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Topological transitions in multi-band superconductors

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ABSTRACT

The search for Majorana fermions has been concentrated in topological insulators or superconductors. In general, the existence of these modes requires the presence of spin–orbit interactions and of an external magnetic field. The former implies in having systems with broken inversion symmetry, while the latter breaks time reversal invariance. In a recent paper, we have shown that a two-band metal with an attractive inter-band interaction has non-trivial superconducting properties, if the k-dependent hybridization is anti-symmetric in the wave-vector. This is the case, if the crystalline potential mixes states with different parities as for orbitals with angular momentum l and $l+1$. In this paper we take into account the effect of an external magnetic field, not considered in the previous investigation, in a two-band metal and show how it modifies the topological properties of its superconducting state. We also discuss the conditions for the appearance of Majorana fermions in this system.

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1. Introduction

The quest for a quantum computer is one of the main challenges and goals of modern science and technology [1]. The achievement of this goal requires among other things finding the right qubits as the basic elements for quantum computation. These qubits should be robust with respect to perturbations and coupling to the environment. Serious candidates which satisfy many of these requirements are Majorana fermions [2] that should exist at the ends of one-dimensional p-wave superconductors [3–5]. The possibility of achieving induced p-wave superconductivity in a normal superconductor has been demonstrated by considering the spin–orbit interaction [5,4] in systems with broken inversion symmetry [4,6,7]. This interaction gives rise to pairing of states with the same *helicity* with the typical wave-vector asymmetry, i.e., $\Delta(-k) = -\Delta(k)$, characteristic of p-wave superconductors [4]. In a recent paper, we demonstrated a new mechanism to achieve many of the properties of spin–orbit coupled superconductors based on the hybridization of orbitals, with different parities, in neighboring sites of a centro-symmetric lattice [8]. In the present paper we investigate a two-band superconductor with asymmetric (odd parity) hybridization in the presence of a longitudinal external Zeeman magnetic field. We show how this Zeeman field gives rise to topological transitions, with linear, Dirac-like dispersion relations close to Fermi points. Furthermore we show how p-wave pairing arises naturally in this system, in the present case associated with intra-band pairing.

Hybridization is a key concept in chemistry and physics. In the former it arises from the mixing of different orbitals by the crystalline potential. This mixing can occur locally, for example, when one hybridizes plane-wave states with any of the harmonics, or among orbitals in different sites. In the latter situation, one possibility is the mixing of orbitals with different parities like those with angular momentum l and $l+1$ in neighboring sites. In this case the k-dependent hybridization becomes asymmetric in k, i.e., $V(-k) = -V(k)$ even in centro-symmetric lattices [9]. In one dimension, for example, one gets $V(k) \propto \sin ka$ with a the lattice spacing. Finally, let us mention that this case of asymmetric $V(k)$ is of great relevance for condensed matter physics as it includes the $d-p$ type of mixing, relevant for the copper oxides [10], for example, and $d-f$ mixing that encompasses many rare-earth systems, the actinides and their compounds [9,11,12].

2. Hamiltonian and methods

We consider a three-dimensional (3D) two-band metal with hybridization between the bands and an attractive interaction *only between quasi-particles in different bands* [13,14]. This situation may arise in metals where one of the bands is a narrow band with strongly repulsive interactions. In cold atom systems where the interactions can be tuned artificially this is one of possible choices. The hybridization occurs due to the mixing of different orbitals in neighboring sites by the crystalline potential and consequently it is k-dependent. Mixing in the same site involving non-orthogonal wave functions is not excluded. The attractive inter-band interaction is treated in the BCS approximation, as usual. Then the Hamiltonian reads,

$$\mathcal{H} = \sum_{k\sigma} \left(\epsilon_k^a a_{k\sigma}^\dagger a_{k\sigma} + \epsilon_k^b b_{k\sigma}^\dagger b_{k\sigma} \right) - \sum_{k\sigma} \left(\Delta_{ab} a_{k\sigma}^\dagger b_{-k-\sigma}^\dagger + \Delta_{ab}^* b_{k-\sigma} a_{k\sigma} \right) + \sum_{k\sigma} \left(V_k a_{k\sigma}^\dagger b_{k\sigma} + V_k^* b_{k\sigma}^\dagger a_{k\sigma} \right), \quad (1)$$

where $\epsilon_k^{a,b} = k^2/2m^{a,b} - \mu_{a,b}$ are the energies of the electrons in the a and b bands. In an obvious notation $a_{k\sigma}^\dagger$ and $b_{k\sigma}^\dagger$ create electrons in these bands, respectively. Notice that hybridization V_k transfers electrons with the *same* spin from one band to another (Fig. 1). The anomalous term that does not conserve the number of particles arises from a BCS decoupling of an attractive interaction, $H_{int} = -g_{ab} \sum_{k,k'} a_{k\sigma}^\dagger a_{k'\sigma} b_{-k-\sigma}^\dagger b_{-k'-\sigma}$ with $g_{ab} > 0$. Sub-dominant interactions, i.e., those that do not determine the ground state of the system are taken into account through a renormalization of the masses, such that $m^{a,b}$ can be considered as effective masses.

In spite of formal similarities [8], there is an important difference between the two-band problem with hybridization that we study in the present paper and that with spin–orbit interactions, where