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Study of finite femionic chains with edge modes using an appropriate momentum representation

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This work is based on the Su-Schrieffer-Heeger model, which describes a system of non-interacting polarized fermions, *i.e*. without spin, moving in a one-dimensional optical superlattice with fixed boundary conditions. Starting from the Hamiltonian of the system in second quantization, in which the optical lattice has discretized the space, and taking into account that the basis that diagonalizes the kinetic energy is the one of momentum, we perform the discrete sine transform type-I, which respects the hard-wall boundary conditions of the system and allows us to express our Hamiltonian in the momentum basis, in such a way that we can think that it is possible to extend the study to an arbitrary number of sites. Finally, we apply the Bogoliubov-de Gennes formalism getting the dispersion relation and the bare vertex function where together they form the couplings matrix. By diagonalizing this matrix, we visualize the parameter set where the system hosts zero-energy modes.

Keywords: Su-Schrieffer-Heeger model; spinless fermions; optical lattices; Bogoliubov-de Gennes formalism.

Este trabajo esta basado en el modelo Su-Schrieffer-Heeger, el cual describe un sistema de fermiones polarizados no interactuantes, *i.e.* sin espín, moviéndose en una superred óptica unidimensional con condiciones fijas de frontera. Empezando con el hamiltoniano del sistema en segunda cuantización, en la cual la red óptica ha discretizado el espacio, y teniendo en cuenta que la base que diagonaliza la energía cinética es la de momento, aplicamos la transformada discreta seno tipo I, la cual respeta las condiciones fijas del sistema y nos permite expresar nuestro hamiltoniano en la base de momento, de tal forma que nos deja pensar que es posible extender el estudio del sistema a un número arbitrario de sitios. Finalmente, aplicamos el formalismo de Bogoliubov-de Gennes obteniendo la relación de dispersión y la función de correlación irreducible de una partícula, las cuales forman la matriz de acoples. Diagonalizando dicha matriz de acoples, se logra visualizar el conjunto de parámetros para el cual el sistema presenta modos de energía cero.

Descriptores: Modelo Su-Schrieffer-Heeger; fermiones sin espín; redes ópticas; formalismo de Bogoliubov-de Gennes.

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1. Introduction

Nowadays, the realization of the quantum computer has awakened a great scientific interest [1]. A quantum computer [2] is basically a physical system that can storage and process a big quantity of information based on one of the fundamental principles of quantum mechanics, the superposition principle [3]. The whole formalism is developed in terms of quantum bits or qubits. A qubit is the coupling of two isolated quantum states; it can be exemplified by considering the coupling between a ground-state and an excited state of a certain atom, which makes it an ideal tool to storage information [4]. Nevertheless, that coupling is not totally convenient because of the finite time of coherence of those states, what causes the information to be lost in time. Several alternatives have been proposed in the field of topological systems, either superconductors [5] or insulators [6–8], whose experimental simulations are feasible in the field of ultracold matter [9,10]. Ultracold atoms are between the intersection of many fields of physics like quantum information, quantum optics, condensed matter, statistical mechanics and non-linear physics, with a strong contribution from the numerical methods [11].

Atoms at temperatures of the order of 10^{-9}K, charged in optical lattices, are quantum simulators that can reproduce physical systems of condensed matter among other fields of physics. The periodic confinement is carried out by counter propagating lasers and magneto-optical traps emulating in this way, the crystalline lattice. In this direction, highly controllable physical systems can be studied and characterized with different theoretical methods [12, 13].

In particular, the present work focuses on the study of the Su-Schrieffer-Heeger (SSH) model [14], which is based on the tunneling of polarized fermions through periodic wells with different probability amplitudes and absence of interactions, making it one of the simplest models that presents edge states with non-trivial topology [15]. We introduce and describe the model in Sec. 2. It is convenient to work out the model in the momentum space; for this purpose, the discrete sine transform type I is used, which preserves the hard-wall boundary conditions that the problem satisfies. It is desirable to be able to analyze the excitation spectrum of the Hamiltonian for this one-dimensional finite lattice. To obtain such spectrum, we propose to work in the frame of the Bogoliubov-de Gennes formalism [16] described in Sec. 3. This is an analytic technique that allows us to decouple the states associated with each internal degree of freedom of the system in the momentum space, such that it is possible to identify under what parameters the system shows zero energy modes, besides allowing a proper writing of the Hamiltonian. In this way, it is easier to obtain the excitation spectrum of

the system, as well as obtaining the numerical solution at low computational cost, being able to extend the study of the system to an arbitrary number of sites.

In Sec. 3, we also present and discuss the results of the excitation eigenvalues for the relevant cases: trivial and topological regimes, the later hosting the zero energy modes. Section 4 is devoted to the conclusions and perspectives of the present work.

2. The SSH model

The Su-Schrieffer-Heeger model, better known as the SSH model [14], was originally proposed in 1980 to describe the behavior of electrons in polymers. Nevertheless, it became widely used as the simplest model in which topological nontrivial phase transitions may occur. The Su-Schrieffer-Heeger model [17] describes polarized fermions, *i.e.* without spin, moving in a one-dimensional chain with staggered hopping amplitudes. The chain (superlattice) consists of N unit cells, each one hosting two sites, one in sublattice A (filled circles), and one in sublattice B (empty circles) as shown in Fig. 1.

Since non-interacting fermions are analyzed, the system is described by the Hamiltonian of a free particle with alternated amplitude probabilities such as

$$\hat{H} = -v \sum_{m=1}^{N} \left(|m,B\rangle\langle A,m| + h.c.\right) - w \sum_{m=1}^{N-1} \left(|m+1,A\rangle\langle B,m| + h.c.\right), \qquad (1)$$

where $|m,\alpha\rangle = \hat{a}^{\dagger}_{m,\alpha}|\oslash\rangle$ with $m \in 1,2,...,N$ and $\alpha \in \{A,B\}$; $\hat{a}^{\dagger}_{m,\alpha}$ creates a particle in the unit cell m and sublattice α, $|\oslash\rangle$ is vacuum or absence of particle and $h.c.$ stands for the hermitian conjugate. For simplicity, we take the hopping amplitudes to be real and nonnegative, $v, w \geq 0$.

The configuration of one particle per unit cell, known as half-filling, is characteristic of the simplest insulators such as polyacetylene, where each carbon atom brings one conduction electron, and so we find one particle per unit cell [15].

The SSH model becomes very simple when the values of the staggered amplitudes are extreme, setting, for example, the intracell hopping to 1 ($v = 1$) while the intercell hopping is set to zero ($w = 0$) or vice versa. In both cases, the SSH chain falls apart to a sequence of unbounded cells, as shown in Fig. 2.

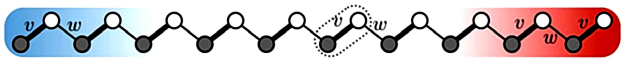

FIGURE 1. Geometry of the SSH model. Filled circles are sites on sublattice A and empty circles are sites on sublattice B, each cell hosting a single fermion, as depicted: the n=6th cell is circled by a dotted line. Hopping amplitudes are staggered: intracell hopping v (thick lines) is different from intercell hopping w (thin lines). The left and right edge regions are indicated by blue and red shaded backgrounds [15].

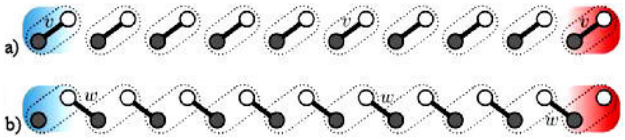

FIGURE 2. Fully disconnected cells limits of the SSH model, where the chain has fallen apart to disconnected dimers. a) For the trivial case (only intracell hopping v), every energy eigenstate is an even or an odd superposition of two sites at the same unit cell. b) In the topological case (only intercell hopping w), dimers are between neighboring unit cells, and there is 1 isolated site per edge, that must contain one zero-energy eigenstate each, as there are no onsite potentials [15].

For the first case, see Fig. 2a), when $v = 1$ and $w = 0$, we have totally disconnected dimers and the particle can jump freely in its cell, being a dimer a compound consisting of two sites linked together either by a strong or a weak manner. This is the state of a free particle in two sites and it is enough to solve this problem and multiply it by the number of disconnected cells that the lattice has. For the other case, see Fig. 2b), when $v = 0$ and $w = 1$, we have a dimer where a monomer is in a cell m while the other is in the cell $m+1$. In this case, the first and last cells (the blue and red shaded edges of the lattice in Fig. 2) have a disconnected site. From now on, we name those disconnected sites like zero energy modes since they are not formally in the Hamiltonian, and to be able to include them they would have to have zero energy in the excitation spectrum. Those modes with zero energy are the ones we want to inspect.

As we know, the Hamiltonian of a free particle is diagonal in momentum space; in addition to that, we have the purpose of extending the study to an arbitrary number of sites, therefore, it is a good idea to carry out a unitary transform that allows us to go to the momentum space. The standard way is to use the Fourier transform which is only valid for infinite systems or for systems with periodic boundary conditions. Nevertheless, the standard Fourier transform is not convenient since it does not respect the boundary conditions of a finite system. This is the reason why we propose the discrete sine transform I, which arises from linear combinations of plane waves, such that the combination satisfies the boundary conditions of our physical system. Such combination turns out to be

$$|\zeta^{-}_{\alpha}\rangle = \hat{a}^{\dagger}_{\zeta,\alpha}|\oslash\rangle = \sqrt{\frac{2}{N+1}} \sum_{m=0}^{N+1} \sin\left(\frac{\zeta\pi m}{N+1}\right) \hat{a}^{\dagger}_{m,\alpha}|\oslash\rangle, \qquad (2)$$

where ζ is the momentum quantum number. Thus, the transformation of ladder operators from the position representation to the one of momentum and vice versa take the following form, respectively

$$\hat{a}^{(\dagger)}_{m,\alpha} = \sqrt{\frac{2}{N+1}} \sum_{\zeta=0}^{N+1} \sin\left(\frac{\pi\zeta m}{N+1}\right) \hat{a}^{(\dagger)}_{\zeta,\alpha},$$

$$\hat{a}^{(\dagger)}_{\zeta,\alpha} = \sqrt{\frac{2}{N+1}} \sum_{m=0}^{N+1} \sin\left(\frac{\pi\zeta m}{N+1}\right) \hat{a}^{(\dagger)}_{m,\alpha}, \qquad (3)$$

and the orthogonality condition of the momentum basis is given by

$$\delta_{\zeta\zeta'} = \frac{2}{N+1} \sum_{m=0}^{N+1} \sin\left(\frac{\pi m\zeta}{N+1}\right) \sin\left(\frac{\pi m\zeta'}{N+1}\right). \qquad (4)$$

After some calculations, the final expression for the Hamiltonian, having used the discrete sine transform type I, is given by

$$\hat{H} = -\sum_{\zeta} \epsilon(\zeta) \left(\hat{a}^{\dagger}_{\zeta,A}\hat{a}_{\zeta,B} + \hat{a}^{\dagger}_{\zeta,B}\hat{a}_{\zeta,A}\right) - \sum_{\zeta\zeta'} F(\zeta,\zeta') \left(\hat{a}^{\dagger}_{\zeta,A}\hat{a}_{\zeta',B} - \hat{a}^{\dagger}_{\zeta,B}\hat{a}_{\zeta',A}\right), \qquad (5)$$

where $\epsilon(\zeta)$ is the dispersion relation and $F(\zeta,\zeta')$ is the bare vertex function which together determine the elements of the couplings matrix. The functional forms of them both are as follow

$$\epsilon(\zeta) = v + w\cos\left(\frac{\pi\zeta}{N+1}\right),$$

$$F(\zeta,\zeta') = \left(\frac{2w}{N+1}\right) \frac{\sin\left(\frac{\pi\zeta}{N+1}\right)\sin\left(\frac{\pi\zeta'}{N+1}\right)}{\cos\left(\frac{\pi\zeta}{N+1}\right) - \cos\left(\frac{\pi\zeta'}{N+1}\right)}. \qquad (6)$$

In Fig. 3, we present the single-excitation dispersion relation $\epsilon(\zeta)$ for a system with $N = 77$ unit cells, $v = 0$, and $w = 0.5$. Notice that v is only a shift on the graph, and w modifies the amplitude of the $\epsilon(\zeta)$ function.

A vertex function is the one particle irreducible correlation function [18]. In our case, the function $F(\zeta,\zeta')$ describes the couplings among the momenta of the system with the constraint $\zeta \pm \zeta' = 2n+1$, with $n \in \mathbb{Z}$. In Fig. 4, we present $F(\zeta,\zeta')$ for $N = 101$ unit cells, fixing $\zeta = 50$, and $w = 0.5$. It can be seen that ζ' gets localized around $\zeta = 50$, and the function, in absolute value, decays rapidly as it gets farther from the localization.

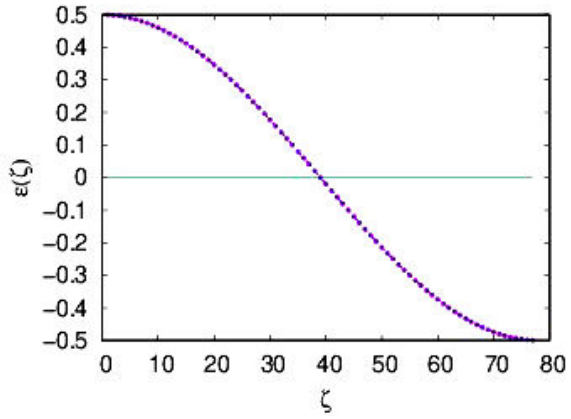

FIGURE 3. Dispersion relation $\epsilon(\zeta)$ for $N = 77$, $v = 0$, and $w = 0.5$.

3. Results

In the present section, it is proposed to work within the framework of the Bogoliubov-de Gennes (BdG) formalism [16] in order to obtain the excitation spectrum as the function of the system parameters and, consequently, the system phase diagram. This mechanism is a generalization of the model proposed by Bogoliubov Valatin, used by Bardeen-Cooper-Schrieffer to describe the superconductivity theory [19], which is a mean field approximation and allows us to rewrite the Hamiltonian as quadratic separated contributions.

Once we have the Hamiltonian of the system in the momentum space, Eq. (5), it can be rewritten in a matrix form such that

$$\hat{H} = \hat{C}^{\dagger}\mathbb{H}_{BdG}\hat{C}, \qquad (7)$$

where $\hat{C}^{\dagger}$ and $\hat{C}$ are the so-called Nambu operators, which should be chosen properly. For a system of N unit cells, the Nambu operator looks like follows

$$\hat{C}^{(\dagger)} = (\hat{a}^{(\dagger)}_{\zeta_1,A}, \hat{a}^{(\dagger)}_{\zeta_1,B}, \hat{a}^{(\dagger)}_{\zeta_2,A}, \hat{a}^{(\dagger)}_{\zeta_2,B}, ..., \hat{a}^{(\dagger)}_{\zeta_N,A}, \hat{a}^{(\dagger)}_{\zeta_N,B}). \qquad (8)$$

$\mathbb{H}_{BdG}$, is the Bogoliubov-de Gennes couplings matrix, which for the case of 4 unit cells presents the following structure

$$\begin{pmatrix}
0 & \epsilon(\zeta_1) & 0 & F(\zeta_1\zeta_2) & 0 & 0 & 0 & F(\zeta_1\zeta_4) \\
\epsilon(\zeta_1) & 0 & -F(\zeta_1\zeta_2) & 0 & 0 & 0 & -F(\zeta_1\zeta_4) & 0 \\
0 & F(\zeta_2\zeta_1) & 0 & \epsilon(\zeta_2) & 0 & F(\zeta_2\zeta_3) & 0 & 0 \\
-F(\zeta_2\zeta_1) & 0 & \epsilon(\zeta_2) & 0 & -F(\zeta_2\zeta_3) & 0 & 0 & 0 \\
0 & 0 & 0 & F(\zeta_3\zeta_2) & 0 & \epsilon(\zeta_3) & 0 & F(\zeta_3\zeta_4) \\
0 & 0 & -F(\zeta_3\zeta_2) & 0 & \epsilon(\zeta_3) & 0 & -F(\zeta_3\zeta_4) & 0 \\
0 & F(\zeta_4\zeta_1) & 0 & 0 & 0 & F(\zeta_4\zeta_3) & 0 & \epsilon(\zeta_4) \\
-F(\zeta_4\zeta_1) & 0 & 0 & 0 & -F(\zeta_4\zeta_3) & 0 & \epsilon(\zeta_4) & 0
\end{pmatrix} \qquad (9)$$

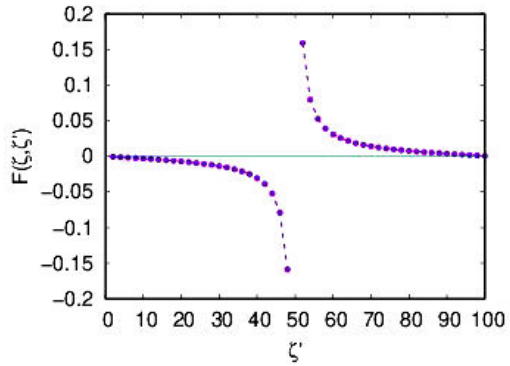

FIGURE 4. Vertex function $F(\zeta, \zeta')$ with $N = 101$, $\zeta = 50$, and $w = 0.5$.

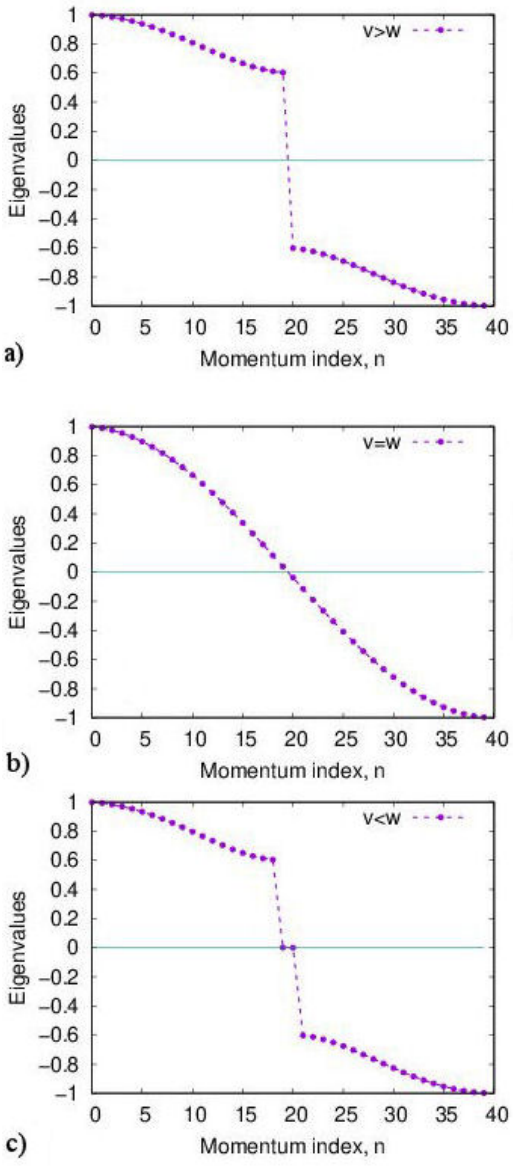

FIGURE 5. Figures a), b), and c) were made for a system with 20 unit cells ($N = 20$). a) Disconnected on-cell dimers: $v = 0.8$ and $w = 0.2$, b) simple and non staggered chain: $v = w = 0.5$, and c) non-trivial dimerized order: $v = 0.2$ and $w = 0.8$.

The eigenvalues of the couplings matrix are the so-called excitation spectrum; among them and under a certain parameter set, the zero-energy modes arise and their associated eigenstates are expected to be located at the edges as Fig. 2b), suggests.

For the first case, shown in Fig. 5a), the intercell hopping probability is smaller than the intracell hopping amplitude, such that a gap in the excitation spectrum has been opened, and in the extreme case when $w = 0$, the system behaves as disconnected on-cell dimers, and the gap opens completely. For the second case, shown in Fig. 5b), both hopping amplitudes have the same value, such that $v = w = 0.5$. For this case, the system behaves as a simple and non-staggered 1-D chain, and the particles move freely, hence there is no gap in the spectrum. For the third and, last case, shown in Fig. 5c), the intercell hopping amplitude is stronger than the intracell hopping amplitude, such that $v < w$, displaying again a gap in the spectrum but now hosting two zero energy modes. Moreover, for the extreme case when $v = 0$, the gap is wide open and we have a non-trivial dimerized order in the system, and zero-energy modes appear at the center of the gap with expected edge wavefunctions. These zero energy modes are known to be robust states making them suitable to be thought as qubits for quantum computation [20].

4. Conclusions

We use the sine transform type I to properly express the Hamiltonian of our system in momentum space. Moreover, we implement the Bogoliubov-de Gennes formalism in order to write it in an adequate way, and to obtain the excitation spectrum as the function of the system parameters, being able to extend the study of the system to an arbitrary number of sites. We obtain the three representative regimes for different values of the hopping amplitudes v and w: disconnected on-cell dimers ($v > w$), simple and non staggered chain ($v = w$) and non-trivial dimerized order ($v < w$), and we visualize the two zero-energy modes in the last case which are located in the middle of the spectrum gap.

The corresponding eigenfunctions of the obtained zero-energy modes must be accomplished, and the comparison with the topological counterpart by using periodic boundary conditions is desirable, since it constitutes a good complement to the present work.

Acknowledgments

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