Magnetic impurities in superconductor-silicene topological.

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We studied a finite sample with honeycomb lattice using the Kane-Mele model with superconductivity and local impurity. We analyzed how it affected the energies levels, the superconducting order parameter and free-energy. We also show that zero-energy mode at the end of the chain, might host Majorana’s fermion.

Abstract

We studied a finite sample with honeycomb lattice using the Kane-Mele model with superconductivity and local impurity. We analyzed how it affected the energies levels, the superconducting order parameter and free-energy. We also show that zero-energy mode at the end of the chain, might host Majorana’s fermion.

Introduction

Topological insulators are materials known to host a metallic edge state in the non-trivial topological phase. The Kane-Mele model is an example of a topological insulator with honeycomb lattice and spin-orbit coupling [1]. This model has been drawing attention, as interesting materials like silicene may hold unusual properties. In 2013, it was showed that silicene may have an induced superconducting state at the metallic edge states when doped [2].

We also know that Majorana’s fermions might appear in systems with spin-orbit coupling and superconductivity, this combined with superconductivity in the edges makes silicene an interesting place to search for Majorana’s fermion in impurities chains localized at the edges.

In this work we study a finite sample of honeycomb lattice with a 10 atoms impurity chain at a zigzag edge. We proceed to analyze how doping and the impurity magnetic strength affects the existence of Majorana’s fermion.

Methods and Results

We used the Kane-Mele Hamiltonian (\(\mathcal{H}_{KM}\)), for spin-orbit coupling in honeycomb lattice. A magnetic impurity term in the xy plane (\(\mathcal{H}_{Imp}\)), similar to Zeeman splitting, and a superconducting term (\(\mathcal{H}_{SC}\)), with the total Hamiltonian being the sum of those three \(\mathcal{H} = \mathcal{H}_{KM} + \mathcal{H}_{SC} + \mathcal{H}_{Imp}\).

\[
\mathcal{H}_{KM} = t \sum_{\langle i,j \rangle} c_{i,\sigma}^\dagger c_{j,\sigma} + \lambda_\sigma \sum_{\langle i,j \rangle} \sigma \cdot \mathbf{e}_\sigma \langle c_i \sigma c_j \sigma^\dagger \rangle + \lambda_\nu \sum_i \xi_i c_{i,\sigma}^\dagger c_{i,\sigma} - \mu \sum_i c_{i,\uparrow}^\dagger c_{i,\downarrow},
\]

\[
\mathcal{H}_{SC} = -U \sum_i c_i^\dagger \sigma c_i \sigma c_i^\dagger \sigma c_i \sigma,
\]

\[
\mathcal{H}_{Imp} = \sum_{i \in \mathcal{I}} J_{Imp} (\mathbf{n}_i \cdot \mathbf{\varepsilon}_\sigma) \langle c_i \sigma \rangle \langle c_i \sigma^\dagger \rangle,
\]

with \(c_{i,\sigma}\) the destruction operator in the site \(i\) with spin \(\sigma\), \(t\) the hopping term, \(\lambda_\sigma\) the spin-orbit coupling, \(\nu_{ij} = (\mathbf{d}_i \times \mathbf{d}_j)_\sigma = \pm 1\) with \(\mathbf{d}_i\) the unitary vectors that connects site \(i\) with site \(j\). \(\lambda_\nu\) is the rasba term and \(\lambda_\sigma\) is an onsite energy with a weight \(\xi_i = \pm 1\) that depends from the sublattice, +1 for sublattice A and -1 for sublattice B and \(\mu\) is the doping. \(U\) is the coupling strength, \(V\) and \(J\) is the strength of the nonmagnetic impurity magnetic strength, \(V\) and \(J\) is the strength of the magnetic impurity in xy-plane and \(s\) is a vector of Pauli matrices associated with spin.

In this work we used a 400 atoms array with 20 atoms at the zigzag edge and 20 atoms at the armchair edge. We considered a 10 atoms impurity chain at the middle of zigzag edge, as shown in the figure below. We also considered the magnetic alignment of impurities rotates from one impurity to the next of a value of \(\theta + \pi\).

\[\text{Figure 1. Sample configuration}\]

To calculate the superconducting term, we used a mean-field approximation, \(\Delta_i = -U c_i \langle c_i \mu, c_i \mu^\dagger \rangle\), and calculated \(\Delta_i\) selfconsistently. All results were done for zero-temperature, \(\lambda_\sigma = 0.5\) t. i.e. a strong spin-orbit regime, no staggering potential, \(\lambda_\nu=0\) and no Rashba coupling \(\lambda_\sigma=0\).

We studied for each \(J\) and \(\mu\) which value of \(\theta\) minimized the difference of free-energy between the superconducting state (\(\Omega_{SC}\)) and the normal state (\(\Omega_N\)). Figure below shows which \(\theta\) minimizes for \(J=1.8t\) and different dopings. A negative value
Table 1. Phase diagram

<table>
<thead>
<tr>
<th>( \mu )</th>
<th>1.45</th>
<th>1.55</th>
<th>1.65</th>
<th>1.75</th>
<th>1.85</th>
<th>1.95</th>
<th>2.05</th>
<th>2.15</th>
<th>2.25</th>
<th>2.35</th>
<th>2.45</th>
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<th>2.75</th>
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<td>-0.93</td>
<td>-0.70</td>
<td>-0.73</td>
<td>-0.77</td>
<td>-0.80</td>
<td>-0.80</td>
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<tr>
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<td>-0.63</td>
<td>-0.67</td>
<td>-0.67</td>
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<td>-0.70</td>
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<tr>
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<td>-0.43</td>
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<td>-0.50</td>
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<td>-0.40</td>
<td>-0.40</td>
<td>-0.40</td>
<td>-0.47</td>
<td>-0.47</td>
<td>-0.47</td>
<td>-0.47</td>
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</tr>
<tr>
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<td>-0.33</td>
<td>-0.30</td>
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<td>-0.23</td>
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<td>-0.43</td>
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<td>0.30</td>
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<td>0.30</td>
<td>0.30</td>
<td>0.30</td>
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<td>0.37</td>
</tr>
<tr>
<td>0.7</td>
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<td>0.37</td>
<td>0.37</td>
<td>0.40+</td>
<td>0.40</td>
<td>0.40</td>
<td>0.40</td>
<td>0.37</td>
<td>0.40+</td>
<td>-0.27</td>
<td>-0.27</td>
<td>-0.23</td>
<td>0.40</td>
</tr>
</tbody>
</table>

means the impurity chains rotates clockwise and a positive value means it rotates anti-clockwise.

Figure 2. Free-energy

Next, we calculated the Majorana number \( \mathcal{M} = P_f(\mathcal{H}) \), using [3], for the \( \theta \) that minimized the difference in free-energy. Table 1, above, show distinct phases of the sample depending on the color. Green and yellow have \( \mathcal{M} = +1 \), red and blue have \( \mathcal{M} = -1 \) showing the existence of Majorana's fermion. The difference in color are to highlight the different rotations showed by the value of \( \theta \) inside the cell.

Cells marked with (*) means that exists another \( \theta' \) that also minimizes the free-energy, inside our computation error, and have a Majorana number different from the one showed in the table, as it can be seen it happens in zones that have a transition.

Discussion

In this work we saw that impurity chains at zigzag edge may form a spiral magnetic chain that depending upon the parameter may or may not host Majorana's fermion. However, this system might not be good for experimentalists as many impurity states have near zero-energy. Finite effects due to small size of the chain can contribute to this difficult in LDOS, even allowing Majorana's from different ends to interact themselves.

We also note that the same procedure was done to the armchair edge, however no Majorana was found, this is due the peculiarities of the armchair in comparison to zigzag.

Acknowledgments

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1. C. L. Kane and E. J. Mele Phys. Rev. Lett, 2005 95(22),