Continue with tight binding model

1. We use the property of the Dirac delta integral. For a single variable $\delta(f(x)-f_0)dx = \frac{1}{|f'(x_0)|}\delta(x-x_0)dx$. This can used in the multi dimensional integral by imagining first that we do a change of variables from d^dk to a $dSdk_\perp$, where dS is the parametrization of the constant energy surfaces and $dk_\perp$ is the orthogonal direction to those constant energy surfaces. This way the integral can be rewritten as

$$\int d^dk\delta(E-E_n(k)) = \int dSdk_\perp\delta(E-E_n(k_\perp)) = \int dSdk_\perp\frac{1}{|E_n'(k_\perp)|}\delta(k_0-k_\perp) \tag{1}$$

   where $|E_n'(k_\perp)| = |\frac{dE_n(k_\perp)}{dk_\perp}|$ which is equivalent $|\nabla E_n(\mathbf{k})|$. (Note that $\nabla E_n(\mathbf{k})$ as a vector in momentum space is orthogonal to the constant energy surfaces.) After that simply carrying out the integral in $k_\perp$, we arrive to Eq. (23) of the exercise sheet.

2. Similarly to the 2D case, after carrying out a Fourier transform we find that the dispersion relation for the 1D chain is $E(k) = -2t\cos(ka)$. The constant energy surfaces in this case are simply pairs of points $\pm k(E)$ for which $-2t\cos(k(E)a) = E$. The gradient of the dispersion relation is $\nabla E(k) = 2ta\sin(ka)$. Thus the density of states can be written as

$$D(E) = \frac{2}{\pi|2ta\sin(k(E)a)|} = \frac{2}{2ta\pi\sqrt{1-\left(\frac{E}{2t}\right)^2}} \tag{2}$$

   Here we simply expressed the $\sin(k(E)a) = \sqrt{1-\cos(k(E)a)^2}$, and expressed the right hand side using the energy. The factor of 2 comes from the $\pm k(E)$ wave numbers. We see that this has a divergence at the edges of the spectrum for $E = \pm 2t$, where the dispersion is flat, i.e. $|\nabla E(k)| = 0$.

3. The dispersion relation of the 2D tight binding model is $E(\mathbf{k}) = -2t(\cos(k_xa) + \cos(k_ya)$ (see on Fig. 2). If we calculate the gradient we find that $\nabla E(\mathbf{k}) = 2ta(\sin(k_xa), \sin(k_ya))$, which is 0 if $k_x, k_y = 0, \frac{\pi}{a}$. $\mathbf{k} = (0,0)$ is the bottom of the spectrum with $E = -4t$, while for $\mathbf{k} = (\frac{\pi}{a}, \frac{\pi}{a})$ the energy is $E = 4t$ at the top of the spectrum. For $\mathbf{k} = (0, \frac{\pi}{a})$ and $(\frac{\pi}{a}, 0)$ cases the energy is $E = 0$. So we can expect divergences at these three energy values. The constant energy surfaces are shown in Fig. 2.

4. Near the bottom of the spectrum $E(\mathbf{k}) \approx -4t + 2t\left(\frac{k_x^2a^2}{2} + \frac{k_y^2a^2}{2}\right) = E_0 + tk^2$, where $k = |\mathbf{k}|$. The constant energy surfaces are circles around $(0,0)$ in $\mathbf{k}$ space. The gradient $|\nabla E(\mathbf{k})| = |2ta(\sin(k_xa), \sin(k_ya))| = 2ta^2k$ The integral for the density of states thus reads as

$$D(E) = \frac{1}{2\pi^2}\int dS\frac{1}{2ta^2k(E)} = \frac{1}{2\pi^2}\frac{2\pi k(E)}{2ta^2k(E)} = const. \tag{3}$$

   We see that actually there is no divergence in this case. There is a singularity still as the density of states is a finite constant for $E > -4t$, but it is 0 for $E < -4t$.

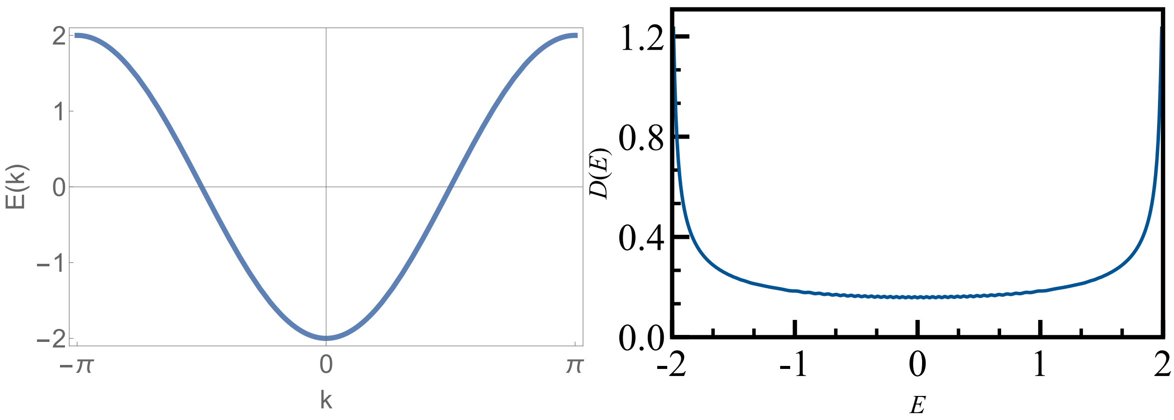

Figure 1: Dispersion relation (left) and density of states (right) of the 1 dimensional nearest neighbour tight binding model. Note that all the plots are done with $a = 1$.

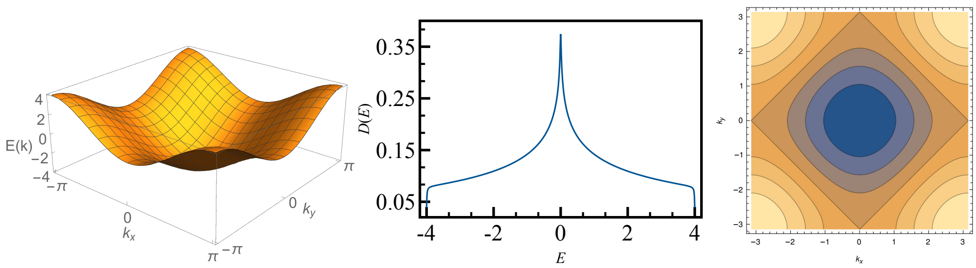

Figure 2: Dispersion relation (left) and density of states (middle) and constant energy surfaces (right) of the 2-dimensional nearest neighbour tight binding model.

5. We can deal with the $E \approx 4t$ case the same way, by writing the wave vector $\mathbf{k} = (\xi_x + \frac{\pi}{a}, \xi_y + \frac{\pi}{a})$, if the energy is close to $4t$ then ξ_x, ξ_y can be considered small, and everything is exactly the same as in the previous case. In fact in general $E(k_x, k_y) = -E(k_x + \frac{\pi}{a}, k_y + \frac{\pi}{a})$, and as a result the density of states is symmetric around 0.

6. $\cos(k_x a) + \cos(k_y a) = 0$ is satisfied if $k_y = \pm k_x \pm \frac{\pi}{a}$. This gives the tilted square contour shown in Fig. 2 in momentum space. Along these lines the $\sin k_y a = \pm \sin k_x a$. Note the relation between dS and dk_x. The density of states reads as

$$D(E) = \frac{1}{2\pi^2} \int\limits_{E=0} dS \frac{1}{\sqrt{2}2ta|\sin k_x a|} = 4\frac{1}{2\pi^2} \int\limits_0^\pi dk_x \frac{1}{2ta \sin k_x a} \tag{4}$$

where we use that the four sides of the square give the same contribution. The integrand on the right hand side diverges as $\frac{1}{k_x}$ near $k_x = 0$ and at $k_x = \pi$ thus the density of state also diverges (as shown in Fig. 2.) The integral can be carried out exactly: $\int \frac{1}{\sin x} = \ln \tan \frac{x}{2}$, this of course also shows that the integral is diverging.

Topological Invariants of Bands

(a) By definition, the Hamiltonian can be explicitly written as

$$H(k) = \begin{pmatrix} E_z & E_x - iE_y \\ E_x + iE_y & -E_z \end{pmatrix} \tag{5}$$

and according to the standard linear algebra, we find the eigenvalues to be

$$\epsilon(k)^2 - E_z^2 - (E_x - iE_y)(E_x + iE_y) = 0, \tag{6}$$

i.e. $\epsilon(k) = \pm\sqrt{E_x^2 + E_y^2 + E_z^2} = \pm|\mathbf{E}(k)|$.

(b) For $\mathbf{E}(k) = (0, -t\sin(k), -t\cos(k) + \mu)$, we have

$$\epsilon(k) = \pm\sqrt{t^2 + \mu^2 - 2\mu t\cos(k)}. \tag{7}$$

Clearly, the gap between the two bands closes when there exists k_0 such that $\epsilon(k_0) = 0$,

- $\mu > 0$: $\epsilon(k)$ can only be zero when $k = 0$ and $t/\mu = 1$.
- $\mu < 0$: $\epsilon(k) = 0$ when $k = \pi$ at $t/\mu = -1$.

(c) Calculate the winding number $\nu = \frac{1}{2\pi}\int_{-\pi}^{\pi} \mathrm{d}k\ \hat{\mathbf{e}}_{\mathbf{x}} \cdot \left(\mathbf{n}(k) \times \frac{\partial \mathbf{n}(k)}{\partial k}\right)$. Notice that in this setup because of $\hat{\mathbf{e}}_{\mathbf{x}}$ the integrand reduces to $n_y\partial_k n_z - n_z\partial_k n_y$.

- $\mu = 0$: In this case, $\mathbf{n}(\mathbf{k}) = (0, -\sin(k), -\cos(k))$, and

$$\begin{aligned}\nu &= \frac{1}{2\pi}\int_{-\pi}^{\pi} \mathrm{d}k\ n_y(k)\partial_k n_z(k) - n_z(k)\partial_k n_y(k) \\ &= -\frac{1}{2\pi}\int_{-\pi}^{\pi} \mathrm{d}k\ [\sin^2(k) + \cos^2(k)] = -1\end{aligned} \tag{8}$$

- $\mu \to \pm\infty$: $\mathbf{n}(\mathbf{k}) = (0, -t\sin(k), -t\cos(k))/\sqrt{t^2 + \mu^2 - 2\mu t\cos(k)}$.
  Notice that now in the expression of $n_y\partial_k n_z - n_z\partial_k n_y$, the denominator has a higher power of μ, so after we take the limit $\mu \to \pm\infty$, the integrand reduces to 0. Therefore, we have $\nu = 0$.

(d) (**optional**) See the Mathematica Notebook