University of Zurich[UZH]

**PHY401**
**Exercise Sheet 7**

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Due on 4 Nov. 2025

Discussion on 4 Nov. 2025

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## 1 Approximating the electronic band structure of Si using a cubic lattice ❖ From 2024

Hidden due to University of Zurich policy.

# The exercises in the following pages are optional.

### Preface

After the following two exercises, you should be able to: (1) Understand the usage of the matrix representation in solving a quantum mechanical problem; (2) Build up a connection between the spin system and the electron system. These two ideas can be generalized to more complex systems. Always try to analyze a system from different perspectives (Dirac notation, matrix representation, etc.). An analogy can sometimes help you understand a new system based on an old one.
The first exercise is a warm-up exercise that familiarizes you with the matrix representation in a spin system. The second exercise (electron system) is more related to the lecture but later you will find similarities between the the two systems.

## 2 Simple spin system ★ New

**Setup** A single spin-1/2 system. The Hamiltonian is given by $H = H_0 + \boldsymbol{\sigma} \cdot \boldsymbol{B}$[1] where

$$H_0 = E_0 \mathbb{I}_{2\times 2} = \begin{pmatrix} E_0 & 0 \\ 0 & E_0 \end{pmatrix}$$

is the free Hamiltonian where both spin-up and spin-down states have the same energy $E_0$. The magnetic field $\boldsymbol{B}$ is given by $\boldsymbol{B} = (B_x, B_y, B_z)$ and the Pauli matrices are given by

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

*Note: We omit physical constants and signs for simplicity.*

(a1) Assuming $\boldsymbol{B} = 0$, write down the matrix form of the Hamiltonian in the basis of $|\uparrow\rangle$ and $|\downarrow\rangle$ (the eigenstates of $\sigma_z$).

(a2) Now we apply a magnetic field along the $x$ axis. Write down the matrix form of the Hamiltonian in the same basis. You should get

$$H = \begin{pmatrix} E_0 & B_x \\ B_x & E_0 \end{pmatrix}$$

(a3) Apparently, with the magnetic field, the spin-up and spin-down states are no longer the eigenstates, meaning that when you are sitting on one state, the magnetic field will try to scatter it and put it into another state. In other words, the two states $|\uparrow\rangle$ and $|\downarrow\rangle$ are no longer stable. Denote $(1,0)$ and $(0,1)$ as the vector form of the $|\uparrow\rangle$ and $|\downarrow\rangle$ states, respectively. Prove that $(1,1)$ and $(1,-1)$ are the eigenstates of the new Hamiltonian. Also prove that the new energy levels are

$$E_+ = E_0 + B_x, \quad E_- = E_0 - B_x.$$

Interestingly, $(1,1)$ and $(1,-1)$ are also the eigenstates of $\sigma_x$. Try to explain your result. And think about why the magnetic field changes the energy?

(b) Now we want to understand the physical interpretation of the diagonal term in the Hamiltonian and the off-diagonal term in the Hamiltonian. You might need to recall the concept of *time-dependent perturbation theory* or *Fermi-Golden Rule*. Please You may use ChatGPT to explore this concept. Here is a prompt that you can use:

[1] Note: In this sheet we set $\hbar = 1$ and absorb the magnetic moment constant into the definition of $\mathbf{B}$, so the Zeeman term is written simply as $\boldsymbol{\sigma} \cdot \mathbf{B}$. The overall sign convention is unimportant for the purpose of this exercise.

> Could you explain the physical meaning of the off-diagonal elements in the Hamiltonian using the time-dependent perturbation theory? You can explain the concept in the two-level system. For example the 2 dimensional Hamiltonian goes like
>
> `E_1 & B \\ B & E_2`
>
> (latex-like syntax). Please think before you answer. I need both relatively rigorous and intuitive answers.

In a word, the diagonal term is the "unperturbed energy" of the system and the off-diagonal term tells you how fast the system is hopping from one state to another.

(c) Now we are adding in a $z$-component of the magnetic field: now the Hamiltonian goes like

$$H = \begin{pmatrix} E_0 + B_z & B_x \\ B_x & E_0 - B_z \end{pmatrix}$$

Using the equation $\det(H - \lambda \mathbb{I}) = 0$, show that the eigenvalues are

$$E_\pm = E_0 \pm \sqrt{B_x^2 + B_z^2} = E_0 \pm |\boldsymbol{B}|$$

Discuss the two limiting cases where $B_z = 0, B_x \neq 0$, and $B_z \neq 0, B_x = 0$ separately. Explain why $B_z$ and $B_x$ have the same effect on the energy. Explain why the energy splitting depends only on the total field magnitude.

(d) Can you make a guess on the resulting energy levels when you add in all three components of the magnetic field, i.e. $x$, $y$ and $z$-components. ? The Hamiltonian now is

$$H = \begin{pmatrix} E_0 + B_z & B_x - iB_y \\ B_x + iB_y & E_0 - B_z \end{pmatrix}$$

Take a minute to think about your result. Does it have anything to do with the rotational symmetry of the system?

## 3 Electron in a periodic potential ★ New

**Setup** A free electron in a periodic potential is described by the Hamiltonian $H = \frac{P^2}{2m} + V(x)$. For convenience, we set $\hbar = 1$ and $2m = 1$. In this convention the Hamiltonian is

$$H = P^2 + V(X)$$

In the case of $V = 0$, the eigenstates are denoted by $|k\rangle$ (Dirac notation) or $\phi_k(x) = e^{ikx}$ (wave function notation) where $k$ is the wave vector. The energy of this state is $k^2$

(a1) Let us set $V(X) = 0$ for now. Sketch the free electron Hamiltonian $H = P^2$ in the $|k\rangle$ basis, assuming that $k$ is discrete. You should get a diagonal matrix. You don't have to write the exact matrix, since there are infinitely many of such states. Just sketch the matrix.

(a2) What is the matrix element of $V(X)$ in the $|k\rangle$ basis? Can you sketch how the entire Hamiltonian $H = P^2 + V(X)$ looks in the $|k\rangle$ basis?[2]

(a3) Plot the free electron energy dispersion relation $\epsilon_k = k^2$. Explain that there is a one-to-one correspondence between the point on the dispersion and the matrix representation of the operator $P^2$.

(b1) Using the results obtained above, explain that within the first Brillouin zone, states cannot scatter into one another, except for the two states right at the boundary.[3]

(b2) Now let us look at the two states at the boundary of the first Brillouin zone. For convenience, we set $a = 1$. The two states are thus $|\pi\rangle$ and $|-\pi\rangle$. Here is the Hamiltonian concerning only these two states:

$$H = \begin{pmatrix} \epsilon & \tilde{V} \\ \tilde{V} & \epsilon \end{pmatrix}$$

where $\epsilon \equiv \pi^2$ is the energy of the two states. The off-diagonal element is the corresponding element of the Fourier transform of the potential $V(X)$. Review the class lecture note if you are not sure about how to get this matrix form. Compare this with the Hamiltonian in the spin system in the previous exercise (a2) with magnetic field along the $x$-axis. Directly write down the energy eigenvalues of this Hamiltonian.

(b3) Using the analogy between this system and the spin system in the previous exercise, try to explain why there is an energy split, intuitively.

(c1) Now consider a state a bit away from the boundary of the first Brillouin zone, say $|\pi - \delta\rangle$ where $\delta$ is small and represents the deviation from the boundary. Due to the periodic potential, this state will be mostly scattered into another state $|-\pi - \delta\rangle$ which is on the opposite side of the Brillouin zone. Prove that the Hamiltonian concerning only these two states is given by

$$H = \begin{pmatrix} \epsilon + 2\pi\delta & \tilde{V} \\ \tilde{V} & \epsilon - 2\pi\delta \end{pmatrix}$$

up to the first order in $\delta$. Note that we also got similar result in the lecture, but in Dirac notation. Here in this exercise, we use another notation, the matrix representation, for the analysis.

(c2) Again try to build up an analogy between this Hamiltonian and the the Hamiltonian in the spin system defined in (c) in the previous exercise. Directly write down the new energy levels (or energy eigenvalues, in another word) of this Hamiltonian. Expand your result up to the second order in $\delta$. You should get the same result as the result obtained in the lecture, just with different coefficients.

*Spoiler: the energy level is quadratic in $\delta$. Therefore you will have a parabolic-like dispersion near the boundary of the Brillouin zone.*

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[2] Hint1: the matrix element using Dirac notation: say $|1\rangle, |2\rangle, |3\rangle$ are three basis vectors. Now we have a 3 by 3 matrix

$$A = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix}$$

as an example, the element $a_{12} = \langle 1|A|2\rangle$.

Hint2: there will be off-diagonal elements in the matrix.

[3] Hint: From the last exercise, you already know the physical interpretation of the off-diagonal elements in the Hamiltonian.

**Bonus Exercise 1** Rewrite the analysis (purely Dirac notation) in the lecture note in the matrix representation.

**Bonus Exercise 2** In exercise 2 (b1) and (c1), we only consider the matrix elements concerning the two states close to the boundary of the Brillouin zone. Why can we do this? What about the other states? Please justify this approximation.

The key takeaways from this sheet are: (1) matrix representation is a powerful tool to solve a quantum mechanical problem; (2) Setting up an analogy between a new system and a system you already know can be helpful.