- This is an individual homework. Each submission must have been worked out and written up by the submitting student.
- This homework is an open-book assessment. Students are permitted to use lecture slides, notes, exercises, and any other provided resource materials to solve the problems.
- Some problems may require students to generate plots. For this, students may utilize any offline or online plotting tools of their choice.
- Each homework set contains questions worth a total of 20 points. You may gain extra point(s) by solving the optional questions. But the maximum you can get in one homework is 20.
- A digital copy of the homework solutions, whether handwritten or typed, must be submitted through the Moodle assignment section by Monday, October 7th, 2024, at 11:59 PM.
- The homework will be assessed within a reasonable timeframe, and students may discuss their assessments during the exercise sessions.

For a 1D monoatomic chain of N sites a nearest-neighbour tight-binding Hamiltonian is given by:

$$H = -t \sum_{j=1}^{N} \left(c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j \right). \tag{1}$$

where t is the hopping amplitude, and $c_i^\dagger$ (c_i) are the fermionic particle creation (annihilation) operators associated to site-i. This is a crucial Hamiltonian in solid state physics, which can be supplemented with additional terms to model a number of effects observed in real systems.

Diatomic tight binding chain

Now let's consider another example by adding alternating onsite potential to the nearest-neighbour tight-binding model with periodic boundary condition (assuming N is even and $v_a < v_b$):

$$H = -t \sum_{j=1}^{N} \left(c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j \right) + v_a \sum_{j=1}^{N/2} n_{2j-1} + v_b \sum_{j=1}^{N/2} n_{2j}, \tag{2}$$

where $n_j = c_j^\dagger c_j$ is the number operator. This Hamiltonian models a diatomic system with two distinct atoms, implied by two different on-site potentials, in each unit cell.

(a) Using the Heisenberg equation of motion, write the equation of motion for $c_i^\dagger c_{i+1}$. **[2 points]**

(b) **Band structure**

Let's now figure out the band structure of such a system.

(i) In order to diagonalize the Hamiltonian Eq. (2), we first label the operators at odd site as $a_j \equiv c_{2j-1}$ and at even site as $b_j \equiv c_{2j}$. Then the corresponding Fourier transformation is

$$\begin{aligned} a_k &\coloneqq \sqrt{\frac{2}{N}} \sum_{j=1}^{N/2} a_j e^{-2ikj},\ a_j = \sqrt{\frac{2}{N}} \sum_{\#k} a_k e^{+2ikj}; \\ b_k &\coloneqq \sqrt{\frac{2}{N}} \sum_{j=1}^{N/2} b_j e^{-2ikj},\ b_j = \sqrt{\frac{2}{N}} \sum_{\#k} b_k e^{+2ikj}; \end{aligned} \tag{3}$$

where $\#k$ indicates the sum is over reduced Brillouin zone $k = \frac{2\pi}{N} n$, $n = -\lfloor \frac{N}{4} \rfloor + 1, -\lfloor \frac{N}{4} \rfloor + 2, \ldots, -\lfloor \frac{N}{4} \rfloor + \frac{N}{2}$, $k \in (\frac{\pi}{2}, \frac{\pi}{2}]$ (we have encountered this in Exercise 3).
Now use Eq. (3) to write the Hamiltonian Eq. (2) in momentum space. **[2 points]**

(ii) Define the grouped operator $\psi_k^\dagger \coloneqq \left(a_k^\dagger, b_k^\dagger\right)$. Write the Hamiltonian into the following matrix form:

$$H = \sum_{\#k} \psi_k^\dagger \mathcal{H}(k) \psi_k. \tag{4}$$

What is the expression of $\mathcal{H}(k)$? **[2 points]**

(iii) Find the unitary transformation U_k to diagonalize $\mathcal{H}(k)$. What are the eigenvalues? And what is the gap Δ (the smallest difference between the two eigenvalues)? **[3 points]**
hint: If a hermitian matrix $\mathcal{H}$ can be written as a linear combination of identity matrix and Pauli matrices σ^x, σ^y and σ^z:

$$\mathcal{H} = h_0 \mathbf{I} + h_1 \sigma^x + h_2 \sigma^y + h_3 \sigma^z = h_0 \mathbf{I} + \vec{h} \cdot \vec{\sigma},$$

we can parameterize $\vec{h}$ as $\vec{h} = |\vec{h}| \left(\cos\varphi \sin\theta,\ \sin\varphi \sin\theta,\ \cos\theta\right)^{\mathrm{T}}$, where $|\vec{h}| = \sqrt{h_1^2 + h_2^2 + h_3^2}$, and then the unitary transformation to diagonalize $\mathcal{H}$ is

$$U = \begin{pmatrix} e^{-i\varphi/2} \cos\frac{\theta}{2} & e^{+i\varphi/2} \sin\frac{\theta}{2} \\ e^{-i\varphi/2} \sin\frac{\theta}{2} & -e^{+i\varphi/2} \cos\frac{\theta}{2} \end{pmatrix}.$$

Finally, we find the diagonalized Hamiltonian as

$$H = \sum_{\#k} \psi_k^\dagger U_k U_k^\dagger \mathcal{H}(k) U_k U_k^\dagger \psi_k = \sum_{\#k} \left(E_\alpha(k) \alpha_k^\dagger \alpha_k + E_\beta(k) \beta_k^\dagger \beta_k \right), \tag{5}$$

where $\left(\beta_k^\dagger, \alpha_k^\dagger\right) = \left(a_k^\dagger, b_k^\dagger\right) U_k$.

(c) **(Optional)** By evaluating the usual anticommutation relations, confirm that α_k and β_k are fermionic as well. **[1 point]**

(d) Analyze the behavior of the lowest energy band near its minima and compare it with the free electron dispersion to determine the "effective" mass of the electrons. **[1 point]**

(e) **(Optional)** Determine the effective mass of the electrons for the lower band at $k = \pi/2$. What does a negative effective mass signify? **[2 points]**

(f) **Exciton**

We can now obtain a simple model for excitons by additionally introducing an interaction between the electrons and holes to Eq. (2). In this task we consider short-range interactions between nearest neighbor sites

$$\hat{U} = u \sum_j n_j n_{j+1}.$$

Express the interaction in the form

$$\hat{U} \approx -\frac{4u}{N} \sum_{\#k,k',q} \cos^2(k-k')\alpha_{q+k}\beta_k^\dagger \beta_{k'}\alpha_{k'+q}^\dagger. \tag{6}$$

Proceed as follows:

(i) Recall the transformation of the operators a_k, b_k into the eigenbasis in the interaction free case (valence, conduction band) with the unitary matrix U:

$$\begin{pmatrix}\beta_k \\ \alpha_k\end{pmatrix} = U^\dagger \begin{pmatrix}a_k \\ b_k\end{pmatrix} = \begin{pmatrix}e^{-i\varphi/2}\cos\frac{\theta}{2} & e^{+i\varphi/2}\sin\frac{\theta}{2} \\ e^{-i\varphi/2}\sin\frac{\theta}{2} & -e^{+i\varphi/2}\cos\frac{\theta}{2}\end{pmatrix} \cdot \begin{pmatrix}a_k \\ b_k\end{pmatrix} \tag{7}$$

We approximate the matrix elements with their value at $k = \pi/2$ in the lower band. Why do we focus on this value of k ? Show that in this case

$$\alpha_k \approx a_k$$
$$\beta_k \approx b_k$$

up to a phase. **[2 points]**

(ii) Under this approximation, rewrite the interaction U by introducing the number operators on even and odd sites n_{2j} and $n_{2j\pm1}$, and then replace them with α's and β's. We neglect here all terms which only contain two β-operators to obtain Eq. (6). Consider the fermionic commutation relations! **[3 points]**

(iii) We now make the Ansatz for an excitonic wave function with momentum q:

$$|\Psi_q\rangle = \sum_{\#k} A_k^q \, \alpha_{q+k}\beta_k^\dagger |\Omega\rangle \ , \tag{8}$$

where Ω denotes the ground state for $\hat{U} = 0$, $|\Omega\rangle = \prod_{\#k} \alpha_k^\dagger |0\rangle$. Within our approximation, one can determine A^q such that the exciton is an eigenstate of $H + \hat{U}$ with energy $E_\Omega + \omega_q$. Here E_Ω denotes the groundstate energy for $\hat{U} = 0$, $H|\Omega\rangle = E_\Omega|\Omega\rangle$. Furthermore, let's do a global shift E_{shift} to the energy spectrum so that $E_\alpha(k) = E_{\text{shift}} - E_k$ and $E_\beta(k) = E_{\text{shift}} + E_k$ (this operation, of course, would not change the physics). What is E_{shift}?
Show that the equation

$$(E_k + E_{k+q} - \omega_q)\, A_k^q = \frac{4u}{N} \sum_{\#k'} A_{k'}^q \cos^2(k-k') \ , \tag{9}$$

must be satisfied. **[4 points]**

(iv) For $u \ll t, |v_a - v_b|$, we can approximate $\cos(k-k') \approx 1$. Show, that Eq. (9) can be simplified to

$$\frac{1}{4u} = \frac{1}{N} \sum_{\#k} \frac{1}{E_k + E_{k+q} - \omega_q} \ . \tag{10}$$

[1 point]

(v) **(Optional)** Find a graphical solution for the equation for fixed v_a, v_b, t and q on a small system (e.g., $N = 10$) with *Mathematica* or any numerical tool you like. Show that a state exists below the energy gap Δ and interpret this result! Discuss the differences compared to the exciton energy structure discussed in the three dimensional situation with a Coulomb interaction in the lecture. **[2 points]**