Topologically protected mid-gap states induced by impurity in one-dimensional superlattices

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Received 13 August 2013, revised 18 January 2014
Accepted for publication 31 January 2014
Published 26 February 2014

Abstract

Based on the discovery of the nontrivial topological properties of one-dimensional superlattices, we show that mid-gap states emerge in such systems induced by a single on-site impurity. Besides the trivial bound state located at the impurity site, these mid-gap states are localized at the adjacent sites of the impurity in the limit of a strongly attractive/repulsive impurity potential, behaving as edge states under open boundary conditions and thus carrying the information of topological properties. This feature makes it possible to reveal the topological properties of superlattices via the impurity effect and to realize the adiabatic pumping between the opposite sides of the impurity in setups of one-dimensional optical lattices or photonic crystals.

Keywords: superlattice, impurity, mid-gap state

(Some figures may appear in colour only in the online journal)

1. Introduction

In recent years, due to the very fast development of cold atom techniques \([1, 2]\), quantum simulation of topological insulators has been attracting more and more attention experimentally and theoretically \([3–7]\). However, while most of the studies mainly focus on the two- or three-dimensional topological systems, one-dimensional (1D) topological insulators are less investigated besides some well-known models, like the Su–Schrieffer–Heeger model \([8]\), Kitaev–Majorana chain \([9]\), Creutz ladder \([10]\) etc. Recently, the discovery of the topological properties of 1D superlattices \([11, 12]\) adds a new member to this family. Because of the realization of quasiperiodic potentials (Aubry–André model \([13]\)) via incommensurate superlattices both in cold atoms \([14, 15]\) and photonic crystals \([12]\), it paves the way for studying the topological properties of 1D superlattices, to date including topological phase transitions \([16, 17]\), fractional topological states \([18]\), Z\(_2\) topological insulators \([19, 20]\), topological Mott insulators \([21, 22]\) and even topological superconductors \([23–27]\).

As it is known that the detection of the topological edge states needs open boundaries of the system \([28, 29]\), in cold atom experiments, the confining harmonic trap blurs such boundaries making the edge states not obvious \([30]\). Goldman et al raise a proposal to detect the chiral edge states in two-dimensional systems using Bragg spectroscopy sensitive to the angular momentum \([31]\). To demonstrate the nontrivial topological properties of the 1D superlattices, several proposals have been given, such as detecting plateaus in the density profile subjected to a harmonic trap in cold atoms \([11]\) and the direct observation of the localized edge states using photonic waveguides \([12]\). In this paper, we study the effect of the impurity potential on the topologically nontrivial 1D superlattices and find that a single on-site impurity can induce mid-gap states. It is interesting that the topologically nontrivial mid-gap states are localized next to the impurity in the limit of the large impurity potential, behaving as the...
edge states under open boundary conditions (OBCs). But these states will not be blurred by the confining trap and may be more easily detected in the interior of the system than the edge states at the boundaries. The pumping of these mid-gap states can also be realized between the opposite sides of the impurity. By the technique of the spatially resolved radio-frequency spectroscopy (SRRFS) [32], the local density of states (LDOS) can be measured directly. Therefore, the impurity supplies an alternative way to study the topological properties of the 1D superlattices.

The paper is organized as follows. After this brief introduction, we introduce the mid-gap states induced by a single on-site impurity in 1D spinless fermionic superlattices and show the relationship of these states to the Z-type topological properties possessed by such superlattices. Then, the behaviour of the mid-gap states can be used to show experiment the topological properties of the superlattices by the technique of the SRRFS in cold atoms to detect the LDOS within the harmonic trap. The similar discussion can be easily generalized to the spin-1/2 case and the relationship between the opposite sides of the impurity. At last, a summary is given.

2. Z-type topological insulators with a single on-site impurity

Firstly, we concentrate on 1D tight-binding superlattices for spinless fermions with L sites, among which the on-site potential is periodically modulated and a single impurity potential is introduced on the site of i = 0. The Hamiltonian is as follows:

\[
H = -t \sum_i (\hat{c}_i^\dagger \hat{c}_{i+1} + \text{H.c.}) + \sum_i V_i \hat{n}_i + F \hat{n}_0, \tag{1}
\]

where \(\hat{c}_i^\dagger (\hat{c}_i)\) is the creation (annihilation) operator for spinless fermions at site \(i\) and \(\hat{n}_i = \hat{c}_i^\dagger \hat{c}_i\) is the particle-number operator. \(t > 0\) is the hopping amplitude and set to be the unit of energy, \(V_i = V \cos(2\pi ax_i + \delta)\) is the on-site modulated potential with \(V\) being the strength, \(1/a\) the periodicity and \(\delta\) the arbitrary phase shift. The lattice constant, \(a\), is taken to be 1 in the following for convenience. \(F\) is the potential of the impurity. Without the loss of generality, we choose an odd number of sites and put the impurity at the centre \((i = 0)\) of the chain in the following discussion.

Without the modulation, there is only one bound state which is exactly localized at the impurity site with its energy lower \((F/t < 0)\) (figure 1(a)) or higher \((F/t > 0)\) (figure 1(b)) than those of the scattering states. After the modulation is turned on, besides the trivial bound states, some states, which are also localized, emerge within the bulk gaps. However, they are not localized right at the impurity site but on the ones next to it (figure 2). Here and hereafter, in order to focus our attentions on these mid-gap states, we adopt periodic boundary conditions instead of OBCs to prevent the emergence of edge states. Because behaviours in cases of \(F/t > 0\) and \(F/t < 0\) are similar except for the trivial bound state above or below the top or bottom of the energy bands, we only discuss the \(F/t < 0\) case below.

Previous studies [11, 12] have shown that the family of 1D superlattices in the absence of the impurity is topologically nontrivial, which is clearly demonstrated from the fact that by adiabatically changing the phase shift \(\delta\) under OBCs, the energies of the edge states will connect the upper and lower bulk bands, and thus these states can be pumped from one end of the chain to the other. A Z-type topological invariant, Chern number [33, 34], can be defined for the \(n\)th band in the \((k, \delta)\) space under PBCs, i.e.,

\[
C_n = \frac{1}{2\pi} \oint_{\delta = \text{const}} \frac{d\delta}{2\pi} \oint_{k = \text{const}} \delta \partial_k [\hat{A}_{n,k} - \hat{A}_{n,k}],
\]

where \(\hat{A}_{n,k} = \text{Re} (\phi_n(k, \delta)) \partial_k \phi_n(k, \delta)\) (\(s = \delta, k\)), \(k\) is the quasimomentum and \(\phi_n(k, \delta)\) is the Bloch wavefunction for the \(n\)th band of the Hamiltonian with fixed \(\delta\). Now let us turn on the impurity and we find that the energies of the emergent mid-gap states also vary with \(\delta\) (figures 3(a) and (e)). As the strength of the impurity potential, \(F\), increases, these states become more and more localized at the adjacent sites of the impurity and their energies with respect to \(\delta\) gradually connect the upper and lower bulk bands, behaving like the energies of the edge states under OBCs (figure 3(e)). The main difference is that the mid-gap states do not transfer from one edge to the other, but from one side of the impurity to the other, when \(\delta\) is tuned. Furthermore, we also find that the number of touches to the lower (or higher) band is equal to the Chern number of the bulk gap, i.e., the summation of the Chern numbers of the bands below the Fermi surface, so we can deduce the Chern numbers experimentally from how many circles (one circle means the mid-gap state transfers from one side of the

Figure 1. The single-particle eigenenergies in ascending order with (a) an attractive \((F = -5t)\) or (b) a repulsive \((F = 5t)\) impurity located at the centre \((i = 0)\) of the 1D tight-binding chain without modulation under PBCs. The insets are density profiles (or probability distributions) of the bound states labelled by blue stars, which are localized at the impurity site with energies (a) lower or (b) higher than that of the scattering continuous. Here, we do the calculation with \(L = 201\) sites.
Figure 2. For the attractive ($F = -5t$) (a)–(d) and the repulsive ($F = 5t$) (e)–(h) impurities with the periodic modulation, $\alpha = 1/3$, the eigenenergies with the mid-gap states labelled by coloured triangles are shown in ascending order. The corresponding density profiles (b)–(d), (f)–(h) of the mid-gap states in the same colour demonstrate the ways of localization on one side of the impurity or at the impurity site. The other parameters are chosen as $L = 201$, $V = 0.5t$, $\delta = \pi/4$ under PBCs.

Figure 3. The eigenenergies versus $\delta$ with a single impurity of a weaker ($F = -3t$) (a)–(d) and a stronger ($F = -10t$) (e)–(h) on-site potentials under the periodic modulation, $\alpha = 1/3$. The mid-gap states are labelled by coloured dots, which tend to connect the upper and the lower bulk bands and to be localized on one side of the impurity in the strong limit of impurity potential. The corresponding density profiles show some specific points of $\delta$s to demonstrate the transfer from one side to the other. The other parameters are chosen as $L = 201$, $V = t$ under PBCs.

Impurity to the other and then transfers back) the mid-gap state transfers as $\delta$ is tuned within a period $[0, 2\pi]$, e.g. in figure 3, the one circle of transfer shows that the Chern number is $\pm 1$ for the two bulk gaps.

To understand this phenomenon, the impurity can be regarded as a kind of boundary, which resembles the open boundaries for the large impurity potential with both boundaries being connected through the impurity. Therefore, all topological properties demonstrated by edge states under OBCs also hold for the mid-gap states localized near the impurity. These states are topologically protected [12, 35] and thus robust against small perturbations. More importantly, they are distributed within a small space around the impurity, which is helpful to the experimental detection, not like the edge states, the signal of which is weakened by the external traps. Therefore, the introduction of impurity provides an alternative tool to investigate the topological properties of the superlattices instead of directly detecting the edge states under OBCs.
Figure 4. LDOS for spinless fermions with a single impurity of a strong on-site potential \((F = −10t)\) within a slowly varying harmonic trap \((V_h = 0.0005t)\). The mid-gap states in the bulk gaps are transferred from one side of the impurity to the other by tuning the phase shift, \((a) \delta = \pi/3, (b) \delta = 2\pi/3, (c) \delta = \pi. \) Here we take \(\sigma = 1/3, L = 201, V = t.\)

3. Detection of mid-gap states in cold atoms

To realize the superlattice Hamiltonian (1) in cold atoms \([14, 15]\), an atomic Fermi gas is firstly loaded into a primary 1D optical lattice potential \(V_1(x) = V_1\cos^2(k_1x)\) with the wave number \(k_1\) and the strength \(V_1\), then a secondary optical lattice potential \(V_2(x) = V_2\cos(k_2x + \delta)\) with the wave number \(k_2\) and the strength \(V_2\) is superimposed on the primary one as a weak perturbation if \(V_1 \gg V_2\). In the framework of the tight-binding approximation, the primary and the secondary optical lattices mainly contribute to the hopping term and the periodically modulated on-site term of the Hamiltonian (1), respectively, as the second lattice shifts the energies in a small range of size but does not change substantially the position of the minima [36]. Here \(\alpha = k_2/k_1\) can be tuned by the wave numbers of the two sets of optical lattices and \(\delta\) is the overall relative phase shift between them [36, 37].

In cold atom experiments, the observation of edge states is difficult due to the existence of a harmonic trap for confining the Fermi gases, which weakens the boundaries and reduces particle densities at both wings of the trap. In the previous section, we show that the impurity can induce mid-gap states, resembling edge states under OBCs in the superlattices without impurity. These states also reflect the topological information of the superlattices and they are localized only in a small space, overcoming the negative effect of the harmonic trap. So the introduction of an impurity in the centre of the harmonic trap is helpful for the detection of the topological mid-gap states in the interior, instead of the boundary of the system, as the impurity-induced mid-gap states have more notable signatures than edge states blurred by the presence of the harmonic trap. To see this, we calculate the LDOS in Lehmann representation at the zero temperature,

\[
\rho(i, \omega) = \sum_n [(|G|c|n\rangle)^2 \delta(\omega - \omega_{n0}) + (|G|c\dagger|n\rangle)^2 \delta(\omega + \omega_{n0})],
\]

(2)

where \(\omega_{n0} = E_n - E_0\) with |\(G\) and |\(n\) being the ground state with energy \(E_0\) and the \(n\)th excited state with energy \(E_n\), respectively. Figure 4 shows the LDOS after adding the harmonic trap term, \(H_h = V_h\delta^2\) with \(V_h\) being the strength of the trap. It is shown that as \(\delta\) is tuned, the mid-gap states are firstly localized on one side of the impurity, then merge into the bulk bands becoming extended and are finally transferred to the other side of the impurity. This quantity can be directly measured experimentally by SRRFS [32]. In [32], the spatial resolution of imaging is about 1.4 \(\mu\m\). However, the common lattice constant is in the order of several hundred nanometers, e.g., the wavelength of the laser beams to generate the optical lattices in [38] is 852 nm. Therefore, if we want to detect the signals of the mid-gap states localized near the impurity, the resolution should be improved at least by one order of magnitude. Alternatively, because our results can be easily generalized from one single impurity into several ones (which can be regarded as a large impurity) doped in the centre of the chain, the mid-gap states will be localized at the sites next to the outermost impurity if the potential of the ‘large’ impurity is strong enough, and thus the current resolution is expected to be able to detect such mid-gap states.

4. \(Z_2\)-type topological insulators with a single on-site impurity

For spin-1/2 fermions, a secondary spin-dependent optical lattice is added with the form of \(V_\sigma(x) = V\cos(2\pi\alpha x + \sigma\delta)\), where \(\sigma = 1(\uparrow)\) or \(-1(\downarrow)\) representing spin-up or spin-down components, respectively. This kind of potential can be implemented by two counter-propagating laser beams with linear polarizations forming an angle 2\(\delta\) [39, 40]. Hamiltonian (1) can be easily generalized to the spin-dependent one by just replacing the spinless operators (\(\hat{c}_i, \hat{c}^\dagger_i, \hat{n}_i\)) and potential (\(V_i\)) by corresponding spin-dependent ones (\(\hat{c}_i^\sigma, \hat{c}^\dagger_i^\sigma, \hat{n}_i^\sigma\), \(V_i^\sigma\)) yielding

\[
H = -t \sum_{\sigma} (\hat{c}_i^\sigma \hat{c}_{i+1, \sigma} + \text{H.c.}) + \sum_{\sigma} V_i^\sigma \hat{n}_i^\sigma + F \sum_{\sigma} \hat{n}_0^\sigma.
\]

(3)
where $V_{\sigma} = V \cos(2\pi \alpha i + \sigma \delta)$. From the same procedure as in the spinless case, without the impurity, this generalized 1D spin-dependent superlattice has been proposed to simulate the quantum spin Hall effect with $Z_2$-type topological properties [19]. Likewise, a spin-dependent Chern number can be defined in the $(k, \delta)$ space under PBCs as $C_{i,\alpha,n} = \frac{1}{i} \int_{0}^{2\pi/\delta} dk \int_{0}^{2\pi} d\delta [\partial_k A_{i,\alpha,n} - \partial_\delta A_{i,\alpha,n}]$ with the spin-dependent Berry connection $A_{i,\alpha,n}$ and the Bloch wavefunction $\phi_{i,\alpha}(k, \delta)$ for fixed $\delta$. Using these spin-dependent Chern numbers, a total $Z_2$ topological invariant is constructed as $\nu_i = (C_{i,\alpha,n} - C_{i,\alpha,n})/2$, which can be used to characterize the $Z_2$-type topological properties. In principle, this formalism is also applicable to spin–orbit superlattice systems where the total spin is no longer conserved. The only change of these definitions for the topological invariants is to replace the Bloch wavefunctions for fermions with spins by those for quasi-fermions with pseudospins, which mix the spin-up and spin-down fermions with helicity conserved. As long as the bulk gap is not closed, the topological properties of the system cannot be changed.

When the impurity is embedded, due to the presence of the spin-dependent potential, it is possible for the system to possess both kinds of fermions simultaneously localized on one side or both sides of the impurity. From the form of the potential, it is easy to prove that the spectra for spin-up and spin-down components are symmetric with respect to $\delta = \pi$ within the interval $\delta \in [0, 2\pi]$. In principle, one can always translate the whole potential by a phase $\delta_0$, i.e., $V_{\sigma} = V \cos(2\pi \alpha i + \sigma \delta - \delta_0)$. Consequently, the spectrum for spin-up (down) will be shifted by $\delta_0$ to the right (left) along the $\delta$-axis. By tuning the whole phase $\delta_0$ and the relative phase $\delta$, one can manipulate the emergence of the mid-gap states on one side or on both sides of the impurity simultaneously or non-simultaneously. For example, without the phase difference of the two components, i.e., $\delta = 0$, the whole spectrum is doubly degenerate and the mid-gap states are always localized on the same side of the impurity for any $\delta_0$. Another case is that one can always make the spectrum for each component mirror symmetric with respect to $\delta = \pi$ by tuning $\delta_0$, e.g. $\delta_0 = \pi/6$ for the case of $\alpha = 1/3$. Thus, the whole spectrum is doubly degenerate for all $\delta$s with mid-gap states of different spins simultaneously localized on the opposite sides separately. Fine tuning both phases, we may obtain much richer physics. Here, we mainly demonstrate the physics of the latter with $\delta_0 = \pi/6$ for the case of $\alpha = 1/3$ to make the whole spectrum mirror symmetric. Within the same harmonic trap independent of spins in cold atom experiments as the spinless one, one can also measure the LDOS for each spin using the SRRFS. As $\delta$ changes, the positions of spin-up and spin-down mid-gap states will be exchanged (figure 5).

5. Photonic crystals and the adiabatic pumping

Following the experiment of detecting and pumping edge states in photonic crystals [12], a similar setup can be used to detect and pump the mid-gap states after adding the impurity in the centre. In the experiment, the superlattice can be implemented by a set of coupled single-mode waveguides and the propagating light can hop between the neighbouring waveguides. The on-site and the hopping terms can be controlled by the refraction index of the waveguides, which can be effectively tuned by changing the width of the waveguides and the spacings between them, respectively. The propagating direction can be used to detect the adiabatic evolution of the injected light with the adiabatic tuning of $\delta$. In this setup, a harmonic trap is not needed and the on-site impurity can be
generated by tuning one waveguide’s refraction index different from those of others. Therefore, the above phenomena of the mid-gap states may also be observed in this photonic crystal setup. If a light is injected into the waveguide nearest to the impurity, a localized or an extended light signal would be observed depending on the value of $\delta$.

To realize the adiabatic pumping of the mid-gap states, it is more convenient to use the ‘off-diagonal’ version of the on-site modulated superlattices [12], which has similar topological properties as the on-site one, because the control of the waveguide spacings along the propagating direction is easier than that of the width of the waveguides to change the refraction index. The Hamiltonian is as follows:

$$H = -\sum_i \left[ (t + t_i) c_{i+1}^\dagger c_i + H.c. \right] + \mathcal{F} \hat{n}_0,$$

where $t_i = V \cos(2\pi\alpha i + \delta)$ and $t$ is set to the unit of energy. To realize the adiabatic pumping in this ‘off-diagonal’ version of superlattices, the propagating axis is used to mimic the change of $\delta$ by slowly varying the spacings of the waveguides along this axis. As the injected light propagates in the waveguides, the hopping strength controlled by $\delta$ varies. Figure 6 shows the spectrum of the Hamiltonian (4) with respect to $\delta$. If a light is injected into the waveguides right-nearest to the impurity at $\delta = 0.5\pi$ in the beginning, it will be localized at this site. As the light propagates, $\delta$ is changed along the propagation direction. Consequently, the light is expanded to other sites at $\delta = \pi$ and localizes on the left side of the impurity at $\delta = 1.5\pi$. Through this process, it is possible to pump the mid-gap states from one side of the impurity to the other.

**6. Summary**

In summary, we show that a single on-site impurity can induce mid-gap states in the 1D topologically nontrivial superlattices. In the limit of the strong impurity potential, these states will be localized next to the impurity and behave like the edge states under OBCs. Based on this character of the mid-gap states, we propose an alternative scheme to detect the topological properties (e.g. Chern numbers) of the 1D superlattices. In cold atom experiments, we calculate the LDOS for the SRRFS measurement to demonstrate the localization and the transfer of the mid-gap states for the spinless and spin-1/2 fermions. Alternatively, the scheme of the photonic crystal is also proposed to demonstrate the feature of these states and can be used to realize the adiabatic pumping.

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