Spectrum of one-dimensional chain with commensurate charge density wave

Arthur Boetes, Bruno Eijsvoogel, Robert Hauer, Geert Kapteijns
Seminar Theoretical Physics
June 2016

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 [1]:

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

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 $\lambda = \frac{q}{p}a$ with q, p coprime integers, $p \leq q$, and a the lattice spacing, the charge order is said to be commensurate, i.e. the charge modulation is periodic in q 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:

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

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:

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

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 the Hamiltonian in matrix form. This will prove to be a more convenient way to perform numerical calculations.

First we group terms in the sum over k into q sums over m.

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

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.

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

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

II. Mapping onto the Hofstadter butterfly

Now we will 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 [3]:

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

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

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. Numerical Calculations and Results

The numerical methods used to create the band structure and the butterfly are discussed here. For this, the matrix in equation 2 is vital. The arguments of the matrix are $\{k, \phi, \Delta, Q, a\}$. For all numerical calculations, the mapping to the Hofdstadter problem ($\Delta = 2t$) is used and a is set to 1. The chemical potential is dependent on Q and a as $\mu = -2t\cos(\frac{Qa}{2})$. As has been mentioned before, we look at cases were $\frac{Qa}{2\pi} = \frac{p}{q}$, with $p \leq q$. For numerical purposes, the matrix is scaled to the hopping parameter t. More scaling is achieved by setting k to qka. With this scaling the allowed energies, setting the chemical potential to zero, are between -4 and 4. For the scaled momenta, k, $0 \leq k \leq 2\pi$.

The matrix has a size of q by q and diagonalizing it yields a spectrum of q eigenvalues which might be degenerate.

A. Band structure

When calculating the band structure, the value of Q is fixed and k is varied. The phase ϕ can also be varied, but is set to zero for convenience. Every value of k yields a matrix and in turn every matrix is diagonalized thus yielding an energy spectrum for every k. Grouping these values correctly results in the band structure.

For the different values of $\frac{Qa}{2\pi} \in \{2/3, 3/5\}$ the band structures are plotted in Fig. 1.

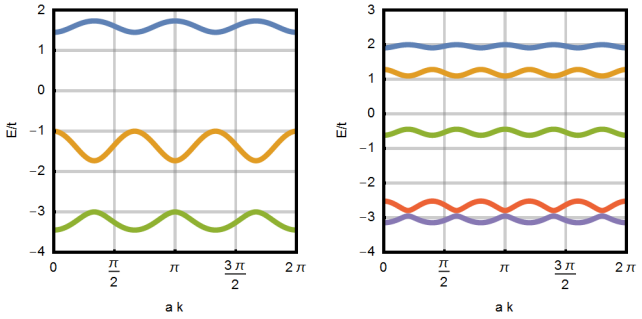

Fig. 1: Band structure of the CDW with phase $\phi = 0$. Left:$p = 2$, $q = 3$ yielding Chern numbers, bottom to top, of -1,1,0. Right:$p = 3$, $q = 5$ yielding Chern numbers, bottom to top, of 2, -1, 1, -2, 0.

B. The CDW butterfly

Mapping the charge density wave to the Hofstadter problem, and setting the chemical potential to zero, the Hofstadter butterfly is retrieved. The butterfly can be constructed by fixing k and ϕ, while varying Q. The relation $\frac{Qa}{2\pi} = \frac{p}{q}$ must be obeyed however and for numerical calculations an upper limit on q must be made. The resulting values for Q result from a list of fractions where $1 \leq p \leq q$ and all the fractions are reduced to the lowest term, making p and q coprime. The requirement of the fractions is that $0 < \frac{p}{q} \leq 1$. For a particular value of $\frac{p}{q}$, there are q eigenvalues or bands, and so a list of fractions and energies is obtained. There is a Chern number associated with every band, which can be used to color the butterfly according to the Chern number.

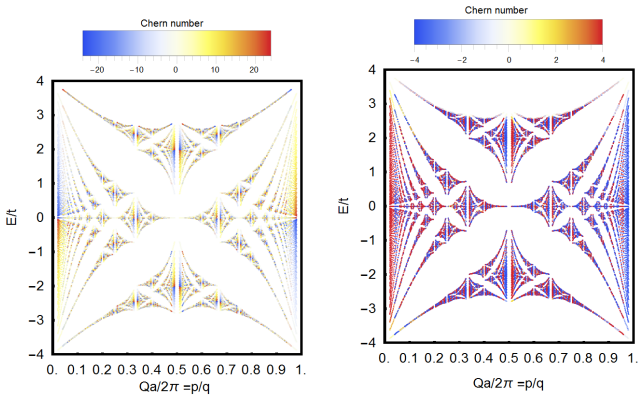

Fig. 2: Allowed energies of the of the CDW Hamiltonian with phase $\phi = 0$ using the method described in this section with a maximum value of $q = 50$. Left: The spectrum colored using the Chern numbers. Right:The energy spectrum where the coloring is done by adding Accumulating the Chern numbers starting at the lowest band and truncating at -4 and 4.

IV. 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 the previous 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 $\frac{p}{q}$ in the Hofstadter butterfly in Fig. 2.

The transport of electrons along the chain is analogous to the transport of electrons in the integer quantum Hall effect.

V. Topological Classification

The charge density wave Hamiltonian in k-space can be divided in different classes [2]. 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 2×2 matrix, exept in the case of half filling, the four Bogoliubov-de Gennes cases. From the three clases left, it must be the one where the Hamiltonian in k space is complex. With this reasoning our Hamiltonian falls into the symmetry-free class.

REFERENCES

[1] Felix Flicker and Jasper van Wezel. Quasiperiodicity and 2d topology in 1d charge-ordered materials. *EPL (Europhysics Letters)*, 111(3):37008, 2015.

[2] Shinsei Ryu, Andreas P Schnyder, Akira Furusaki, and Andreas WW Ludwig. Topological insulators and superconductors: tenfold way and dimensional hierarchy. *New Journal of Physics*, 12(6):065010, 2010.

[3] Nobuyuki Yoshioka, Hiroyasu Matsuura, and Masao Ogata. Distribution of chern number by landau level broadening in hofstadter butterfly. In *Journal of Physics: Conference Series*, volume 603, page 012019. IOP Publishing, 2015.