Spectrum of commensurate charge density waves on a one-dimensional lattice

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June 2016

***Abstract*— Lorem ipsum dolor sit amet, consectetur adipisicing elit, sed do eiusmod tempor incididunt ut labore et dolore magna aliqua. Ut enim ad minim veniam, quis nostrud exercitation ullamco laboris nisi ut aliquip ex ea commodo consequat. Duis aute irure dolor in reprehenderit in voluptate velit esse cillum dolore eu fugiat nulla pariatur. Excepteur sint occaecat cupidatat non proident, sunt in culpa qui officia deserunt mollit anim id est laborum.**

I. One-dimensional charge density waves

Materials in which the electron density $\rho(x)$ is modulated with a wave of wavelength $\lambda = \frac{2\pi}{Q}$ are said to contain a charge density wave. In this paper, we will treat a simple model for a one-dimensional chain of atoms containing such a charge density wave:

$$H = -t\sum_x (c_x^\dagger c_{x+a} + c_x^\dagger c_{x-a}) + \sum_x (\mu + \Delta\cos(Qx+\phi))c_x^\dagger c_x \tag{1}$$

The first term describes hopping between sites, and the second term contains the chemical potential and the charge density wave. From the fact that a band gap opens at μ, it follows that $\mu = -2t\cos(\frac{Qa}{2})$.

If $\lambda = na$ with n integer and a the lattice spacing, the charge order is said to be commensurate, i.e. the charge modulation is neatly periodic in n lattice sites. Otherwise, the charge order is called incommensurate.

After imposing periodic boundary conditions, commensurate charge order is the only option, and the total amount of lattice sites N must equal a multiple of λ.

To diagonalize H, we first apply the canonical Fourier transform:

$$c_x = \frac{1}{\sqrt{N}} \sum_{0\le k<\frac{2\pi}{a}} e^{ikx} c_k$$

The hopping term and the chemical potential both give contributions diagonal in k. After writing $\cos(Qx+\phi) = \frac{1}{2}(e^{i(Qx+\phi)} + e^{-i(Qx+\phi)})$, we see that the charge wave in real space gives an off-diagonal contribution in k. The resulting Hamiltonian in Fourier space is:

$$H = \sum_{0\le k<\frac{2\pi}{a}} (\frac{1}{2}\varepsilon_k c_k^\dagger c_k + \Delta_\phi c_k^\dagger c_{k+Q} + \text{H.c.})$$

Where $\varepsilon_k = -2t\cos(ka) + \mu$ and $\Delta_\phi = \Delta e^{i\phi}$, i.e. Δ acquires a phase corresponding to the offset of the charge distribution.

A. Matrix Form Hamiltonian

We will take a few steps to put this Hamiltonian in Matrix form. This will prove to be a more convinient way to perform numerical calculations.
First we group terms in the sum over k into q sums over m.

$$\begin{aligned} H &= \sum_{0\le k<\frac{2\pi}{a}} (\frac{1}{2}\varepsilon_k c_k^\dagger c_k + \Delta_\phi c_k^\dagger c_{k+Q} + \text{H.c.}) \\ &= \sum_{0\le k<\frac{2\pi}{qa}} \sum_{m=0}^{q-1} (\frac{1}{2}\varepsilon_{k+\frac{2\pi m}{qa}} c_{k+\frac{2\pi m}{qa}}^\dagger c_{k+\frac{2\pi m}{qa}} + \Delta_\phi c_{k+\frac{2\pi m}{qa}}^\dagger c_{k+\frac{2\pi m}{qa}+Q} + \text{H.c.}) \end{aligned}$$

Since our case is commensurate, we can express $Q = \frac{2\pi}{qa}$. Furthermore we can shift the sum over m by 1, since k and $k+\frac{2\pi}{a}$ are equivalent points in k-space.

$$\begin{aligned} &= \sum_{0\le k<Q} \sum_{p=1}^{q} (\frac{1}{2}\varepsilon_{k+Qm} c_{k+Qm}^\dagger c_{k+Qm} + \Delta_\phi c_{k+Qm}^\dagger c_{k+Q(m+1)} + \text{H.c.}) \\ &= \sum_{0\le k<Q} (c_{k+Q}^\dagger, c_{k+2Q}^\dagger, \ldots, c_{k+qQ}^\dagger)\tilde{H}_k (c_{k+Q}, c_{k+2Q}, \ldots, c_{k+qQ})^T \end{aligned}$$

$$\tilde{H}_k = \begin{bmatrix} \varepsilon_{k+Q} & \Delta_\phi & 0 & \ldots & 0 & \Delta_\phi^* \\ \Delta_\phi^* & \varepsilon_{k+2Q} & \Delta_\phi & 0 & \ldots & 0 \\ 0 & \Delta_\phi^* & \ddots & \ddots & & \vdots \\ \vdots & 0 & \ddots & & & 0 \\ 0 & \vdots & & & & \Delta_\phi \\ \Delta_\phi & 0 & \ldots & 0 & \Delta_\phi^* & \varepsilon_{k+qQ} \end{bmatrix} \tag{2}$$

II. Chern numbers and Electron transport

Varying the phase of the CDW, does not necessarily transport the electrons along the chain. The transport depends on the chemical potential. For $\mu(Q = \frac{ap}{q}) = 0$, we have *no* electron transport. This corresponds to our Chern numbers being 0. This is in agreement with the calculations of section **???**. The important connection to make is that the Chern

numbers are antisymmetric at the same point as the chemical potential is. This is the point for which the electron transport changes directions. The antisymmetry of the Chern numbers is easily seen in the antisymmetry around $\frac{1}{2}$ of the colouring of the spectrum as a function of $\frac{p}{q}$ ie the Hofstadter Butterfly figure **???**.

The transport of electrons along the chain is analogous to the transport of electrons in the integer quantum Hall effect. In the next subsection we look more carefully at this comparison.

A. The Hofstadter Hamiltonian vs CDW

The CDW spectrum is a Hofstadter butterfly [**?**]. It turns out that the CDW is very similar to that where the butterfly originally arose. So let's compare our real-space Hamiltonian to that of the tight-binding model on an isotropic square lattice under a vertical uniform magnetic field in k-space [**?**]:

$$\mathscr{H} = -t \sum_{k_x,k_y} (c_1^\dagger(\mathbf{k}), c_2^\dagger(\mathbf{k}), \ldots, c_q^\dagger(\mathbf{k})) \tilde{\mathscr{H}_k} (c_1(\mathbf{k}), c_2(\mathbf{k}), \ldots, c_q(\mathbf{k}))$$

$$\tilde{\mathscr{H}_k} = \begin{bmatrix} E_{k_y+2\pi\Phi} & 1 & 0 & \ldots & 0 & e^{-iqk_x} \\ 1 & E_{k_y+4\pi\Phi} & 1 & 0 & \ldots & 0 \\ 0 & 1 & \ddots & \ddots & & \vdots \\ \vdots & 0 & \ddots & & & 0 \\ 0 & \vdots & & & & 1 \\ e^{iqk_x} & 0 & \ldots & 0 & 1 & E_{k_y+2\pi q\Phi} \end{bmatrix}$$

With $E_{k_y+2\pi m\Phi} = 2\cos(k_y + 2\pi m\Phi)$. Where Φ is in units of the magnetic flux quantum.

This is how to map this situation onto that of the CDW.

$$k_y \leftrightarrow \phi$$
$$\Phi \leftrightarrow \frac{Q}{2\pi}$$

The x-sum in the CDW case goes from sites 1 to q. The length of the chain q is the same as the length of the magnetic unit cells in the lattice. The phase due to the flux in the lattice case gives us the complex exponential in the corners of our matrix. Finally to make the mapping work we need to set $\Delta = 2t$ and $a = 1$.

III. Topological classification

The charge density wave Hamiltonian in k-space can be divided in different classes. Originally the classification was developed for translational or rotational invariant systems, but because the dihedral group is the only nontrivial space group another classification is made. When symmetries are taken into account a topological classification can be made. If a system behaves in the same way when time is reversed on can say that the system has a time symmetry. For time symmetry there are 3 options. Either the system is not time symmetric $(T = 0)$, or it is time symmetric $(T^2 = 1)$ or the system is time anti-symmetric $(T^2 = -1)$. Another symmetry is charge conjugation C. When this is observed as particle-hole symmetry one can distinguish an occupation of the hole or an empty hole. When there is a symmetry the charge conjugation can be plus $(C^2 = 1)$ or minus $(C^2 = -1)$ and when there is no symmetry the charge conjugation number is zero $(C = 0)$. Because both the time reversal operator T and the charge conjugation number C are topological invariant their multiplication $S = T * C$ is also a topological invariant. As a first guess one would find $3*3 = 9$ topological invariant sectors. But when there is no time reversal $(T = 0)$ and no charge conjugation $(C = 0)$, S can have two values. When a system is symmetric in the combination of time and particle hole symmetry S is given the value of 1. When it is not symmetric in the combination of them the value is 0. All together there are than 10 different topological sectors where S is an invariant. This Tenfold Way classifies the allowed topologies of all gapped, disordeblack, quadratic fermion theories into ten classes based on the dimension of the parameter space, see ???. The advantage of this classification is that these sectors have edge states which are classified by a nonzero Chern number. Because these edge states do not depend on small perturbations in the bulk of the material it is possible to measure variables at the edge that give information of the whole material. To classify our Hamiltonian we see that there are no zero's on the diagonal, which exclude the 3 chiral cases. Because the Hamiltonian can be expressed as a 2x2 matrix, exept in the case of half filling, the four Bogoliubov-de Gennes cases. From the three

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IV. CONCLUSIONS

A conclusion section is not requiblack. Although a conclusion may review the main points of the paper, do not replicate the abstract as the conclusion. A conclusion might elaborate on the importance of the work or suggest applications and extensions.