ICFP M2 2022/2023

Condensed Matter Theory

Homework Assignment - Solutions

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A. The Rice-Mele model

The Rice-Mele (RM) model is defined on the same chains as the Su-Schrieffer-Heeger (SSH) model. As a reminder from exercise sheet 4, the SSH model is defined on a finite one-dimensional chain of N unit cells, with each consist of two sites, A and B. The SSH Hamiltonian reads as

$$\mathcal{H}_N = t\sum_{j=1}^{N}(|j,A\rangle\langle j,B| + \text{h.}c.) + t'\sum_{j=1}^{N-1}(|j+1,A\rangle\langle j,B| + \text{h.}c.).$$

The RM model is obtained by adding the term

$$\mathcal{H}_{N,m} = m\sum_{j=1}^{N}\left(|j,A\rangle\langle j,A| - |j,B\rangle\langle j,B|\right)$$

to the SSH model assuming $m \neq 0$.

(a) Find the RM matrix $\hat{\mathcal{H}}_N^{\text{RM}}(k) = \hat{\mathcal{H}}_N(k) + \hat{\mathcal{H}}_{N,m}(k)$. Find the bandstructure of $\hat{\mathcal{H}}_N^{\text{RM}}(k)$ and the bandgap. Assuming $m \neq 0$, is there still a transition in the model?
We first go to momentum-space, $\hat{\mathcal{H}}_N^{\text{RM}}(k) = \hat{\mathcal{H}}_N(k) + \hat{\mathcal{H}}_{N,m}(k)$ with

$$\begin{cases}\hat{\mathcal{H}}_N(k) = & \text{Re}(f_k)\sigma_x + \text{Im}(f_k)\sigma_y, \quad f_k = t + t'e^{ika} \\ \hat{\mathcal{H}}_{N,m}(k) = & m\sigma_z\end{cases}$$

in the basis $\{|k,A\rangle,|k,B\rangle\}$. Diagonalizing the Hamiltonian leads to two bands:

$$E_\pm(k) = \pm\sqrt{m^2 + |f_k|^2}.$$

So for a finite 'mass' $m \neq 0$, the system is gapped for all values of k with a band gap of $\Delta = 2\sqrt{m^2 + (t-t')^2}$ at $k/a = \pm\pi$. Since the band gap cannot be closed by varying the hopping parameters, there is no transition in the model.

(b) Does this Hamiltonian anticommute with any k-independent matrix ? What are the implications for topological properties as we discussed for the SSH model?
For the SSH model ($m = 0$) we have shown in exercise sheet 4 that $\{\hat{\mathcal{H}}_N(k),\sigma^z\} = 0$. We furthermore introduced the operator $\hat{\mathcal{P}} = \sum_{j=1}^{n}(|j,A\rangle\langle j,A| - |j,B\rangle\langle j,B|) = \frac{1}{m}\hat{\mathcal{H}}_m$ and found $\{\hat{\mathcal{H}}_N,\hat{\mathcal{P}}\} = 0$. Here, however, $\{\hat{\mathcal{H}}_N^{\text{RM}}(k),\hat{\mathcal{P}}\} = 2$, which indicates that the "chiral symmetry" is broken. So we expect not to have any protected edge states.
Another way to see this is to note the finite gap for all values of $t',t \in \mathbb{R}$: There is no gap closing, so no topological transition possible at which the winding number could change - the system is always in the same (topologically trivial) class with $\nu = 0$.
When visualising $\hat{\mathcal{H}}_N^{\text{RM}}(k)$ in the Bloch sphere representation, it is no longer located on the equator as soon as $m \neq 0$. This means that the winding number is ill-defined, the map is $C^1 \xrightarrow{\hat{\mathcal{H}}_N^{\text{RM}}(k)} S^2$, so the homotopy group is trivial.

(c) To study a single eigenstate with both $t,t' > 0$, we consider a half-infinite SSH chain defined by $\mathcal{H}_\infty = \lim_{N\to\infty} \mathcal{H}_N$. Assume that there is an eigenstate $|\psi_0\rangle$ at zero energy, and find it explicitly. [Hint: Write $|\psi_0\rangle$ as a linear combination of the states $|n,\alpha\rangle$ with $\alpha = A,B$ and $n = 1,\cdots,\infty$ and solve the Schroedinger equation as a system of linear equations in the coefficients]. For which regime of t,t' is this a valid state? What is the value of exponential decay length $\xi(t,t')$ of $|\psi_0\rangle$? Discuss the behavior of $\xi(t,t')$ near $t = t'$.
Let's assume the existence of $|\psi_0\rangle$ such that $\hat{\mathcal{H}}_\infty|\psi_0\rangle = 0$. Writing the state as a linear combination of states $|j,A\rangle$,$|j,B\rangle$, $|\psi_o\rangle = \sum_{i\geq 1}^{\infty}(a_i|i,A\rangle + b_i|i,B\rangle)$, we observe that $\forall i \geq 1$ $\langle i, A/B|\hat{\mathcal{H}}_\infty|\psi_0\rangle = 0$. So let's inspect the terms one by one, starting with the first unit cell:

$$\langle 1,A|\hat{\mathcal{H}}_\infty|\psi_0\rangle = 0 \quad \Rightarrow t\langle 1,B|\psi_0\rangle = 0 \quad \Rightarrow b_1 = 0$$

$$\langle 1,B|\hat{\mathcal{H}}_\infty|\psi_0\rangle = 0 \quad \Rightarrow \left(t\langle 1,A|\psi_0\rangle + t'\langle 2,A|\right)|\psi_0\rangle = 0 \quad \Rightarrow ta_1 + t'a_2 = 0$$

$$\langle 2,A|\hat{\mathcal{H}}_\infty|\psi_0\rangle = 0 \quad \Rightarrow \left(t\langle 2,B|\psi_0\rangle + t'\langle 1,B|\right)|\psi_0\rangle = 0 \quad \Rightarrow tb_1 + t'b_2 = 0 \quad \Rightarrow b_2 = 0$$

$$\langle 2,B|\hat{\mathcal{H}}_\infty|\psi_0\rangle = 0 \quad \Rightarrow \left(t\langle 2,A|\psi_0\rangle + t'\langle 3,A|\right)|\psi_0\rangle = 0 \quad \Rightarrow ta_2 + t'a_3 = 0$$

$$\vdots$$

One can show by recursion that $\forall i \geq 1$ $b_i = 0$ and $ta_i + t'a_{i+1} = 0$. This means that $a_i = \left(-\frac{t}{t'}\right)^{i-1} a_1$, where a_1 is fixed by the normalization of $|\psi_0\rangle$. We rewrite the overlap of $|\psi_0\rangle$ with a state $|n,A\rangle$:

$$|\langle n,A|\psi_o\rangle| = |a_n| = |a_1|e^{(n-1)\ln(t/t')} = |a_1|\frac{t'}{t}e^{-n\ln(\frac{t'}{t})} = |a_1|\frac{t'}{t}e^{-n/\xi}$$

with $\xi = \frac{1}{\ln\frac{t'}{t}}$. For the state to be normalizable, we require $\xi > 0$, which implies $t' > t$. In other words, this is the condition for $|\psi_0\rangle$ to exist.
We therefore recover a bulk-boundary correspondence: Near criticality ($t = t'$), $\xi \to \infty$ and the bound state delocalizes.

(d) Find the exact change in energy of the edge state (when $t' > t$) in the RM model $\mathcal{H}_\infty^{\mathrm{RM}} \equiv \mathcal{H}_\infty + \lim_{N\to\infty}\mathcal{H}_{m,N}$, considering $\mathcal{H}_{m,N}$ as a perturbation. Is it still a zero mode?
Let's calculate the energy eigenvalue of the $|\psi_0\rangle$ state. We note that $\langle\psi_0|\hat{\mathcal{H}}_\infty|\psi_0\rangle = 0$, so

$$\langle\psi_0|\hat{\mathcal{H}}_\infty^{\mathrm{RM}}|\psi_0\rangle = \langle\psi_0|\hat{\mathcal{H}}_{m,\infty}|\psi_0\rangle = m\sum_{i\geq 1}|a_i|^2 = m|\psi_0|^2 = m \neq 0$$

So $|\psi_0\rangle$ is no longer a zero mode - the edge state has been destroyed.

B. Spinful graphene

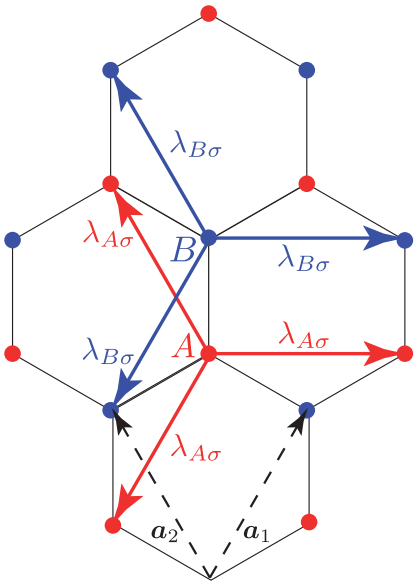

Figure 1: Graphene lattice in real space, with arrow depicting all the spin-dependent next-nearest-neighbor hoppings assigned to one unit-cell (the marked A,B). An arrow pointing from site i to site j, labeled by $\lambda_{\alpha\sigma}$ represents the term $\lambda_{\alpha\sigma}c^\dagger_{\alpha,j,\sigma}c_{\alpha,i,\sigma}$, where $\alpha \in \{A,B\}$ is the type of sites i,j.

In this problem we consider a more realistic model of graphene by addressing the spin-1/2 nature of electrons and by adding next-nearest neighbor hoppings. Together these features allow us to better study transitions in Dirac systems, and the role of spin-orbit coupling in graphene. We will use the tight-binding lattice model Hamiltonian $H = H_t + H_m + H_\lambda$, with:

$$H_t = \sum_{\sigma=\uparrow,\downarrow}\sum_{R,\delta} t_\sigma c^\dagger_{B,R+\delta,\sigma}c_{A,R,\sigma} + h.c. \tag{1}$$

$$H_m = \sum_{\sigma=\uparrow,\downarrow}\sum_{R} m_\sigma (c^\dagger_{A,R,\sigma}c_{A,R,\sigma} - c^\dagger_{B,R,\sigma}c_{B,R,\sigma}) \tag{2}$$

$$H_\lambda = \sum_{\sigma=\uparrow,\downarrow}\sum_{\langle\langle R,R'\rangle\rangle} \lambda_{\alpha\sigma}c^\dagger_{\alpha,R',\sigma}c_{\alpha,R,\sigma} + h.c., \tag{3}$$

where the operator $c^\dagger_{\alpha,R,\sigma}$ creates an electron on site $\alpha = A,B$ in unit-cell $\vec{R}$, and with spin $\sigma = \uparrow, \downarrow$. We further focus on spin-independent nearest-neighbor hopping $t_\sigma \equiv t > 0$ and on-site potential terms ($m_\sigma \equiv m$, so that $H_t + H_m$ becomes two independent copies of the spinless graphene you studied in TD and main lecture. More precisely: $R \equiv \vec{R} \equiv \vec{R}_A$ is the position of the unit-cell defined to coincide with the position of A atom in that unit-cell (hence use the inverse Fourier transform $c^\dagger_{\alpha,k,\sigma} = \int_{BZ}\frac{d^2k}{2\pi}\exp(-i\vec{k}\cdot\vec{R})c^\dagger_{\alpha,k,\sigma}$); the sum over $\vec{\delta}$ ensures that hoppings to all three nearest neighbors of A are included. However, the H_λ adds four new complex spin-dependent next-nearest neighbor hoppings $\lambda_{\alpha\sigma} \in \mathbb{C}$, $\alpha = A,B$, $\sigma = \uparrow, \downarrow$, and the precise definition of the next-nearest neighbor terms $\langle\langle R,R'\rangle\rangle$ is in Fig. 1.

(a) What is the Hamiltonian in momentum space? What is the 2x2 matrix spin-dependent Hamiltonian h^σ_k for momentum k?
We recall equation (3) of exercise sheet 3, where we diagonalized H_t, and introduce $\psi_{\mathbf{k},\sigma} =$

$\begin{pmatrix} c_{A\mathbf{k}\sigma} \\ c_{B\mathbf{k}\sigma} \end{pmatrix}$:

$$H_t = \sum_{\mathbf{k},\sigma} \psi^\dagger_{\mathbf{k},\sigma} h_{t,\sigma} \psi_{\mathbf{k},\sigma}, \text{ with } h_{t,\sigma}(\mathbf{k}) = \begin{pmatrix} 0 & f(\mathbf{k}) \\ f^*(\mathbf{k}) & 0 \end{pmatrix},$$

where $f(\mathbf{k}) = t\left(1 + e^{i\mathbf{k}\mathbf{a}_1} + e^{i\mathbf{k}\mathbf{a}_2}\right)$ for $\mathbf{a_{1/2}} = \frac{a}{2}(\pm 1, \sqrt{3})$. The mass term is diagonal in this representation with

$$h_{m,\sigma}(\mathbf{k}) = \begin{pmatrix} m & 0 \\ 0 & -m \end{pmatrix},$$

such that for $\lambda_{\alpha\sigma} = 0$ the spectrum is given by $\epsilon_\sigma(\mathbf{k}) = \pm\sqrt{m^2 + |f(\mathbf{k})|^2}$, which is independent of spin σ. The Dirac points are present only for $m \neq 0$, and are defined by $\epsilon_\sigma(\mathbf{k}) = 0$, which implies $|f(\mathbf{k})| = 0$. The latter leads to the condition $1 + 2e^{ik_y a\sqrt{3}} \cos(\frac{ak_x}{2}) = 0$, so we find two inequivalent Dirac points at $\mathbf{K} = (\frac{4\pi}{3}, 0)$ and $\mathbf{K}' = (-\frac{4\pi}{3}, 0)$. Taking into account spin, we have 4 Dirac points, 2 at $\mathbf{K}$ and 2 at $\mathbf{K}'$.
For finite values of m, the A and B sublattices become inequivalent, which breaks inversion symmetry, and the protection of the Dirac points is lost, thereby opening a gap.
Now assume $\lambda_{\alpha\sigma} \neq 0$ and inject in the Hamiltonian $c^\dagger_{A,\mathbf{R},\sigma} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{R}} c^\dagger_{A,\mathbf{k},\sigma}$:

$$\begin{aligned} H_\lambda &= \sum_{\sigma,\alpha} \sum_{\mathbf{k}} \lambda_{\alpha,\sigma} \left(\underbrace{e^{i\mathbf{k}\cdot(\mathbf{a}_1 - \mathbf{a}_2)} + e^{i\mathbf{k}\cdot\mathbf{a}_2} + e^{-i\mathbf{k}\cdot\mathbf{a}_1}}_{g(\mathbf{k})} \right) c^\dagger_{\alpha,\mathbf{k},\sigma} c_{\alpha,\mathbf{k},\sigma} + \text{h.c.} \\ &= \sum_{\sigma,\alpha} \sum_{\mathbf{k}} 2\text{Re}\left(\lambda_{\alpha\sigma} g(\mathbf{k})\right) c^\dagger_{\alpha,\mathbf{k},\sigma} c_{\alpha,\mathbf{k},\sigma} \end{aligned}$$

The Hamiltonian for momentum k reads therefore

$$h_\sigma(\mathbf{k}) = \begin{pmatrix} m + 2\text{Re}\left(\lambda_{A\sigma} g(\mathbf{k})\right) & f(\mathbf{k}) \\ f^*(\mathbf{k}) & -m + 2\text{Re}\left(\lambda_{B\sigma} g(\mathbf{k})\right) \end{pmatrix}.$$

Note that the Hamiltonian is now spin-dependent.

(b) The antiunitary time-reversal operator $\mathcal{T}$ for spin$-\frac{1}{2}$ electrons acts in the following way:

$$\mathcal{T} z c_{\alpha,R,\uparrow} \mathcal{T}^\dagger = +z^* c_{\alpha,R,\downarrow}, \tag{4}$$
$$\mathcal{T} z c_{\alpha,R,\downarrow} \mathcal{T}^\dagger = -z^* c_{\alpha,R,\uparrow}, \tag{5}$$

for a complex number z. What are the constraints on t,m,$\lambda_{\alpha\sigma}$ when time-reversal symmetry is imposed on the Hamiltonian?
From the definition of the action of $\mathcal{T}$ it follows

$$\mathcal{T} z \begin{pmatrix} c_{\alpha\mathbf{R}\uparrow} \\ c_{\alpha\mathbf{R}\downarrow} \end{pmatrix} \mathcal{T}^{-1} = z^* (is^y) \begin{pmatrix} c_{\alpha\mathbf{R}\uparrow} \\ c_{\alpha\mathbf{R}\downarrow} \end{pmatrix},$$

where s^y denotes the Pauli matrix. In spin space $\mathcal{T} = is^y\mathcal{K}$, so

$$\begin{aligned} \mathcal{T} c^\dagger_{\alpha\mathbf{k}\uparrow} \mathcal{T}^{-1} &= c^\dagger_{\alpha,-\mathbf{k},\downarrow} \\ \mathcal{T} c^\dagger_{\alpha\mathbf{k}\downarrow} \mathcal{T}^{-1} &= -c^\dagger_{\alpha,-\mathbf{k},\uparrow} \end{aligned}$$

We use now our definition of Fourier transformation to obtain

$$\begin{aligned} \mathcal{T} z \psi^\dagger_{\mathbf{k},\uparrow} \mathcal{T}^{-1} &= \mathcal{T} \begin{pmatrix} z c^\dagger_{A,\mathbf{k}\uparrow} \\ z c^\dagger_{B,\mathbf{k}\uparrow} \end{pmatrix} \mathcal{T}^{-1} = z^* \begin{pmatrix} c^\dagger_{A,-\mathbf{k}\downarrow} \\ c^\dagger_{B,-\mathbf{k}\downarrow} \end{pmatrix} = z^* \psi^\dagger_{-\mathbf{k}\downarrow} \\ \mathcal{T} z \psi^\dagger_{\mathbf{k},\downarrow} \mathcal{T}^{-1} &= -z^* \begin{pmatrix} c^\dagger_{A,-\mathbf{k}\uparrow} \\ c^\dagger_{B,-\mathbf{k}\uparrow} \end{pmatrix} = -z^* \psi^\dagger_{-\mathbf{k}\uparrow} \end{aligned}$$

We assume time-reversal symmetry, i.e. $\mathcal{T}H\mathcal{T}^{-1} = H$. Let's start again with $H_t + H_m$:

$$\begin{aligned}\mathcal{T}(H_t + H_m)\mathcal{T}^{-1} &= \sum_{\mathbf{k}} \left[\mathcal{T}\psi^\dagger_{k\uparrow}\mathcal{T}^{-1}\mathcal{T}h_\uparrow(\mathbf{k})\mathcal{T}^{-1}\mathcal{T}\psi_{\mathbf{k}\uparrow}\mathcal{T}^{-1} + \mathcal{T}\psi^\dagger_{k\downarrow}\mathcal{T}^{-1}\mathcal{T}h_\downarrow(\mathbf{k})\mathcal{T}^{-1}\mathcal{T}\psi_{\mathbf{k}\downarrow}\mathcal{T}^{-1}\right] \\ &= \sum_{\mathbf{k}} \left[\psi^\dagger_{-\mathbf{k}\downarrow}h^*_\uparrow(\mathbf{k})\psi_{-\mathbf{k}\downarrow} + \psi^\dagger_{\mathbf{k}\uparrow}h^*_\downarrow(-\mathbf{k})\psi_{\mathbf{k}\uparrow}\right]\end{aligned}$$

Since without H_λ we have $h_\sigma(\mathbf{k}) = h(\mathbf{k})$, and furthermore

$$h^*(-\mathbf{k}) = \begin{pmatrix} m^* & f^*(-\mathbf{k}) \\ f(-\mathbf{k}) & -m^* \end{pmatrix} = \begin{pmatrix} m & f(\mathbf{k}) \\ f^*(\mathbf{k}) & -m \end{pmatrix} = h(\mathbf{k}),$$

so $H_t + H_m$ is time-reversal symmetric (TRS).
We repeat the calculation now for H_λ, where TRS imposes $h^*_\downarrow(-\mathbf{k}) = h_\uparrow(\mathbf{k})$, so

$$\mathrm{Re}(\lambda_{\alpha,\uparrow}g(\mathbf{k})) = \mathrm{Re}(\lambda^*_{\alpha,\downarrow}g^*(-\mathbf{k})), \quad \lambda_{\alpha\sigma} \in \mathbb{C}$$

For $g(\mathbf{k})$ we know that Re $g(\mathbf{k})$ = Re $g(-\mathbf{k})$ and Im $g(\mathbf{k}) = -$Im $g(-\mathbf{k})$, so Re $(\lambda_{\alpha,\uparrow}g(\mathbf{k}))$ − Im $(\lambda_{\alpha,\uparrow}g(\mathbf{k}))$ = Re $(\lambda_{\alpha,\downarrow}g(-\mathbf{k}))$ − Im $(\lambda_{\alpha,\downarrow}g(-\mathbf{k}))$ = Re $(\lambda_{\alpha,\downarrow}g(\mathbf{k}))$ + Im $(\lambda_{\alpha,\downarrow}g(\mathbf{k}))$. That means that $\mathrm{Re}(\lambda_{\alpha,\uparrow}) = \mathrm{Re}(\lambda_{\alpha,\downarrow})$ and $\mathrm{Im}(\lambda_{\alpha,\uparrow}) = -\mathrm{Im}(\lambda_{\alpha,\downarrow})$, or $\lambda_{\alpha\uparrow} = \lambda^*_{\alpha\downarrow}$ independent of α, $\lambda_{\alpha\uparrow} = \lambda_\uparrow \in \mathbb{C}$.
So for the Hamiltonian this implies $t^* = t$, $m = m^*$ (this follows directly from the hermiticity of H_t and H_m) and $\lambda_{\alpha,\sigma} = \lambda^*_{\alpha,\bar{\sigma}}$.

(c) What is the 2x2 matrix $\mathcal{H}^{\sigma,\xi}_q$ for the time-reversal symmetric Hamiltonian at small momenta $|\vec{q}| \ll |\vec{K}_D|$ near the Dirac points $\xi\vec{K}_D$, $\xi = \pm 1$?
We need to expand $\mathbf{k}$ around $\xi\mathbf{K}_D$, i.e. $\mathbf{k} = \xi\mathbf{K}_D + \mathbf{q}$.
We use $e^{i\mathbf{k}\cdot\mathbf{a}_1} = e^{i(\xi\mathbf{K}_D+\mathbf{q})\cdot\mathbf{a}_1} = w^\xi e^{i\mathbf{q}\cdot\mathbf{a}_1}$ with $w = e^{2\pi i/3}$ and $e^{i\mathbf{k}\cdot\mathbf{a}_2} = w^{-\xi}e^{i\mathbf{q}\cdot\mathbf{a}_2} \simeq w^{-\xi}(1 + i\mathbf{q}\cdot\mathbf{a}_2)$. Thereby we get

$$\begin{aligned} f(\mathbf{k}) &\simeq t(1 + w^\xi(1 + i\mathbf{q}\cdot\mathbf{a}_1) + w^{-\xi}(1 + i\mathbf{q}\cdot\mathbf{a}_2)) \\ &= t(-a\frac{\sqrt{3}}{2}q_x\xi - ia\frac{\sqrt{3}}{2}q_y) = -at\frac{\sqrt{3}}{2}\xi(q_x + i\xi q_y) \\ g(\mathbf{k}) &= w^{-\xi}e^{i\mathbf{q}(\mathbf{a}_1-\mathbf{a}_2)} + w^{-\xi}e^{i\mathbf{q}\mathbf{a}_2} + +w^{-\xi}e^{-i\mathbf{q}\mathbf{a}_1} \\ &\simeq w^{-\xi}(3 + i\mathbf{q}\cdot(\mathbf{a}_1 - \mathbf{a}_2) + i\mathbf{q}\mathbf{a}_2 - i\mathbf{q}\cdot\mathbf{a}_1) = 3w^{-\xi}\end{aligned}$$

So

$$H_{\lambda\uparrow} = \sum_{\mathbf{q}}\sum_{\alpha}(3w^{-\xi}\lambda_\alpha c^\dagger_{\alpha\mathbf{q}\uparrow}c_{\alpha\mathbf{q}\uparrow} + \text{h.c.}) = \sum_{\mathbf{q}}\sum_{\alpha} \underbrace{2\mathrm{Re}\,(3w^{-\xi}\lambda_\alpha)}_{-3\mathrm{Re}\lambda_\alpha + 3\sqrt{3}\xi\mathrm{Im}\lambda_\alpha} c^\dagger_{\alpha\mathbf{q}\uparrow}c_{\alpha\mathbf{q}\uparrow}$$

and

$$H_{\lambda\downarrow} = \sum_{\mathbf{k}}\sum_{\alpha}(-3\mathrm{Re}\lambda_\alpha - 3\sqrt{3}\xi\mathrm{Im}\lambda_\alpha)c^\dagger_{\alpha\mathbf{k}\downarrow}c_{\alpha\mathbf{k}\downarrow}$$

Gathering all terms, we do obtain the equations:

$$h_\uparrow(\mathbf{q}) = \begin{pmatrix} t'_A + \xi\eta_A + m & -\xi v_F(q_x + i\xi q_y) \\ -\xi v_F(q_x - i\xi q_y) & t'_B + \xi\eta_B - m \end{pmatrix}$$

and

$$h_\downarrow(\mathbf{q}) = \begin{pmatrix} t'_A - \xi\eta_A + m & -\xi v_F(q_x + i\xi q_y) \\ -\xi v_F(q_x - i\xi q_y) & t'_B - \xi\eta_B - m \end{pmatrix}$$

with $t'_\alpha = -3\mathrm{Re}\lambda_\alpha$, $\eta_\alpha = 3\sqrt{3}\mathrm{Im}\lambda_\alpha$ and $v_F = at\sqrt{3}/2$.

(d) What is the energy dispersion of $\mathcal{H}_q^{\sigma,\xi}$?
Diagonalizing the equations and assuming that t' is sublattice independent, we get $\epsilon_\uparrow(\mathbf{q}) = t' + \xi\bar{\eta} \pm \sqrt{v_F^2\mathbf{q}^2 + \bar{\eta}^2 - (\xi\eta_A + m)(\xi\eta_B - m)}$ with $\bar{\eta} = \frac{\eta_A+\eta_B}{2}$ and $\epsilon_\downarrow(\mathbf{q}) = t' - \xi\bar{\eta} \pm \sqrt{v_F^2\mathbf{q}^2 + \bar{\eta}^2 - (\xi\eta_A - m)(\xi\eta_B + m)}$.

(e) The unitary spatial inversion operator $\mathcal{I}$ for spin$-\frac{1}{2}$ electrons acts in the following way:

$$\mathcal{I} z c_{A/B,k,\sigma} \mathcal{I}^\dagger = +z c_{B/A,-k,\sigma}, \tag{6}$$

for a complex number z. What are the constraints on t,m,$\lambda_{\alpha\sigma}$ for the spin-dependent Hamiltonian h_k^σ to be inversion-symmetric as well as time-reversal symmetric? Can a gap open at the Dirac points under these conditions? What can you say about the symmetry protection of the Dirac cones in presence of spin?
Inversion does not act on the spin, so let us look at the 2×2 matrix $h_{\uparrow,\xi}(\mathbf{q})$. Inversion imposes $(h_{\uparrow,\xi}(\mathbf{q}))_{11} = (h_{\uparrow,-\xi}(-\mathbf{q}))_{22}$ and $(h_{\uparrow,\xi}(\mathbf{q}))_{12} = (h_{\uparrow,-\xi}(-\mathbf{q}))_{21}$. The second condition is always satisfied, but the first one imposes

$$m + t'_A + \xi\eta_A = -m + t'_B - \xi\eta_B \quad \forall m, \mathrm{Re}\lambda_\alpha, \mathrm{Im}\lambda_\alpha.$$

Therefore $m = 0$ and $\eta_A = -\eta_B = \eta$ and $t'_A = t'_B = t'$. As we see below, a gap can open at the Dirac points even if there is $\mathcal{T}$ and $\mathcal{I}$ symmetry.

(f) As the Hamiltonian parameters $m, \lambda_{\alpha\sigma}$ vary, a topological band transition (TBT) leading to a change of topological properties of the bands, can only occur when bands touch at a certain momentum k_0. A transition requires a mixing among band states as parameters change, hence we can disregard crossings of bands with different conserved quantum numbers and crossings due to rigid shifts of bands, i.e., due to Hamiltonian terms $\propto \mathbb{1}$. At which parameter values and at which momenta are TBT possible in the time-reversal and inversion symmetric low-energy Hamiltonian $\mathcal{H}_q^{\sigma,\xi}$? How many topologically different phases of gapped graphene do you think there are?
Suppose the spinful Hamiltonian has both $\mathcal{T}$ and $\mathcal{I}$ symmetry, i.e. $\epsilon_\sigma(\mathbf{q}) = t' \pm \sqrt{\eta^2 + v_F^2 q^2}$. Despite these symmetries, the Dirac points are now gapped as soon as $\eta \neq 0$. η corresponds to complex spin-dependent next nearest-neighbor hoppings. We thus see that $\mathcal{T} + \mathcal{I}$ no longer protect the Dirac points. However, such a gap phase is different from a standard insulator. Suppose $m \neq 0$ but still $\eta_A = -\eta_B$, $t'_A = t'_N = t'$

$$h_\sigma = \pm i\xi(\mathbf{q}) = t' + \begin{pmatrix} m + \xi\sigma\eta & -\xi v_F(q_x + i\xi q_y \\ -\xi v_F(q_x - i\xi q_y) & -m - \xi\sigma\eta \end{pmatrix}$$

So $\epsilon_{\sigma,\xi}(\mathbf{q}) = t' \pm \sqrt{(m + \xi\sigma\eta)^2 + v_F^2 q^2}$. The gap is closing for $m = -\xi\sigma\eta$. Such a transition can occur via gap closing at $+\mathbf{K}_D$ for spin $\uparrow$ and at $-\mathbf{K}_D$ for spin $\downarrow$, or vice versa since $\xi\sigma = \text{const}$. This is a topological transition though time-reversal symmetry. For large $|m| > |\eta|$ one obtains a standard insulator, for small $|m| < |\eta|$ it amounts to a topological insulator first predicted by Kane and Mele[1]. Such insulator is different from a quantum Hall insulator as it respects time reversal symmetry. It is a 2D quantum **spin** Hall insulator. It has spin-dependent, counter-propagating edge states, which was a major discovery.

[1] C.L. Kane & E.J. Mele, *Phys. Rev. Lett.* **95**, 226801 (2005)

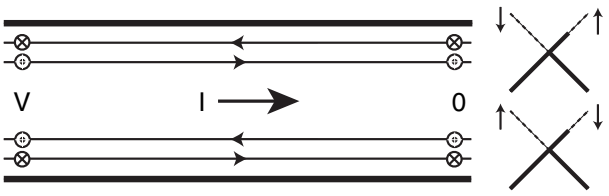

Figure 2: Schematic diagram showing the effect of a charge current I on the population of the edge-states (shown in the diagrams to the right). Figure taken from *Phys. Rev. Lett.* **95**, 226801 (2005).

C. Green's functions

(a) Consider electrons of a one-dimensional chain of Hydrogen atoms (with periodic boundary conditions) within a tight-binding approximation retaining nearest-neighbor hopping t, as in the lecture. In second quantized notation denote the creation/annihilation operators by $(c^\dagger_{i,\sigma}, c_{i,\sigma})$, where i is the site index of the chain and σ is the spin of the electron. Consider the retarded Green's function

$$G^R(\mathbf{k},\sigma,t) \equiv -i\theta(t)\langle\{c_{\mathbf{k},\sigma}(t)\,,\, c^\dagger_{\mathbf{k},\sigma}(0)\}\rangle,$$

where $\mathbf{k}$ is the wave-vector of the electrons, $\langle\hat{\mathcal{O}}\rangle \equiv (1/Z)\sum_n e^{-\beta E_n}\langle n|\mathcal{O}|n\rangle$, and $|n\rangle$ are the energy eigenstates of the Hamiltonian. Neglecting any Coulomb interactions, calculate the Fourier transform of the above quantity,

$$G^R(\mathbf{k},\sigma,\omega) = \int_{-\infty}^{\infty} dt e^{i\omega t} G^R(\mathbf{k},\sigma,t),$$

for this system by at least two different methods of your choice. (You may e.g. use the Lehmann representation, or you may calculate G^R in time and then Fourier transform etc...). Calculate the spectral function and make a sketch of what you would expect to measure during a photoemission or inverse photoemission experiment.
A small caveat : The retarded Green's function slightly differs from the time-ordered Green's function defined during the lecture. How does the Lehmann representation for the retarded one look like?
A one-dimensional chain of Hydrogen atoms of length N with periodic boundary conditions ($N+1\hat{=}1$) without any Coulomb interaction amounts to the tight-binding chain

$$H = t\sum_{i=1}^{N}\sum_{\sigma}\left(c^\dagger_{i,\sigma}c_{i+1,\sigma} + \text{h.c.}\right) - \mu\sum_i n_i$$

Here, the sums run over all Hydrogen sites i, which should be spaced with distance a. Since we aim at the Green's function in k-space, we Fourier transform the Hamiltonian using $c_{k,\sigma} = \frac{1}{\sqrt{N}}\sum_{j=1}^{N} e^{ikja}c_{j,\sigma}$, which leads to

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

For non-interacting particles, we can write down the expression for $c^\dagger_{k,\sigma}(t) = c^\dagger_{k,\sigma}e^{i\xi_k t}$, where we defined the dispersion $\xi_k = 2t\cos(ka) - \mu = \epsilon(k) - \mu$. So calculating the retarded Green's function amounts to calculating G^R in time and then Fourier transforming to frequency space:

$$\begin{aligned} G^R(k,\sigma,t) &= -i\theta(t)\langle c_{k,\sigma}(t)c^\dagger_{k,\sigma}(0) + c^\dagger_{k,\sigma}(0)c_{k,\sigma}(t)\rangle \\ &= -i\theta(t)e^{-i(\epsilon_k-\mu)t}\underbrace{\langle c_{k,\sigma}c^\dagger_{k,\sigma} + c^\dagger_{k,\sigma}c_{k,\sigma}\rangle}_{=1} \end{aligned}$$

The Fourier transform then needs a convergence parameter $\eta \longrightarrow 0^+$ to ensure convergence. Here, we rather follow the route outlined in Exercise Sheet 5 and insert the definition of

the Heaviside step function, which includes this parameter η:

$$\begin{aligned} G^R(k,\sigma,t) &= -i\int_{-\infty}^{\infty} \mathrm{d}t\; e^{i\omega t}\theta(t)e^{-i(\epsilon_k-\mu)t}, \quad \theta(t) = -\lim_{\eta\to 0^+}\frac{1}{2\pi i}\int_{-\infty}^{\infty}\mathrm{d}\tau\frac{e^{-i\tau t}}{\tau+i\eta} \\ &= \frac{1}{2\pi}\lim_{\eta\to 0^+}\int_{-\infty}^{\infty}\mathrm{d}\tau\;\frac{1}{\tau+i\eta}\underbrace{\int_{-\infty}^{\infty}\mathrm{d}t e^{i(\omega-\xi_k-\tau)t})}_{2\pi\delta(\omega-\xi_k-\tau)} \\ &= \lim_{\eta\to 0^+}\int_{-\infty}^{\infty}\mathrm{d}\tau\;\frac{\delta(\omega-\xi_k-\tau)}{\tau+i\eta} \\ &= \frac{1}{\omega-\xi_k+i0^+} \end{aligned}$$

We can instead also use the Lehmann representation to calculate G^R. In that case, we write down the definition of the retarded Green's function and insert explicitly the expressions of the operator averages:

$$\begin{aligned} G^R(k,\sigma,t) &= -i\theta(t)\left(\sum_{n,m}\frac{e^{-\beta E_n}}{Z}\langle n|c_{k,\sigma}(t)|m\rangle\langle m|c^\dagger_{k,\sigma}|n\rangle\right. \\ &\qquad \left. +\sum_{m,n}\frac{e^{-\beta E_m}}{Z}\langle m|c^\dagger_{k,\sigma}|n\rangle\langle n|c_{k,\sigma}(t)|m\rangle\right) \\ &= -i\theta(t)e^{-i\xi_k t}\left(\sum_n\frac{e^{-\beta E_n}}{Z}\langle n|c_{k,\sigma}c^\dagger_{k,\sigma}|n\rangle + \sum_m\frac{e^{-\beta E_m}}{Z}\langle m|c^\dagger_{k,\sigma}c_{k,\sigma}|m\rangle\right) \\ &= -i\theta(t)e^{-i\xi_k t}\sum_n\frac{e^{-\beta E_n}}{Z}\langle n|\left(\underbrace{c_{k,\sigma}c^\dagger_{k,\sigma}+c^\dagger_{k,\sigma}c_{k,\sigma}}_{=1}\right)|n\rangle \\ &= -i\theta(t)e^{-i\xi_k t} \end{aligned}$$

Applying the Fourier transformation as before leads then to the same result.
As discussed on Exercise Sheet 5, the spectral function $A(k,\omega) = -\frac{1}{\pi}G^R(k,\sigma,\omega)$ is in this case simply

$$A(k,\omega) = \delta(\omega-\xi_k).$$

In a photoemission experiment one would measure the electron-like part of the spectrum, i.e. the spectral function at negative energies. In case of inverse photoemission, electrons can be only absorbed if they match the empty spectrum, i.e. the spectral function at positive energies, see Fig. 3.

(b) Consider now a single-site problem (i.e., not a chain) with an isolated Hydrogen atom whose electrons are described by the Hamiltonian $H = \epsilon(n_\uparrow + n_\downarrow) + U(n_\uparrow - \frac{1}{2})(n_\downarrow - \frac{1}{2})$. Give an interpretation of the two terms. Convince yourself that for $\epsilon = 0$ the system is half-filled. Calculate the retarded Green's function of this system which is given by

$$G^R(\sigma,t) \equiv -i\theta(t)\langle\{c_\sigma(t)\,,\,c^\dagger_\sigma(0)\}\rangle,$$

and its Fourier transform $G^R(\sigma,\omega)$. Note, since this is a single-site problem there is no site index, or wave-vector index. Calculate also the corresponding non-interacting ($U = 0$) Green's function $G^R_0(\sigma,\omega)$ and deduce the self-energy (defined by $\Sigma(\sigma,\omega) = G^R_0(\sigma,\omega)^{-1} - G^R(\sigma,\omega)^{-1}$). Calculate the spectral function and make a sketch of what you would expect to measure during a photoemission or inverse photoemission experiment.
The Hamiltonian of the isolated Hydrogen atom describes in its first term the on-site energy

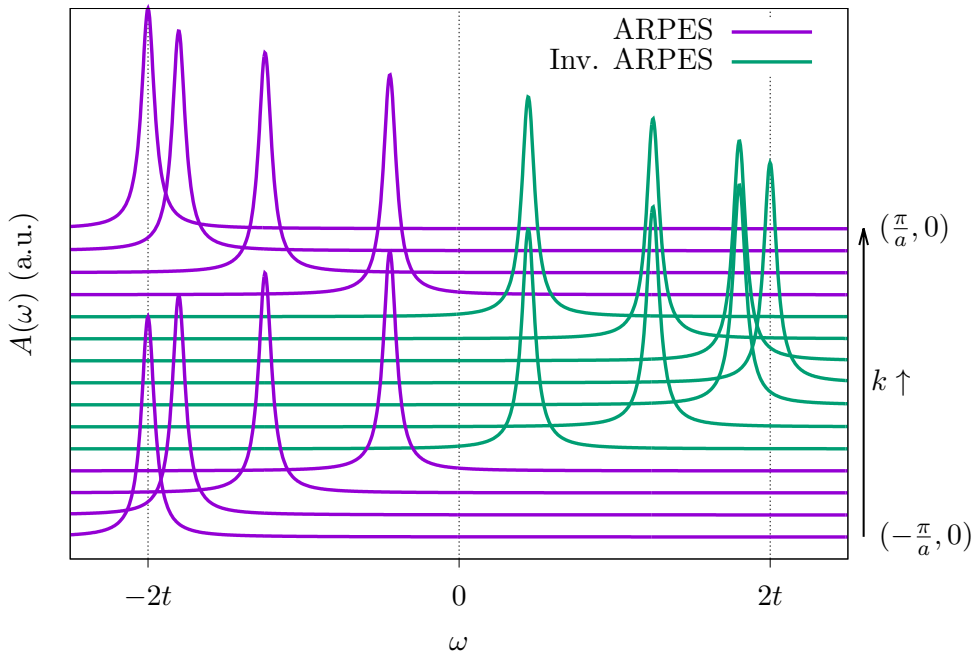

Figure 3: Spectral function of the non-interacting Hydrogen chain as probed by angle-resolved photoemission spectroscopy (ARPES) as well as inverse photoemission.

of an electron of $\uparrow$ or $\downarrow$ spin on the Hydrogen atom. The second term describes a repulsive interaction term between two electrons placed at the same time on the Hydrogen atom. By redefining the particle number operators, a term corresponding to a chemical potential has been implicitly included:

$$U\left(n_\uparrow - \frac{1}{2}\right)\left(n_\downarrow - \frac{1}{2}\right) = U n_\uparrow n_\downarrow - \frac{U}{2}(n_\uparrow + n_\downarrow) + \frac{U}{4}$$

In this form, the second term of the Hamiltonian is particle-hole symmetric, which means that for $\epsilon = 0$ the system is half-filled, $\langle \hat{n} \rangle = 1$. To show this, we write down the Hilbert space of the Hydrogen atom $\mathcal{H} = \{|0\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle\}$. These states are eigenstates of the Hamiltonian with energies $E = \frac{U}{4}, \epsilon - \frac{U}{4}, \epsilon - \frac{U}{4}, 2\epsilon + \frac{U}{4}$ respectively. We now evaluate the expectation value

$$\begin{aligned}\langle \hat{n} \rangle &= \frac{1}{Z}\sum_m e^{-\beta E_m}\langle m|\hat{n}|m\rangle = \frac{e^{-\beta E_{|\uparrow\rangle}} + e^{-\beta E_{|\downarrow\rangle}} + 2e^{-\beta E_{|\uparrow\downarrow\rangle}}}{e^{-\beta E_{|0\rangle}} + e^{-\beta E_{|\uparrow\rangle}} + e^{-\beta E_{|\downarrow\rangle}} + e^{-\beta E_{|\uparrow\downarrow\rangle}}} \\ &= 2\frac{e^{-\beta(\epsilon - \frac{U}{4})} + e^{-\beta(2\epsilon + \frac{U}{4})}}{e^{-\beta\frac{U}{4}} + 2e^{-\beta(\epsilon - \frac{U}{4})} + e^{-\beta(2\epsilon + \frac{U}{4})}}\end{aligned}$$

For $\epsilon = 0$ we obtain $\langle \hat{n} \rangle = 1$, which is half-filling.
To calculate the retarded Green's function, we can again explicitly use the eigenstates $|n\rangle$

of the single site:

$$\begin{aligned}
G^R(\sigma,t) &= -i\theta(t)\frac{1}{Z}\sum_n e^{-\beta E_n}\langle n|\left(e^{iHt}c_\sigma e^{-iHt}c_\sigma^\dagger + c_\sigma^\dagger e^{iHt}c_\sigma e^{-iHt}\right)|n\rangle \\
&= -i\theta(t)\frac{1}{Z}\Big(e^{-\beta E_{|0\rangle}}(e^{iE_{|0\rangle}t}e^{-iE_{|\sigma\rangle}t}) \\
&\quad + e^{-\beta E_{|\uparrow\rangle}}(\delta_{\sigma,\uparrow}e^{iE_{|0\rangle}t}e^{-iE_{|\uparrow\rangle}t} + \delta_{\sigma,\downarrow}e^{iE_{|\uparrow\rangle}t}e^{-iE_{|\uparrow\downarrow\rangle}t}) \\
&\quad + e^{-\beta E_{|\downarrow\rangle}}(\delta_{\sigma,\uparrow}e^{iE_{|\downarrow\rangle}t}e^{-iE_{|\uparrow\downarrow\rangle}t} + \delta_{\sigma,\downarrow}e^{iE_{|0\rangle}t}e^{-iE_{|\downarrow\rangle}t}) \\
&\quad + e^{-\beta E_{|\uparrow\downarrow\rangle}}(e^{iE_{|0\rangle}t}e^{-iE_{|\uparrow\downarrow\rangle}t})\Big) \\
&= -i\theta(t)\frac{1}{Z}\left(e^{i(E_0-E_1)t}(e^{-\beta E_0}+e^{-\beta E_1}) + e^{i(E_1-E_2)t}(e^{-\beta E_1}+e^{-\beta E_2})\right) \\
&= -i\theta(t)\frac{1}{Z}\left(e^{-it(\epsilon-\frac{U}{2})}(e^{-\beta\frac{U}{4}}+e^{-\beta(\epsilon-\frac{U}{4})}) + e^{-it(\epsilon+\frac{U}{2})}(e^{-\beta(\epsilon-\frac{U}{4})}+e^{-\beta(2\epsilon+\frac{U}{4})})\right)
\end{aligned}$$

where we abbreviated $E_{|\uparrow\rangle} = E_{|\downarrow\rangle} = E_1$ and $E_{|0\rangle} = E_0$. We now Fourier transform into frequency space as before and obtain

$$\begin{aligned}
G^R(\sigma,\omega) &= \frac{1}{Z}\left(\frac{e^{-\beta\frac{U}{4}}+e^{-\beta(\epsilon-\frac{U}{4})}}{\omega+i0^+-(\epsilon-\frac{U}{2})} + \frac{e^{-\beta(\epsilon-\frac{U}{4})}+e^{-\beta(2\epsilon+\frac{U}{4})}}{\omega+i0^+-(\epsilon+\frac{U}{2})}\right). \\
&= \frac{\alpha}{\omega+i0^+-(\epsilon-\frac{U}{2})} + \frac{\beta}{\omega+i0^+-(\epsilon+\frac{U}{2})}, \\
&\quad \alpha = \frac{e^{-\beta\frac{U}{4}}+e^{-\beta(\epsilon-\frac{U}{4})}}{Z},\quad \beta = \frac{e^{-\beta(\epsilon-\frac{U}{4})}+e^{-\beta(2\epsilon+\frac{U}{4})}}{Z}
\end{aligned}$$

So the Green's function has two poles at $\epsilon \pm \frac{U}{2}$ causing for $\epsilon = 0$ a splitting of the peaks of the spectral function of $\Delta = U$.
For the non-interacting Green's function we obtain

$$\begin{aligned}
G_0^R(\sigma,\omega) &= \frac{1}{Z}\left(\frac{1+e^{-\beta\epsilon}}{\omega+i0^+-\epsilon} + \frac{e^{-\beta\epsilon}+e^{-2\beta\epsilon}}{\omega+i0^+-\epsilon}\right) \\
&= \underbrace{\frac{(1+e^{-\beta\epsilon})^2}{Z}}_{=1}\frac{1}{\omega+i0^+-\epsilon}, \qquad Z_{U=0} = 1+2e^{-\beta\epsilon}+e^{-2\beta\epsilon}
\end{aligned}$$

We note that $\alpha+\beta = (e^{\beta U/4}+2e^{-\beta(\epsilon-U/4)}+e^{-\beta(2\epsilon+U/4)})/Z = 1$, which is the sum rule discussed on exercise sheet 5, and with which we simplify the expression to

$$G^R(\sigma,\omega) = \frac{\omega+i0^+-\epsilon+\frac{U}{2}(\alpha-\beta)}{(\omega+i0^+-\epsilon)^2-\frac{U^2}{4}}$$

This allows us to calculate the self-energy $\Sigma^R(\sigma,\omega) = G_0^R(\sigma,\omega)^{-1} - G^R(\sigma,\omega)^{-1}$.

$$\begin{aligned}
\Sigma^R(\sigma,\omega) &= \omega+i0^+-\epsilon - \frac{(\omega+i0^+-\epsilon)^2-\frac{U^2}{4}}{\omega+i0^+-\epsilon+\frac{U}{2}(\alpha-\beta)} \\
&= \frac{U}{2}\frac{\frac{U}{2}+(\alpha-\beta)(\omega+i0^+-\epsilon)}{\omega+i0^+-\epsilon+\frac{U}{2}(\alpha-\beta)}
\end{aligned}$$

In the limit $U \longrightarrow 0$, we have (as expected) $\Sigma^R \longrightarrow 0$. Furthermore, at half-filling (i.e. $\epsilon = 0$) we see that $\alpha = \beta$ and therefore

$$\Sigma^R_{\langle\hat{n}\rangle=1}(\sigma,\omega) = \frac{U^2/4}{\omega+i0^+}$$

So the self-energy has a pole at $\omega = 0$ with weight $U^2/4$. The Green's function takes at half-filling the simple form

$$G^R_{\langle\hat{n}\rangle=1}(\sigma,\omega) = \frac{1}{2}\left(\frac{1}{\omega + i0^+ - \frac{U}{2}} + \frac{1}{\omega + i0^+ + \frac{U}{2}}\right)$$

So the spectral function consists of two delta peaks at $\pm\frac{U}{2}$ with equal weight $\frac{1}{2}$. In a photoemission experiment, one would measure the occupied part of the spectrum, i.e. the the peak at $\omega = -\frac{U}{2}$. With inverse photoemission, the unoccupied part of the spectrum will be accessed, i.e. the peak at $\omega = \frac{U}{2}$, see Fig. 4.

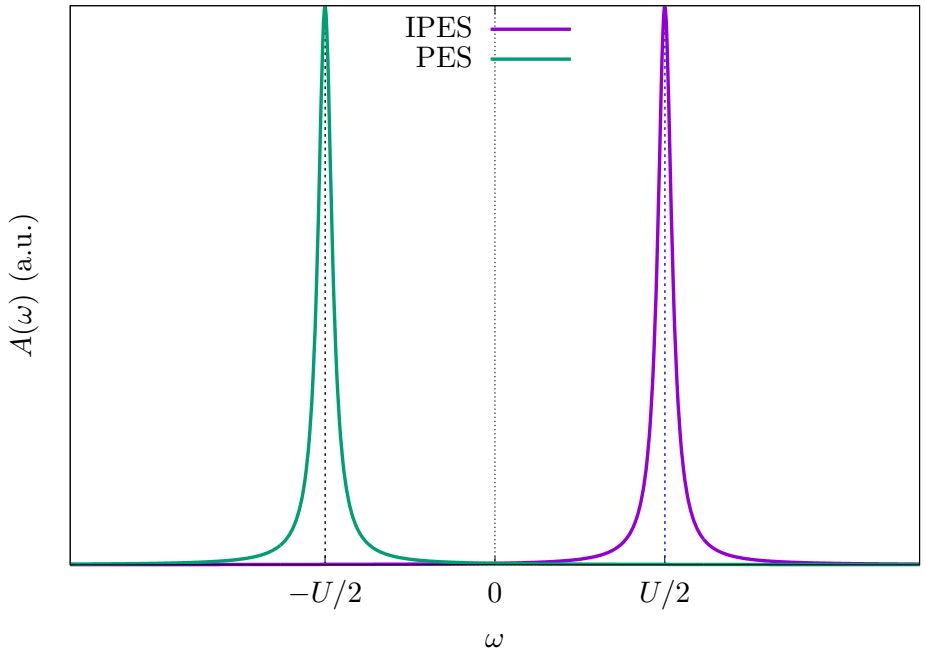

Figure 4: Sketch of the expected photoemission (PES) and inverse PES (IPES) spectrum for the interacting single-site problem

(c) Assume now that the self-energy calculated in the previous task (b) can be used as an approximation to the self-energy of an interacting 1d chain problem. Write down the retarded Green's function $G^R(\mathbf{k},\sigma,\omega)$ of the 1d chain resulting from making this approximation. Can you determine its poles? Calculate and sketch the spectral function. Comment on the approximation made. Under which circumstances would you expect it to describe your system qualitatively correctly?
We add the self-energy of the single-site problem at half-filling to the 1d chain at half-filling ($\mu = 0$, i.e. $\xi_k = \epsilon_k$). This leads to the retarded Green's function

$$G^R(k,\sigma,\omega) = \frac{1}{(\omega - \epsilon_k + i0^+) - \frac{U^2}{4}\frac{1}{\omega+i0^+}}$$

To calculate its poles we use $\frac{1}{\omega+i0^+} = \mathcal{P}\frac{1}{\omega} + i\pi\delta(\omega)$ and rewrite

$$G^R(k,\sigma,\omega) = \frac{1}{(\omega - \epsilon_k - \mathcal{P}\frac{U^2/4}{\omega}) + i(0^+ - \pi\frac{U^2}{4}\delta(\omega))}$$

The poles of the Green's function are then obtained by solving $\omega - \epsilon_k - \mathcal{P}\frac{U^2/4}{\omega} = 0$ leading to

$$\omega_\pm = \frac{\epsilon_k \pm \sqrt{\epsilon_k^2 + U^2}}{2}$$

Since $G^R(k,\sigma,\omega = 0) = 0$ for finite U, we can simplify now the Green's function for $\omega \neq 0$ to

$$G^R(k,\sigma,\omega) = \frac{1}{\omega - \epsilon_k - \frac{U^2/4}{\omega} + i\eta} = \underbrace{\frac{\omega - \epsilon_k - \frac{U^2}{4}}{\eta^2 + (\omega - \epsilon_k - \frac{U^2}{4\omega})^2}}_{\longrightarrow \frac{1}{\omega - \epsilon_k - \frac{U^2}{4\omega}}} - i \underbrace{\frac{\eta}{\eta^2 + (\omega - \epsilon_k - \frac{U^2}{4\omega})^2}}_{\longrightarrow \pi\delta(\omega - \epsilon_k - \frac{U^2}{4\omega})}$$

For the spectral function it follows

$$A(k,\omega) = \delta\left(\omega - \epsilon_k - \frac{U^2}{4\omega}\right)$$

In order to simplify this expression and since we already know the two roots $\omega_\pm$ of $f(\omega) = \omega - \epsilon_k - \frac{U^2}{4\omega}$, we will use that the composition of the Delta distribution with a continuously differentiable function $f(x)$ is given by[2] $\delta(f(x)) = \sum_i \frac{\delta(x - x_i)}{|f'(x_i)|}$, where the sum runs over all roots of $f(x)$, which are assumed to be simple (which is the case here). Here, $f'(\omega) = 1 + \frac{U^2}{4\omega^2}$, so we rewrite the spectral function as

$$A(k,\omega) = \frac{\delta(\omega - \omega_+)}{1 + \frac{U^2}{4\omega_+^2}} + \frac{\delta(\omega - \omega_-)}{1 + \frac{U^2}{4\omega_-^2}} \tag{7}$$

$$= \frac{\left(\epsilon_k + \sqrt{\epsilon_k^2 + U^2}\right)^2}{U^2 + \left(\epsilon_k + \sqrt{\epsilon_k^2 + U^2}\right)^2}\delta(\omega - \omega_+) + \frac{\left(\epsilon_k - \sqrt{\epsilon_k^2 + U^2}\right)^2}{U^2 + \left(\epsilon_k - \sqrt{\epsilon_k^2 + U^2}\right)^2}\delta(\omega - \omega_-) \tag{8}$$

We see that not only the position of the delta peaks, but also the spectral weights change as a function of interaction strength U. A sketch of the resulting spectral function for different values of U is shown in Figure 5.

The approximation of using an atomic self-energy neglects any k-dependence of the self-energy, which is a good approximation for localized systems at large $U \gg 1$. As a more refined version of an approximation using a local self-energy, the dynamical mean-field theory (DMFT) was used with quite some success over the past 20 years for strongly correlated systems.

(d) Now make a different approximation to the self-energy of the retarded Green's function. Assume it to have the form $\Sigma^R(k,\omega) = C + Z_{\mathbf{k}}^{-1}\omega - i\Gamma\omega^2$. What are the dimensions of the parameters $(C, Z_{\mathbf{k}}, \Gamma)$? Determine whether Γ is a positive or negative quantity. Assuming the system is in the "normal Fermi liquid regime", what can you say about the coefficients C and Z_k^{-1} Calculate the retarded Green's function $G^R(\mathbf{k},\sigma,\omega)$ of the 1d chain using this self-energy. Deduce the spectral function.

By assuming the form $\Sigma^R(k,\omega) = C + Z_{\mathbf{k}}^{-1}\omega - i\Gamma\omega^2$ for the self-energy, we see that C should be of dimension of frequency (or energy since we set $\hbar = 1$), Z_k should have dimension of 1, and Γ needs to have dimension of time.

To decide how to choose Γ, we write down the retarded Green's function and calculate the corresponding spectral function:

$$G^R(k,\sigma,\omega) = \frac{1}{(1 - Z_k^{-1})\omega - (\xi_k + C) + i(\Gamma\omega^2 + 0^+)}$$

[2]For more details, see e.g. *I. M Gel'fand, N. Y. Vilekin* "Generalized Functions, Volume 1", AMS Chelsea Publishing (1964)

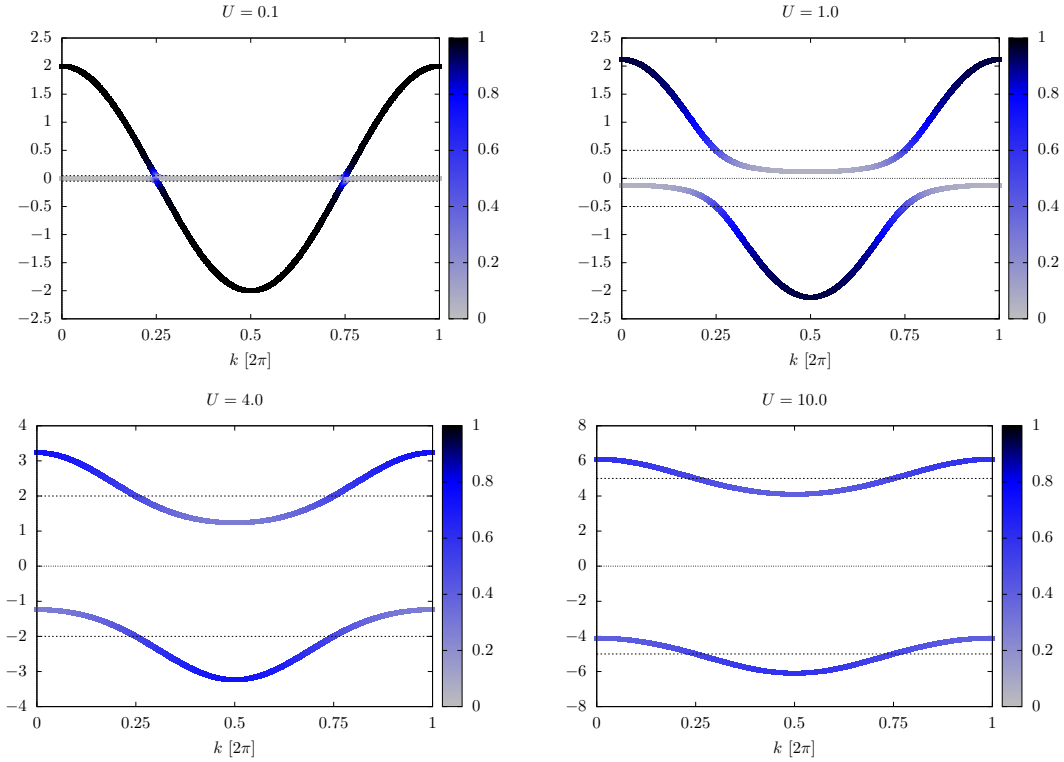

Figure 5: Spectral function according to equation (8). We plot here the positions of the delta-peaks and encode the weight via a color map. The dashed lines indicate the energies $-U/2$, 0, $U/2$.

$$A(k,\omega) = -\frac{1}{\pi}\mathrm{Im}\; G^R(k,\sigma,\omega) = \frac{1}{\pi}\frac{\Gamma\omega^2}{\Gamma^2\omega^4 + ((1-Z_k^{-1})\omega - \xi_k - C)^2}$$

Since the spectral weight needs to be non-negative, we conclude that $\Gamma \geq 0$. This actually corresponds to a finite lifetime of the quasiparticles.
We now assume that the system is in the normal Fermi liquid regime. To obtain the standard FL expression, we define the quasiparticle residue $\tilde{Z}_k = (1-Z_k^{-1})^{-1}$, the dispersion $\tilde{\epsilon}(k) = \tilde{Z}_k(\xi_k + C)$ and the inverse quasiparticle lifetime $\tilde{\eta}_k(\omega) = 1/\tilde{\tau}_k(\omega) = \tilde{Z}_k(\Gamma\omega^2 + 0^+)$ to arrive at

$$G^R(k,\sigma,\omega) = \frac{\tilde{Z}_k}{\omega - \tilde{\epsilon}_k + i\tilde{\eta}_k(\omega)}$$

$$A(k,\omega) = \frac{\tilde{Z}_k}{\pi}\frac{\tilde{\eta}_k(\omega)}{(\omega-\tilde{\epsilon}_k)^2 + (\tilde{\eta}_k(\omega))^2}$$

By these redefinitions it becomes clear that the constant C corresponds to a shift of the quasiparticle energies and that Z_k has direct consequences on the quasiparticle weight $\tilde{Z}_k$. The line-width of the spectral function is finally given by $\tilde{\eta}_k(\omega)$, which includes Γ.

In reality, the 1d chain system is not in the Fermi liquid regime. Nevertheless, the above form allows us to understand the modifications brought about by Fermi liquid-like self-energies onto band-like systems.
The approximation of using an atomic-like self-energy as in part c above is known under the name "Hubbard-1" approximation[3].

[3] J. Hubbard, *Proc. Roy. Soc. London A* **276** 238 (1963)