Roma la Sapienza
Solid State Physics

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Esercitazione °5: Spontaneous polarisation, Berry phase and Wannier functions

Exercise I : Spontaneous polarisation of a 2-atom linear chain

1. Definitions - system

   Let's consider a one-dimensional periodic chain, with period a, with two atoms, the first of type A in $-a/4$, the second of type B in $+a/4$. We describe the system with a tight-binding (TB) Hamiltonian, using one basis function per atom $\{|\alpha R\rangle\}_{\alpha=\{A,B\},R=ja}$, with j an integer. Namely, the $|\alpha R\rangle$ basis function is located at the position $(\tau_\alpha + R)$ where $\tau_A = -a/4$ and $\tau_B = +a/4$. We suppose the TB basis to be orthonormal. The hopping integral of the Hamiltonian is non-zero between neighbouring atoms and equal to $-t$ with $t > 0$. The onsite terms are $\langle AR|H|AR\rangle = -\Delta$ and $\langle BR|H|BR\rangle = +\Delta$. From now on (if the opposite is not specified) we suppose that $\Delta > 0$. We also suppose that each atom provides an electron to the chain.

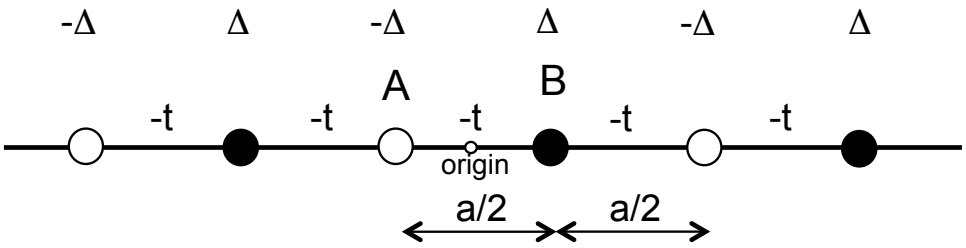

Figure 1: Two-atom linear chain

2. Bands

   Rewrite the Hamiltonian using the Bloch-like basis $\{|\alpha k\rangle = \sum_R \frac{e^{i(\tau_\alpha+R)k}}{\sqrt{N}}|\alpha R\rangle\}_{\alpha=\{A,B\},k}$. Find the eigenenergies of the Hamiltonian, plot the band structure in the first Brillouin zone. Is the system metallic or insulating? Which band is occupied ?

3. Bloch eigenstates

   Compute the Bloch (normalised in the N cells) eigenstates of the occupied band, $\{|Ok\rangle\}_k$. We will look for a phase convention for the Bloch eigenstates such that for $-\pi/a \leq k < \pi/a$ the $|Ok\rangle$ is continuous and differentiable with respect to the variable k. Verify if $|Ok\rangle$ is continuous also at the zone border, namely if

$$|O\left(-\frac{\pi}{a}\right)\rangle = |O\frac{\pi}{a}\rangle. \tag{1}$$

If this is not the case, modify the phase convention of the eigenstates by multiplying them by a k dependent phase factor e^{ibk}, where the constant b is chosen in such a way that, with the new resulting phase-convention, Eq. (1) is satisfied. Note that the condition of Eq. (1) should be satisfied if we want to use the Bloch function to compute the Berry phase from the k-derivative of the periodic part of the Bloch states.

4. Periodic part of Bloch eigenstates

   Consistently with a TB approximation, the position operator r should be considered to be diagonal in the $\{|\alpha R\rangle\}_{\alpha=\{A,B\},R=ja}$ basis, namely

$$r|\alpha R\rangle = (\tau_\alpha + R)|\alpha R\rangle. \tag{2}$$

   Demonstrate using Eq. (2), that if we write the Bloch state found at the end of the previous point as:

$$|Ok\rangle = \sum_R \sum_\alpha \frac{e^{i(\tau_\alpha+R)k}}{\sqrt{N}} c_{\alpha k}|\alpha R\rangle \tag{3}$$

   the corresponding periodic part is:

$$|u_k\rangle = \sum_R \sum_\alpha c_{\alpha k}|\alpha R\rangle. \tag{4}$$

5. Spontaneous polarisation of the occupied band

   We recall that in one dimension the electronic contribution to the polarisation is equal to:

$$P = \frac{-2|e|r_W}{a}, \tag{5}$$

   were r_W is the centroid of the Wannier function associated to the occupied band. We recall also that

$$r_W = a\int_{-\pi/a}^{\pi/a} \frac{dk}{2\pi} i\langle u_k|\frac{|u_k\rangle}{dk}. \tag{6}$$

   Using Eq. (6) and the results of the previous two points compute r_W. Is this result compatible with the mirror and translational symmetries present in the systems? If yes why? Is the location of r_W univocally fixed by the symmetries of our system? If not, is the result expected based on qualitatively (hand-waving) arguments?

   Consider what is happening for $\Delta < 0$. Plot r_W as a function of Δ considering a finite interval of Δ-values symmetric around 0. What is happening for $\Delta = 0$? Why?

Exercise 2 : Wannier fuctions of a 2-atom linear chain

Here we plan to compute numerically the Wannier function of the occupied band of the system discussed in the previous exercise. We consider the particular case where $t = 10$ eV and $\Delta = 1$ eV. We recall that the Wannier function centred in the unit cell with $R = 0$ is defined as:

$$|W_0\rangle = \sum_k \frac{1}{\sqrt{N}}|Ok\rangle \tag{7}$$

1. Phase convention for the Bloch state

   Consider the coefficients $c_{\alpha k}$ defined in Eq. (3). For one of the two atoms the coefficient is different from zero in all the interval $-\pi/a \leq k < \pi/a$ (we call this atom D), for the other atom (we call it nD) the coefficient can be zero in one k-point. Identify the two types of atoms. The basis function of the atom D in the unit cell centred in the origin is $|D0\rangle$ and the basis function of the atom nD in the unit cell centred in the origin is $|nD0\rangle$. We fix two phase conventions for the Bloch states. We fix the phase convention D by choosing the phase in such a way that $\langle D0|Ok\rangle$ is real and positive for $-\pi/a \leq k < \pi/a$. We fix the phase convention nD by choosing the phase in such a way that $\langle D0|Ok\rangle$ is real and positive (or zero) for $-\pi/a < k < \pi/a$. Determine the Bloch states in the two conventions.

2. Compute the Wannier functions

   The shape and localisation of Wannier function depends on the phase convention used for Bloch states. For the two different phase conventions determined at the previous point, write a short computer-code to compute numerically and to plot the Wannier function using Eq.(7) for the three cases $N = 11$, $N = 31$, $N = 111$. Restrict the k summation in the first Brillouin zone. Notice that if N is odd:

$$k = \frac{j}{N}\frac{2\pi}{a} \qquad j = -\frac{N-1}{2}, -\frac{N-1}{2}+1, ..., \frac{N-1}{2} \tag{8}$$

   and we do not have in the summation, the $k = -\pi/a$ and $k = \pi/a$ values. For the 6 cases ($N = 3$, $N = 11$, $N = 31$ and the two phase conventions) plot the real part (and eventually the imaginary part if it is non-zero) of

$$\langle \alpha R|W_0\rangle \tag{9}$$

   as a function of $(\tau_\alpha + R)$ in the interval $-2Na < (\tau_\alpha + R) < 2Na$. Compare and comment the results.