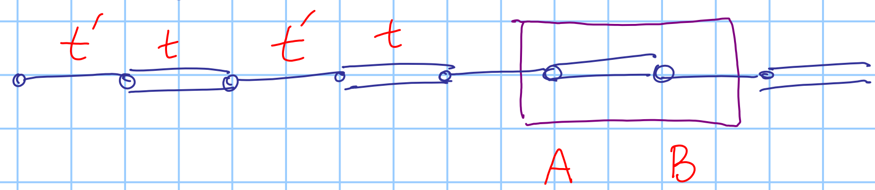
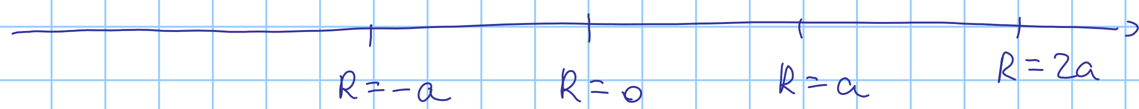
Topology in band structure, SSH model.

Note Title 2/13/2013

We consider a model of dimerized hopping, the so-called SSH model.





We look for wavefunctions of the form

$$\psi(r) = \sum_R e^{ikR}\left[C_A \phi_A(r-R) + C_B \phi_B(r-R)\right]$$

We assume

$$\int \phi_A^*(r)\,\phi_B(r)\,dr = 0$$

$$\int \phi_A^*(r)\,\phi_B(r+a)\,dr = 0$$

We take

$$\int \phi_A^*(r)\,\Delta U(r)\,\phi_B(r) = -t$$

$$\int \phi_A^*(r)\,\Delta U(r)\,\phi_B(r+a) = -t'$$

Following our general formalism we obtain

$$E_0 C_A + C_B \int \phi_A^*(r)\, \Delta U(r)\, \phi_B(r)$$

$$+ C_B e^{-ik\cdot a} \int \phi_A^*(r)\, \Delta U(r)\, \phi_B(r-a)$$

$$= \varepsilon(k) \cdot C_A$$

$$\boxed{\left(\varepsilon(k) - E_0\right) C_A = \left(-t - t' e^{-ika}\right) C_B}$$

$$E_0 C_B + C_A \cdot \int \phi_B^*(r)\, \Delta U(r)\, \phi_A(r)$$

$$+ C_A e^{ika} \int \phi_B^*(r)\, \Delta U(r)\, \phi_A(r-a)$$

$$= \varepsilon(k) \cdot C_B$$

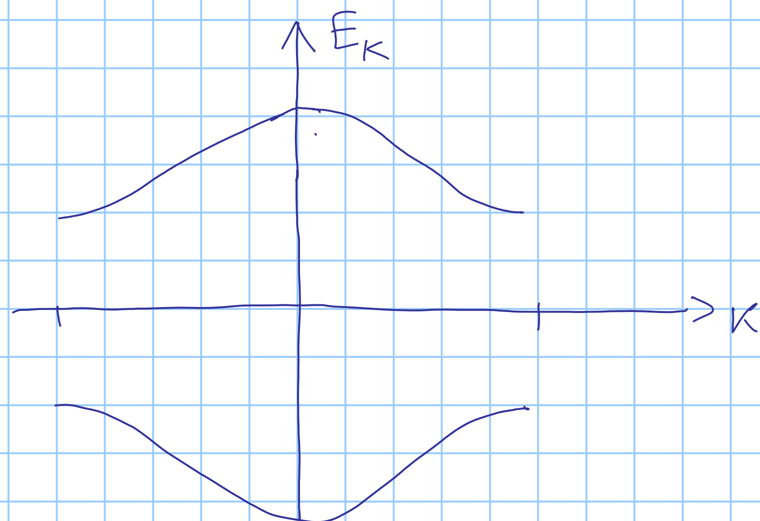
$$\boxed{\left(\varepsilon(k) - E_0\right) C_B = \left(-t - t' e^{ika}\right) C_A}$$

Hence we can write with $E_0 = 0$ and assuming ϕ_A and ϕ_B to be real

$$\hat{\mathcal{H}} = \begin{bmatrix} 0 & -t - t' e^{-ika} \\ -t - t' e^{ika} & 0 \end{bmatrix}$$

We set $a \equiv 1$.

$$\hat{\mathcal{H}} = (-t - t'\cos k)\,\hat{\sigma}_x - t'\sin k\,\hat{\sigma}_y$$



Let us look at eigenstates

$$\mathcal{H} = -E_k\left(\cos\theta_k\,\hat{\sigma}_x + \sin\theta_k\,\hat{\sigma}_y\right)$$

$$\tan\theta_k = \frac{\sin k}{t + t'\cos k}$$

Eigenvalues $\quad \varepsilon_k = \pm E_k$

$$E_k^2 = (t + t'\cos k_x)^2 + (t'\sin k)^2$$

Equation on the eigenstate for $\varepsilon_k = -E_k$

$$\begin{bmatrix} -E_k & E_k\cos\theta_k - iE_k\sin\theta_k \\ E_k\cos\theta_k + iE_k\sin\theta_k & -E_k \end{bmatrix}\begin{pmatrix} C_A \\ C_B \end{pmatrix} = 0$$

$$\begin{pmatrix} -1 & e^{-i\theta_k} \\ e^{i\theta_k} & -1 \end{pmatrix}\begin{pmatrix} C_A \\ C_B \end{pmatrix} = 0$$

Eigenstate for $\varepsilon_k = -E_k$

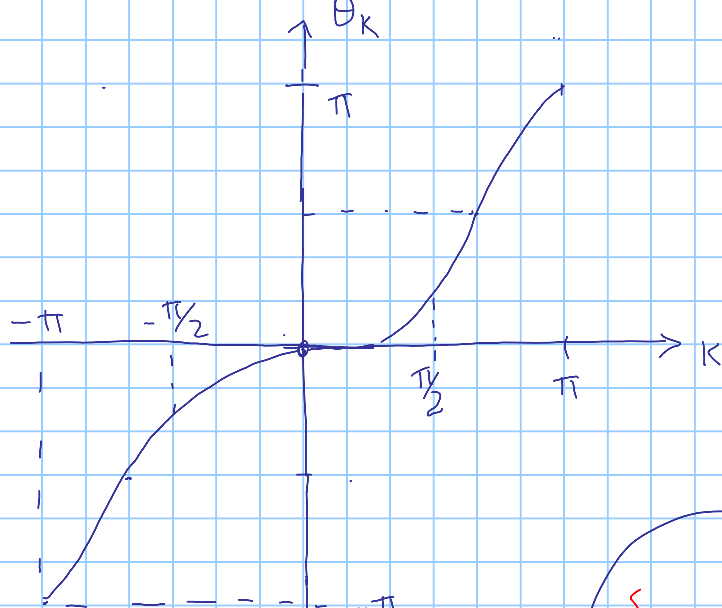
$$\psi_k = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-i\theta_k} \\ 1 \end{pmatrix}$$

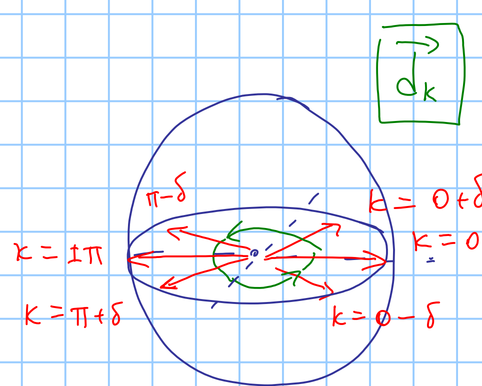
We can write the Hamiltonian as

$$\boxed{H_k = -\vec{d}_k \, \vec{\sigma}.}$$

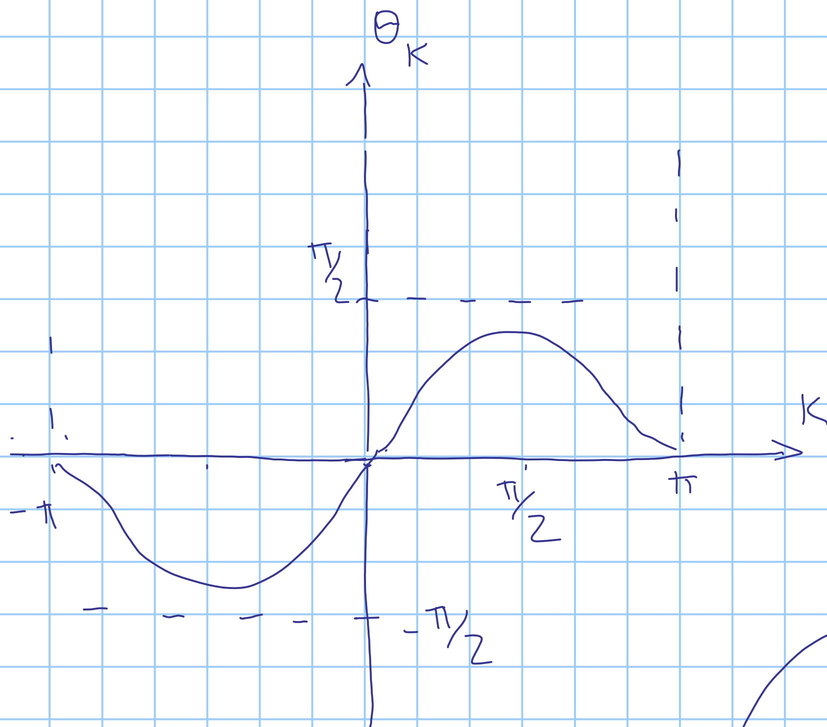
Vector $\vec{d}$ has only x and y component, i.e. it has to lie in the xy plane. Consider a change in the vector $\vec{d}_k$ as k changes in the Brillouin zone $-\pi \le k < \pi$

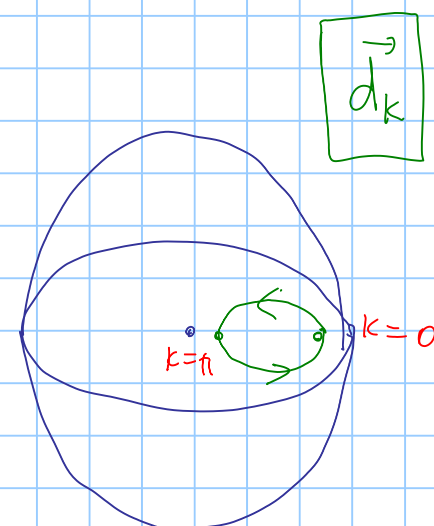
Take $t' > t$





Take $t' < t$



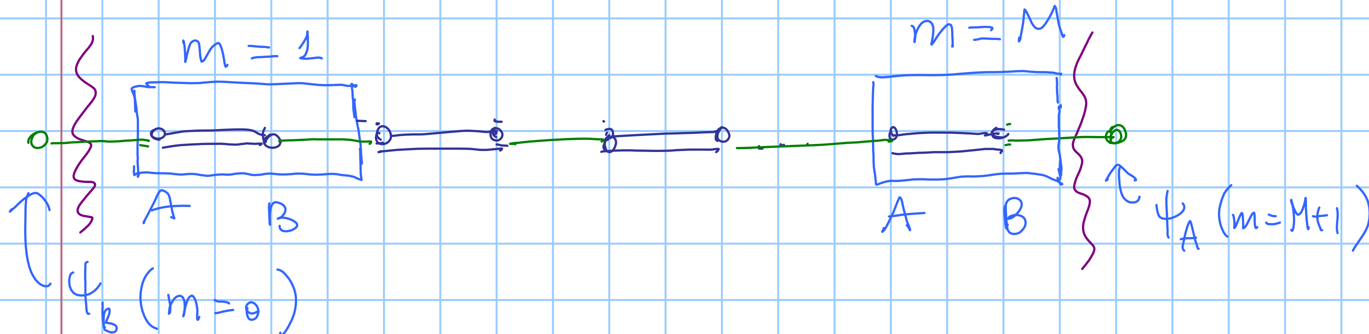


There is topological difference between the two trajectories: the first one encircles $d_k = 0$ and the second one does not. We can not have $d_k = 0$ since this would mean closing the gap.

Mathematically the difference between the two trajectories shows up in the Zak/Berry phase

$$\frac{1}{i}\int_{-\pi}^{\pi} \langle u_k | \partial_k u_k \rangle \, dk = \begin{cases} -\pi, & t' > t \\ 0, & t' < t \end{cases}$$

Regime $t' > t$ is topologically distinct from vacuum. This leads to existence of zero energy edge states. Consider a finite chain that starts with A site and ends with a B site.



We have integer number of unit cells of the topologically non-trivial state. Hence we expect edge states. This can be checked by the direct calculation. We can use our plane wave states

$$\psi_{k\mp} = e^{ikR}\begin{bmatrix} e^{i\theta_k} \\ \pm 1 \end{bmatrix}$$

to construct states satisfying boundary conditions

$$\psi_B(m=0) = 0$$

$$\psi_A(m=M+1) = 0$$

$$\tilde{\psi}_k = \left(\psi_{k\pm} - \psi_{-k\pm}\right)$$

Obviously $\tilde{\psi}_k(R=0)=0$ and k will be fixed by requiring $\psi_A(m=M+1)=0$.

It is easy to check that when $t'>t$ we have $N = 2(M-1)$ solutions of type $\tilde{\psi}_k$ (bulk states. Remember to count both $\pm E_k$ states). And 2 solutions are zero energy edge states. On the other hand when $t'<t$ we will find $N=2M$ bulk states and no edge states.

One can give a simple cartoon of this by considering $t \to 0$ limit with t' finite.