(A.) *The tight-binding* model on a square lattice.

1. The simplest way is to start by reversing the relationship, that is, writing the N states $|j\rangle$ according to the N states $|\mathbf{k}\rangle$. Let's not forget that $\mathbf{k}$ belongs to the first Brillouin zone, that is, $\mathbf{k} = \big(-\frac{\pi}{a} + \frac{2\pi}{L}n_x\big)\mathbf{e_x} + \big(-\frac{\pi}{a} + \frac{2\pi}{L}n_y\big)\mathbf{e_y}$, with $n_x = 1...\frac{L}{a}$ et $n_y = 1...\frac{L}{a}$, where L is the length of the lattice so that $L^2 = Na^2$. We have (simple inversion of Fourier transform):

$$|i\rangle = \frac{1}{\sqrt{N}}\sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r_i}}|\mathbf{k}\rangle \tag{1}$$

It is verified that:

$$\begin{aligned}|\mathbf{k}\rangle &= \frac{1}{\sqrt{N}}\sum_i e^{-i\mathbf{k}\cdot\mathbf{r_i}}\Big(\frac{1}{\sqrt{N}}\sum_{\mathbf{k}'} e^{i\mathbf{k}'\cdot\mathbf{r_i}}|\mathbf{k}'\rangle\Big)\\ &= \frac{1}{N}\sum_{\mathbf{k}'}\underbrace{\Big(\sum_i e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r_i}}\Big)}_{=N\delta_{\mathbf{k},\mathbf{k}'}}|\mathbf{k}'\rangle = |\mathbf{k}\rangle.\end{aligned} \tag{2}$$

Let's use Eq. (**??**) to rewrite the Hamiltonian.

$$\begin{aligned}H &= -t\sum_{\langle i,j\rangle}\big(|i\rangle\langle j| + |j\rangle\langle i|\big)\\ &= -t\sum_i\Big(\sum_{j\text{ , neighbours of }i}|i\rangle\langle j|\Big)\\ &= -\frac{t}{N}\sum_{\mathbf{k}',\mathbf{k}}\sum_i\Big(\sum_{j\text{ , neighbours of }i}e^{i(\mathbf{k}\cdot\mathbf{r_i}-\mathbf{k}'\cdot\mathbf{r_j})}\Big)|\mathbf{k}\rangle\langle\mathbf{k}'|\\ &= -\frac{t}{N}\sum_{\mathbf{k}',\mathbf{k}}\eta(\mathbf{k}')\underbrace{\Big(\sum_i e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r_i}}\Big)}_{=N\delta_{\mathbf{k},\mathbf{k}'}}|\mathbf{k}\rangle\langle\mathbf{k}'|,\end{aligned} \tag{3}$$

where $\eta(\mathbf{k}') = e^{ia\mathbf{k}'\cdot\mathbf{e_x}} + e^{-ia\mathbf{k}'\cdot\mathbf{e_x}} + e^{ia\mathbf{k}'\cdot\mathbf{e_y}} + e^{-ia\mathbf{k}'\cdot\mathbf{e_y}} = 2(\cos(k'_x a) + \cos\big(k'_y a\big))$.
We then obtain:

$$H = \sum_{\mathbf{k}}\mathcal{E}_{\mathbf{k}}|\mathbf{k}\rangle\langle\mathbf{k}|,$$

with $\mathcal{E}_{\mathbf{k}} = -2t(\cos(k_x a) + \cos(k_y a))$.

2. Taking inspiration from the previous question, we can introduce the creation operator:

$$c^\dagger_{\mathbf{k},\sigma} = \frac{1}{\sqrt{N}}\sum_i e^{-i\mathbf{k}\cdot\mathbf{r_i}}c^\dagger_{i,\sigma}. \tag{4}$$

By taking the hermitian conjugate, one must necessarily have

$$c_{\mathbf{k},\sigma} = \frac{1}{\sqrt{N}} \sum_i e^{i\mathbf{k}\cdot\mathbf{r_i}} c_{i,\sigma}. \tag{5}$$

To be acceptable, these operators must follow the fermionic anti-commutations relations:

$$\left\{c_{\mathbf{k},\sigma}, c^\dagger_{\mathbf{k}',\sigma'}\right\} = \frac{1}{N}\sum_{i,j} e^{i(\mathbf{k}\cdot\mathbf{r_i}-\mathbf{k}'\cdot\mathbf{r_j})} \underbrace{\left\{c_{i,\sigma}, c^\dagger_{j,\sigma'}\right\}}_{=\delta_{i,j}\delta_{\sigma,\sigma'}} = \frac{1}{N}\underbrace{\sum_i e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r_i}}}_{=N\delta_{\mathbf{k},\mathbf{k}'}} \delta_{\sigma,\sigma'} = \delta_{\mathbf{k},\mathbf{k}'}\delta_{\sigma,\sigma'}. \tag{6}$$

And also, $\left\{c^\dagger_{\mathbf{k}',\sigma'}, c^\dagger_{\mathbf{k},\sigma}\right\} = \left\{c_{\mathbf{k}',\sigma'}, c_{\mathbf{k},\sigma}\right\} = 0$.
We then repeat the same calculations as in Eq. (**??**) to get:

$$H = -t \sum_{\langle i,j\rangle,\sigma} \left(c^\dagger_{i,\sigma} c_{j,\sigma} + c^\dagger_{j,\sigma} c_{i,\sigma}\right) = \sum_{\mathbf{k},\sigma} \mathcal{E}_{\mathbf{k}} c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma}.$$

(B.)

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

$$\int d^dk \delta(E - E_n(k)) = \int dSdk_\perp \delta(E - E_n(k_\perp)) = \int dSdk_\perp \frac{1}{|E_n'(k_\perp)|}\delta(k_0 - k_\perp) \tag{7}$$

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. (2) 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

$$D(E) = \frac{2}{\pi|2ta\sin(k(E)a)|} = \frac{2}{2ta\pi\sqrt{1 - \left(\frac{E}{2t}\right)^2}} \tag{8}$$

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 $E(\mathbf{k}) = -2t(\cos(k_x a) + \cos(k_y a)$ (see on Fig. **??**). If we calculate the gradient we find that $\nabla E(\mathbf{k}) = 2ta(\sin(k_x a), \sin(k_y a))$, 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. **??**.

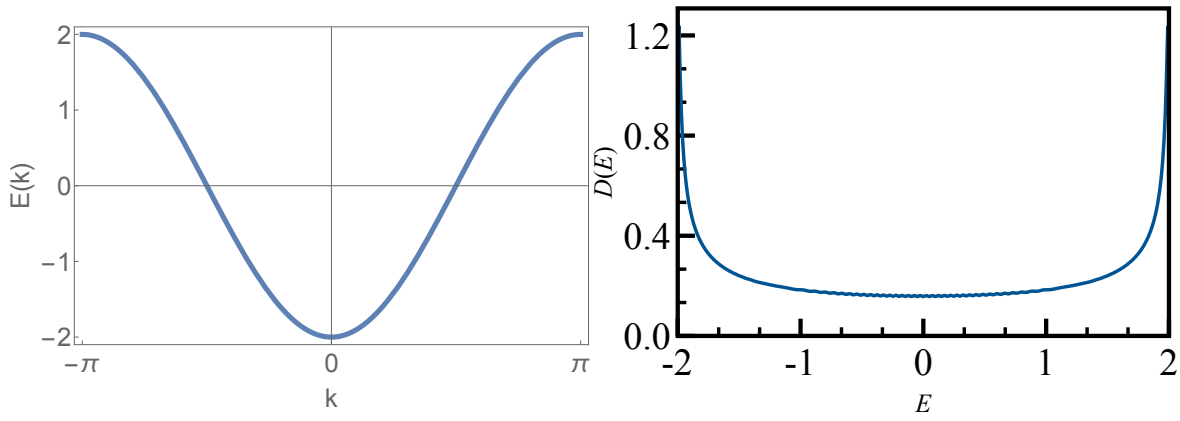

Figure 1: Dispersion relation (left) and density of states (right) of the 1 dimensional nearest neighbour tight binding model. Note that all the plots are done with $a = 1$.

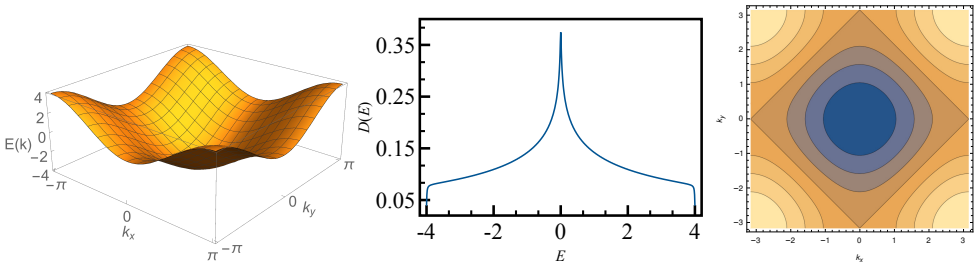

Figure 2: Dispersion relation (left) and density of states (middle) and constant energy surfaces (right) of the 2-dimensional nearest neighbour tight binding model.

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

$$D(E) = \frac{1}{2\pi^2}\int dS \frac{1}{2ta^2 k(E)} = \frac{1}{2\pi^2}\frac{2\pi k(E)}{2ta^2 k(E)} = const. \tag{9}$$

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 $E < -4t$.

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. **??** 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

$$D(E) = \frac{1}{2\pi^2}\int\limits_{E=0} dS \frac{1}{\sqrt{2}2ta|\sin k_x a|} = 4\frac{1}{2\pi^2}\int\limits_0^{\pi} dk_x \frac{1}{2ta\sin k_x a} \tag{10}$$

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. **??**.) 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.

(C.)

1. Considering only H_U, the configurations of minimum energy (zero energy) with N sites and N electrons are those for which there is one electron per site. The subspace of energy U consists of the configurations with a single site with two electrons (and thus a single empty site).

2. P_0 is the projection operator on zero energy configurations. Hence $P_0 H_U P_0 = 0$. Besides, $\forall |\Psi\rangle$ belonging to the eigen subspace of H_U of zero energy, $H_t|\Psi\rangle$ will be a linear combination of states with a doubly occupied site (and therefore also an empty site). That is, $H_t|\Psi\rangle$ will be part of the eigen subspace of H_U of energy U. So by orthogonality of the eigen-subspaces, $P_0 H_t|\Psi\rangle = 0$, $\forall |\Psi\rangle$ belonging to the eigen subspace of H_U of zero energy and $P_0 H_t P_0 = 0$.

3. As we have just seen, $\forall |\Psi\rangle$ belonging to the eigen subspace of H_U of zero energy, $H_t|\Psi\rangle$ will be part of the eigen subspace of H_U of energy U. This implies that $P_n H_t|\Psi\rangle = 0\,,\ \forall n > 1$ also by orthogonality of the different eigen subspaces of H_U. We have just shown that

$$\frac{P_0 H_t P_n H_t P_0}{E_0 - E_n} = \sum_{\langle i,j\rangle,\langle k,l\rangle} \frac{P_0 H^t_{(k,l)} P_1 H^t_{(i,j)} P_0}{E_0 - E_1}.$$

In fact, $\forall |\phi\rangle$ in the Hilbert space, $H^t_{(i,j)} P_0 |\phi\rangle$ can only give a ket state that is a superposition of configurations with the site i doubly occupied and the site j empty or vice-versa. Likewise for any bra $\langle\phi'|$, $\langle\phi'|P_0 H^t_{(k,l)}|$ can only be a bra superposition of configurations with the site k doubly occupied and the site l empty or vice-versa. Hence $P_1 H^t_{(i,j)} P_0|\phi\rangle = H^t_{(i,j)} P_0|\phi\rangle$. Besides, as P_1 is the identity for any state of the proper subset of H_U of energy U (by definition of a projector), $P_1 H^t_{(i,j)} P_0|\phi\rangle = H^t_{(i,j)} P_0|\phi\rangle$. We thus have:

$$\sum_{n\neq 0} \frac{P_0 H_t P_n H_t P_0}{E_0 - E_n} = \sum_{\langle i,j\rangle} \frac{P_0 H^t_{(i,j)} P_1 H^t_{(i,j)} P_0}{E_0 - E_1}.$$

In the second order, we realize that the different pairs of sites do not communicate by the hopping term. Let us thus focus on the Hubbard model on 2 sites:

$$\begin{aligned} H &= -t \sum_{\langle i,j\rangle,\sigma} (c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{j\sigma} c_{i\sigma}) + U \sum_i n_{i\uparrow} n_{i\downarrow} \\ &= \underbrace{-t(c^\dagger_{1\uparrow} c_{2\uparrow} + c^\dagger_{2\uparrow} c_{1\uparrow} + c^\dagger_{1\downarrow} c_{2\downarrow} + c^\dagger_{2\downarrow} c_{1\downarrow})}_{=H_t} + \underbrace{U\,(n_{1\uparrow} n_{1\downarrow} + n_{2\uparrow} n_{2\downarrow})}_{=H_U} \end{aligned}$$

4. There are 6 possible states for two electrons:

$$\begin{aligned} |1\rangle &= c^\dagger_{1\uparrow} c^\dagger_{2\uparrow} |0\rangle \\ |2\rangle &= c^\dagger_{1\downarrow} c^\dagger_{2\downarrow} |0\rangle \\ |3\rangle &= c^\dagger_{1\uparrow} c^\dagger_{2\downarrow} |0\rangle \\ |4\rangle &= c^\dagger_{1\downarrow} c^\dagger_{2\uparrow} |0\rangle \\ |5\rangle &= c^\dagger_{1\uparrow} c^\dagger_{1\downarrow} |0\rangle \\ |6\rangle &= c^\dagger_{2\uparrow} c^\dagger_{2\downarrow} |0\rangle \end{aligned}$$

We have (see course)

$$\begin{aligned} H_U|1\rangle &= 0 \\ H_U|2\rangle &= 0 \\ H_U|3\rangle &= 0 \\ H_U|4\rangle &= 0 \\ H_U|5\rangle &= U|5\rangle \\ H_U|6\rangle &= U|6\rangle \end{aligned}$$

The ground state of H_U (energy $E_0 = 0$) is four-fold degenerate $\{|1\rangle, |2\rangle, |3\rangle, |4\rangle\}$ and the excited state (energy $E_1 = U$) is two-fold degenerate $\{|5\rangle, |6\rangle\}$. The projector on the ground states is given by

$$P_0 = \sum_{m=1}^{4} |m\rangle\langle m|$$

and the projector on the first excited states

$$P_1 = \sum_{p=5}^{6} |p\rangle\langle p|$$

5. We have

$$\begin{aligned} \langle 5|H_t|1\rangle &= 0 \\ \langle 6|H_t|1\rangle &= 0 \\ \langle 5|H_t|2\rangle &= 0 \\ \langle 6|H_t|2\rangle &= 0 \\ \langle 5|H_t|3\rangle &= -t \\ \langle 6|H_t|3\rangle &= -t \\ \langle 5|H_t|4\rangle &= t \\ \langle 6|H_t|4\rangle &= t \end{aligned}$$

Therefore, the only non-zero matrix elements of $H_{\text{eff}}^{(2)}$ are

$$\begin{aligned}
\langle 3|H_{\text{eff}}^{(2)}|3\rangle &= \sum_{p=5,6} \frac{\langle 3|H_t|p\rangle\langle p|H_t|3\rangle}{E_0 - E_1} \\
&= -\frac{1}{U}\left(\langle 3|H_t|5\rangle\langle 5|H_t|3\rangle + \langle 3|H_t|6\rangle\langle 6|H_t|3\rangle\right) \\
&= -\frac{2t^2}{U} \\
\langle 3|H_{\text{eff}}^{(2)}|4\rangle = \langle 4|H_{\text{eff}}^{(2)}|3\rangle &= \sum_{p=5,6} \frac{\langle 3|H_t|p\rangle\langle p|H_t|4\rangle}{E_0 - E_1} \\
&= -\frac{1}{U}\left(\langle 3|H_t|5\rangle\langle 5|H_t|4\rangle + \langle 3|H_t|6\rangle\langle 6|H_t|4\rangle\right) \\
&= \frac{2t^2}{U} \\
\langle 4|H_{\text{eff}}^{(2)}|4\rangle &= \sum_{p=5,6} \frac{\langle 4|H_t|p\rangle\langle p|H_t|4\rangle}{E_0 - E_1} \\
&= -\frac{1}{U}\left(\langle 4|H_t|5\rangle\langle 5|H_t|4\rangle + \langle 4|H_t|6\rangle\langle 6|H_t|4\rangle\right) \\
&= -\frac{2t^2}{U}
\end{aligned}$$

and in the basis $\{|1\rangle, |2\rangle, |3\rangle, |4\rangle\}$ the matrix of $H_{\text{eff}}^{(2)}$ is given by

$$\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{2t^2}{U} & \frac{2t^2}{U} \\ 0 & 0 & \frac{2t^2}{U} & -\frac{2t^2}{U} \end{pmatrix}$$

By diagonalising this matrix we obtain a ground state of energy $E = -\frac{4t^2}{U}$

$$\frac{1}{\sqrt{2}}(|3\rangle - |4\rangle)$$

and three degenerate excited states of energy $E = 0$

$$\begin{aligned}
&|1\rangle \\
&|2\rangle \\
&\frac{1}{\sqrt{2}}(|3\rangle + |4\rangle)
\end{aligned}$$

6. The ground states of H_U are states with one electron per site. Denoting $|\sigma_1, \sigma_2\rangle$ the state with an electron of spin σ_1 at site 1 and an electron of spin σ_2 at site 2, we have

$$\begin{aligned}
|1\rangle &= c_{1\uparrow}^\dagger c_{2\uparrow}^\dagger |0\rangle \\
&= |\uparrow,\uparrow\rangle \\
|2\rangle &= c_{1\downarrow}^\dagger c_{2\downarrow}^\dagger |0\rangle \\
&= |\downarrow,\downarrow\rangle \\
|3\rangle &= c_{1\uparrow}^\dagger c_{2\downarrow}^\dagger |0\rangle \\
&= |\uparrow,\downarrow\rangle \\
|4\rangle &= c_{1\downarrow}^\dagger c_{2\uparrow}^\dagger |0\rangle \\
&= |\downarrow,\uparrow\rangle
\end{aligned}$$

and the eigen states of H_{eff} read:

$$\begin{aligned} |1\rangle &= |\uparrow,\uparrow\rangle \\ |2\rangle &= |\downarrow,\downarrow\rangle \\ \frac{1}{\sqrt{2}}(|3\rangle + |4\rangle) &= \frac{1}{\sqrt{2}}(|\uparrow,\downarrow\rangle + |\downarrow,\uparrow\rangle) \\ \frac{1}{\sqrt{2}}(|3\rangle - |4\rangle) &= \frac{1}{\sqrt{2}}(|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle) \end{aligned}$$

Summary The degeneracy of the ground state of H_U is partially lifted by the perturbation H_t. The energy level is split into the ground state of energy $-\frac{4t^2}{U}$ (singlet) and three states of energy 0 (triplets).

(D.) Using the following expansion for the square root $\sqrt{1+x^2} \approx 1 + 1/2x^2$ we find the energy in the second order:

$$\begin{aligned} &E_\pm = \tfrac{U \pm \sqrt{U^2+16t^2}}{2} = \tfrac{U \pm U\sqrt{1+16t^2/U^2}}{2} \approx \tfrac{U \pm U(1+8t^2/U^2)}{2} \\ &E_+ \approx U + 4t^2/U \\ &E_- \approx -4t^2/U \\ &E_0 = 0 \end{aligned}$$

For the spectrum close to 0 in the limit $t \ll U$ we find the same energies as obtained with the effective Hamiltonian.