there are van Hove singularities at $E = \pm t$. Note that for the honeycomb lattice

$$E_\pm(\Gamma) = \pm 3t \quad , \quad E_\pm(K) = 0 \quad , \quad E_\pm(M) = \pm t$$

In the vicinity of either of the two inequivalent zone corners K and K', if we write $\vec{k} = \vec{K} + \vec{q}$ or $\vec{k} = \vec{K}' + \vec{q}$, we have $E = \pm \hbar v_F |\vec{q}|$ with $v_F = \frac{\sqrt{3}}{2} ta/\hbar$. This is a 2D Dirac spectrum, and K and K' are the locations of Dirac points.

Lecture 2 (Jan. 7): How to go flux yourself

Simple model: spinless s-orbitals in a 2D crystal

The Hamiltonian is

$$H = -\sum_{\vec{r}<\vec{r}'} \left(t_{\vec{r}\vec{r}'} c^\dagger_{\vec{r}} c_{\vec{r}'} + t^*_{\vec{r}\vec{r}'} c^\dagger_{\vec{r}'} c_{\vec{r}} \right)$$
$$= -\sum_{\vec{r}<\vec{r}'} \left(t_{\vec{r}\vec{r}'} |\vec{r}\rangle\langle\vec{r}'| + t^*_{\vec{r}\vec{r}'} |\vec{r}'\rangle\langle\vec{r}| \right)$$

The notation $\vec{r} < \vec{r}'$ means that each pair $(\vec{r}, \vec{r}')$ is included only once in the sum. We may write

$$t_{\vec{r}\vec{r}'} = t^*_{\vec{r}'\vec{r}} = |t_{\vec{r}\vec{r}'}| \, e^{iA_{\vec{r}\vec{r}'}} \qquad (A_{\vec{r}\vec{r}'} \text{ defined mod } 2\pi)$$

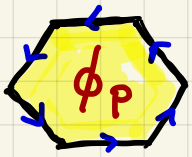
where $A_{\vec{r}\vec{r}'}$ is a gauge field living on the link $(\vec{r}, \vec{r}')$. Note $A_{\vec{r}'\vec{r}} = -A_{\vec{r}\vec{r}'}$. The tight-binding Hamiltonian exhibits a **gauge invariance**,

$$c_{\vec{r}} \to e^{i\alpha_{\vec{r}}} c_{\vec{r}} \quad (\text{or } |\vec{r}\rangle \to e^{-i\alpha_{\vec{r}}} |\vec{r}\rangle)$$

$$t_{\vec{r}\vec{r}'} \to e^{i(\alpha_{\vec{r}} - \alpha_{\vec{r}'})} t_{\vec{r}\vec{r}'}, \quad \text{i.e.} \quad A_{\vec{r}\vec{r}'} \to A_{\vec{r}\vec{r}'} + \alpha_{\vec{r}} - \alpha_{\vec{r}'}$$

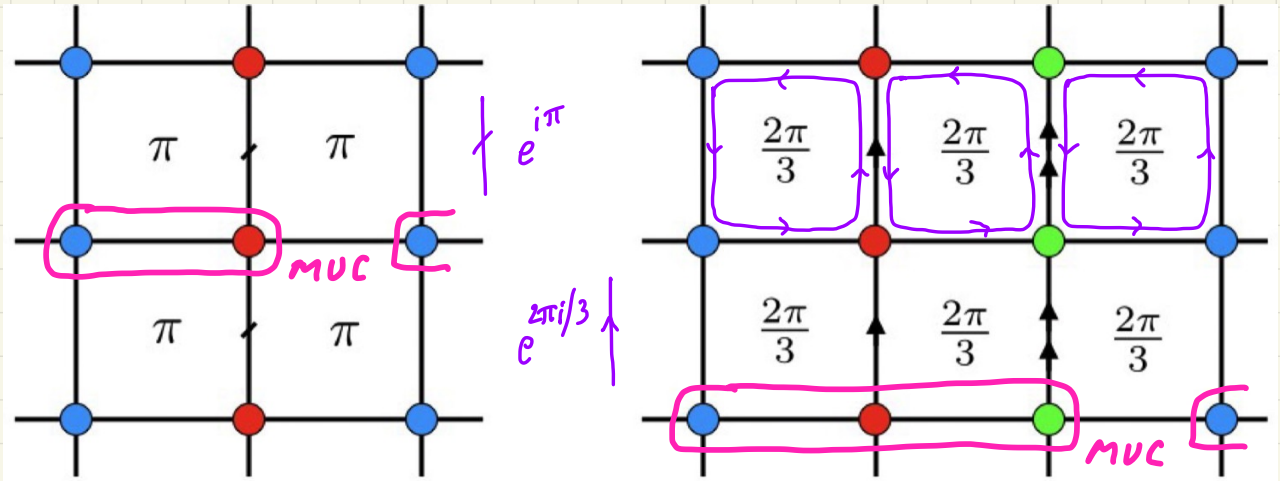
The U(1) flux ϕ_p through any plaquette p is given by

$$\phi_p = \sum_{\langle \vec{r}\vec{r}' \rangle \in \partial p} A_{\vec{r}\vec{r}'}$$



I.e. it is a directed sum of $A_{\vec{r}\vec{r}'}$ along all links $\langle \vec{r}\vec{r}' \rangle$ in the boundary ∂p of the plaquette p. Consequently, each plaquette flux ϕ_p is <u>invariant</u> under a gauge transformation. On a Bravais lattice $\mathcal{L}$, the tight-binding model with uniform flux ϕ in every elementary plaquette is known as the **Hofstadter model**.

It is clear that any configuration with $\phi \neq 0$ must be described by a gauge field configuration $\{A_{\vec{r}\vec{r}'}\}$ which breaks the lattice translational invariance, because opposite sides of any plaquette are traversed in opposite directions, and their respective phase factors cancel. Consider next the following:

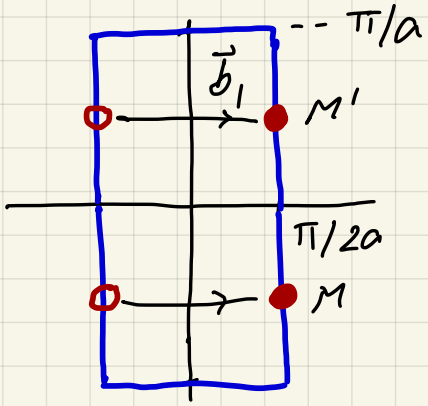


For $\phi = \pi$, we have a **magnetic unit cell** which contains two lattice sites (A/blue and B/red), while for $\phi = \frac{2\pi}{3}$ the magnetic unit cell contains three sites (A/blue, B/red, C/green). Consider the $\phi = \pi$ model. The magnetic Bravais lattice is rectangular, with $\vec{a}_1 = 2a\hat{x}$ and $\vec{a}_2 = a\hat{y}$. We then have

$$t_{AA}(\vec{R}) = t\,\delta_{\vec{R},\vec{a}_2} + t\,\delta_{\vec{R},-\vec{a}_2} \Rightarrow \hat{t}_{AA}(\vec{k}) = 2t\cos(\vec{k}\cdot\vec{a}_2)$$

$$t_{BB}(\vec{R}) = -t\,\delta_{\vec{R},\vec{a}_2} - t\,\delta_{\vec{R},-\vec{a}_2} \Rightarrow \hat{t}_{BB}(\vec{k}) = -2t\cos(\vec{k}\cdot\vec{a}_2)$$

$$t_{AB}(\vec{R}) = t\,\delta_{\vec{R},0} + t\,\delta_{\vec{R},-\vec{a}_1} \Rightarrow \hat{t}_{AB}(\vec{k}) = t\left(1 + e^{i\vec{k}\cdot\vec{a}_1}\right)$$



Thus,

$$H(\vec{\theta}) = -t\begin{pmatrix} 2\cos\theta_2 & 1+e^{i\theta_1} \\ 1+e^{-i\theta_1} & -2\cos\theta_2 \end{pmatrix} \begin{matrix} \text{A} \\ \text{B} \end{matrix} \qquad \begin{matrix} \text{A} & \text{B} \end{matrix}$$

$$E_\pm(\vec{\theta}) = \pm 2t\sqrt{\cos^2\left(\tfrac{1}{2}\theta_1\right) + \cos^2\theta_2}$$

The two bands touch at $E_\pm(\vec{\theta}) = 0$ for $(\theta_1, \theta_2) = (\pi, \pm\frac{1}{2}\pi)$, and writing $(\theta_1, \theta_2) = (\pi + \delta_1, \pm\frac{\pi}{2} + \delta_2)$, we find

$$E_\pm(\vec{\theta}) = \pm 2t\sqrt{\sin^2\left(\tfrac{1}{2}\delta_1\right) + \sin^2\delta_2}$$

$$= \pm 2ta\sqrt{q_1^2 + q_2^2} + \mathcal{O}(|\vec{q}|^3)$$

where $\vec{q} = \vec{k} - \vec{k}_D$ is measured from either of the touching points. These are Dirac points!

(NB: $\phi = 0 \Rightarrow$ single band with $\mathcal{E}(\vec{\theta}) = -2t\left[\cos\theta_1 + \cos\theta_2\right]$)

When $\phi = \frac{2\pi}{3}$, we have

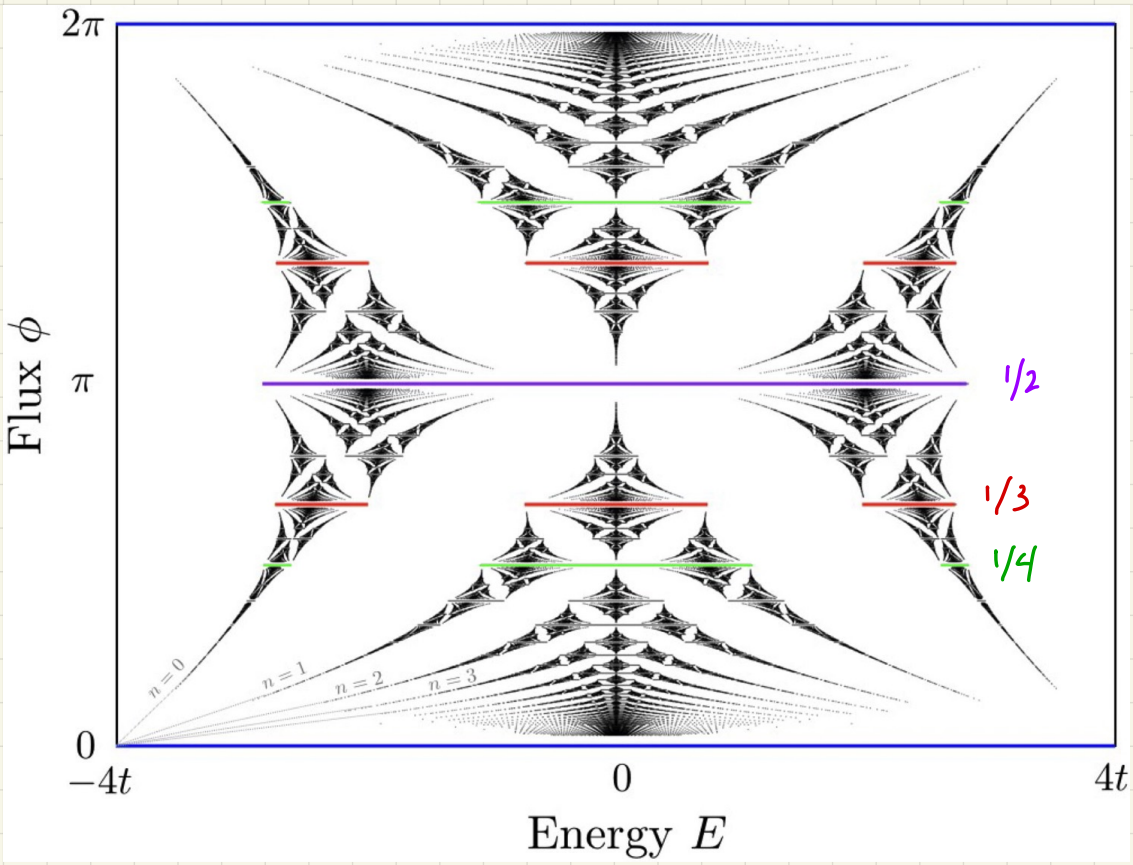
$$H(\vec{\theta}) = -t \begin{pmatrix} 2\cos\theta_2 & 1 & e^{i\theta_1} \\ 1 & 2\cos(\theta_2 + \frac{2\pi}{3}) & 1 \\ e^{-i\theta_1} & 1 & 2\cos(\theta_2 + \frac{4\pi}{3}) \end{pmatrix} \begin{matrix} A \\ B \\ C \end{matrix}$$

(A, B, C)

For flux $\phi = 2\pi p/q$ (p, q relatively prime), ($q \times 1$ muc)

$$H = -t \begin{pmatrix} 2\cos\theta_2 & 1 & 0 & \cdots & e^{i\theta_1} \\ 1 & 2\cos(\theta_2 + \frac{2\pi p}{q}) & 1 & & \vdots \\ 0 & 1 & \ddots & \ddots & 0 \\ \vdots & & \ddots & \ddots & 1 \\ e^{-i\theta_1} & 0 & \cdots & 1 & 2\cos(\theta_2 + \frac{2\pi(q-1)p}{q}) \end{pmatrix}$$

The energy bands versus flux ϕ have a fractal structure, known as Hofstadter's butterfly:



When the denominator q is large, we expect to recover the continuum Landau level spectrum $E_n = (n+\frac{1}{2})\hbar\omega_c$. For $B=0$,

$$\begin{aligned} E(\vec{k}) &= -2t\cos(k_x a) - 2t\cos(k_y a) \\ &= -4t + t\vec{k}^2 a^2 + \ldots \end{aligned}$$

whence we identify $ta^2 = \hbar^2/2m \Rightarrow m = \hbar^2/2ta^2$. The magnetic field is $B = \phi\hbar c/ea^2$ and so

$$\hbar\omega_c = \frac{\hbar eB}{mc} = \frac{\hbar e}{c} \times \frac{\phi\hbar c}{ea^2} \times \frac{2ta^2}{\hbar^2} = 2\phi t$$

which describes the corners of the Hofstadter butterfly, where continuum Landau levels radiate out from the energies $E = \pm 4t$, with

$$E_n(\phi) = \pm\big(4t - (2n+1)\phi t\big)$$

$$E_n(\phi) = \pm\big(4t - (2n+1)(2\pi - \phi)t\big)$$

and $\phi \ll \pi$.

- **Topological band structures**

This subject has received an enormous amount of attention during the past decade. Usually in physics when a parameter, such as pressure or unit cell size, is varied continuously, the system responds continuously. However, in some cases there are robust features, such as the

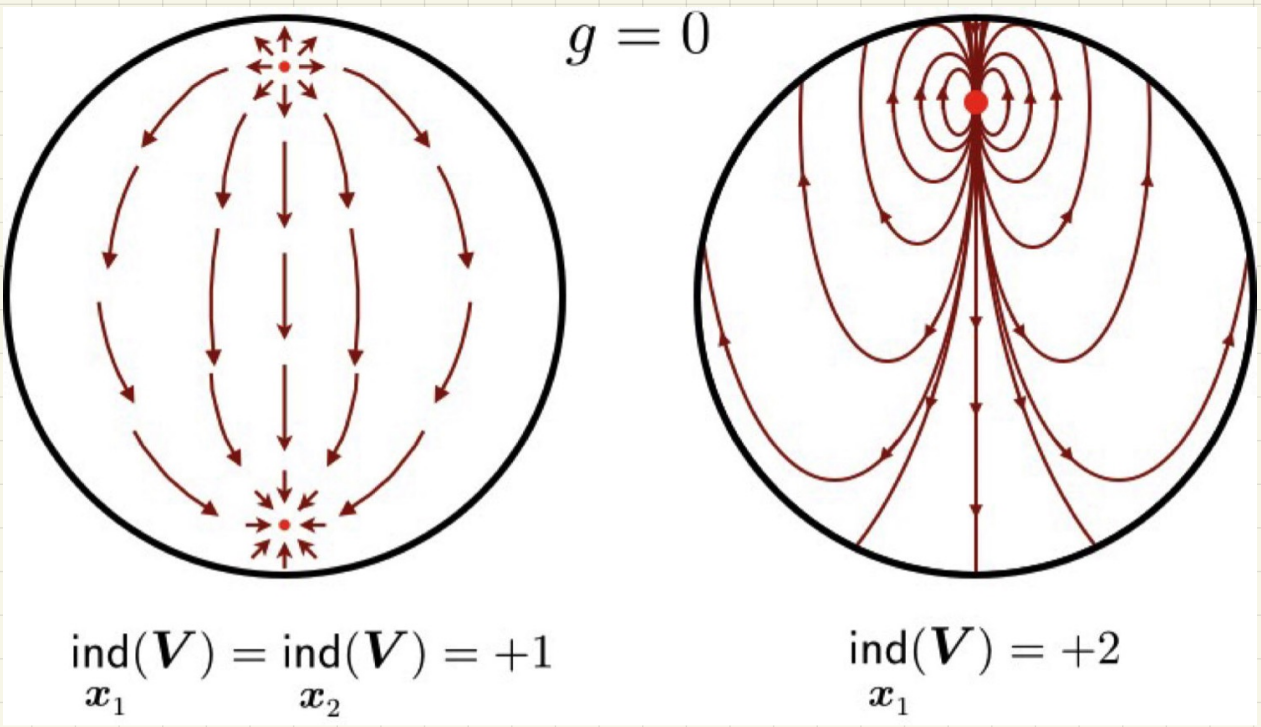
presence of bound states or edge states, and sometimes an observable response, such as the Hall conductivity σ_{xy} in $d=2$, is quantized throughout an entire phase of matter. In mathematics, there are deep connections between geometry, which is a local property, and topology, which leads to global characterizations. An example is the famous Gauss-Bonnet theorem, which says

$$\int_M dS\, K = 2\pi\chi(M) = 2\pi \sum_i \operatorname*{ind}_{\vec{x}_i}(\vec{V})$$

where M is an orientable two-dimensional manifold (such as a sphere S^2 or a torus T^2), K is the local **Gaussian curvature**, given by $K = (R_1 R_2)^{-1}$, where $R_{1,2}$ are the local principal radii of curvature, $\chi(M) \in \mathbb{Z}$ is M's **Euler characteristic**, given by $\chi(M) = 2 - 2g_M$ where g_M is the **genus** of M, which is the number of holes (or handles), $\vec{V}$ is any smooth vector field on M, and $\operatorname*{ind}_{\vec{x}_i}(V)$ is the **index** of $\vec{V}$ at the position $\vec{x}_i$ of its i^{th} singularity, where $\vec{V}(\vec{x}_i) = 0$:

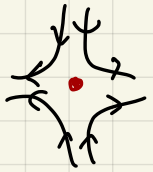
$$\operatorname*{ind}_{\vec{x}_i}(\vec{V}) = \oint_C d\vec{x} \cdot \vec{\nabla} \tan^{-1}\left(\frac{V_2(\vec{x})}{V_1(\vec{x})}\right)$$

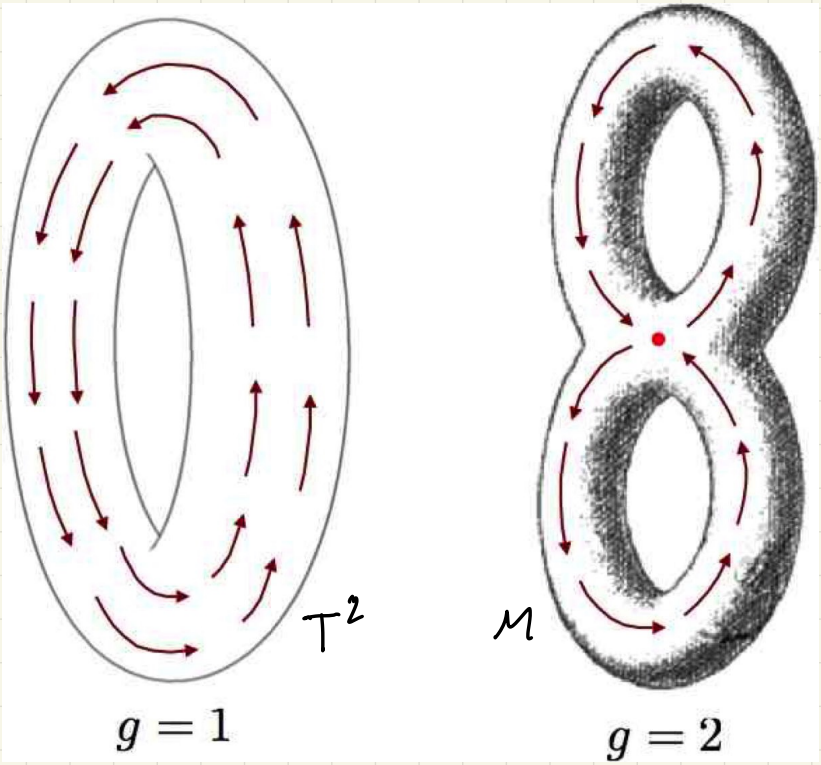
I.e. the index is a **winding number**. As an example, consider the case of the sphere, S^2:

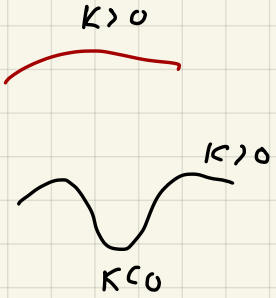


The sphere has genus $g=0$, so $\chi(S^2) = 2$, which must be the sum of indices of any smooth vector field $\vec{V}(\vec{x})$ on S^2 at its singularities.

Other examples, with $g > 0$:







If you take any 2-manifold M, you can continuously

deform it, changing its local geometry and thus its local Gaussian curvature $K(\vec{x})$, but the integral

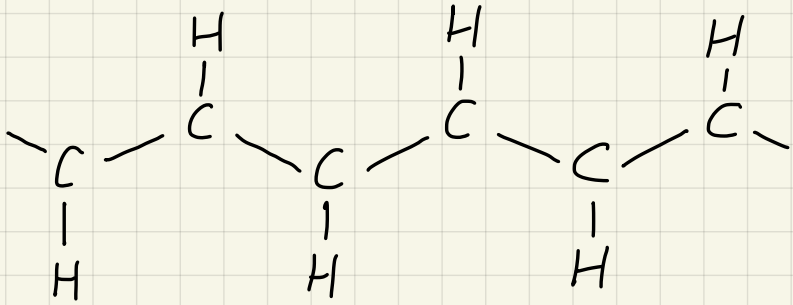
$$\frac{1}{2\pi}\int_M dS\, K(\vec{x}) = 2 - 2g_M$$

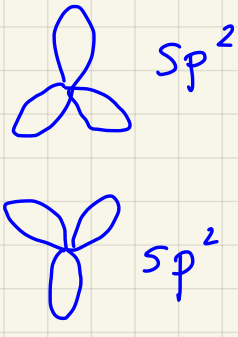
remains constant (and quantized), so long as one does not violate M. Gilbert's Two Commandments of Topology:

I. Thou shalt not cut.
II. Thou shalt not glue.

- **Su-Schrieffer-Heeger (SSH) model**

This is a model for the long chain polymer $(CH)_x$, known as polyacetylene ($x \sim 10^4$ is not difficult to achieve). The electronic structure of carbon is $1s^2 2s^2 2p^2$. In $(CH)_x$, the 1s electrons are tightly bound. The 2s, $2p_x$, and $2p_y$ orbitals engage in planar sp^2 hybridization, resulting in the backbone structure



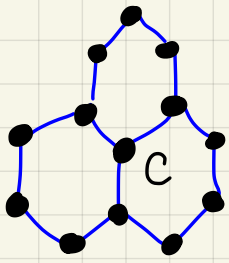


Each single bond represents a shared electron pair.

We now have one more e^- per carbon to assign, from the p_z (or π) orbital. Where do these electrons want to go? If we model the backbone as a $d=1$ chain along which the π-electrons hop, then

$$H = -t \sum_{n,\sigma} (c^\dagger_{n\sigma} c_{n+1\,\sigma} + c^\dagger_{n+1\,\sigma} c_{n\sigma})$$

$$= -2t \sum_{k,\sigma} \cos(ka)\, c^\dagger_{k\sigma} c_{k\sigma}$$

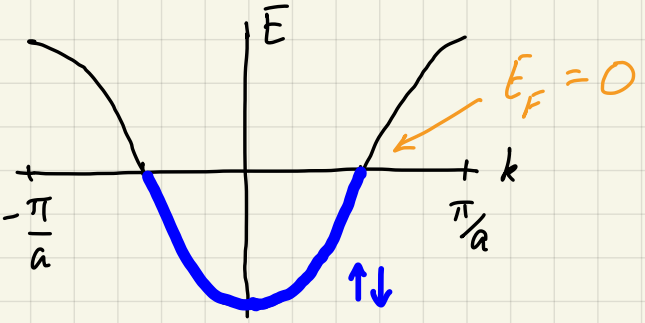


graphene

and thus $\varepsilon(k) = -2t\cos(ka)$. We populate this band with $\uparrow$ and $\downarrow$ π-electrons so that it is half-filled, corresponding to one electron per site:

This is a $d=1$ metal, with $k_F = \frac{\pi}{2a}$ and all states $k \in [-k_F, +k_F]$ filled.

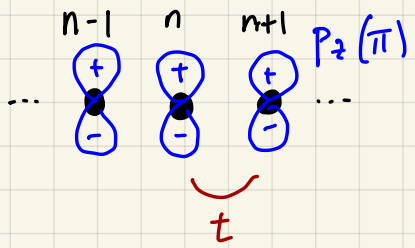
The ground state energy is then



$$E_0 = 2 \sum_{k=-\pi/a}^{+\pi/a} \varepsilon(k) = -4tNa \int_{-\pi/a}^{\pi/a} \frac{dk}{2\pi} \cos(ka) = -\frac{4Nt}{\pi}$$

spin

But we can do even better if we consider the effect of phonons. Let the displacement (along the backbone) of the n^{th} C atom be given by u_n with respect to the uniform spacing configuration. This means that the distance between C atoms n and $n+1$ is given by $u_{n+1} - u_n$. The hopping integral t should depend exponentially on this difference, i.e.



$$t_{n,n+1} = t\, e^{-\alpha(u_{n+1}-u_n)} \approx t\left(1-\alpha(u_{n+1}-u_n)+\dots\right)$$

We thus consider the following model,

$$H_{SSH} = -t\sum_n \left(1-\alpha(u_{n+1}-u_n)\right)\left(c^\dagger_{n\sigma}c_{n+1\sigma} + c^\dagger_{n+1\sigma}c_{n\sigma}\right) + \sum_n\left(\frac{p_n^2}{2M} + \frac{1}{2}K(u_{n+1}-u_n)^2\right)$$

modulation of hopping amplitude

carbon mass

phonon Hamiltonian

This is the SSH model. It describes interacting electrons and acoustic photons in a $d=1$ chain. We now entertain the possibility of **spontaneous dimerization**, writing

$$u_n = (-1)^n\zeta + \delta u_n$$

We will determine the dimerization amplitude ζ by energy minimization. The phonon Hamiltonian then becomes

$$H_{ph} = \underbrace{\sum_n\left[\frac{p_n^2}{2M} + \frac{1}{2}K(\delta u_{n+1}-\delta u_n)^2\right]}_{H^0_{ph}} + 2NK\zeta^2 + 4K\zeta\sum_n(-1)^n\delta u_n$$

We can express H^0_{ph} in terms of ladder operators, viz.

$$H^0_{ph} = \sum_k \hbar\omega_k\left(A^\dagger_k A_k + \frac{1}{2}\right)$$

where

$$A_k = \frac{1}{\sqrt{2\hbar M w_k}}\hat{p}_k + \sqrt{\frac{M w_k}{2\hbar}}\,\delta\hat{u}_k$$

with

$$\begin{Bmatrix}\hat{p}_k \\ \delta\hat{u}_k\end{Bmatrix} = \frac{1}{\sqrt{N}}\sum_n e^{-ikna}\begin{Bmatrix}p_n \\ \delta u_n\end{Bmatrix}$$

Let's now make the variational Ansatz $|\Psi_{var}\rangle = |\Psi_0^{el}\rangle \otimes |\Psi_0^{ph}\rangle$, where $|\Psi_0^{ph}\rangle$ is the ground state of H_{ph}^0, whose energy eigenvalue is

$$E_0^{ph} = \frac{1}{2}\sum_k \hbar w_k = 4N\hbar\sqrt{\frac{K}{M}}$$

Note that $\langle\Psi_0^{ph}|\delta u_n|\Psi_0^{ph}\rangle = 0$, and thus

$$\begin{aligned} H_{eff} &= \langle\Psi_0^{ph}|H_{SSH}|\Psi_0^{ph}\rangle \\ &= E_0^{ph} + 2NK\zeta^2 - \sum_\sigma\sum_{j=1}^{N/2}\left(t_1\, a_{j\sigma}^\dagger b_{j\sigma} + t_2\, b_{j\sigma}^\dagger a_{j+1,\sigma} + H.c.\right) \\ &= 4N\hbar\sqrt{\frac{K}{M}} + 2NK\zeta^2 + \sum_{q,\sigma}\begin{pmatrix}a_{q\sigma}^\dagger & b_{q\sigma}^\dagger\end{pmatrix}\begin{pmatrix}0 & t_1+t_2e^{-iq\tilde{a}} \\ t_1+t_2e^{iq\tilde{a}} & 0\end{pmatrix}\begin{pmatrix}a_{q\sigma} \\ b_{q\sigma}\end{pmatrix} \end{aligned}$$

where $a_{j\sigma} = c_{2j-1,\sigma}$, $b_{j\sigma} = c_{2j,\sigma}$, $\tilde{a} = 2a$, $q \in \left[-\frac{\pi}{\tilde{a}}, \frac{\pi}{\tilde{a}}\right]$ is the "reduced Brillouin zone", and $t_{1,2} = (1 \mp 2\alpha\zeta)t$. We now diagonalize H_{eff}, obtaining

$$H_{eff} = 4N\hbar\sqrt{\frac{K}{M}} + 2NK\zeta^2 + \sum_{q,\sigma}|t_1+t_2e^{-iq\tilde{a}}|\left(\gamma_{+q\sigma}^\dagger\gamma_{+q\sigma} - \gamma_{-q\sigma}^\dagger\gamma_{-q\sigma}\right)$$

with $\gamma_{\pm q\sigma} = \frac{1}{\sqrt{2}}(a_{q\sigma} \pm b_{q\sigma})$. The ground state energy of H_{eff} is

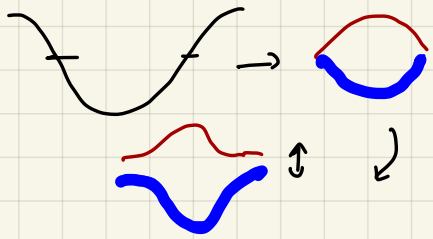
$$E^0_{var}(\zeta) = 4Nt\sqrt{\frac{K}{M}} + 2NK\zeta^2 - \frac{N}{4\pi}\int_{-\pi}^{\pi} d\theta \sqrt{t_1^2 + t_2^2 + 2t_1 t_2 \cos\theta}$$

where the subscript "var" reminds us this is a variational energy, i.e. $E^0_{var} = \langle \Psi_{var} | H_{SSH} | \Psi_{var} \rangle$. In the limit where $\alpha^2 t \ll K$, we have

$$\frac{E_0^{var}(\zeta)}{N} = 4t\sqrt{\frac{K}{M}} + 2K\zeta^2 - \frac{4t}{\pi} - \frac{8t}{\pi}\alpha^2\zeta^2 \ln\left(\frac{2}{\sqrt{e}\,\alpha\zeta}\right) + \cdots$$

and minimizing wrt ζ gives

$$\zeta^* = \frac{2}{\sqrt{e}\,\alpha} e^{-\pi K/4\alpha^2 t}$$



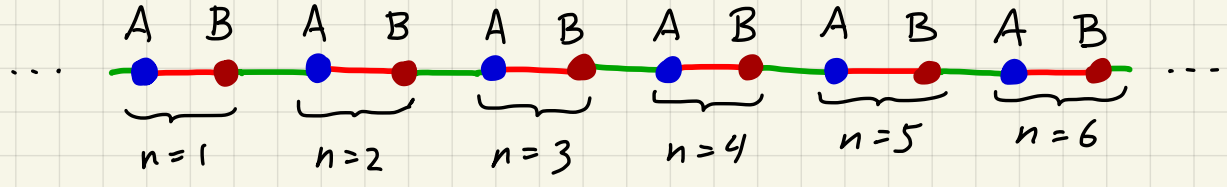
Thus, the system prefers to spontaneously dimerize!

Lecture 3 (Jan. 12) : Edge states in the SSH model

The effective Hamiltonian for the fermionic sector of the SSH model is

$$H = -\sum_{n=1}^{N_c} \left(t_1 a_n^\dagger b_n + t_2 b_n^\dagger a_{n+1} + H.C. \right)$$

where $N_c = \frac{1}{2}N$ is the number of unit cells, each of which contains one A site and one B site:



hopping amplitudes: t_1, t_2