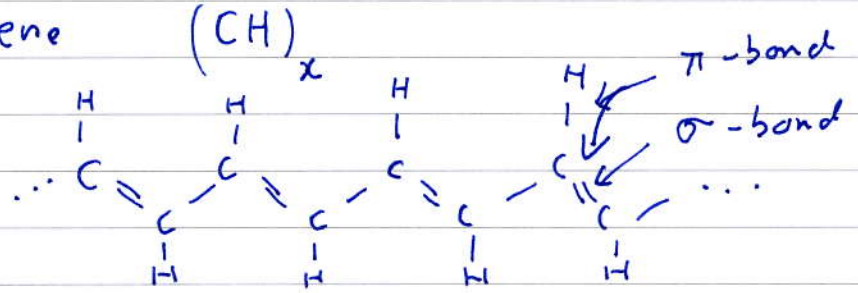
4 Aug 2018

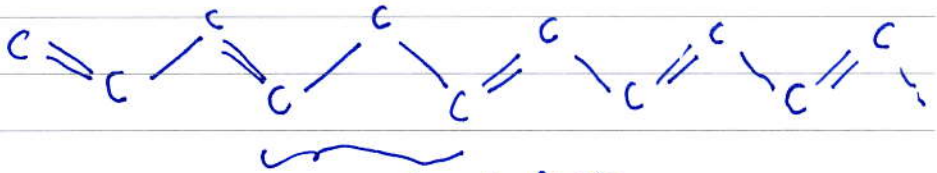
Su, Schrieffer, & Heeger (SSH) model
PRL 42, 1698 (1979).

The SSH model was proposed as a model for polyacetylene $(CH)_x$



This is called "conjugated" because of double / single bond alternation.

" "
Domain wall



topological defect.

Is this a phonon degree or electron degree or both?

For mathematical & conceptual simplicity we consider "spinless" electrons — the spin degeneracy merely gives a factor of 2

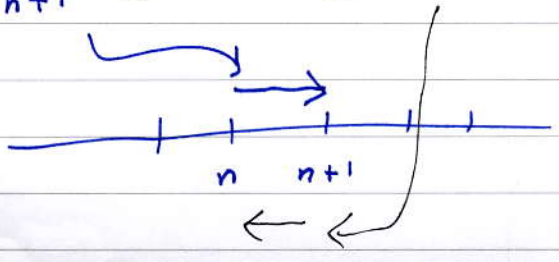
The Hamiltonian consists of

$$\hat{H} = \hat{H}_e + \hat{H}_p + \hat{H}_{ep}$$

Electron is tight-binding nearest hopping

$$\hat{H}_e = -t_0 \sum_{n=1}^{N} \left(c_{n+1}^{+} c_n + c_n^{+} c_{n+1} \right)$$

Here π-bond treated as electrons explicitly.



the term $C^+_{n+1} C_n$ means electron hops from the site n to $n+1$, its hermitian conjugate $(C^+_{n+1} C_n)^+ = C^+_n C_{n+1}$ denotes the reverse hop from $n+1$ to n.

Alternately we can write $\hat{H}_e = C^+ H C$

with $C = \begin{pmatrix} C_1 \\ C_2 \\ \vdots \\ C_n \\ \vdots \\ C_N \end{pmatrix}$ $H = \begin{bmatrix} \ddots & & & \\ & 0 & -t_0 & 0 \\ & -t_0 & 0 & -t_0 \cdots \\ & 0 & -t_0 & 0 \cdots \end{bmatrix}$

we may use periodic boundary condition $C_{n+N} \equiv C_n$

The existence of phonon is because σ-bond, treated adiabatically.

The phonon part is $H_p = \sum_n \frac{1}{2} M (\dot{x}_n)^2 + \frac{1}{2} \sum_n \tilde{K} (x_{n+1} - x_n)^2$

x is displacement M is mass, $\tilde{K}$ is force constant.

$[\tilde{K} x]$ = Newton's force. The site "n" denotes the -CH- as a whole, not separately C or H. Mass $M \simeq$ mass of carbon.

Let introduce $u_n = \sqrt{M}\, x_n$

then we prefer the mass normalized displacement u_n. Then

$$H_p = \sum_n \frac{1}{2} \dot{u}_n^2 + \frac{1}{2} K \sum_n (u_{n+1} - u_n)^2$$

Note $K = \frac{\tilde{K}}{M}$ which has units of ω^2 or $\frac{1}{\text{time}^2}$

Note $\dot{u}_n \equiv p_n$ is the conjugate momentum of u_n

The electron-phonon interaction term

$$\hat{H}_{ep} = \sum_n \alpha \left(u_{n+1} - u_n\right) c^\dagger_{n+1} c_n + h.c.$$

$$= \sum_{\ell n k} M^{\ell}_{nk} c^\dagger_n c_k u_\ell$$

M^{ℓ}_{nk} is the general form. For SSH model we take

$$M^{\ell}_{nk} = \begin{cases} \alpha & \text{if } n = k+1, \ \ell = n \\ & \text{or if } n+1 = k \quad \ell = k \\ -\alpha & \ldots \quad \ell = k \\ & \qquad\qquad\quad \ell = n \\ 0 & \text{otherwise} \end{cases}$$

Note. My α is not SSH PRL 'α' as my u is $\sqrt{M}\times$ so the α's differ by $\sqrt{M}$.

There are three parameters in the SSH model

hopping t_0

Spring constant normalized by $\sqrt{\text{Mass}}$ K

Electron-phonon coupling α

What values to take for polyacetylene? we can ask Tianqi to do a first-principles calculation to find out.

SSH ~~My~~ rough estimate $t_0 \sim 2.5\,eV = \frac{10}{4}\,eV$

$$\tilde{K} = M\underline{K} = 21\ eV/\text{Å}^2$$

Mass of carbon is $M = 12\,u$ $\quad u = 1.66\times10^{-27}\ kg$

↑ atomic mass unit

So $K = \frac{21}{12} = 1.75\ eV/(u\,\text{Å}^2)$

According to SSH : $\frac{\alpha\sqrt{M}}{t_0} = 1.65\ \text{Å}^{-1}$ v.s.

or $\alpha = 1.65 \times 2.5 \times \sqrt{12}$ eV/(√u Å)

$= 14.3$ eV·√u·Å

$= \frac{1.65 \times 2.5}{\sqrt{12}} = 1.19$ eV(√u Å)

It appears a natural set of units is

Energy	E_0	$= 1\text{eV}$	$= 1.6 \times 10^{-19}$ J
length	L_0	$= 1\text{Å}$	$= 10^{-10}$ m
mass	M_0	$= 1\text{u}$	$= 1.66 \times 10^{-27}$ Kg

In this units we have

$t_0 = 2.5$ $\quad M = 12$

$K = 1.75$

$\alpha = 1.19$

} all numbers are order 1. However $\hbar \neq 1$

We also need $\hbar$. in e.g. $i\hbar\frac{\partial\psi}{\partial t} = H\psi$

what is $\hbar$ in eV, Å, u units ?

$\hbar = 1.0546 \times 10^{-34}$ J s

$= \frac{1.0546 \times 10^{-34}\ \text{J s}}{E_0 \cdot \sqrt{\frac{M_0 L_0^2}{E_0}}} = 0.064\ \sqrt{\text{eV u}\cdot\text{Å}^2}$

$\hbar \approx 0.064$ ← bad thing about $\hbar \neq 1$ is

E and ω don't have the same value $E = \hbar\omega$.

t_0, K, α in atomic units. 5 Aug 2018

In atomic unit $E_0 = 27.2$ eV = 1 hartree

$$t_0 = \frac{2.5}{27.2} = 0.092 \text{ hartree}$$

$$K = 1.75 \frac{\frac{1}{27.2} \text{ hartree}}{1836 m_e \cdot \left(\frac{1}{0.53} a_0\right)^2}$$

$a_0 = 0.53$ Å

m_e : electron mass

$$= 0.0000098 \text{ hartree}/(m_0 a_0^2)$$

$$\approx 10^{-5} \text{ atomic units (very small)}$$

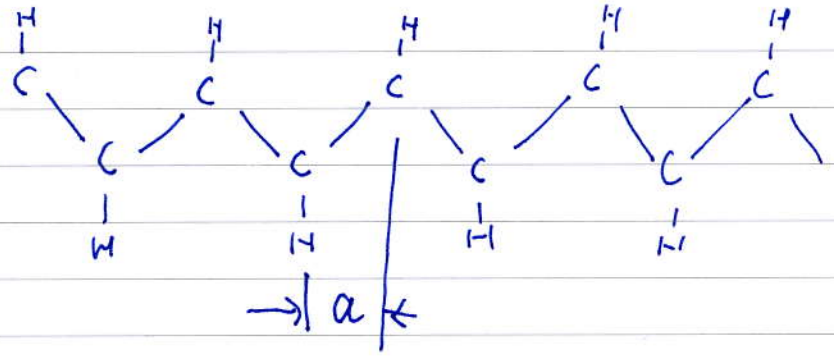
a_0 : Bohr radius

$$\alpha = 1.19 \text{ eV}(\sqrt{u}\ \text{Å}) \quad \text{hartree}\sqrt{m_e}\, a_0$$

$$= 1.19 \frac{1}{27.2} \sqrt{1836} \cdot \frac{1}{0.53}$$

$$\approx 9.62 \text{ atomic units.}$$

The lattice constant $a = 1.22$ Å



a is the value before dimerization with one unit of CH group per cell.

Born-Oppenheimer approximation / peierls instability.

In the SSH original PRL and in PRB, 22, 2099 (1980), they are interested in the soliton, which is the phonon degree of freedom

Here, we are interested in the electronic degree of freedom and considers the phonons as a thermal bath.

We consider two situations

1) $\mu = 0$ we have a lot of electrons, i.e. at $\mu = 0$ we have $\frac{1}{2}$ electron per site (our electron has no spin). This is the real polyacetylene at no doping situation

2) We have very low electron concentration. so low so that practically, we have only 1 electron in an infinite lattice. In such low carrier concentration regime we can use diffusion to study electron transport.

i.e. $\sigma = en\mu$, $\mu = \beta e D$, $D = \frac{\langle x^2 \rangle}{2t}$ $t \to \infty$

D is diffusion constant, $e = |e| > 0$ is charge
μ is mobility
σ is conductivity
n is carrier density $n = \frac{N}{AL}$ or Δn is # of electron per unit length.

In the low n limit electrons do not dimerize. No π electrons, only σ (system) electrons

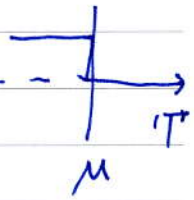
However, if $n \neq 0$, a uniform chain is unstable with respect to the charge of ion positions. This is known as Peierls instability.

We need to solve the "Born-Oppenheimer" problem first. which is find the ground state of electrons fixing u_n

$$E(u_n) = \sum_k \varepsilon_k f_k + \text{potential energy} \quad \beta \to \infty$$

subject to $\sum_k f_k = N$

here we take $T = 0$ and f_k is a step function



since u_n is fixed, $\dot{u}_n = 0$ we need to diagonalize the Hamiltonian

$$\tilde{H} = -\sum_n \left(t_0 - \alpha(u_{n+1} - u_n)\right) c^+_{n+1} c_n + h.c.$$

electron + electron-phonon interaction

$$\tilde{H}\varphi_k = \varepsilon_k \varphi_k$$

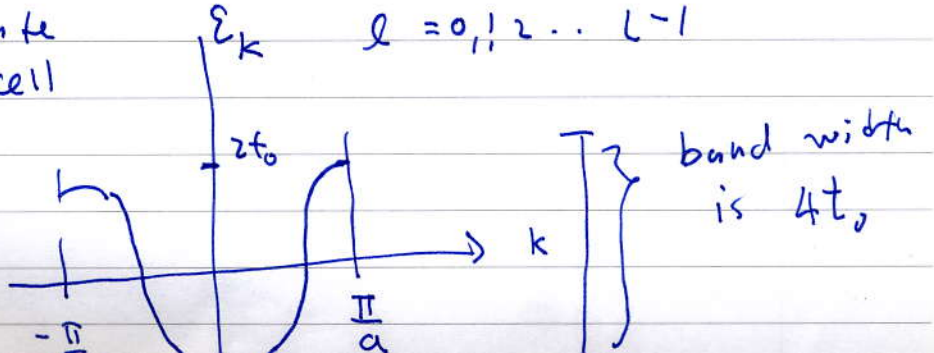
the potential energy is $\frac{1}{2} K \sum_n (u_{n+1} - u_n)^2$

If $\alpha = 0$, then it is clear the true ground state of the full system is (equilibrium lattice $u_n \equiv 0$) and electron state is to fill the band to the fermi-level.

When $\alpha = 0$ $\quad \tilde{H} = -t_0 \sum_n c^+_{n+1} c_n + h.c.$

$$\varepsilon_k = -2t_0 \cos(ka) \qquad k = \frac{2\pi l}{L \cdot a}$$

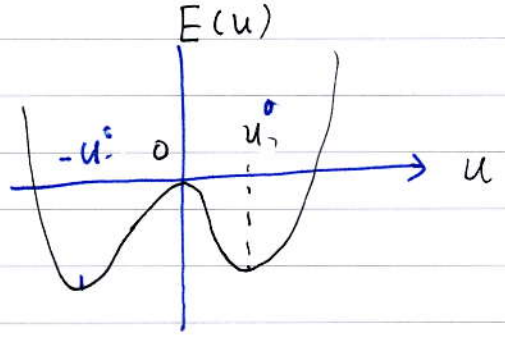
We assume a finite system of L unit cell



When $\alpha \neq 0$, we really need to solve the eigenvalue problem for electrons but that is not really possible analytically. Let make good guess. We assume the over all ground state of the whole system is at

$$u_n = (-1)^n u^0$$

And E v.s. u^0 takes the form so $u_n \equiv 0$ is a maxima instead of a minima. There are two minima located at



$$\pm \frac{u^0}{\sqrt{M}} = \pm 0.04 \text{ Å} \quad \text{is small}$$

problem: Find the functional form of $E(u)$, determine u^0 by $\frac{\partial E}{\partial u} = 0$.

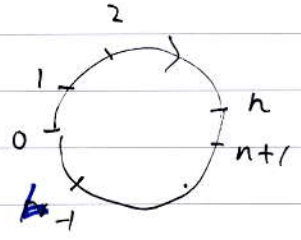
Take periodic boundary condition such that site n and site $n+L$ are the same, $C_n \equiv C_{n+L}$

then

$$\hat{H}^e = -t\, C_0^\dagger C_1 - t C_1^\dagger C_2 - t C_2^\dagger C_3 - \cdots + h.c.$$

$C_{L-1}^\dagger C_0$

before dimerization ($\alpha = 0$)



Let $C_n = \frac{1}{\sqrt{L}} \sum_k e^{inak} C_k$

this is plane wave $e^{i\vec{k}\cdot\vec{R}}$

$k \in 1BZ$ with L points

so $-t \sum_n C_n^\dagger C_{n+1} = -t \frac{1}{L} \sum_{n,k,k'} e^{-inak} e^{i(n+1)ak'} C_k C_{k'}$

$= -t e^{iak'} \frac{1}{L} \sum e^{ina(k'-k)} C_k^\dagger C_{k'} = \sum -t e^{iak} C_k^\dagger C_k$

"hermitian conjugate"

$-te^{ika}$ + h.c.

Adding h.c. part we get

$$\hat{H}_0 = -t\sum_n c_n^+ c_{n+1} + h.c. = \sum_k \varepsilon_k c_k^+ c_k$$

$$\varepsilon_k = -2t\cos(ka)$$

Hamilt is digd automatically by Fourr transform.

When we have a dimerized phonon ground state,

$u_n = (-1)^n u^0$

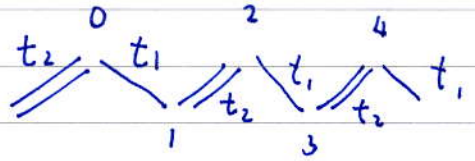
or $u_0 = u^0$ $u_1 = -u^0$, $u_2 = u^0$, $u_3 = -u^0$, etc

the hopping is $t_{01} = t^0 - \alpha(u_0 - u_1) = t^0 - 2\alpha u^0 \equiv t_1$

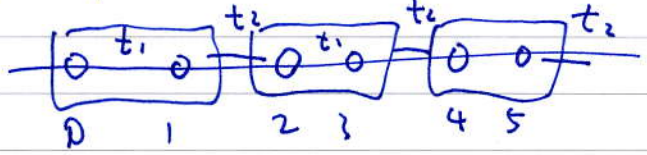
$t_{12} = t^0 - \alpha(u_1 - u_2) = t^0 + 2\alpha u^0 \equiv t_2$

or Hamilt of electron becomes

$$H_e = -t_1 c_0^+ c_1 - t_2 c_1^+ c_2 - t_1 c_2^+ c_3 - t_2 c_3^+ c_4 \cdots + h.c.$$



To diagonalize this Hamilton we need take two degrees per cell.



so let $c_{2n} = \frac{1}{\sqrt{L/2}} \sum_{k \in \text{half of orig BZ}} e^{i(2n)a\cdot k} c_k^e$ ← even

$c_{2n+1} = \frac{1}{\sqrt{L/2}} \sum_k e^{i(2n)a\cdot k} c_k^o$ ← odd

$k = \frac{2\pi l}{(L/2)\cdot 2a}$ $l = 0, 1, 2 \ldots \frac{L}{2} - 1$

Then the Hamiltonian in k-space is

$$H^e = -\left[\sum_{n=0}^{L/2} t_1 \left(C_{2n}^{\dagger} C_{2n+1}\right) + t_2 C_{2n+1}^{\dagger} C_{2n+2}\right] + h.c.$$

$$\sum_{n=0}^{L/2} C_{2n}^{\dagger} C_{2n+1} = \frac{1}{L/2} \sum_{kk'} \sum_{n} e^{-i 2n a k + i(2n) a \cdot k'} C_k^{e\dagger} C_{k'}^{o}$$

$$= \frac{1}{L/2} \sum_{kk'} \sum_{n} \underbrace{e^{i(2n)a(k'-k)}}_{\delta_{kk'} \cdot L/2} \quad \text{in } C_k^{e\dagger} C_{k'}^{o}$$

$$= \sum_k C_k^{e\dagger} C_k^{o} + C_k^{o\dagger} C_k^{e}$$

$$\sum_{n=0}^{L/2} C_{2n+1}^{\dagger} C_{2n+2} = \frac{1}{L/2} \sum_{kk'} \sum_{n} e^{-i 2n a k} e^{i(2n+2) a \cdot k'} \left(C_k^{o}\right)^{\dagger} C_{k'}^{e}$$

$$= \sum_k e^{i 2 a k} \left(C_k^{o}\right)^{\dagger} C_k^{e} + e^{-i 2 a k} \left(C_k^{e}\right)^{\dagger} C_k^{o}$$

so we have in k space (even sites ↙)

$$H^e = \sum_k \begin{pmatrix} C_k^{e\dagger} & C_k^{o\dagger} \end{pmatrix} \begin{pmatrix} 0 & -t_1 - t_2 e^{-i 2 a k} \\ -t_1 - t_2 e^{i 2 a k} & 0 \end{pmatrix} \begin{pmatrix} C_k^{e} \\ C_k^{o} \end{pmatrix} \leftarrow \text{odd sites}$$

$$H(k) = \begin{pmatrix} 0 & -t_1 - t_2 e^{-i 2 a k} \\ -t_1 - t_2 e^{i 2 a k} & 0 \end{pmatrix} \qquad 2ak = 2\pi$$

we see $H(k) = H\left(k + \frac{\pi}{a} l\right)$ is periodic with period $\frac{\pi}{a}$

$$H^e = \sum_k C^{\dagger}(k) H(k) C(k)$$

$C(k)$: 2×1 vector

The Hamiltonian of the electrons can be further diagonalized by $(H(k) - \varepsilon)\psi_k = 0$ $\psi_k = \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$

or $\det \begin{pmatrix} -\varepsilon & -(t_1 + t_2 e^{-i2ak}) \\ -(t_1 + t_2 e^{i2ak}) & -\varepsilon \end{pmatrix} = 0$

or $\varepsilon^2 - (t_1 t_2 e^{-i2ak})(t_1 + t_2 e^{i2ak}) = 0$

$$\rightarrow \quad \varepsilon_k = \pm \sqrt{t_1^2 + t_2^2 + 2 t_1 t_2 \cos(2ak)}$$

If $t_1 = t_2 = t_0$ then $\varepsilon_k = \pm 2 t_0 \cos(ak)$ which is correct result.

use $t_1 = t^0 - 2\alpha u$ u is amplitude in $u_n = (-1)^n u$

$t_2 = t^0 + 2\alpha u$

we also have

$$\varepsilon_k = \pm \sqrt{(t^0 - 2\alpha u)^2 + (t^0 + 2\alpha u)^2 + 2(t^0 - 2\alpha u)(t^0 + 2\alpha u)\cos(2ak)}$$

$$= \pm \sqrt{2 t_0^2 + 8\alpha^2 u^2 + 2(t_0^2 - 4\alpha^2 u^2)\cos(2ak)}$$

$$= \pm \sqrt{2 t_0^2 (1 + \cos(2ak)) + 8\alpha^2 u^2 (1 - \cos(2ak))}$$

$$= \pm \sqrt{4 t_0^2 \cos^2(ak) + 16 \alpha^2 u^2 \sin^2(ak)} \equiv \pm \sqrt{(\varepsilon_k^0)^2 + \Delta_k^2}$$

here $\varepsilon_k^0 = -2 t_0 \cos(ak)$ is the dispersion when $\alpha = 0$

$\Delta_k = 4\alpha u \sin(ak)$ is the gap.

we used the trigonomic relation

$$\frac{1+\cos(2\theta)}{2} = \cos^2\theta = \left[\frac{e^{i\theta}+e^{-i\theta}}{2}\right]^2$$

$$\frac{1-\cos(2\theta)}{2} = \sin^2\theta$$

Let the diagonized Hamilton be

$$H^e = \sum_{k\,m} \varepsilon_{km}\, \tilde{c}^{+}_{km}\, \tilde{c}_{km}$$ to find the relation

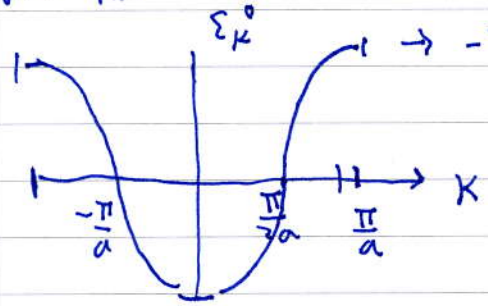
between $\tilde{c}_{km}$ $m=1,2$ for the two braches to

c^e_k and c^o_k we need the eigenvectors of $H(k)$.

Band structure

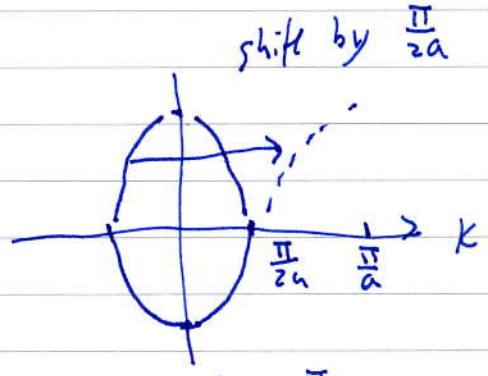
If $\alpha = 0$ and use unit cell of latte constant a

we have one branch



$\equiv$

shift by $\frac{\pi}{2a}$



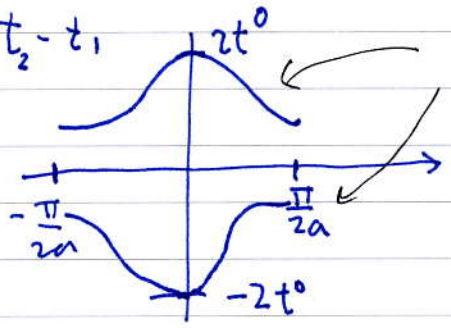
two branch $\to \pm\varepsilon_k$

If $\alpha \neq 0$ a gap devep at BZ bound $ak = \frac{\pi}{2}$

$\Delta = 4\alpha u = t_2 - t_1$

$\pm\sqrt{(\varepsilon^o_k)^2 + \Delta_k^2}$

gap is 2Δ

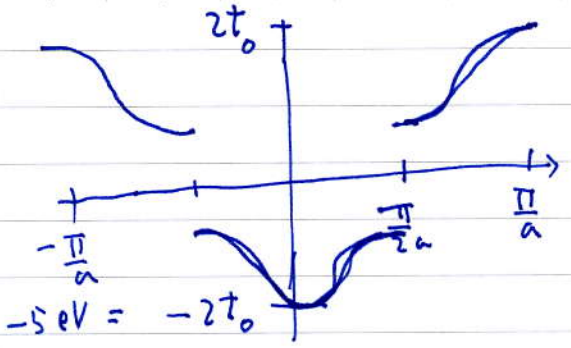


$\leftarrow$ latte is $(2a)$

Due to gap, metal becomes an insulator.

Note $E_g = 2\Delta = 8\alpha u = 2(t_2 - t_1)$ is the band gap!

We could represent the band with 2 branches by the extended BZ of $-\frac{\pi}{a}$ to $\frac{\pi}{a}$, then



gap $= 2\Delta = 8\alpha u = 1.4$ eV

for polyacetylene $t_0 = 2.5$ eV

To determine the stable u, we need to compute $E(u)$ and find minimum u. μ is fermi energy

$$E(u) = \sum_k \varepsilon_k \theta(\mu - \varepsilon_k) + \frac{1}{2} K \sum_n (u_{n+1} - u_n)^2$$

electron energy — potential of phonon

$u_{n+1} - u_n = \pm 2u$

$$= L \cdot a \int_{-\frac{\pi}{a}}^{+\frac{\pi}{a}} \left(\frac{dk}{2\pi}\right) \varepsilon_k \theta(\mu - \varepsilon_k) + 2K u^2 \cdot L$$

we use extended BZ as shown above

$$= L \cdot a \int_{-\infty}^{\mu} d\varepsilon\, D(\varepsilon)\, \varepsilon + 2K u^2 \cdot L$$

Here $D(\varepsilon)$ is the density of state associated with the dispersion relation $\varepsilon_k = \pm \sqrt{(\varepsilon_k^0)^2 + \Delta_k^2}$.

$$D(\varepsilon) = \frac{1}{L \cdot a} \sum_k \delta(\varepsilon - \varepsilon_k)$$

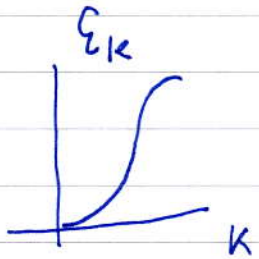
density of state per unit length.

See page 167 for a type shape of $E(u)$.

The integral $\int_{-\infty}^{\mu} d\varepsilon \ldots$ can be performed analytically and can be related to elliptical integral.

Density of state $D(\varepsilon)$ in 1D is proportional to the group velocity $v_{k(\varepsilon)}$

Let $\int \frac{dk}{2\pi} F(\varepsilon_k) = \int d\varepsilon\, D(\varepsilon) F(\varepsilon)$



here $F(x)$ is some arbitrary function.

Focusing on the $k>0$ part of the dispersion curve ε_k, we have a unique $k \leftrightarrow \varepsilon$ relation

so $d\varepsilon_k = \frac{\partial \varepsilon_k}{\partial k} dk$ (k is wave vector $[k] = \frac{1}{a}$)

$= \frac{\partial \varepsilon_k}{\partial \hbar k} \hbar dk = v_k \hbar dk$ $\hbar k = p$ is momentum

$v_k = \frac{\partial}{\hbar \partial k} \varepsilon_k$ is group velocity. If $\varepsilon_k = \frac{(\hbar k)^2}{2m}$

$v_k = \frac{\partial \varepsilon_k}{\partial \hbar k} = \frac{\hbar k}{m} = \frac{p}{m}$

so $\int \frac{dk}{2\pi} F(\varepsilon_k) = \int \frac{d\varepsilon_k}{2\pi \hbar v_k} F(\varepsilon_k) = \int d\varepsilon \frac{1}{2\pi \hbar v_k} F(\varepsilon)$

Since $k \leftrightarrow \varepsilon$ is one to one we should invert the relation to find $v_k \equiv v_{k(\varepsilon)} = v(\varepsilon)$

i.e. group velocity as a function of energy.

However, for each ε, we have two wavevector $-k$ and $+k$. So the # of states is two times larger i.e.

$$D(\varepsilon) = \frac{1}{2\pi \cdot \hbar v(\varepsilon)} \cdot 2 = \frac{1}{\pi \hbar v(\varepsilon)}.$$

Uniform 1D electron chain $a \equiv 0$ then

$\varepsilon_k = -2t \cos(ak)$ with hopping t

Group velocity is $\frac{\partial \varepsilon}{\hbar \partial k} = (-2t)\frac{(-a)}{\hbar} \sin(ak)$

So uniform 1D chain $V_k = \frac{2ta}{\hbar}\sin(ka)$

But we need to express V_k as a function of energy

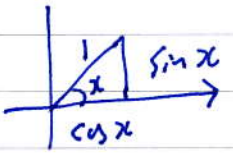
$\varepsilon = -2t\cos(ak)$

$\sin(ka) = \sqrt{1-\cos^2(ka)}$

$k>0$

$\sin^2(x)+\cos^2(x)=1$

$\sin(ka) = \sqrt{1-\left(\frac{\varepsilon}{2t}\right)^2}$



So $V(\varepsilon) = \frac{2ta}{\hbar}\sqrt{1-\left(\frac{\varepsilon}{2t}\right)^2}$

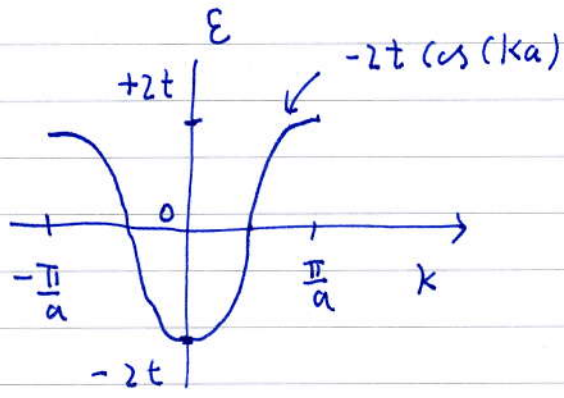
so the uniform 1D chain (not counting spin degeneracy) is

$$D(\varepsilon) = \frac{1}{2\pi\hbar V(\varepsilon)}\cdot 2 = \frac{1}{\pi\hbar}\cdot\frac{1}{\sqrt{1-\left(\frac{\varepsilon}{2t}\right)^2}}\cdot\frac{1}{\frac{2ta}{\hbar}}$$

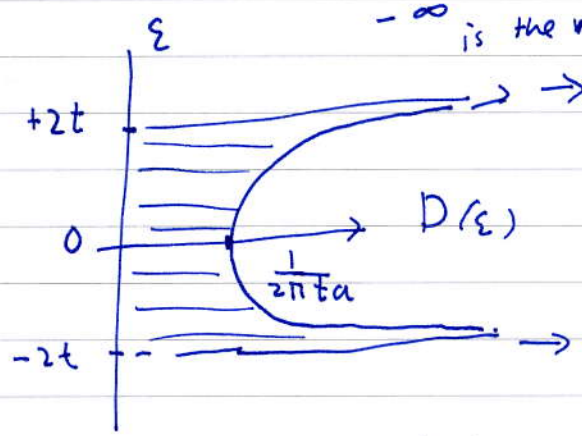
$$= \frac{1}{2\pi}\cdot\frac{1}{ta}\frac{1}{\sqrt{1-\left(\frac{\varepsilon}{2t}\right)^2}} = \frac{1}{2\pi ta}\frac{1}{\sqrt{\left(1-\frac{\varepsilon}{2t}\right)\left(1+\frac{\varepsilon}{2t}\right)}}$$

$D(\varepsilon)$ diges as $\frac{1}{\sqrt{x}}$ at $\varepsilon = \pm 2t$

$\int_{-\infty}^{+\infty} D(\varepsilon)\,d\varepsilon = \frac{1}{a}$ is the normalization



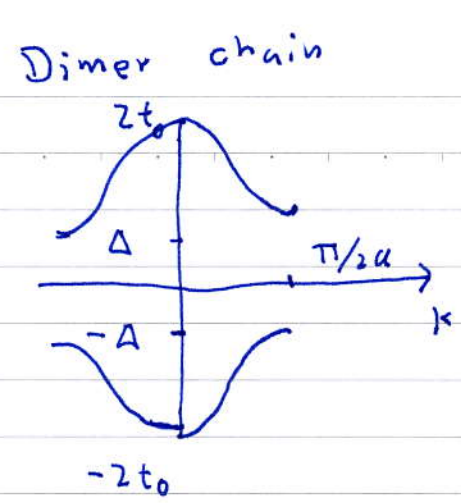
Dispersion relation
ε vs k

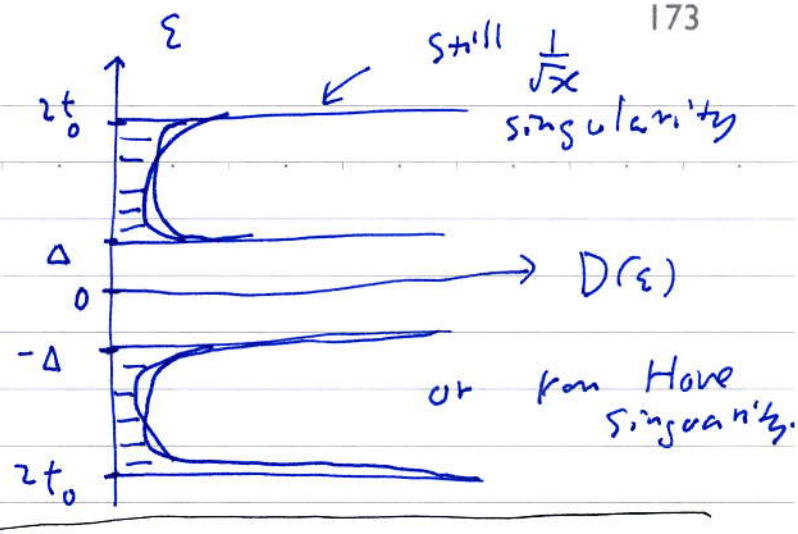


density of state
ε vs D

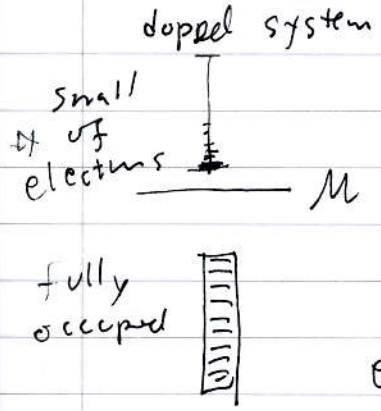
Density of state for the dimerized chain with $\alpha \neq 0$ is (work this out using group velocity)

$$D(\varepsilon) = \begin{cases} \frac{1}{\pi a}\cdot\frac{|\varepsilon|}{\sqrt{(4t_0^2-\varepsilon^2)(\varepsilon^2-\Delta^2)}} & \Delta \le |\varepsilon| \le 2t_0 \\ \Delta = 4\alpha u & \text{otherwise} \end{cases}$$





What is electron, phonon, ep interaction in this case when system is dimerized?



If μ is in the gap, gap is large, then the electron in the valence band do not conduct, we have very few carriers that contribute to electric current. So the valence band with energy $\varepsilon < 0$ should be treated "adiabatically", ie. they contribute to phonon potential only. Since the system is dimerized, we expect phonon should at least have two bands.

$$K_1 \quad K_2 \quad K_1 \quad K_2 \quad K_1$$
$$\sim\!\!\sim O \sim\!\!\sim O \sim\!\!\sim O \sim\!\!\sim O \sim\!\!\sim O \cdots$$

What is K_1, K_2 ??

$$\text{or} \quad K_{ij} = \frac{\partial E^{tot}(\Delta u_1, \Delta u_2 \cdots)}{\partial \Delta u_i \, \partial \Delta u_j} \; ?$$

How to compute the force constant?

$$u_n = u_n^0 + \Delta u_n$$
$$\uparrow \text{ dimer equation position}$$

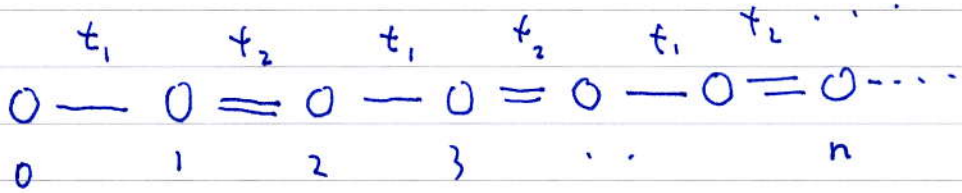
What is EPI ?

See arXiv: 1509.02295
Asbóth, Oroszlány, Pályi "A short course on Topological Insulators"

7 Aug 2018

SSH model as a topological insulator

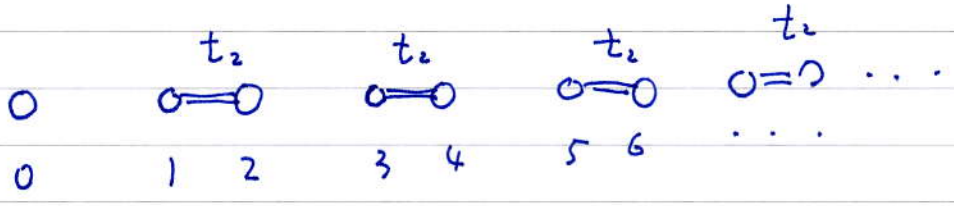
Consider a semi-infinite SSH chain with sites 0, 1, 2, 3 . .



$t_1 = t^0 - 2\alpha u^0$ we assue $t_1 < t_2$
$t_2 = t^0 + 2\alpha u^0$ $(\alpha > 0 \quad u^0 > 0)$

$$H = -t_1 c_0^\dagger c_1 - t_2 c_1^\dagger c_2 - t_1 c_2^\dagger c_3 - \cdots \text{h.c.}$$

Let's consider the limit case of $t_1 = 0$, $t_2 > 0$
then the model becomes



then the Hamilton is

$$\hat{H} = C^\dagger H C = -t_2 c_1^\dagger c_2 - t_2 c_3^\dagger c_4 \cdots \text{h.c.}$$

or $C = \begin{bmatrix} c_0 \\ c_1 \\ c_2 \\ \vdots \\ c_n \\ \vdots \\ \infty \end{bmatrix}$

$$H = \begin{array}{c} \\ 0 \\ 1 \\ 2 \\ 3 \\ 4 \\ \vdots \end{array} \begin{array}{c} \begin{array}{ccccc} 0 & 1 & 2 & 3 & 4 \end{array} \\ \begin{bmatrix} 0 & 0 & 0 & \cdot & \cdot \\ 0 & 0 & -t_2 & & \\ 0 & -t_2 & 0 & 0 & 0 \\ \cdot & 0 & 0 & 0 & -t_2 \\ \cdot & & & -t_2 & 0 \\ \cdot & & & 0 & 0 \end{bmatrix} \end{array}$$

We see the Hamilton is block diagonal with

$H_0 = (0) = (0)$ $\qquad H_n = \begin{pmatrix} 0 & -t_2 \\ -t_2 & 0 \end{pmatrix}$ ∞ times

The eigen system of the semi-infinite hamiltonian

$$H = \begin{bmatrix} 0 & 0 & \cdots \\ 0 & 0 & -t_2 \; 0 \; 0 \\ & -t_2 & 0 \quad 0 \; 0 \\ 0 & 0 & 0 \quad 0 \; -t_2 \\ & & -t_2 \; 0 \end{bmatrix}$$

is eigenvalue $\varepsilon_0 = 0$, eigen vector $\psi_0 = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$

$$H\psi_0 = 0\psi_0$$

This is the zero-energy mode.

For the $\begin{bmatrix} 0 & -t_2 \\ -t_2 & 0 \end{bmatrix}$ block $\rightarrow (H-\varepsilon)\psi = 0$

$$\det \begin{bmatrix} \varepsilon & t_2 \\ t_2 & \varepsilon \end{bmatrix} = 0 \qquad \varepsilon^2 - t_2^2 = 0 \rightarrow \varepsilon = \pm t_2$$

$\det \begin{pmatrix} a & b \\ c & d \end{pmatrix} = ad - cb$ eigenvector is $\begin{bmatrix} \varepsilon & t_2 \\ t_2 & \varepsilon \end{bmatrix} \begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$

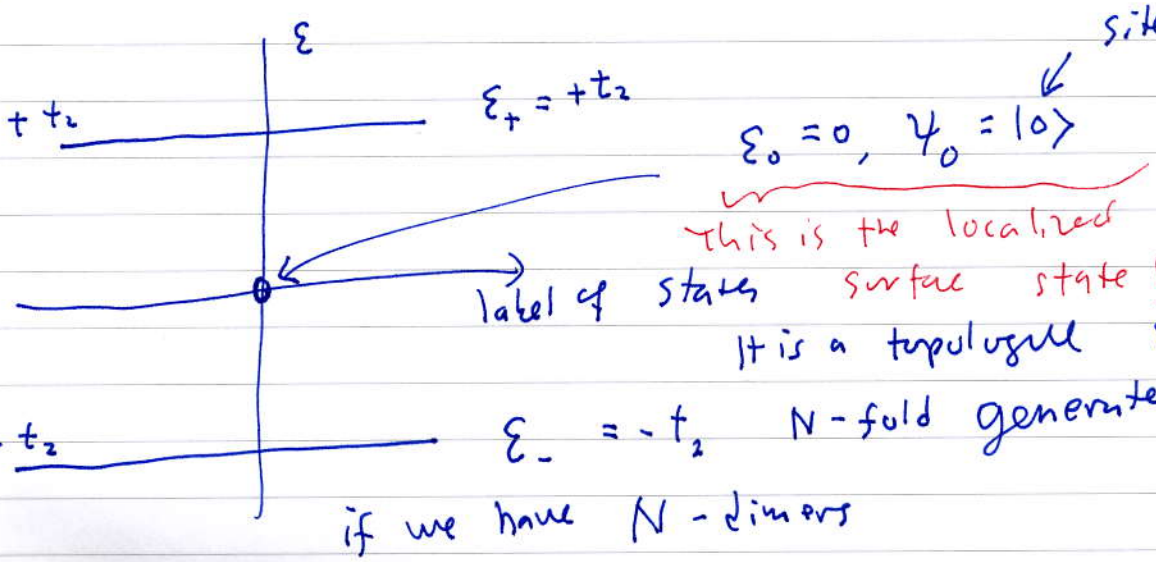
If $\varepsilon = -t_2$ $\begin{bmatrix} -t_2 & t_2 \\ t_2 & -t_2 \end{bmatrix} \begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \rightarrow \psi_1 - \psi_2 = 0 \rightarrow$

$$\psi_- = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

if $\varepsilon = t_2$ $\begin{bmatrix} t_2 & t_2 \\ t_2 & t_2 \end{bmatrix} \begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \rightarrow \psi_1 + \psi_2 = 0$ $\quad \psi_+ = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix}$

$$\langle \psi_- | \psi_+ \rangle = 0$$

We can use the following "band" diagram to describe the situation



if we have N-dimers

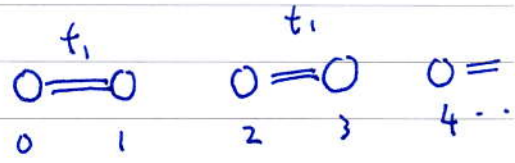
$\varepsilon = \varepsilon_- = -t_2$ $\psi_- = \frac{1}{\sqrt{2}} (|n\rangle + |n+1\rangle)$ $\quad n = 1, 3, 5, 7 \cdots$

Opposite limit $t_1 > 0$, $t_2 = 0$

$$\hat{H} = -t_1 c_0^\dagger c_1 - t_1 c_2^\dagger c_3 - t_1 c_4^\dagger c_5 \cdots + h.c.$$

$$H = \begin{array}{c} \\ 0 \\ 1 \\ 2 \\ 3 \\ \vdots \end{array} \begin{array}{c} \begin{array}{cccc} 0 & 1 & 2 & \cdots \end{array} \\ \begin{bmatrix} 0 & -t_1 & 0 & 0 & \\ -t_1 & 0 & 0 & 0 & \\ 0 & 0 & 0 & -t_1 & \cdots \\ 0 & 0 & -t_1 & 0 & \\ & & \vdots & & \end{bmatrix} \end{array}$$

For this case we have



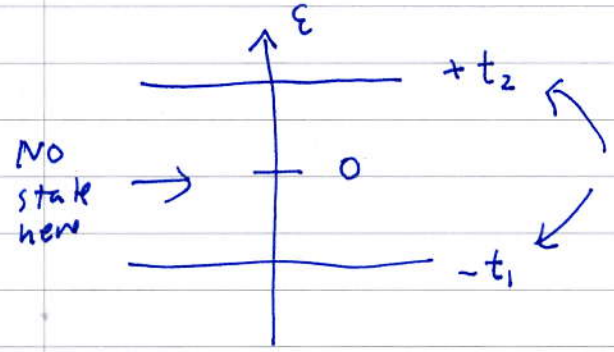
We have no isolated single site. all of them are dimers with Hamiltonian block $\begin{bmatrix} 0 & -t_1 \\ -t_1 & 0 \end{bmatrix}$

so Eigen energy is $\epsilon_- = -t_1$ $\psi_- = \frac{1}{\sqrt{2}}(|n\rangle + |n+1\rangle)$

$\epsilon_+ = +t_1$ $\psi_+ = \frac{1}{\sqrt{2}}(|n\rangle - |n+1\rangle)$

$n = 0, 2, 4, \cdots$

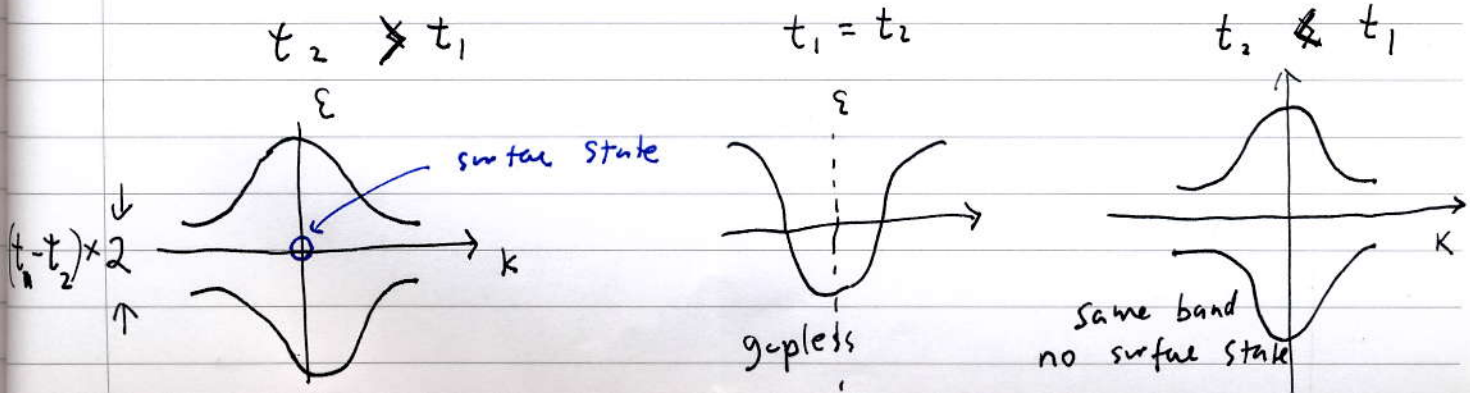
The dispersion (band structure) is



← This case is topologically trivial

We can consider the horizontal axis as K so it is a flat-band. but it is just any label e.g. site n.

The general cases



Winding number of the Hamiltn $H(k)$ and edge state — why the local real edge states is topological?

Take into account translational invariance with periodic boundary condition, the Hamiltn can be expressed in k space as

$$\hat{H} = \sum_k C^\dagger(k)\, H(k)\, C(k)$$ see page 161

Here $C(k) = \begin{pmatrix} c^e(k) \\ c^o(k) \end{pmatrix}$ ← even site ← odd site

and $H(k)$ is 2×2. Since we have two degres of freedom per unit cell.

$$H(k) = \begin{bmatrix} a(k) & c^*(k) \\ c(k) & b(k) \end{bmatrix} = \alpha_0(k) I + d_x(k)\sigma_x + d_y(k)\sigma_y + d_z(k)\sigma_z$$

are the most general hamiltn. So the space or manifold of Hamiltnis of this form is 4 dimensional in real space. However fr SSH model we have

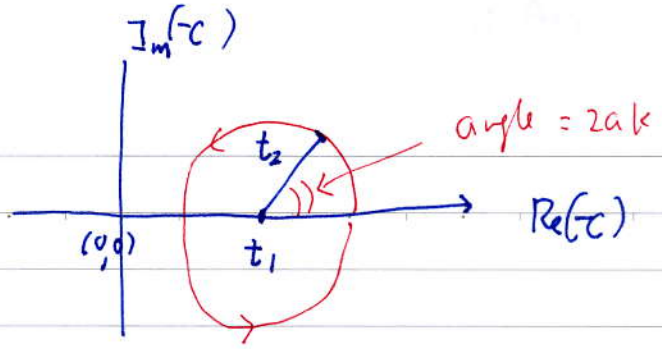
$$a(k) = b(k) = 0, \qquad c(k) = -t_1 - t_2 e^{2i a k}$$

$H(k) = H\left(k + \frac{2\pi}{2a}\right)$ ← lattice constant is $2a$

1 BZ is $k \in \left[-\frac{\pi}{2a}, \frac{\pi}{2a}\right]$ We see the Hamiltn of SSH model is two-dimensional! Only 2D space winding # is meaningful.

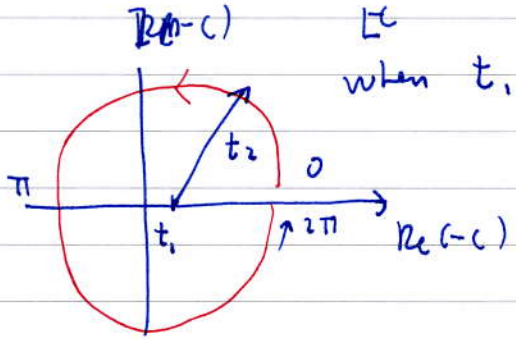
Winding #

use $-C = t_1 + t_2 e^{i2ak}$



As k varies fm 0 to $\frac{2\pi}{2a}$ or 2ak fm 0 to 2π -C traces out a circle.

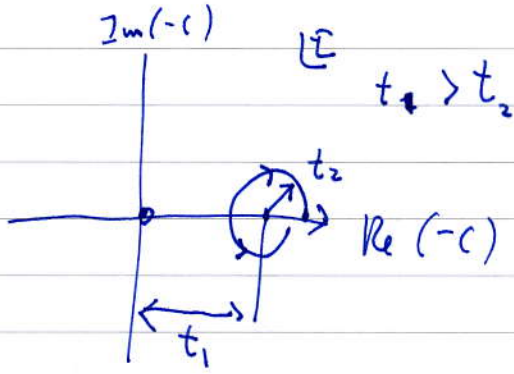
The winding # is defined as how many times the origin $Z = 0 = 0 + i0$ is enclosed!



when $t_1 < t_2$

winding # is 1

model system is "topologized"

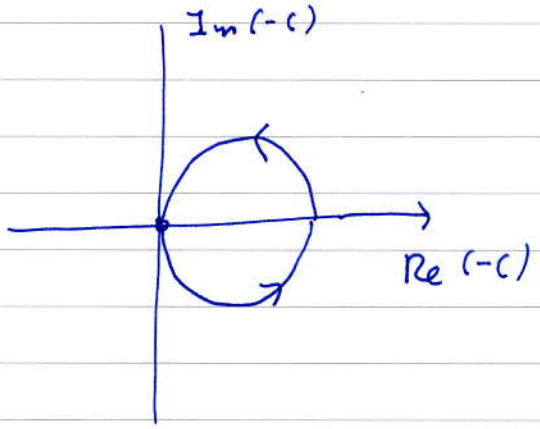


did not wind 0

isolate is "trivial"

topologically

when $t_1 = t_2$



When the curve passes 0 exactly the winding number is not defined!

We could define the winding number algebraically by the contour integral

$$\nu = \frac{1}{2\pi i} \oint \frac{1}{z}\, dz$$

(contour integral is on the path $Z = C(K)$ generated by $C(k)$ $0 \le K \le \frac{2\pi}{2a}$.

Bulk - edge correspondence (how to prove this)

winding number ν = # of edge states on site A
− # of edge state on site B.

For SSH model, there is no state on site B, only on site A. So

when $t_1 < t_2$ $\nu = 1$, $N_A = 1$

when $t_1 > t_2$ $\nu = 0$, $N_A = 0$

Surface Green's function of SSH model

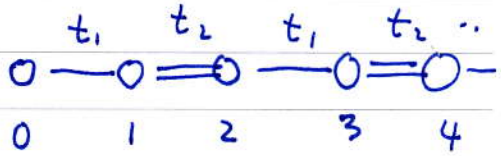
We take a look of the surface Green's function which is defined by a semi-infinite single particle Hamiltonian. We look at the "surface" density of states defined by the imaginary part of the surface Green's function. localized surface state should show up as a δ-function peak.

(retained)

The surface Green's function satisfies the equation

$$((E + i\eta)I - H)\, g = I$$

$$H = \begin{matrix} & 0 & 1 & 2 & \\ 0 & 0 & -t_1 & 0 & \\ 1 & -t_1 & 0 & -t_2 & 0 \\ 2 & 0 & -t_2 & 0 & -t_1 \to \infty \\ & 0 & 0 & -t_1 & 0 \\ & \downarrow & & & \\ & \infty & & & \end{matrix}$$



Our naming convention is shown above, start this with site 0, and bond hopping t_1.

In component form, the first few linear equations are

$$(E+i\eta)g_{00} + t_1 g_{01} = 1$$

$$t_1 g_{10} + (E+i\eta)g_{11} + t_2 g_{12} = 0$$

$$t_2 g_{21} + (E+i\eta)g_{22} + t_1 g_{23} = 0$$

$$t_1 g_{32} + (E+i\eta)g_{33} + t_2 g_{34} = 0$$

use periodicity focus on 2×2 block

$$H = \begin{bmatrix} H_{00} & V & 0 & 0 \\ V^T & H_{00} & V & 0 \\ 0 & V^T & H_{00} & V \\ 0 & 0 & V^T & \ddots \end{bmatrix} \qquad H_{00} = \begin{bmatrix} 0 & -t_1 \\ -t_1 & 0 \end{bmatrix}$$

$$V = \begin{bmatrix} 0 & 0 \\ -t_2 & 0 \end{bmatrix} \qquad V^T = \begin{bmatrix} 0 & -t_2 \\ 0 & 0 \end{bmatrix}$$

$$g = \begin{bmatrix} g_{00} & g_{01} \\ g_{10} & \ddots \\ g_{20} & \end{bmatrix}$$

here $g_{00} = \begin{bmatrix} a & b \\ c & d \end{bmatrix}$ is 2×2

$$[(E+i\eta)I - H]\,g = I \rightarrow \text{focus on 0th column}$$

$$(E+i\eta)I - H_{00})g_{00} + V g_{10} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

2×2

$$-V^T g_{j-1,0} + \left((E+i\eta)\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - H_{00}\right) g_{j0} + V g_{j+1,0} = 0$$

use periodicity we consider solution of the form

$$g_{j0} = A\lambda^j \qquad j = 0, 1, 2, \ldots \qquad A \text{ is } 2\times 2 \text{ matrix}$$

If $j > 0$ $\quad -V^T \frac{1}{\lambda} + \left((E+i\eta)I - H_{00}\right) - V\lambda = 0$

a matrix equation need to be solved.

For $j = 0$ $\quad ((E+i\eta)I - H_{00})A - VA\lambda = I$

$$-V^T \frac{1}{\lambda} + \left((E+i\eta) I - H_{00} \right) - V\lambda = 0$$

or $\begin{pmatrix} 0 & t_2 \frac{1}{\lambda} \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} E+i\eta & t_1 \\ t_1 & E+i\eta \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ \lambda t_2 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}$ don't work!!

$E + i\eta = 0$ $\quad t_1 + \lambda t_2 = 0$ etc.

these equations don't make sense!

Equations for the first column of $g = \begin{bmatrix} g_0 & \cdots \\ g_1 \\ g_2 \\ \vdots \end{bmatrix}$

0: $(E+i\eta) g_0 + t_1 g_1 = 1$

1: $t_1 g_0 + (E+i\eta) g_1 + t_2 g_2 = 0$

2: $t_2 g_1 + (E+i\eta) g_2 + t_1 g_3 = 0$

⋮

try the following solution

$\left.\begin{matrix} g_0 \\ g_2 \\ g_4 \end{matrix}\right\}$ + $g_{2n} = A\lambda^n$ $\quad$ $\left.\begin{matrix} g_1 \\ g_3 \\ \vdots \end{matrix}\right\}$ $g_{2n+1} = B\lambda^n$ $\quad$ $n = 0, 1, 2, \cdots$ ← different amplitude on even & odd sites

Then $\begin{cases} t_1 A + (E+i\eta) B + t_2 A\lambda = 0 \\ t_2 B + (E+i\eta) A\lambda + t_1 B\lambda = 0 \end{cases}$

$g_0 = A, \quad g_2 = A\lambda, \quad g_4 = A\lambda^2$

$g_1 = B, \quad g_3 = B\lambda, \quad g_5 = B\lambda^2$

write as matrix eq. $\begin{pmatrix} t_1 + \lambda t_2 & E+i\eta \\ (E+i\eta) & t_1 + \frac{t_2}{\lambda} \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$

No solution Unless $\det \begin{pmatrix} t_1 + \lambda t_2 & E+i\eta \\ (E+i\eta) & t_1 + t_2/\lambda \end{pmatrix} = 0$

or $(t_1 + \lambda t_2)(t_1 + \frac{t_2}{\lambda}) - (E+i\eta)^2 = 0$

or $t_1^2 + t_2^2 - (E+i\eta)^2 + t_1 t_2 \left(\lambda + \frac{1}{\lambda}\right) = 0$

this is a quadratic equation in λ,

$$\lambda^2 t_1 t_2 + (t_1^2 + t_2^2 - (E+i\eta)^2)\lambda + t_1 t_2 = 0$$

We take the solution such that $|\lambda| < 1$ because we need the boundary condition $g_j \to 0$ as $j \to \infty$.

Determine A & B.

$$(E+i\eta)A + t_1 B = 1, \quad (E+i\eta)B = -t_1 A - t_2 A\lambda$$

$$(E+i\eta)A + t_1\left(\frac{-t_1 - \lambda t_2}{E+i\eta}\right)A = 1$$

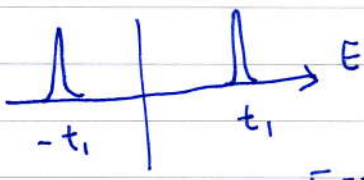
$$g_{00} = A = \frac{E+i\eta}{\underbrace{(E+i\eta)^2}_{\| \; t_1^2 + t_2^2 + t_1 t_2(\lambda + \frac{1}{\lambda})} - t_1^2 - \lambda t_1 t_2} = \frac{E+i\eta}{t_2^2 + t_1 t_2 \frac{1}{\lambda}}$$

use the expression $A = \dfrac{E+i\eta}{(E+i\eta)^2 - t_1^2}$

special case $t_2 = 0$

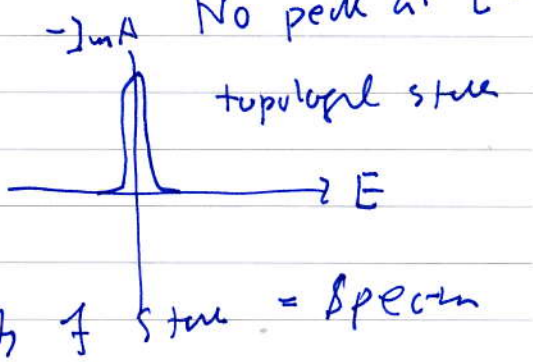
dimer limit

topological trivial case $E = \pm t_1$



opposite limit $t_1 = 0$

$$A = \frac{E+i\eta}{(E+i\eta)^2} = \frac{1}{E+i\eta} = P\frac{1}{E} - i\pi\delta(E)$$



imagin part of $A = -\mathrm{Im}\, g$ = density of state = spectrum has one peak at $E = 0$.

What is $-\int_{-\infty}^{+\infty} 2\,\mathrm{Im}\, g_{00}(E)\,\frac{dE}{2\pi} = ?$ $= 1$?

9 Aug 2018

Let use t_0 and Δ such that

$t_1 = t_0 - \frac{\Delta}{2}$ $\quad t_2 - t_1 = \Delta$ = half of gap $E_g > 0$

$t_2 = t_0 + \frac{\Delta}{2}$ $\quad = 4\alpha u^0$

See if we can get a nice formula for λ or not.

Equation for λ on page 191 is

$$t_1^2 + t_2^2 - (E + i\eta)^2 + t_1 t_2 \left(\lambda + \frac{1}{\lambda}\right) = 0$$

$$\| \quad (t_0 - \tfrac{\Delta}{2})^2 + (t_0 + \tfrac{\Delta}{2})^2 - (E+i\eta)^2 + (t_0 - \tfrac{\Delta}{2})(t_0 + \tfrac{\Delta}{2})\left(\lambda + \tfrac{1}{\lambda}\right)$$

$$= 0$$

$$2t_0^2 + \frac{\Delta^2}{4} \cdot 2 - (E+i\eta)^2 + \left(t_0^2 - \frac{\Delta^2}{4}\right)\left(\lambda + \frac{1}{\lambda}\right) = 0$$

or $(E+i\eta)^2 = t_0^2\left(2 + \lambda + \frac{1}{\lambda}\right) + \frac{\Delta^2}{4}\left(2 - \lambda - \frac{1}{\lambda}\right)$

Let $\lambda = e^{2iq}$ here q can be complex

$$= 4t_0^2\left(\frac{1 + (e^{2iq} + e^{-2iq})/2}{2}\right) + \frac{4\Delta^2}{4}\left(\frac{1 - (e^{2iq} + e^{-2iq})/2}{2}\right)$$

$$= 4t_0^2 \cos^2(q) + \Delta^2 \sin^2(q)$$

If $\Delta \le |E| \le t_0$ i.e. energy is in the band

$|\lambda| < 1$ $\quad \eta \to 0^+$ $\quad |\lambda| = 1$ $\quad q$ is real

we have propagating wave $\quad g_j = A\lambda^j$

$= A e^{iqj}$

The above equation is just the dispersion relation $\quad \Delta_q = \Delta \sin(q)$

$$E = \pm\sqrt{\varepsilon_q^2 + \Delta_q^2} \qquad q \equiv ak$$

$\eta \to 0^+$ $\quad q$ is dimensionless.

See page 163.

The quadratic equation for λ

$$\lambda^2 + \frac{(t_1^2 + t_2^2 - (E+i\eta)^2)}{t_1 t_2}\lambda + 1 = 0$$

has two solution λ_+, λ_-. From the Volta theorem we get

$$(\lambda - \lambda_+)(\lambda - \lambda_-) = 0$$

$$\lambda^2 - (\lambda_+ + \lambda_-)\lambda + \lambda_- \lambda_+ = 0$$

Compare we must have

$$\lambda_+ \lambda_- = 1 \quad \text{or} \quad |\lambda_+ \lambda_-| = 1$$

if $|\lambda_-| < 1$ then $|\lambda_+| > 1$

$$\lambda_+ + \lambda_- = -\frac{t_1^2 + t_2^2 - (E+i\eta)^2}{t_1 t_2}$$

This equation fails it t_1 or $t_2 = 0$.

$\lambda \equiv$ the one with $|\lambda| < 1$.

Explicit expression for λ

$$\left(t_0^2 - \frac{\Delta^2}{4}\right)\lambda^2 + \left(2t_0^2 + \frac{\Delta^2}{2} - (E+i\eta)^2\right)\lambda + \left(t_0^2 - \frac{\Delta^2}{4}\right) = 0$$

$$\lambda = \frac{-\left(2t_0^2 + \frac{\Delta^2}{2} - (E+i\eta)^2\right) \pm \sqrt{\left(2t_0^2 + \frac{\Delta^2}{2} - (E+i\eta)^2\right)^2 - 4\left(t_0^2 - \frac{\Delta^2}{4}\right)^2}}{2\left(t_0^2 - \frac{\Delta^2}{4}\right)}$$

We take the sign $\pm$ such that $|\lambda| <$, $\eta > 0$.

λ is real (when $\eta \to 0^+$) if

$$\left(2t_0^2 + \frac{\Delta^2}{2} - (E)^2\right)^2 > 4\left(t_0^2 - \frac{\Delta^2}{4}\right)^2$$

or when $\left|2t_0^2 + \frac{\Delta^2}{2} - E^2\right| > 2\left|t_0^2 - \frac{\Delta^2}{4}\right|$

or $E^2 > 2t_0^2 + \frac{\Delta^2}{2} \to E^2 - 2t_0^2 - \frac{\Delta^2}{2} \gtrless 2t_0^2 - \frac{\Delta^2}{2}$

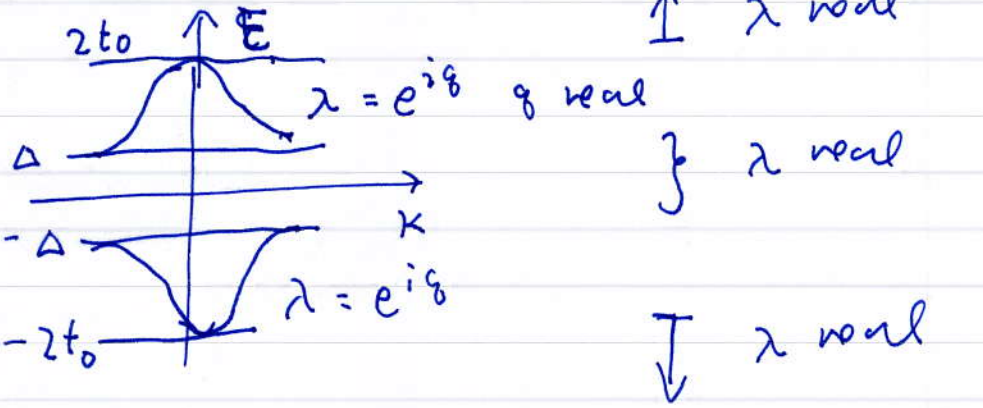
or $E^2 \gtrless 4t_0^2 \quad |E| > 2t_0$

or If E is small

$$\cancel{2}t_0^2 + \frac{\Delta^2}{2} - E^2 > \cancel{2}t_0^2 - \frac{\Delta^2}{2}$$

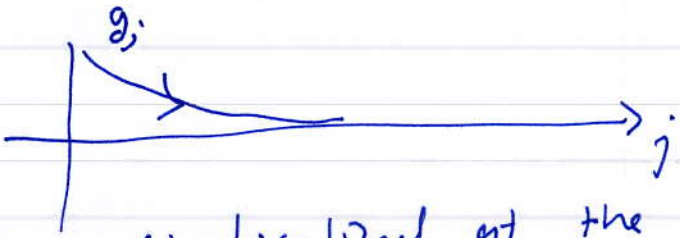
$$\Delta^2 > E^2 \quad \text{or} \quad |E| < \Delta$$

Thus the condition $\sqrt{\cdots}$ is real, or λ is real is the same as E is outside the band



Since when λ is real or when $\Delta \leq |E| \leq 2t_0$ is false, or when $|E| > 2t_0$, or $|E| < \Delta$ λ is real, this means, since $|\lambda| < 1$

$g_j = A\lambda^j$ must decay exponentially



i.e. when energy is in the gap, the Green's function $g_{j0}(E)$ must localized at the edge.

What is the difference of topologically nontrivial localized state at $E=0$, v.s. other localized state in the gap?

Surface Green's function in term of t_0, Δ

$$g_{00} = A = \frac{E + i\eta}{(E+i\eta)^2 - t_1^2 - \lambda t_1 t_2}$$

$$g_{oo} = \frac{E+i\eta}{(E+i\eta)^2 - (t_o - \frac{\Delta}{2})^2 - \lambda\,(t_o - \frac{\Delta}{2})(t_o + \frac{\Delta}{2})}$$

$$(t_o - \tfrac{\Delta}{2})(t_o + \tfrac{\Delta}{2}) = t_o^2 - \left(\tfrac{\Delta^2}{4}\right)$$

$$= \frac{E+i\eta}{(E+i\eta)^2 - (t_o - \frac{\Delta}{2})^2 - \frac{1}{2}\left[-\left(2t_o^2 + \frac{\Delta^2}{2} - (E+i\eta)^2\right) \pm \sqrt{\left(2t_o^2 + \frac{\Delta^2}{2} - (E+i\eta)^2\right)^2 - 4\left(t_o^2 - \frac{\Delta^2}{4}\right)}\right]}$$

$$= \frac{E+i\eta}{\frac{1}{2}(E+i\eta)^2 + \Delta\cdot t_o \mp \frac{1}{2}\sqrt{(E+i\eta)^4 - (E+i\eta)^2(4t_o^2 + \Delta^2) + 4t_o^2\Delta^2}}$$

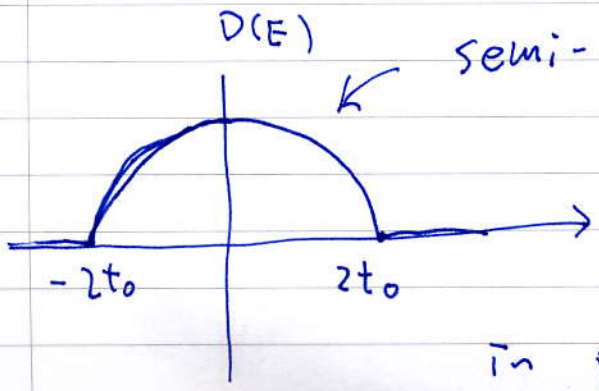
This is still complicated. Let's consider the special case of $\Delta = 0$, no gap then

$$g_{oo}(\Delta = 0) = \frac{1}{2}\left[\frac{1}{E+i\eta \pm \sqrt{(E+i\eta)^2 - 4t_o^2}}\right]$$

$$= \frac{1}{2}\,\frac{(E+i\eta) \mp \sqrt{(E+i\eta)^2 - 4t_o^2}}{(E+i\eta)^2 - (E+i\eta)^2 + 4t_o^2} = \frac{E+i\eta \pm \sqrt{(E+i\eta)^2 - 4t_o^2}}{8t_o^2}$$

$D = -2\,\mathrm{Im}\,g_{oo}$ = "density of state" on surface

$$= \begin{cases} \dfrac{1}{4t_o^2}\sqrt{4t_o^2 - E^2} & \eta \to 0^+ \\ 0 \quad \text{if} \quad |E| > 2t_o \end{cases}$$



semi-circle.

What happen to this graph when $\Delta \neq 0$ in particular when $\Delta = \pm 2t_o$?

When $\Delta = \pm 2t_0$ we have

must take "+" why

$$g_{00} = \frac{E + i\eta}{\frac{1}{2}(E+i\eta)^2 \pm 2t_0^2 \mp \frac{1}{2}\sqrt{(E+i\eta)^2 - 4t_0^2}}$$

↑ which sign to take

If $\Delta = +2t_0$, $t_1 = 0$ $t_2 = 2t_0$ it is topological

t_0^2 terms cancel we get $\frac{1}{2} + \frac{1}{2}$

$$g_{00} = \frac{E + i\eta}{(E+i\eta)^2} = \frac{1}{E+i\eta} = P\frac{1}{E} - i\pi\delta(E)$$

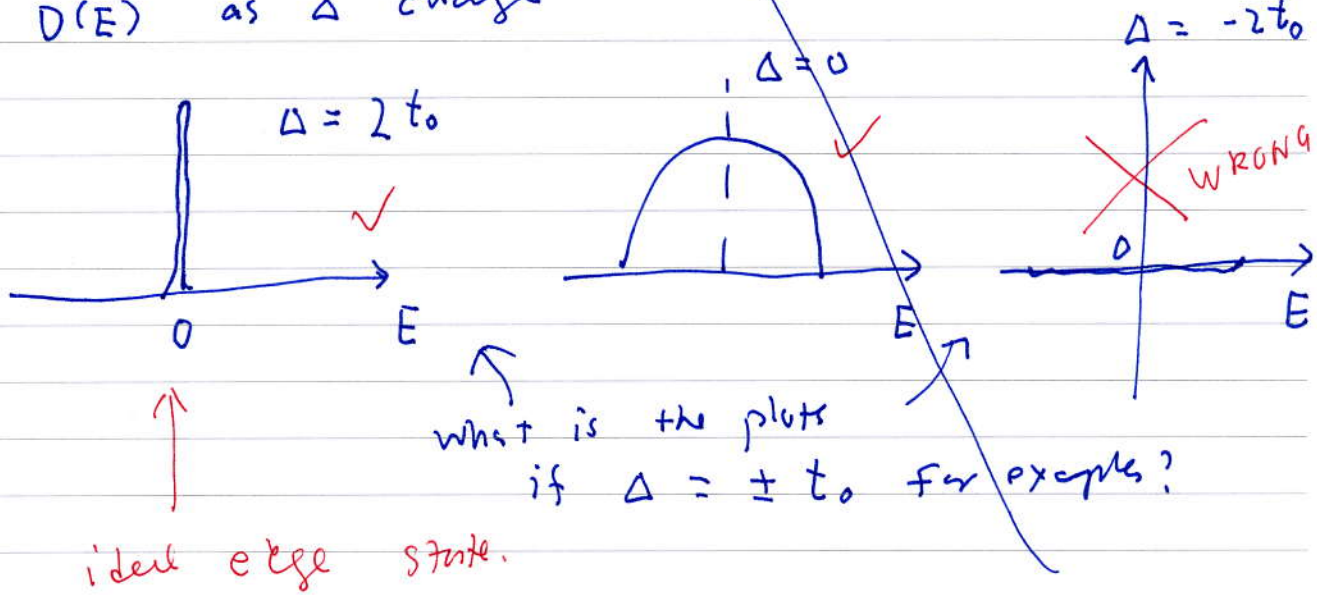
If $\Delta = -2t_0$ $t_1 = 2t_0$ $t_2 = 0$ trivial case

$$g_{00} = \frac{E+i\eta}{4t_0^2} \qquad \mathrm{Im}\, g_{00} = 0 \qquad \eta \to 0$$

WRONG

WRONG

$D(E)$ as Δ change



ideal edge state.

what is the plots if $\Delta = \pm t_0$ for example?

See also page 191

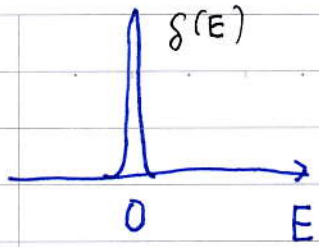
$$g_{00} = \frac{E+i\eta}{(E+i\eta)^2 \pm (2t_0^2) - 2t_0^2}$$

If $\Delta = 2t_0$ we take + sign $\quad g_{00} = \frac{1}{E+i\eta}$

If $\Delta = -2t_0$ we take − sign $\quad g_{00} = \frac{E+i\eta}{(E+i\eta)^2 - 4t_0^2}$

$E = \pm 2t_0$ has peaks

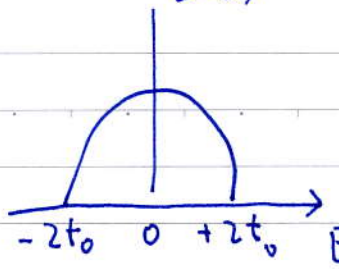
$\Delta = \pm 2t_0$ $t_1 = 0$



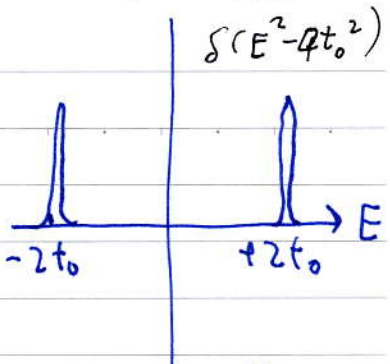
topological state

$\Delta \equiv 0$

$D(E) = -2 \operatorname{Im} g_{00}$



$\Delta = -2t_0, t_2 = 0$



topologically trivial

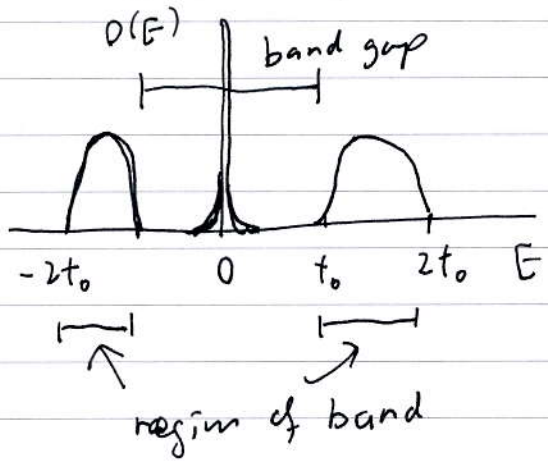
what happen in between
for example $\Delta = \pm t_0$??

We should make plots with "Mathematica" for $-2 \operatorname{Im} g_{00}$ for arbitrary Δ fixing $t_0 = 1$.

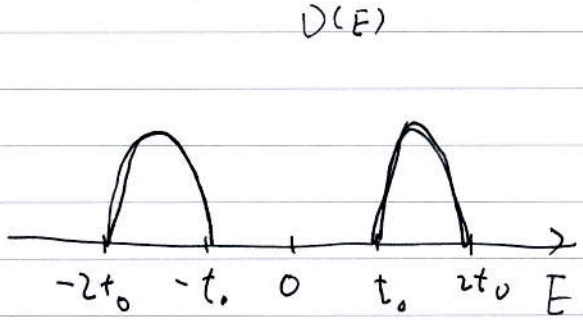
The above pictures are consistent with what I have said on page 191.

How the divergent case $\Delta = \pm 2t_0$ is smoothly connected to the non-divergent case of $\Delta = 0$?

if $\Delta = +t_0$



if $\Delta = -t_0$



NO peak at $E = 0$.

If $\Delta > 0$ localized states at $E = 0$ always exists

if $\Delta < 0$ no localized edge state until at the extreme limit (atomic limit).

10 Aug 2018

Berry phase & SSH model

In quantum mechanics, an overall phase has no physical significance. ψ and $e^{i\alpha}\psi$, $\alpha \in \mathbb{R}$, $i=\sqrt{-1}$ denote the same physical state. We say system is represented by a ray instead of a vector in Hilbert space.

Alternatively, we can use density matrix $\rho_\psi = |\psi\rangle\langle\psi|$

density matrix is unique as when $\psi \to e^{i\alpha}\psi$

$$\rho_{e^{i\alpha}\psi} = e^{i\alpha}|\psi\rangle\langle\psi|e^{-i\alpha} = |\psi\rangle\langle\psi| = \rho_\psi$$

Gauge transformation does not have an effect on density matrix.

Consider two wave functions ψ_1 and ψ_2

clearly $\langle\psi_1|\psi_2\rangle = z_{12} \in \mathbb{C}$ is a complex number.

We write $z_{12} = \langle\psi_1|\psi_2\rangle = |z_{12}|\, e^{-i\gamma_{12}}$

$\gamma_{12} \in \mathbb{R}$.

$$|z| \equiv \sqrt{z z^*} = \sqrt{(\mathrm{Re}\, z)^2 + (\mathrm{Im}\, z)^2}$$

The relative phase is physically significant, e.g. overlapping integrals. However, γ_{12} is not local gauge invariant

$$\psi_1 \to e^{i\alpha_1}\psi_1$$

$$\psi_2 \to e^{i\alpha_2}\psi_2$$

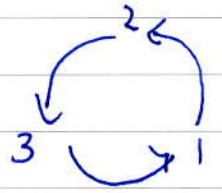
then $\langle\psi_1|\psi_2\rangle = |z_{12}|\, e^{-i\gamma_{12}} \to e^{-i\alpha_1 + i\alpha_2}\langle\psi_1|\psi_2\rangle$

$$= |z_{12}|\, e^{-i(\gamma_{12} + \alpha_1 - \alpha_2)}$$

relative phase

$\gamma_{12} \to \gamma_{12} + \alpha_1 - \alpha_2$ is not invariant.

Now consider three states ordered cyclically



$$\langle\psi_1|\psi_2\rangle\langle\psi_2|\psi_3\rangle\langle\psi_3|\psi_1\rangle$$

$$= z_{12} z_{23} z_{31} = |z_{12} z_{23} z_{31}| e^{-i(\gamma_{12}+\gamma_{23}+\gamma_{31})}$$

Under local gauge transfm $\psi_1 \to e^{i\alpha_1}\psi_1$

$\psi_2 \to e^{i\alpha_2}\psi_2$

$\psi_3 \to e^{i\alpha_3}\psi_3$

the total phase

$$\gamma = \gamma_{12}+\gamma_{23}+\gamma_{31} \to \gamma_{12} + \alpha_1 - \alpha_2 + \gamma_{23} + \alpha_2 - \alpha_3 + \gamma_{31} + \alpha_3 - \alpha_1 \equiv \gamma$$

The total phase in a cyclic order is a gauge invariant quantity so should have a physical significance. This total phase over a "loop" is called Berry phase.

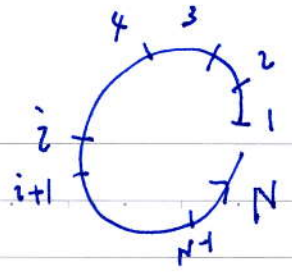
Note that we can also write

$$\langle\psi_1|\psi_2\rangle\langle\psi_2|\psi_3|\psi_3|\psi_1\rangle = \mathrm{Tr}(|\psi_2\rangle\langle\psi_2|\psi_3\rangle\langle\psi_3| |\psi_1\rangle\langle\psi_1|)$$

$$= \mathrm{Tr}(\rho_{\psi_2}\rho_{\psi_3}\rho_{\psi_1}) = \mathrm{Tr}(\rho_{\psi_1}\rho_{\psi_2}\rho_{\psi_3})$$

since ρ_{ψ_i} is gauge invant so is the trace.

We generalize this finite loop to many states and state with contins variables.



$N \to \infty$

$$\langle \psi_i | \psi_{i+1} \rangle = |z_{i,i+1}| e^{-i\gamma_{i,i+1}}$$

$$\gamma = \sum_{i=1}^{N} \gamma_{i,i+1}$$ periodic B.C. $N+1$ is same as 1.

Let $N \to \infty$ the parameter becomes a continuous var, say k, ψ_k $0 \le k \le 2\pi$

We assume ψ_k varies with k smoothly locally, (this can be proved to be so because of the Schrödinger eq)

Discretize k with equal spacing Δk

$$\frac{\langle \psi_k | \psi_{k+\Delta k} \rangle}{|\langle \psi_k | \psi_{k+\Delta k} \rangle|} = e^{-i\Delta\gamma_k}$$

Δk is small, we Taylor expand the left-hand side

$$\psi_{k+\Delta k} = \psi_k + \frac{\partial \psi_k}{\partial k}\Delta k + O(\Delta k^2) \qquad \langle \psi_k | \psi_k \rangle = 1$$

so $$\langle \psi_k | \psi_{k+\Delta k} \rangle = 1 + \langle \psi_k | \frac{\partial \psi_k}{\partial k} \rangle \Delta k + \cdots$$

$$|\langle \psi_k | \psi_{k+\Delta k} \rangle| = \sqrt{\left(1 + \langle \psi_k | \tfrac{\partial \psi_k}{\partial k} \rangle \Delta k\right)\left(1 + \langle \psi_k | \tfrac{\partial \psi_k}{\partial k} \rangle \Delta k\right)^*}$$

$$= |z_{k,k+\Delta k}|^2 = \sqrt{z\, z^*}$$

$$= \sqrt{1 + \underbrace{\left(\langle \psi_k | \tfrac{\partial \psi_k}{\partial k} \rangle + \langle \tfrac{\partial \psi_k}{\partial k} | \psi_k \rangle\right)}_{=0} \Delta k + O(\Delta k)^2} = 1 + O(\Delta k^2)$$

$$\langle \psi_k | \psi_k \rangle = 1 \to \frac{\partial}{\partial k}\langle \psi_k | \psi_k \rangle = 0$$

$$\langle \psi | \varphi \rangle = \langle \varphi | \psi \rangle^*$$

Thus we see $\dfrac{\langle \psi_k | \psi_{k+\Delta k}\rangle}{|\langle \psi_k | \psi_{k+\Delta k}\rangle|} = 1 + \langle \psi_k | \dfrac{\partial \psi_k}{\partial k}\rangle \Delta k + O(\Delta k^2)$

↑ correction to the normalization is 2nd order

but $e^{-i\Delta\gamma_k} = 1 - i\Delta\gamma_k + O(\Delta\gamma_k^2)$

compare we find

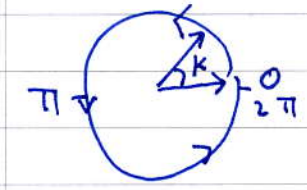
$$\Delta\gamma_k = i\langle \psi_k | \frac{\partial \psi_k}{\partial k}\rangle \Delta k = i\langle \psi_k | \left(\frac{\partial}{\partial k} | \psi_k\rangle\right) \Delta k$$

Adding all contributions in a loop

$$\gamma = i\int_0^{2\pi} dk \langle \psi_k | \frac{\partial}{\partial k} | \psi_k\rangle$$

integration over one period

This is a standard formula for Berry phase defined on a loop!



$\psi_k \equiv \psi_{k+2\pi}$ is assumed.

we don't have a Stoke's theorem as we are strictly in 1D manifold.

Let us apply the Berry phase concept to SSH model

here H should be the k-space one.

using dimensionless $q = 2ak$ $\quad 0 \le q \le 2\pi$

we have, from page 161

$$H(q) = \begin{pmatrix} 0 & c^* \\ c & 0 \end{pmatrix} \qquad -c \equiv t_1 + t_2 e^{iq}$$

$$\hat{H}\psi = \varepsilon\psi \qquad (\varepsilon I - H)\psi = \begin{pmatrix}0\\0\end{pmatrix}$$

$$\det \begin{pmatrix} \varepsilon & -c^* \\ -c & \varepsilon \end{pmatrix} = 0 \qquad \varepsilon^2 - |c|^2 = 0$$

Eigenvalue is $\varepsilon_\pm = \pm|c| = \pm\sqrt{(t_1 + t_2 e^{iq})(t_1 + t_2 e^{-iq})}$

$= \pm\sqrt{t_1^2 + t_2^2 + 2t_1 t_2 \cos q}$

The wave function for $\mathcal{E}_+ = +\sqrt{\cdots} = +|c|$

$$\begin{pmatrix} \mathcal{E} & -c^* \\ -c & \mathcal{E} \end{pmatrix}\begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \qquad \mathcal{E}\psi_1 - c^*\psi_2 = 0$$

or $-c\psi_1 + \mathcal{E}\psi_2 = 0$

or if $\mathcal{E} = \mathcal{E}_+$ $\quad |c|\psi_1 - c^*\psi_2 = 0$

$$-c\psi_1 + |c|\psi_2 = 0$$

$$\psi_2 = \frac{c}{|c|}\psi_1 \qquad \text{so } \psi_+ = \begin{pmatrix} 1 \\ \frac{c}{|c|} \end{pmatrix}\frac{1}{\sqrt{1+1}} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ e^{i\alpha} \end{pmatrix}$$

here $c = |c|e^{i\alpha}$

α is the phase of c

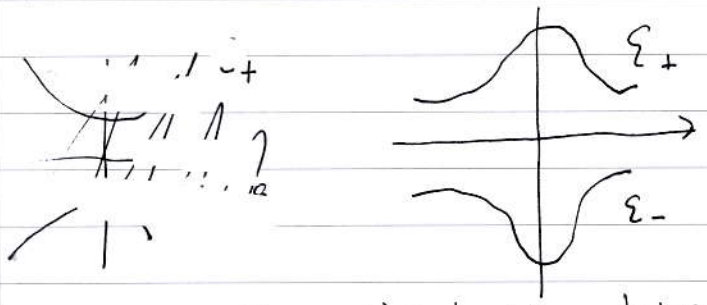
If $\mathcal{E} = \mathcal{E}_- = -|c|$ the eqn is $-c\psi_1 - |c|\psi_2 = 0$

$$\psi_2 = \frac{-c}{|c|}\psi_1$$

or $\psi_- = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -e^{i\alpha} \end{pmatrix}$ $\qquad \langle\psi_-|\psi_+\rangle = \frac{1}{2}(1, -e^{-i\alpha})\begin{pmatrix} 1 \\ e^{i\alpha} \end{pmatrix}$

$= 0$

the Eigenvectors are orthogonal!



$|c| = \sqrt{(\quad)(\quad)}$

$-\frac{1}{2} - t$

$-\frac{3}{2}$

Focus on $\mathcal{E}_+$ the bottom branch with $\psi_+ = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ e^{i\alpha} \end{pmatrix}$

$$c = -t_1 - t_2 e^{iq} \qquad e^{i\alpha} = \frac{c}{|c|}$$

$$\frac{\partial \psi_+}{\partial q} = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ \frac{\partial}{\partial q}\frac{c}{|c|} \end{pmatrix} \qquad \frac{\partial}{\partial q}\frac{c}{|c|} = \frac{\partial}{\partial q}\left[\frac{-t_1 - t_2 e^{iq}}{\sqrt{(t_1 + t_2 e^{iq})(t_1 + t_2 e^{-iq})}}\right]$$

$$= \frac{-t_2 e^{iq}}{|c|} i + c\left(-\tfrac{1}{2}\right)\frac{1}{|c|^3}\left[it_2 e^{iq}(-c^*) + (-c)(-it_2 e^{-iq})\right]$$

$$= \frac{-it_2 e^{iq}}{|c|} + \frac{1}{2}\frac{1}{|c|}it_2 e^{iq} + \frac{1}{2}\frac{ic^2}{|c|^3}t_2 e^{-iq}$$

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$$\frac{\partial \psi_+}{\partial q} = \left[-\frac{1}{2\sqrt{2}} \frac{i t_2}{|c|} e^{iq} + \frac{1}{2\sqrt{2}} \frac{i c^2}{|c|^3} t_2 e^{-iq} \right]$$

$$\langle \psi_+ | \frac{\partial}{\partial q} \psi_+ \rangle = \frac{1}{2} \left[-\frac{1}{2} \frac{i t_2}{|c|} e^{iq} \frac{c^*}{|c|} + \frac{i}{2} \underbrace{\frac{c^2 c^*}{|c|^3 |c|}}_{\frac{c}{|c|}} t_2 e^{-iq} \right]$$

$$i \langle \psi_+ | \frac{\partial}{\partial q} | \psi_+ \rangle = \frac{1}{4} \frac{t_2}{|c|^2} c^* e^{iq} - \frac{1}{4} \frac{c}{|c|^2} t_2 e^{-iq}$$

How to do integral $\int_0^{2\pi} dq$ then?

The integral $\int_0^{2\pi} dq \ldots$ looks complicated. Let first look at simpler case of the special limits:

1) $t_2 = 0 \quad c = t_1 \rightarrow \psi_+ = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$

so $\frac{\partial \psi_+}{\partial q} = 0 \qquad \langle \psi_+ | \frac{\partial \psi_+}{\partial q} \rangle = 0$

$$\gamma = i \int dq \langle \psi_+ | \frac{\partial}{\partial q} \psi_+ \rangle = 0$$

This is the topological trivial case with 0 Berry phase.

2) $t_1 = 0, \quad c = -t_2 e^{iq} \qquad \psi_+ = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -e^{iq} \end{pmatrix}$

$$\langle \psi_+ | \frac{\partial}{\partial q} | \psi_+ \rangle = \underbrace{\frac{1}{\sqrt{2}} (1, -e^{-iq})}_{\psi^*} \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ -i e^{iq} \end{pmatrix} = i \frac{1}{2}$$

$$\gamma = -\int_0^{2\pi} \frac{1}{2} dq = -\pi \mod(2\pi) = \pi$$

This is the topological state. Since is defined only up to mod 2π, $-\pi$ and π are equivalent.?

General case

$$\gamma = i \int_0^{2\pi} dq \langle \psi_+ | \frac{\partial}{\partial q} | \psi_+ \rangle$$

$$= \frac{t_2}{4} \int_0^{2\pi} dq \left[\frac{c^* e^{iq}}{|c|^2} + \text{c.c.} \right]$$

$$= \frac{t_2}{4} \int_0^{2\pi} dq \frac{(-t_1 - t_2 e^{-iq}) e^{iq} + \text{c.c}}{t_1^2 + t_2^2 + 2 t_1 t_2 \cos q} \quad \Big\} \text{ same as } \mathcal{E}_\pm^2$$

$$= \frac{t_2}{4} \int_0^{2\pi} dq \frac{1}{\mathcal{E}_+^2} \left[-t_1 e^{iq} - t_2 - t_1 e^{-iq} - t_2 \right]$$

$$= -\frac{t_2}{4} \int_0^{2\pi} dq \frac{2 t_1 \cos q + 2 t_2}{t_1^2 + t_2^2 + 2 t_1 t_2 \cos q}$$

$$= -\frac{1}{4} \int_0^{2\pi} dq \left[\frac{2 t_1 t_2 \cos q + t_1^2 + t_2^2 + t_2^2 - t_1^2}{2 t_1 t_2 \cos q + t_1^2 + t_2^2} \right]$$

$$= -\frac{1}{4} \int_0^{2\pi} dq \left[1 + \frac{t_2^2 - t_1^2}{2 t_1 t_2 \cos q + t_1^2 + t_2^2} \right]$$

$$\gamma = \frac{t_2}{4} \int_0^{2\pi} dq \frac{c^* e^{iq}}{|c|^2} + \text{c. c.} \qquad |c|^2 = c\, c^*$$

$$= \frac{t_2}{4} \int_0^{2\pi} dq \frac{c^* e^{iq}}{c\, c^*} + \text{c. c.}$$

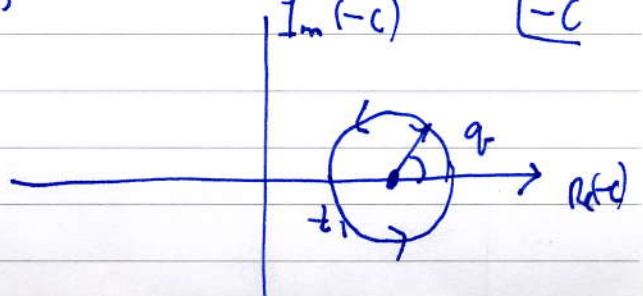
$$= \frac{t_2}{4} \int_0^{2\pi} dq \frac{e^{iq}}{c} + \text{c.c.}$$

here the complex number $c = -t_1 - t_2 e^{iq}$

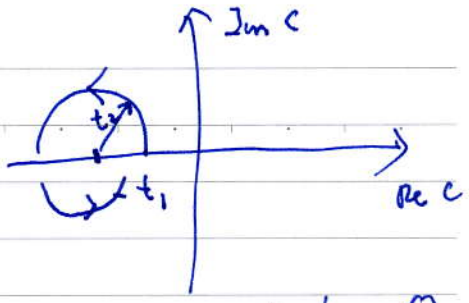
when q varies from 0 to 2π

c traces a circle centered around $-t_1$ of radius t_2

so $dc = -t_2 e^{iq} i\, dq$



$i\,dc = t_2\, e^{i\phi}\, d\phi$



So $\gamma = +\frac{i}{4} \oint_{C \in \text{circle}} \frac{dc}{c} + c.c.$

Now apply the residue theorem

$$\oint \frac{dc}{c} = 2\pi i \,(\text{Res}\ \tfrac{1}{c}) = \begin{cases} 2\pi i & \text{path includes } 0 \\ 0 & \text{path does not includes } 0 \end{cases}$$

$$\gamma = \frac{i}{4} \begin{cases} 2\pi i \\ 0 \end{cases} + c.c. = \begin{cases} \pi & t_2 > t_1 \\ 0 & \text{otherwise} \end{cases}$$

Compare with the winding number expression ν on pge 183

$$\nu = \frac{1}{2\pi i} \oint_{z=C(q)} \frac{dz}{z}$$ we see the Berry phase and winding number are essentially the same for SSH model: they are determined by the same residue theorem on complex plane of c.

$$\gamma = \frac{i}{2} \oint_{z=C(q)} \frac{dz}{z} = -\pi\nu$$

Berry phase ↓ about the phase of ψ_k

winding numb ↑ about the Hamilton $H(k)$ itself

This is well-known. See e.g. arXiv: 1701.08416 Nascimento

Relaxation time τ for Boltzmann equation of SSH model

We assume dimerization does not occur, this is correct when $\mu \to -\infty$ and carrier density $n \to 0$.

The unperturbed electrons and phonons are free ones

$$H_e = -t\sum_{n=1}^{N} c_n^\dagger c_{n+1} + h.c. \qquad \text{periodic B.C. } c_{N+1} \equiv c_1$$

$$= \sum_k \varepsilon_k c_k^\dagger c_k \qquad \varepsilon_k = -2t\cos(ka)$$

$$k = \frac{2\pi l}{aN} \qquad l = 0, 1, 2, \ldots N-1$$

there are exactly N possible k values in the 1st B.Z.

Here $c_n = \frac{1}{\sqrt{N}}\sum_k c_k e^{ina\cdot k}$ ($na \equiv R_n$)

in 3D this is $\vec{R}\cdot\vec{k}$

Similarly for phonon (cap k)

$$\hat{H}_p = \frac{1}{2}\sum_{n=1}^{N} p_n^2 + \frac{1}{2}K\sum_{n=1}^{N}(u_{n+1}-u_n)^2 \qquad u_{n+N} = u_n$$

$$= \sum_q \hbar\omega_q\left(a_q^\dagger a_q + \frac{1}{2}\right) \qquad q = \frac{2\pi m}{aN}$$

q is wave vector of phonon; same as k, N possible values $m = 0, 1, 2, \ldots N-1$

$$\omega_q^2 = 2K(1-\cos aq)$$

$$\to \omega_q = \sqrt{4K}\left|\sin\left(\frac{q_q a}{2}\right)\right| \geq 0$$

we define ω_q such that it is not negative

The equation of motion is

$$\ddot{u}_n = K u_{n-1} - 2K u_n + K u_{n+1}$$

Try plane wave solution $u_n = A e^{ina q - i\omega t}$

$$-\omega^2 = K e^{iaq} - 2K + K e^{-iaq}$$

$$\to \omega^2 = 2K - 2K\cos(qa) = 2K(1-\cos aq)$$

The relation between a_q and u_n is

$$u_n = \sum_q \sqrt{\frac{\hbar}{2\omega_q N}}\, a_q e^{inaq} + h.c.$$

(A is amplitude)

We need to check this is correct.

$$p_n = \dot{u}_n = \sqrt{\frac{\hbar}{2\omega_q N}}\, \dot{a}_q e^{inaq} + h.c.$$

$$= \sqrt{\frac{\hbar}{2\omega_q N}}\,(-i\omega_q)\, a_q e^{inaq} + h.c.$$

we have used $\dot{a}_q \equiv \frac{1}{i\hbar}[a_q, \hat{H}_q] = -i\omega_q a_q$

$$a_q(t) = e^{-i\omega_q t} a_q$$

use $(u_n)^+ = u_n$

$$= (\dot{u}_n)^+ u_n$$

The kinetic energy $= \frac{1}{2}\sum_{n=1}^{N} \dot{u}_n^2 = \frac{1}{2}\sum_{nqq'} \omega_q \sqrt{\frac{\hbar}{2\omega_q}} \left(a_q^+ e^{-inaq} + \right.$

$\left. -i\omega_q a_q e^{inaq} \right) \sqrt{\frac{\hbar}{2\omega_{q'}}} \left(-i\omega_{q'} a_{q'} e^{+inaq'} + i\omega_q a_q^+ e^{-inaq'} \right)$

since $\sum_n e^{inaq} = N\delta_{q0}$ we get 4 terms

$$= \frac{1}{2N}\sum_q \frac{\hbar}{2\omega_q}\omega_q^2 \left[a^+_q a_q + a_q a_q^+ - a_q^+ a_{-q}^+ - a_q a_{-q} \right] N$$

↑ minus sign because i^2

Note we used $\omega_q = \omega_{-q}$

$$= \frac{1}{4}\sum_q \hbar\omega_q \left(a_q^+ a_q + a_q a_q^+ + a_q^+ a_{-q}^+ - a_q a_{-q} \right)$$

The potential energy term is

$$\frac{1}{2}\sum_n K (u_{n+1} - u_n)^2 = \frac{1}{2} K \sum_n (u_{n+1} - u_n)^+ (u_{n+1} - u_n)$$

$$= \frac{1}{2} K \sum_{n,q,q'} \frac{\hbar}{2\omega_q N} \left(\left(e^{-iaq} - 1\right)\left(a_q^+ e^{-inaq}\right) + \left(e^{iaq} - 1\right) a_q e^{inaq} \right)$$

$$\left(\left(e^{iq'a} - 1\right) a_{q'} e^{inaq'} + \left(e^{-iq'a} - 1\right) a_{q'}^+ e^{-inaq'} \right)$$

Sum over n first use the orthogonal relation we find

$$\text{Kinetic energy} = \frac{1}{4} K \sum_{q} \frac{\hbar}{\omega_q} \Big[(e^{-iaq}-1)(e^{iqa}-1)\left(a_q^+ a_q + a_q a_q^+ + a_q^+ a_{-q}^+ + a_q a_{-q}\right)$$

$$(e^{-iaq}-1)(e^{iaq}-1)$$

$$= e^{-i\frac{aq}{2}}\left(e^{-i\frac{aq}{2}} - e^{i\frac{aq}{2}}\right) e^{i\frac{aq}{2}}\left(e^{i\frac{aq}{2}} - e^{-i\frac{aq}{2}}\right)(2i)^2$$

$$= 4 \sin^2\left(q\frac{a}{2}\right) \qquad \omega_q^2 = 4K \sin^2\left(\frac{qa}{2}\right)$$

So Kinetic energy $= \frac{1}{4} \sum_q \hbar\omega_q \left(a_q^+ a_q + a_q a_q^+ + a_q^+ a_{-q}^+ + a_q a_{-q}\right)$

Adding the two terms we see a^+a^+ and aa term cancelled

$$\hat{H}_p = \frac{1}{2} \sum_q \hbar\omega_q \left(a_q^+ a_q + a_q a_q^+\right) \qquad \text{use } [a, a^+] = 1$$

$$= \sum_q \hbar\omega_q \left(a_q^+ a_q + \frac{1}{2}\right).$$

In Summary to go from real space to wave vector Fourier space we need the Transformation for 1D chain

$$c_n = \frac{1}{\sqrt{N}} \sum_k C_k e^{ikna} \qquad n = 1, 2 \ldots N$$

$$u_n = \sum_q \sqrt{\frac{\hbar}{2\omega_q N}}\, a_q e^{iqna} + \text{h.c.} \qquad q, k = \frac{2\pi l}{aN} \quad l = 0, 1, 2 \ldots N-1$$

We need this to get the interest term. electron phonon interaction is

$$H_{ep} = \sum_n \alpha (u_{n+1} - u_n) c_{n+1}^+ c_n + \text{h.c.}$$

$$= \alpha \sum_n \left(\sum_q \sqrt{\frac{\hbar}{2\omega_q N}} \left((e^{iq\cdot a} - 1) e^{iqna} a_q + (e^{-iqa} - 1) e^{-iqna} a_q^+ \right) \right.$$

$$\left. \sum_k \frac{1}{\sqrt{N}} C_k^+ e^{-ik(n+1)a} \sum_{k'} \frac{1}{\sqrt{N}} C_{k'} e^{ik'na} \right) + \text{h.c.}$$

Sum over n we get momentum conservation factors.

$$H_{ep} = \alpha \frac{1}{\sqrt{N}} \sum_{q k k'} \sqrt{\frac{\hbar}{2\omega_q}} (e^{iqa} - 1) e^{-ika} \delta(q - k + k') \, a_q \, c_k^\dagger c_{k'}$$
$$+ \sqrt{\frac{\hbar}{2\omega}} (e^{-iqa} - 1) e^{-ika} \delta(-q - k + k') \, a_q^\dagger c_k^\dagger c_{k'}$$

the h.c. $= \alpha \frac{1}{\sqrt{N}} \sum_{q k k'} \sqrt{\frac{\hbar}{2\omega_q}} (e^{-iqa} - 1) e^{ika} \delta(q - k + k') \, a_q^\dagger c_{k'}^\dagger c_k$ + h.c.

add this two terms: $q \to -q$

$+ \alpha \frac{1}{\sqrt{N}} \sum_{q k k'} \sqrt{\frac{\hbar}{2\omega_q}} (e^{iqa} - 1) e^{ika} \delta(-q - k + k') \, a_q \, c_{k'}^\dagger c_k$ (swap $k \leftrightarrow k'$)

$$= \alpha \frac{1}{\sqrt{N}} \sum_{q k k'} \sqrt{\frac{\hbar}{2\omega_q}} (e^{-iqa} - 1) e^{ik'a} \delta(q - k' + k) \, a_q^\dagger c_k^\dagger c_{k'}$$
$$+ \alpha \frac{1}{\sqrt{N}} \sum_{q k k'} \sqrt{\frac{\hbar}{2\omega_q}} (e^{iqa} - 1) e^{ik'a} \delta(-q - k' + k) \, a_q \, c_k^\dagger c_{k'}$$

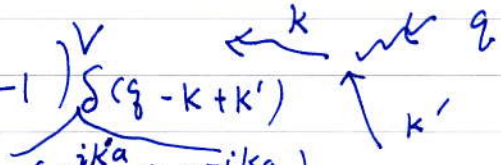
Note $\delta(-k) = \delta(k)$ is symmetric; flip $q \to -q$ for $a^\dagger$ term

$$H_{ep} = \frac{\alpha}{\sqrt{N}} \sum_{q k k'} \sqrt{\frac{\hbar}{2\omega_q}} (e^{+iqa} - 1) \underbrace{(e^{ik'a} + e^{-ika})}_{\text{V}} \delta(q - k + k') \, c_k^\dagger c_{k'} (a_q + a_{-q}^\dagger)$$

See Giustino RMP, 89, 015003 (2017)

$$= \frac{1}{\sqrt{N}} \sum_{q k k'} g_{k k'}^q \, \delta(q - k + k') \, c_k^\dagger c_{k'} (a_q + a_{-q}^\dagger)$$

$$g_{kk'}^q \equiv \alpha \sqrt{\frac{\hbar}{2\omega_q}} \underbrace{(e^{iqa} - 1)(e^{ika} + e^{-ika})}_{V} \delta(q - k + k')$$



Since $H_{ep}^\dagger = H_{ep}$ is hermitian we must have

$$\left(g_{kk'}^q\right)^* = g_{k'k}^{-q}$$

$[\delta(\cdots)]^2 = \delta(\cdots)$

δ - is Kronecker-δ

What we need in the Fermi-golden rule is

$$|g_{kk'}^q|^2 = 4 \frac{\hbar \alpha^2}{2\omega_q} \left| \underbrace{e^{i\frac{qa}{2}}}_{\text{modul}} \cancel{\left(e^{i\frac{qa}{2}} - e^{-i\frac{qa}{2}}\right)} \right|^2 = \frac{4\hbar\alpha^2}{2\omega_q} 4 \sin^2\left(\frac{qa}{2}\right)$$

WRONG!

$$\left|g^q_{kk'}\right|^2 = \frac{4^2 \hbar\alpha^2 \sin^2\left(\frac{qa}{2}\right)}{2\cdot\sqrt{4K\sin^2\left(\frac{qa}{2}\right)}}\,\delta(q-K+k')$$

$$= \left(2\cdot\frac{2}{K}\cdot\delta(\quad +k')\right) = \quad \cdot$$

$$= 4\,\frac{\hbar\alpha^2}{\sqrt{K}}\cdot\left|\sin\left(\frac{qa}{2}\right)\right|\,\delta(q-K+k')$$

$$\left(e^{iqa}-1\right)\left(e^{-ika}+e^{ika}\right)$$

$$= 2i\left(\sin(ka) - \sin(k'a)\right)$$

units for q is energy $\left[\frac{\hbar\alpha^2}{\sqrt{K}}\right] = \left[\frac{E\cdot t\cdot}{\sqrt{\frac{1}{t^2}}}\left(\frac{E}{L\sqrt{M}}\right)^2\right]$

↑ frequency

$$= \left[E\cdot t^2\cdot\frac{E^2}{L^2 M}\right] = [E^2]$$ unit check

$|g|^2 \propto q$ for small q.

$$g^q_{kk'} = \alpha\sqrt{\frac{\hbar}{2\omega_q}}(2i)\left(\sin(ka) - \sin(k'a)\right)\delta(q-K+k')$$

The deformation potential form is

$$g^q_{kk'} = +i\sqrt{\frac{\hbar}{2\omega_q M}}\cdot q\cdot E_1$$

E_1 is the deformation potential term

I think Guistino made a sign error should be $+$ because $u = \sum_q a e^{iq\cdot R}$, $\nabla u \propto iq$

compare if q is small $e^{iqa} - 1 \approx iqa$

so $g^q_{kk'} \approx 2\alpha\sqrt{M}\sqrt{\frac{\hbar}{2\omega_q M}}\,iqa$

we find $\boxed{E_1 \simeq +2\alpha a\sqrt{M}}$ is the deformation potential <0

$\alpha\cdot a$ is energy a is lattice constant, α is electron-phonon coupling. Deformation approximation is correct, if only small qs are important

Deformation potential E_1 from band structure point of view. Let $u_n \equiv 0$ $H_{ep} = 0$

If we deform the lattice slightly, according to

$$u_n = \lambda n \cdot a = \delta u_n \quad \text{or} \quad \lambda = \epsilon n \cdot a\sqrt{M}$$

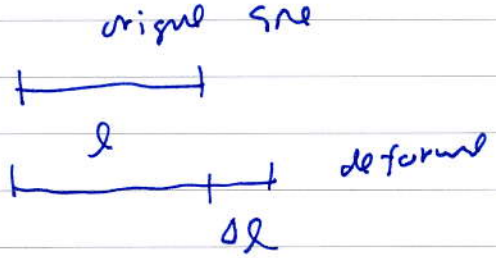
ϵ: strain

$\frac{\delta u_n}{na} = \epsilon$ is the strain

How much band shift? $\Delta\mathcal{E}_{k=0} = E_1 \epsilon$

we focus at band bottom $k=0$ only

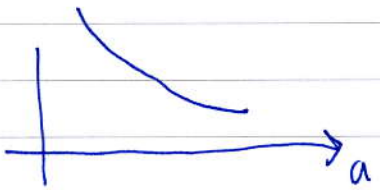
$$\epsilon = \frac{\Delta l}{l}$$



If $u_n = \epsilon \cdot n \cdot a$

the hopping parameter t is change do

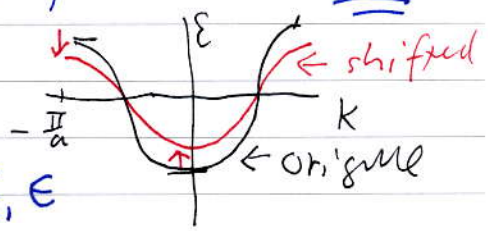
$$t \to \alpha(u_{n+1} - u_n) = t - \alpha(\epsilon a)\sqrt{M}$$



large size small t if $\epsilon > 0$

This means the band bottom is changed

from $-2t$ to $-2(t - \alpha\epsilon a) = -2t + 2\alpha a \cdot \epsilon$



Band bottom shift is

$$\Delta\mathcal{E} = 2\alpha a\sqrt{M}\,\epsilon = E_1 \epsilon$$

$E_1 = 2\alpha a\sqrt{M}$ Except the sign E_1 is correct

$-2t\cos(ka) \to (-2t + \sqrt{M}2\alpha a\epsilon)\cos(ka)$ $g^q_{kk'}$ consideration so the

$E_1 = 2\alpha a\sqrt{M}\cos(ka)$ see page 253.

k-depent E_1 is g carries meaning in wave vector space

Having obtained for the SSH model, assuming no dimerization,

$$\left|g^q_{kk'}\right|^2 = \frac{4\hbar\alpha^2}{\sqrt{K}}\left|\sin\left(\frac{qa}{2}\right)\right|\delta(q - k + k')$$

$$\frac{4\alpha^2\hbar}{2\omega_q}\left(\sin(ka) + \sin(k'a)\right)^2\delta(q - k + k')$$

We can use the formula for τ, that is

$$-\mathrm{Im}\Sigma^r(\varepsilon_k) = \frac{\hbar}{2\tau_k}, \quad \Sigma^r \text{ is obtained from}$$

IVEGF from the diagram 

$$\frac{1}{\tau_p} = \frac{+2\pi}{\hbar N}\sum_{qk}|g^q_{pk}|^2\Big\{(N_q+1-f_k)\,\delta(\varepsilon_p-\varepsilon_k-\hbar\omega_q) + (N_q+f_k)\,\delta(\varepsilon_p-\varepsilon_k+\hbar\omega_q)\Big\}$$

[See my notes Boltzmann-part2.pdf × polaron-physics.pdf]

using the expression for g we get

Kronecker δ

$$\frac{1}{\tau_p} = \frac{2\pi}{\hbar N}\sum_{qk}\underbrace{\frac{4\hbar\alpha^2}{\sqrt{k}}\left|\sin\left(\frac{qa}{2}\right)\right|}_{|g|^2}\delta(q-p+k)\Big\{(N_q+1-f_k)\,\delta(\varepsilon_p-\varepsilon_k-\hbar\omega_q) + (N_q+f_k)\,\delta(\varepsilon_p-\varepsilon_k+\hbar\omega_q)\Big\}$$

↑ Dirac-δ

Here p is fixed,
q is summed, because $\delta(q-p+k)$ we have

$$k = p-q$$

$$\frac{1}{\tau_p} = \frac{2\pi}{\hbar N}\sum_{q}\underbrace{\frac{4\hbar\alpha^2}{\sqrt{k}}\left|\sin\left(\frac{qa}{2}\right)\right|}_{\text{write}}\Big\{(N_q+1-f_{p-q})\,\delta(\varepsilon_p-\varepsilon_{p-q}-\hbar\omega_q) + (N_q+f_{p-q})\,\delta(\varepsilon_p-\varepsilon_{p-q}+\hbar\omega_q)\Big\}$$

We let $N\to\infty$

$$\frac{1}{N}\sum_q \to a\int\frac{dq}{2\pi} \qquad \Delta q = \frac{2\pi}{Na} \qquad a = \text{lattice constant.}$$

$$\frac{1}{\tau_p} = \frac{a}{\hbar}\int_{1BZ}dq\,\underbrace{\frac{4\hbar\alpha^2}{\sqrt{k}}\left|\sin\left(\frac{qa}{2}\right)\right|}_{\text{write } \varepsilon_p-\varepsilon_{p-q}}\Big((N_q+1-f_{p-q})\,\delta(\varepsilon_p-\varepsilon_{p-q}-\hbar\omega_q) + (N_q+f_{p-q})\,\delta(\varepsilon_p-\varepsilon_{p-q}+\hbar\omega_q)\Big)$$

We Taylor expand $\varepsilon_p - \varepsilon_{p-q} \mp \hbar\omega_q$

at the point(s) $\varepsilon_p - \varepsilon_{p-q} \mp \hbar\omega_q = 0$ fixing p

Call the solution q_0 ~ 0

Then $\varepsilon_p - \varepsilon_{p-q} \mp \hbar\omega_q = \varepsilon_p - \varepsilon_{p-q_0} \mp \hbar\omega_{q_0}$

$$- \frac{\partial \varepsilon}{\partial (p-q_0)} (-\delta q) \mp \frac{\partial \hbar\omega_q}{\partial \varepsilon} \delta q \Big|_{q=q_0}$$

$$= V(p-q_0)\,\hbar\,\delta q \mp \frac{\partial \hbar\omega_q}{\partial q}\Big|_{q_0} \delta q + \cdots$$

$V_p \equiv \frac{\partial \varepsilon_p}{\partial \hbar p}$ is the group velocity of electron

Now integration over q is trivial $\delta(aq) = \frac{1}{|a|}\delta(q)$

we find

Clearly $q_0 = 0$ is a solution of $\varepsilon_p - \varepsilon_{p-q} \pm \hbar\omega_q = 0$ but this corresponds to no scattering and should not be counted.

$$\frac{1}{\tau_p} = \frac{4a\alpha^2}{\sqrt{k}} \left[\sum_{q_0} |\sin(q_0 \tfrac{a}{2})| \, \frac{(N_{q_0} + 1 - f_{p-q_0})}{|\hbar V_{p-q_0} - \frac{\partial \hbar\omega_q}{\partial q}|_{q_0}} \right.$$

sum over all the solutions q_0

↑ soln of $\varepsilon_p - \varepsilon_{p-q} - \hbar\omega_q = 0$

$|q|^2$ value is wrong here!

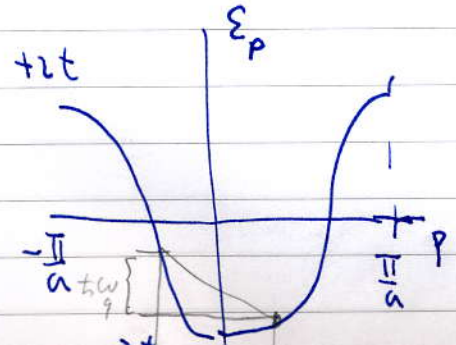
$$\left. + \sum_{q_0} |\sin(q_0 \tfrac{a}{2})| \, \frac{N_{q_0} + f_{p-q_0}}{|\hbar V_{p-q_0} + \frac{\partial \hbar\omega_q}{\partial q}|_{q_0}} \right]$$

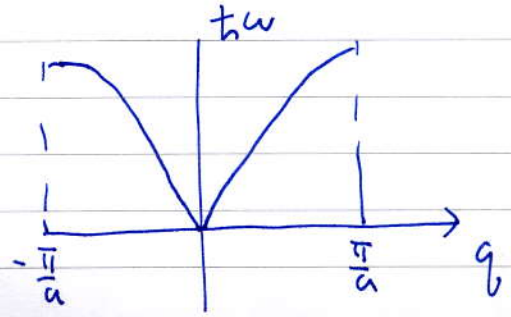
soln of $\varepsilon_p - \varepsilon_{p-q} + \hbar\omega_q = 0$

we can take $f \to 0$, $\mu \to -\infty$

We need to find the solution to equation

given each p: $\varepsilon_p - \varepsilon_{p-q} \pm \hbar\omega_q = 0$





Once the relaxation time τ_p is obtained, the diffusion constant D is then from the formula

$$D = \langle v^2 \tau \rangle = \frac{\sum_p v_p^2 \tau_p \left(-\frac{\partial f_p}{\partial p}\right)}{\sum_p -\frac{\partial f_p}{\partial \varepsilon}} \qquad \mu \to -\infty$$

$$f_p = \frac{1}{e^{\beta(\varepsilon_p - \mu)} + 1} \approx e^{-\beta(\varepsilon_p - \mu)} \qquad \frac{\partial f_p}{\partial \varepsilon_p} = -\beta f_p$$

$\mu \to -\infty$

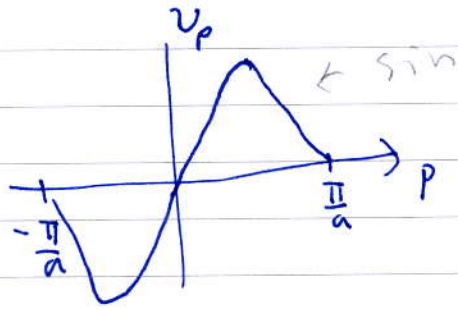
in the limit $\mu \to -\infty$, μ can be cancelled from the numerator & denominator so we just do Boltzmann averages

$$D = \frac{\sum_p v_p^2 \tau_p e^{-\beta \varepsilon_p}}{\sum_p e^{-\beta \varepsilon_p}}, \qquad v_p = \frac{\partial \varepsilon_p}{\partial \hbar p}$$

$\mu \to -\infty$

remember p is wave-vector $\quad \varepsilon_p = -2t \cos(pa)$

$$v_p = \frac{\partial \varepsilon_p}{\hbar \partial p} = \frac{2ta}{\hbar} \sin(pa) \quad \text{is group velocity}$$



$$N = \frac{1}{e^{\beta \hbar \omega} - 1} \approx \frac{1}{\beta \hbar \omega}$$

Deformation potential result:
we assume only long wave matter, Thus we take $q_0 \to 0$ and assume scattering is elastic, in the sense $\hbar \omega_q \approx 0$. then we get

$$\frac{1}{\tau_p} \approx \frac{8 a \alpha^2}{\sqrt{K}} \frac{q_0 a}{2} \frac{1}{\hbar V_p} \left(\frac{\hbar \omega_q}{k_B T}\right)_0^{-1} \leftarrow N_q \text{ classical approx.}$$

$f \to 0$

So the deformation potential result is two solutions for q_0

$$\frac{1}{\tau_p} = \frac{8\,a\,\alpha^2}{\sqrt{K}}\,\frac{1}{\hbar v_p}\,\left(\frac{q_0 a}{2}\right)\,\frac{k_B T}{\hbar\sqrt{4K\left|\sin\frac{q_0 a}{2}\right|}} \times 2$$

$$= \frac{8\,a\,\alpha^2}{K\,\hbar^2 |v_p|}\cdot k_B T \quad \cdots \quad \text{(classical limit in large } T \text{ used)}$$

The denominator has $\left|\hbar V_{q-q_0} - \frac{\partial \hbar\omega_q}{\partial q}\Big|_{q=q_0}\right|$

$\frac{\partial \omega_q}{\partial q} = C$ = sound velocity $\neq 0$ as $q \to 0$

So I think it is wrong to assume $\hbar\omega_q \equiv 0$!

Deformation potential method for SSH model

We follow Barden & Shockley Phys. Rev. 80, 72 (1950) and in particular, Wang, Shi, Chen, Xi, & Shuai. Phys. Chem. Chem. Phys. 14 16505 (2012).

First we determine the deformation potential E_1 for SSH model

$$E_1 = 2\alpha a\sqrt{M}$$

a: lattice const
M: mass

According to elastic scattering theory / Fermi-golden rule, the "transport" relaxation time is

$$\frac{1}{\tau_k} = \frac{1}{N}\sum_{k'} \frac{2\pi}{\hbar}\,|M(k,k')|^2\,\underbrace{\delta(\varepsilon_k - \varepsilon_{k'})}_{\text{energy is conserved, } \hbar\omega_q \equiv 0}\,(1-\cos\theta_{kk'})$$

$$|M(k,k')|^2 = \frac{k_B T\, E_1^2}{C_{ii}}$$

C_{ii} is diagonal elastic constant.

Here C_{ii} is defined in such a way so that it has a dimension of energy $[C_{ii}] = E$. by

$$E/N = \frac{1}{2} C_{ii} \epsilon^2 = \frac{1}{2} C_{ii} \left(\frac{\Delta l}{l}\right)^2 \qquad \epsilon = \frac{\Delta l}{l} \text{ is strain}$$

N is the number of unit cells and $\frac{E}{N}$ gives the energy per cell. This differs from the usual one which is $\frac{E}{V} = \frac{1}{2} C_{ii} \epsilon^2$ in 3D and $\frac{E}{L}$ in 1D.

The Advantage of this definition is that it works in any dimensions with the same formula.

For the SSH model, in the limit $\mu \to -\infty$, electron contribution to total energy is 0, so

$$E = \frac{1}{2} K \sum_{n=1}^{N} (u_{n+1} - u_n)^2$$ is potential energy of coordinate only. Consider uniform dilatation

$$u_n = \sqrt{M} \cdot \underbrace{\epsilon \cdot n a}_{x_n}$$ we get $(n+1) - n = 1$

$$E = \frac{1}{2} KN \left(\sqrt{M}\, \epsilon \cdot a\right)^2 = \frac{1}{2} KMa^2 \epsilon^2 N = \frac{1}{2} C_{ii} \epsilon^2 N$$

Compare with the definition of C_{ii} we find

$$C_{ii} = KMa^2$$

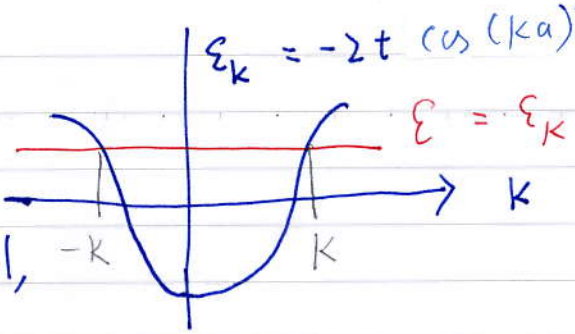
We can compute inverse relaxation time now as

$$\frac{1}{\tau_k} = \frac{1}{N} \sum_{k'} \frac{2\pi}{\hbar} \frac{k_B T E_1^2}{KMa^2} \delta(\varepsilon_k - \varepsilon_{k'}) (1 - \cos\theta_{kk'})$$

$\delta(\varepsilon_k - \varepsilon_{k'})$ means k' can only be such $\varepsilon_k = \varepsilon_{k'}$ k is fixed. i.e. Scattering is elastic. Since ε_k is even, $\varepsilon_k = \varepsilon_{-k}$.

The only way we can have $\varepsilon_k = \varepsilon_{k'}$ is

$k' = k$, or $-k$



But is $k' = k$

$\cos\theta_{kk'} = \cos 0 = 1$,

$1 - \cos\theta = 0$.

Thus the only possible contribution is the back scattering $k' = -k$. then $1 - \cos\pi = 2$

As a result, having the $1-\cos\theta$ factor or not the result is the same.

$$\delta(\varepsilon_k - \varepsilon_{k'}) = \delta\left(\varepsilon_k - \left(\varepsilon_{\underset{-k}{k}} + \frac{\partial \varepsilon_k}{\partial k}(k'-k) + \cdots\right)\right)$$

$$= \frac{1}{\left|\frac{\partial \varepsilon_k}{\partial k}\right|}\delta(k'-k) = \frac{1}{\hbar|V_k|}\delta(k'-k)$$

so

$$\frac{1}{\tau_k} = a\cdot\int \frac{dk'}{2\pi}\cdot\frac{2\pi}{\hbar}\frac{K_B T E_1^2}{KMa^2}\frac{1}{\hbar|V_k|}\delta(k'-k)\cdot 2$$

$1-\cos\theta$ gives 2

$$= 2\cdot a\cdot\frac{1}{\hbar}\frac{K_B T E_1^2}{KMa^2}\frac{1}{\hbar|V_k|} \qquad E_1 = 2\alpha a\sqrt{M}$$

$$= 2\cdot a\,\frac{1}{\hbar}\frac{K_B T\, 4\alpha^2 a^2 M}{KMa^2}\frac{1}{\hbar|V_k|} = \frac{8a\alpha^2 K_B T}{\hbar^2 K|V_k|}$$

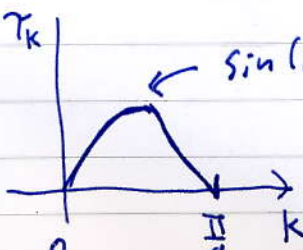
This agrees with that on page 239, obtained by

$$-\mathrm{Im}\,\Sigma^r = \frac{\hbar}{2\tau}.$$

$$\tau_k = \frac{\hbar^2 K|V_k|}{8a\alpha^2 K_B T}$$

check units (velocity)

$$[\tau]_k = \frac{E^2\tau^2\left(\frac{E}{Ma^2}\right)\left(\frac{a}{\tau}\right)}{a\left(\frac{E}{\sqrt{M}a}\right)^2 E} = \tau \quad \checkmark$$



units ok.

$$V_k = \frac{\partial \varepsilon_k}{\partial k} = \frac{2ta}{\hbar}\sin(ka)$$

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Since density of state $D(\varepsilon) \propto \frac{1}{v}$ new $v = v(\varepsilon)$ is group velocity $\frac{\partial \varepsilon}{\partial \hbar k}$ at every ε, we see that, in the deformation potential approximation the relaxation rate

$$\frac{1}{\tau_k} \propto D(\varepsilon_k)$$

This is a general result for elastic scattering. Since $D(\varepsilon)$ diverges at $\varepsilon = 0$ as $\frac{1}{\sqrt{\varepsilon}}$, we see the relaxation time converge to 0 at $\varepsilon \to 0$ $\tau \sim \sqrt{\varepsilon}$.

I am the opinion that at Γ point, $k=0$, and $\varepsilon = 0$, $\tau \to 0$ rather than ∞ is wrong. But I'm not so sure. We should make a comparison with the $-\mathrm{Im}\Sigma^r$ result.

Since we got an anytic formula $\tau_k = \frac{\hbar^2 k |V_k|}{8 a \alpha^2 k_B T}$ we can compute the diffusion constant D, under deformation potential approximation as

$$D = \frac{\sum_k (v_k)^2 \tau_k e^{-\beta \varepsilon_k}}{\sum_k e^{-\beta \varepsilon_k}} = \frac{\int_0^{\pi/a} dk\, (v_k)^2 \tau_k e^{-\beta \varepsilon_k}}{\int_0^{\pi/a} dk\, e^{-\beta \varepsilon_k}}$$

Note $\int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} dk = 2 \int_0^{\frac{\pi}{a}}$, 2 is cancelled by the denominator

clearly $d\varepsilon = \frac{\partial \varepsilon}{\partial \hbar k} \hbar\, dk = v_k \hbar\, dk$

$$\int_0^{\pi a} dk \left(v_k\right)^2 \tau_k e^{-\beta \varepsilon_k} = \int_{-at}^{+at} d\varepsilon \frac{1}{\hbar |V_k|} \left(v_k^2\right) \frac{\hbar^2 k |V_k|}{8 a \alpha^2 k_B T} e^{-\beta \varepsilon}$$

$$\int dk\,(v_k)^2 \tau_k e^{-\beta\varepsilon} = \int_0^\infty d\varepsilon \frac{2\varepsilon}{m} e^{-\beta\varepsilon} \cdot \frac{K \cdot \hbar}{8 a \alpha^2 K_B T}$$

Due to the Boltzmann distribution $e^{-\beta\varepsilon}$, most important contributions are at band bottom, we make an approximation to the dispersion to $\varepsilon = \frac{\hbar^2 k^2}{2m}$ where m is effective mass $\frac{1}{m} = \frac{\partial^2 \varepsilon}{\partial(\hbar k)^2}$

$$\int_0^\infty d\varepsilon \cdot \varepsilon e^{-\beta\varepsilon} = \int_0^\infty \varepsilon \, d(e^{-\beta\varepsilon}) \cdot \frac{1}{(-\beta)}$$

$$= -\frac{1}{\beta}\left[\varepsilon e^{-\beta\varepsilon}\Big|_0^\infty - \int_0^\infty e^{-\beta\varepsilon} d\varepsilon\right] = \frac{1}{\beta^2} = (K_B T)^2$$

So $\int dk\, v^2 \tau e^{-\beta\varepsilon} \approx \frac{K \cdot K_B T \cdot \hbar}{4 a \alpha^2 m}$ $\qquad \varepsilon \approx \frac{\hbar^2 k^2}{2m}$

Denominator $\int dk\, e^{-\beta\varepsilon} \approx \int_0^\infty dk\, e^{-\beta \frac{\hbar^2 k^2}{2m}} = \sqrt{\pi}\sqrt{\frac{m}{\beta\hbar^2}}$

So my prediction (approximate result) is $D \approx \frac{K \cdot \sqrt{K_B T} \cdot \hbar^2}{4 a \alpha^2 m^{3/2} \sqrt{\pi}} \propto \sqrt{T}$ $\qquad$ " m " is mass of electron.

Since the actual dispersion relation is $\varepsilon_k = -2t\cos(ka)$

$$\frac{p_k}{m} = v_k = \frac{\partial \varepsilon_k}{\partial \hbar k} = \frac{2ta}{\hbar}\sin(ka)$$

$$\frac{1}{m} = \frac{\partial^2 \varepsilon_k}{\partial(\hbar k)^2} = \frac{\partial v_k}{\partial \hbar k} = \frac{2t a^2}{\hbar^2}\cos(ka) \approx \frac{2ta^2}{\hbar^2} \quad (k \to 0)$$

or $m = \frac{\hbar^2}{2ta^2}$.

Alternatively $\varepsilon_k = -2t\cos(ka) \approx -2t\left[1 - \frac{(ka)^2}{2}\right]$

$$= \text{const} + \frac{1}{2}\left(\frac{2ta^2}{\hbar^2}\right)(\hbar k)^2$$

$$= \frac{p^2}{2m} \qquad p = \hbar k$$

so $\frac{1}{m} = \frac{2ta^2}{\hbar^2}$

$$\int_{-\infty}^{\infty} e^{-\frac{x^2}{2}} dx = \sqrt{2\pi}$$

We obtained an explicit equation for the diffusion constant

$$D = \langle v^2 \tau \rangle \approx \frac{\hbar^2 K \sqrt{k_B T}}{4\sqrt{\pi}\, m^{3/2} a \alpha^2}, \qquad m = \frac{\hbar^2}{2ta^2}$$

This result is correct if $k_B T \ll t$, which is usually true since $t \approx 2$ eV, $k_B T \approx 0.03$ eV.

Using the Einstein relation, we find the mobility is

$$\mu = \beta e D = \frac{eD}{k_B T} = \frac{e\hbar^2 K}{4\sqrt{\pi}\, m^{3/2} a \alpha^2 \sqrt{k_B T}}$$

why $\mu \propto \frac{1}{\sqrt{T}}$ not $\frac{1}{T}$? ↑ Is this $\mu \propto \frac{1}{\sqrt{T}}$ agreement with experiments? at least at high T?

The 1D conductivity is $\sigma = e n \mu$. This differs from 3D conductivity in units because n is linear density

$$n = \frac{\#\text{ of electrons}}{L: \text{length of system}} \qquad [n] = \frac{1}{a}$$

$$n = \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} \frac{dk}{2\pi} f = \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} \frac{dk}{2\pi} \frac{1}{e^{\beta(\varepsilon_k - \varepsilon_F)} + 1}$$

If ε_F is sufficiently below the band we can make the approximation $\varepsilon_k = -2t\cos(ka) \approx -2t + \frac{\hbar^2 k^2}{2m} + \dots$

We can redefine $\varepsilon = 0$ as at the band bottom then

$$n = \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} \frac{dk}{2\pi} e^{-\beta\left(\frac{\hbar^2 k^2}{2m} - \tilde{\varepsilon}_F\right)}$$

now $\tilde{\varepsilon}_F = 0$ means at band bottom

$$\approx \int_{-\infty}^{+\infty} \frac{dk}{2\pi} e^{-\beta\left(\frac{\hbar^2 k^2}{2m}\right)} e^{\beta \tilde{\varepsilon}_F} \leftarrow \text{is OK if } k_B T \ll t$$

$$n = \frac{1}{2\pi}\int_{-\infty}^{+\infty} dk\; e^{-\frac{\beta\hbar^2 k^2}{2m}} e^{\beta\tilde{\xi}_F} \qquad \text{let } x = \sqrt{\frac{\beta}{m}}\hbar k$$

$$= \frac{1}{2\pi}\sqrt{\frac{m}{\beta}}\frac{1}{\hbar}\underbrace{\int_{-\infty}^{\infty} dx\, e^{-\frac{x^2}{2}}}_{\sqrt{2\pi}} e^{\beta\tilde{\xi}_F} = \frac{1}{\sqrt{2\pi}}\sqrt{\frac{m}{\beta\hbar^2}}\, e^{\beta\tilde{\xi}_F}$$

$$\beta = \frac{1}{k_B T}$$

$m = \frac{\hbar^2}{2ta^2}$ is effective mass

$$\frac{m}{\frac{1}{E}\cdot t} \quad \frac{E\cdot t}{E} = \frac{m}{ma^2 t^2} = \frac{m}{\frac{a^2}{t^2}} \checkmark$$

Thus we find

$$\sigma = en\mu = e\frac{1}{\sqrt{2\pi}}\sqrt{\frac{m}{\beta}}\cdot\frac{1}{\hbar}\exp(\beta\xi_F)\frac{e\hbar^2 K'}{4\sqrt{\pi}\, m^{3/2} a\alpha^2\sqrt{\frac{1}{\beta}}}$$

$$= \frac{e^2\hbar K' \exp(\beta\xi_F)}{m\cdot a\cdot\alpha^2}\cdot\frac{1}{4\sqrt{2}\cdot\pi} \qquad \xi_F < 0$$

check units. in 1D σ is defined by $I = \sigma_{1D}E = \sigma_{1D}\frac{\Delta V}{L}$

I is current (not current density) so unit of

$$[\sigma_{1D}] = \frac{A}{V}L = S\cdot\text{meter} \qquad S: \text{Seemans} = \frac{1}{\text{Ohm}}$$
$$= \text{meter/Ohm} \qquad m: \text{meter}$$

Alternatively we see the dimension of σ is

$$[\sigma] = \left[\frac{I}{V}\cdot L\right] = \left[\frac{e}{\tau\frac{E}{e}}\cdot L\right] \leftarrow \text{energy} = \left[\frac{e^2}{E\tau}\cdot L\right] = \left[\frac{e^2}{ma^2}\cdot a\right]$$

$$= K \qquad [\alpha u] = E$$

$$\left[\frac{e^2\hbar K}{ma\alpha^2}\right] = \left[\frac{e^2 E\cdot\tau\cdot\left(\frac{E}{ma^2}\right)}{ma\left(\frac{E}{\sqrt{m}a}\right)^2}\right] = \left[\frac{e^2\tau}{ma}\right] = \left[\frac{e^2 n\tau}{m}\right] \checkmark = [\sigma]$$

this is correct

so the units checked!

We see $\sigma \propto \frac{Kt}{\alpha^2}$

K: Spring constant
t: electron hopping
α: electron-phonon interaction

If we use the formula for $\frac{1}{\tau}$ from the imaginary part of self energy, Equation on page 235. we need to solve the equation

$$\varepsilon_p - \varepsilon_{p-q} \pm \hbar\omega_q = 0$$

here p is given, and q is to be found. Note $q=0$ is a solution. Should the solution be included in the sum $\sum_q$. I think yes.

$$\varepsilon_p = -2t\cos(pa)$$

$$\omega_q = \sqrt{4K'}\left|\sin\left(\frac{qa}{2}\right)\right|$$

So

$$-2t\left[\cos(pa) - \cos((p-q)a)\right] \pm 2\sqrt{K}\left|\sin\left(\frac{qa}{2}\right)\right| = 0$$

How to solve this equation efficiently!

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from page 227 & 229a

$$g^q_{kk'} = 2i\alpha\sqrt{\frac{\hbar}{2\omega_q}}\left(\sin(ka) - \sin(k'a)\right)\delta(q-k+k')$$

In the deformation potential limit $q \to 0$

but since $\delta(q-k+k')$ imposes $q-k+k' = 0$

when $q \to 0$, $k \approx k'$

So when q is small

$$\sin(ka) - \sin(\underbrace{(k-q)}_{k'}a) = \cos(ka)\cdot qa$$

$$g^q_{kk'} = -i\sqrt{\frac{\hbar}{2\omega M}}\cdot q \underbrace{\sqrt{M}(-2)\alpha a\cdot\cos(ka)}$$

$K \to 0$ take Γ-point only

$$E_1 = +2\alpha\sqrt{M}\,a\cdot\cos(ka)$$