neq j, \\ \hat{c}_i |n\rangle &= |n-1\rangle \cdot \hat{n}_i |n\rangle = n |n\rangle. \end{aligned} \quad (2)$$

Note that the eigenvalue of \hat{n}_i can be any integer n , and \hat{c}_i is not the standard fermionic operator.

In our effective Hamiltonian (1) (see Fig. 1), Δ is the induced pairing energy on the magnetic dot. U is the effective Coulomb repulsion on the dot. The effect of chemical potential or gate voltage is summarized by n_0 . t is the electron hopping amplitude between neighboring dots and J is the Josephson coupling between the dots and the superconducting substrate. Since the dots are magnetic, the spin degree of freedom is assumed to be frozen. We also assume the dots are ferro- or anti-ferro-magnetically ordered, so that there is no spatial dependence in t .

To understand the phase diagram of the above interaction 1+1D fermionic system on an *open chain*, we may perform a Jordan-Wigner transformation

$$\hat{c}_i^\dagger = \hat{n}_i^+ \prod_{j<i} (-1)^{\hat{n}_j} \quad \hat{c}_i = \hat{n}_i^- \prod_{j<i} (-1)^{\hat{n}_j}, \quad (3)$$

where the action of these operators are as follows

$$\begin{aligned} \hat{n}_i |n\rangle &= n |n\rangle \\ \hat{n}_i^+ |n\rangle &= |n+1\rangle \\ \hat{n}_i^- |n\rangle &= |n-1\rangle \end{aligned} \quad (4)$$

Our bosonic effective Hamiltonian then takes the form

$$\begin{aligned} H = \sum_i \left[U(\hat{n}_i - n_0)^2 + \Delta \frac{(-1)^{\hat{n}_i} - 1}{2} \right. \\ \left. + (J\hat{n}_i^+ \hat{n}_i^+ + h.c.) + (t\hat{n}_i^+ (-1)^{\hat{n}_i} \hat{n}_{i+1}^- + h.c.) \right] \end{aligned} \quad (5)$$

The FNP Z_2^f transformation is generated by $(-)^{\sum_i \hat{n}_i}$, which is a symmetry of the above effective Hamiltonian.

III. THE PHASE DIAGRAM

A. Small t limit

When t is small, we can solve the one-site Hamiltonian

$$H_i = U(\hat{n}_i - n_0)^2 + \Delta \frac{(-1)^{\hat{n}_i} - 1}{2} + (J\hat{n}_i^+ \hat{n}_i^+ + h.c.)$$

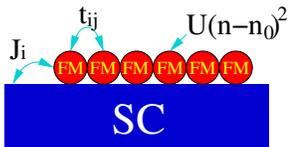


FIG. 1. The geometry of the device: a chain of ferromagnetic dots on a fully gapped superconductor.

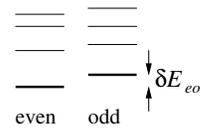


FIG. 2. The many-body energy levels on a single dot, with even and odd electron numbers.

first. Let us assume the the two lowest energy eigenstates of H_i are formed by one even-fermion state $|\uparrow\rangle$ and one odd-fermion state $|\downarrow\rangle$ (see Fig. 2). In this lowest energy subspace, H_i becomes $H_i = h_z \sigma_i^z$, where $\sigma_i^{x,y,z}$ are the Pauli matrices acting on $|\uparrow\rangle, |\downarrow\rangle$. In the subspace $|\uparrow\rangle, |\downarrow\rangle$, $(-)^{\hat{n}_i} = \sigma_i^z$ and \hat{n}_i^+ has a form $\hat{n}_i^+ = e^{i\phi} (h_x \sigma_i^x + i h_y \sigma_i^y)$, where $h_{x,y} \sim O(1)$ are real and positive. Therefore, H in eqn. (5) becomes

$$\begin{aligned} H = \sum_i \left[h_z \sigma_i^z + 2\text{Re}(t) h_x h_y (\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y) \right. \\ \left. + 2\text{Im}(t) (h_x^2 \sigma_i^y \sigma_{i+1}^x - h_y^2 \sigma_i^x \sigma_{i+1}^y) \right] \end{aligned} \quad (6)$$

We can use mean-field theory to find the phase diagram of the above spin-1/2 Hamiltonian by assuming a uniform spin order if $\text{Re}(t) < 0$:

$$\boldsymbol{\sigma}_i = \cos(\phi) \sin(\theta) \mathbf{x} + \sin(\phi) \sin(\theta) \mathbf{y} - \cos(\theta) \mathbf{z} \quad (7)$$

The corresponding average ground state energy per site is given by

$$\begin{aligned} \frac{\langle H \rangle}{N} = -h_z \cos(\theta) + 2\text{Re}(t) h_x h_y \sin^2(\theta) \\ + \text{Im}(t) (h_x^2 - h_y^2) \sin(2\phi) \sin^2(\theta) \end{aligned} \quad (8)$$

Assuming some typical values $h_x = 2/3$, $h_y = 1/3$, and $\text{Re}(t) = \text{Im}(t)$, we have

$$\frac{\langle H \rangle}{N} = -h_z \cos(\theta) + \frac{7}{9} \text{Re}(t) \sin^2(\theta), \quad \sin(2\phi) = 1,$$

and the Z_2^f symmetry breaking happens when $-\frac{\text{Re}(t)}{h_z} > \frac{9}{14}$.

We note that when t is real, the effective theory has a $U(1)$ symmetry generated by $e^{i\theta \sum_i \sigma_i^z}$, where Z_2^f is part of the $U(1)$. In this case $U(1)$ and Z_2^f symmetry breaking cannot happen when we include the quantum fluctuations beyond the mean-field theory. Even when t is complex, we still require $h_x - h_y$ to be large which requires $|J| \gtrsim |h_z|$. We conclude that Z_2^f symmetry breaking or 1+1D topological order can appear if

- (1) the electron hopping t_{ij} between dots is larger than the energy splitting $\delta E_{eo} = 2h_z$ between states of even and odd electrons on a dot,
- (2) the Josephson coupling J_i between the superconducting substrate and the dot satisfy $|J_i| \gtrsim \delta E_{eo}$,
- (3) the electron hopping amplitude t_{ij} is complex, or more precisely, the phase of the gauge invariant combination $J_i t_{ij}^2 J_j^*$ is not zero.

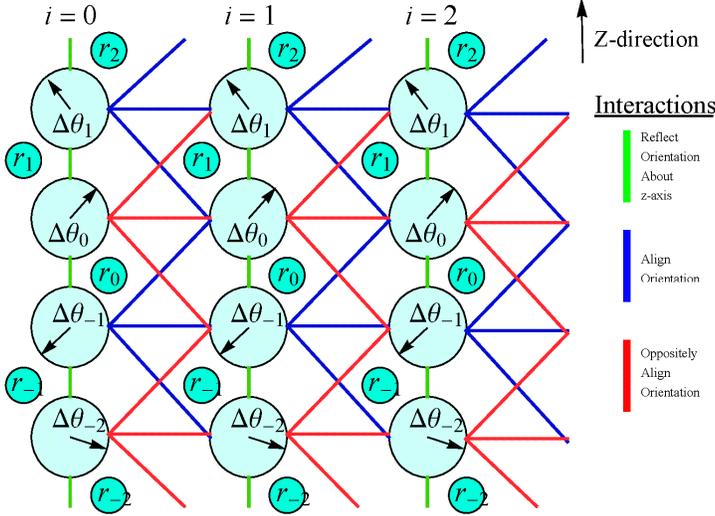


FIG. 3. Ground state energy minimization model.

Note that we can tune the energy splitting between the states of even and odd electrons to zero by tuning the gate voltage. In this case, we only require the electron hopping t_{ij} to be larger than the fluctuation of the energy splitting between even and odd states (caused by randomness). In other words, the electron hopping t_{ij} should overcome the localization effect (at the Josephson coupling energy scale).

B. Mean-field theory for generic case

In the small t limit, only two states per dot are involved. For large t , we need to use the more general model (5), where many states on each dot are included. We can also employ a mean-field approximation for the general model (5) by assuming that the trial ground state of this Hamiltonian takes the form

$$|\psi\rangle = \prod_j |\psi_j\rangle$$

$$|\psi_i\rangle = \sum_n r_n^i e^{i\theta_n^i} |n\rangle, \quad \sum_n (r_n^i)^2 = 1, \quad r_n^i \geq 0. \quad (9)$$

Since the total phase of the quantum wave function is unphysical, $|\psi_i\rangle$ is actually labeled by $(r_n^i, \Delta\theta_n^i)$ [not by (r_n^i, θ_n^i)], where

$$\Delta\theta_n^i = \theta_{n+1}^i - \theta_n^i \quad (10)$$

It is straightforward to show that this assumption gives

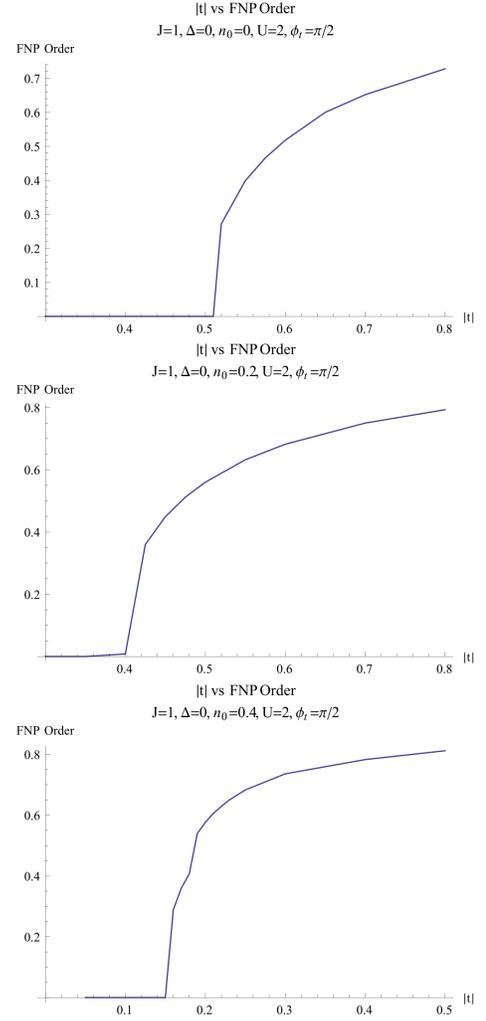


FIG. 4. For $U = 2$, $\phi_t = \pi/2$, $J = 1$, $\Delta = 0$, and $n_0 = 0, 0.2, 0.4$, we find a phase transition at $|t| = 0.5, 0.4, 0.15$ respectively.

us the following energy expectation value:

$$\langle H \rangle = \sum_{in} \left(U(n - n_0)^2 + \Delta \frac{(-1)^n - 1}{2} \right) (r_n^i)^2$$

$$+ \sum_{in} J r_{n+2}^i r_n^i \cos(\Delta\theta_n^i + \Delta\theta_{n+1}^i) \quad (11)$$

$$+ 2t \sum_{i,m,n} (-1)^n r_{n+1}^i r_{m+1}^{i+1} r_n^i r_m^{i+1} \cos(\Delta\theta_n^i - \Delta\theta_m^{i+1} + \phi_t),$$

where ϕ_t is the phase of the hopping amplitude $t = |t|e^{i\phi_t}$.

We can visualize this as in Fig. 3, a 2 dimensional classical system which extends infinitely in one direction (z -direction in the case of Fig. 3), with interactions between the $\Delta\theta$ sites, and the strength of those interactions determined by the occupation of the r sites.

We note that the model (11) has the FNP Z_2^f symme-

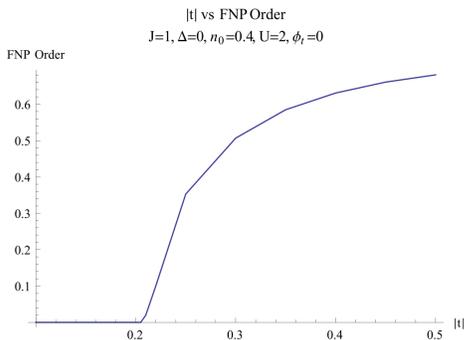


FIG. 5. For $U = 2$, $\phi_t = 0$, $J = 1$, $\Delta = 0$, and $n_0 = 0.4$, we find a phase transition at $|t| = 0.2$.

try

$$\Delta\theta_n^i \rightarrow \Delta\theta_n^i + \pi. \quad (12)$$

When $J = 0$, the model also has the fermion-number conservation $U(1)$ symmetry

$$\Delta\theta_n^i \rightarrow \Delta\theta_n^i + \phi. \quad (13)$$

If we include quantum fluctuations, a $U(1)$ symmetry cannot be spontaneously broken in 1+1D. So, when $J = 0$, the FNP symmetry Z_2^f cannot be spontaneously broken. However, when $J \neq 0$, we only have Z_2^f symmetry, which can be spontaneously broken in 1+1D. Such a Z_2^f symmetry breaking state is a 1+1D fermionic topologically ordered state, that has a topological ground state degeneracy on an open line segment. The Z_2^f symmetry breaking order parameter can be chosen to be

$$\text{FNP order} = \left(\sum_{n=\text{even}} r_n^i \right) \left(\sum_{n=\text{odd}} r_n^i \right) \quad (14)$$

Employing simulated annealing to find the ground state of equation (11) we observe phase transitions in this model. Choosing $U = 2$, $\phi_t = \pi/2$, $J = 1$, $\Delta = 0$, and $n_0 = 0, 0.2, 0.4$ (note that in terms of our energy expression 11 n_0 is defined modulo 0.5), we find a phase transition at $|t| = 0.5, 0.4, 0.15$ respectively (see Fig. 4). The Z_2^f symmetry breaking appears for large t . Also in this case, we observe that the Z_2^f symmetry breaking ground state is discrete.

Choosing $U = 2$, $\phi_t = 0$, $J = 1$, $\Delta = 0$, and $n_0 = 0.4$ (*i.e.* for real t), we can also find a phase transition at $|t| = 0.2$ (see Fig. 5). But in this case, the Z_2^f symmetry breaking ground state is not discrete and is parametrized by a phase variable ϕ . More specifically, by observing the lowest energy configurations of our simulated system we find that the lowest energy configuration for real t takes the following approximate form:

$$|\psi\rangle = \prod_j |\psi_j\rangle \quad (15)$$

$$|\psi_j\rangle = \sum_{n=\text{even}} i^n E(n)|n\rangle + (-1)^j e^{i\phi} \sum_{n=\text{odd}} i^{n+1} O(n)|n\rangle$$

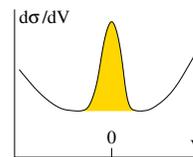


FIG. 6. The weight W of the zero-bias tunnelling peak is represented by the shaded area.

In this case, after we include the quantum fluctuation of ϕ , Z_2^f symmetry breaking will be restored. So the Z_2^f symmetry breaking observed in the real t case is an artifact of the mean-field theory and there is no Z_2^f symmetry breaking beyond the mean-field theory for $\phi_t = 0$.

IV. DISCUSSION

The Princeton group has constructed a chain of magnetic iron atoms on superconducting lead.² The iron atoms on the chain are separated by $\sim 4.2\text{\AA}$ and there is also 21\AA -period modulation in the atomic separations. The superconducting coherent length of Pb is $\xi = 830\text{\AA}$, which is much longer than the total length of the chain which is about 200\AA . So the Josephson coupling should have a non-local form $\sum_{i,j>i} J\hat{c}_i\hat{c}_j$, instead of the local form used in eqn. (1). Because of this, the results in this paper do not apply to Princeton's device. However, if the iron chain is much longer than the superconducting coherence length ξ and if the chain is formed by short segments of length ξ (which can be viewed as dots), then the chain can be viewed as coupled dots. In this case, our approach can be applied to such a system of coupled dots.

The weight W of the zero-bias tunnelling peak into an end of the chain (see Fig. 6) measures the FNP symmetry order parameter. If we can drive a zero-temperature phase transition by tuning, for example, the gate voltage V , we expect $W \sim (V - V_c)^\beta$ near the transition with $\beta = 1/8$ if there is no other gapless channel on the chain. ($\beta = 1/8$ is the critical exponent of 2D Ising transition). Such a feature can be used as a smoking gun to detect the 1+1D fermionic topological order.

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