Condensed Matter Theory I WS 2022/2023

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Sheet 6
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Category A

1. Landau levels in graphene (10 + 10 + 10 = 30 Points)

Let us consider Dirac electrons in graphene. If we consider both Dirac points ($K_{\pm}$-points), we describe quasiparticles in graphene using a Bloch function with 4 components:

$$\Phi = (\phi_{A,K_+}, \phi_{B,K_+}, \phi_{B,K_-}, \phi_{A,K_-}).$$

Here $K_{\pm}$ denotes the two Dirac points located at the edges of the Brillouin zone and $A(B)$ are the two subgrids. In this basis the effective Hamiltonian operator of an electron is

$$\mathcal{H} = v\boldsymbol{\Sigma}\cdot\boldsymbol{p},$$

where

$$\Sigma_x = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \end{pmatrix}, \qquad \Sigma_y = \begin{pmatrix} 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \end{pmatrix}.$$

We consider the electron in an external magnetic field with potential vector $\boldsymbol{A}(\boldsymbol{r}, t)$). We use the minimal coupling

$$\boldsymbol{p} \to \boldsymbol{p}_{kin} = \boldsymbol{p} - (e/c)\boldsymbol{A} \quad ,$$

and consider the gauge:

$$\boldsymbol{A} = (-By, 0).$$

(a) The two valleys ($K_{\pm}$) are not coupled. First, consider the solutions for the K_+-valley. Here the Schrödinger equation couples the two components ϕ_{A,K_+} und ϕ_{B,K_+}. Write the corresponding equations. Show that it can be express in terms of the operator $\hat{a}$ and its hermitian conjugate $\hat{a}^\dagger$ satisfying the commutation relation $[\hat{a}, \hat{a}^\dagger] = \mathbb{I}$, the so-called ladder operator

Solution:

First, we define the magnetic length $\ell_B^2 = \dfrac{\hbar c}{|e|B}$. We can write the Hamiltonian operator around the K_+ valley as:

$$H_{K^+} = v \begin{pmatrix} 0 & \Pi \\ \Pi^\dagger & 0 \end{pmatrix}$$

where

$$\Pi = p_x - ip_y - \frac{\hbar y}{\ell_B^2}, \qquad \Pi^\dagger = p_x + ip_y - \frac{\hbar y}{\ell_B^2}, \qquad \left[\Pi, \Pi^\dagger\right] = 2\frac{\hbar^2}{\ell_B^2}.$$

Therefore

$$\hat{a} = \frac{\ell_B \Pi}{\hbar\sqrt{2}}, \qquad \hat{a}^\dagger = \frac{\ell_B \Pi^\dagger}{\hbar\sqrt{2}}, \qquad [\hat{a}, \hat{a}^\dagger] = \mathbb{I}$$

The Hamiltonian operator reads now

$$H_{K_+} = \hbar\omega_c \begin{pmatrix} 0 & a \\ a^\dagger & 0 \end{pmatrix}, \qquad \omega_c = \sqrt{2}v/\ell_B,$$

(b) Use the known solutions of the oscillator equation to find the Landau levels as well as the eigenstate. Do the same derivation for the valley K_-.

Solution: From the oscillator equation, we know that the hermitian number operator $N = a^\dagger a$ has eigenvectors is such that:

$$N|n\rangle = n|n\rangle, \text{ with } n \in \mathbb{N}$$

The raising and lowering operators act on these states as follow:

$$a|n\rangle = \sqrt{n}\,|n-1\rangle, \qquad a^\dagger|n\rangle = \sqrt{n+1}\,|n+1\rangle$$

We deduce from this algebra that the solutions are

$$|\Psi_{\lambda,n}\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} |n-1\rangle \\ \lambda|n\rangle \end{pmatrix} \qquad \text{with energies } \epsilon_{\lambda,n} = \lambda\hbar\omega_c\sqrt{n}, \qquad \lambda = \pm 1, \qquad n = 1, 2, 3, ...$$

For $n = 0$, we also have a solution

$$|\Psi_0\rangle = \begin{pmatrix} 0 \\ |0\rangle \end{pmatrix} \qquad \text{with energy } \epsilon_0 = 0.$$

Note that the first Landau level does not depend on the magnetic field while the others have a square root dependence.
For the Dirac point K_-, we obtain the Hamiltonian operator:

$$H_{K_-} = -\hbar\omega_c \begin{pmatrix} 0 & a^\dagger \\ a & 0 \end{pmatrix},$$

and

$$|\Psi_{\lambda,n}\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} |n\rangle \\ \lambda|n-1\rangle \end{pmatrix}, \qquad \epsilon_{\lambda,n} = -\lambda\hbar\omega_c\sqrt{n}, \qquad \text{with } \lambda \pm 1$$

$$|\Psi_0\rangle = \begin{pmatrix} |0\rangle \\ 0 \end{pmatrix}, \qquad \epsilon_0 = 0.$$

(c) Add a Dirac-mass $m\sigma_z$ to the Hamiltonian and re-calculate the energy of the Landau levels. How would the result differ at the points K_+ and K_- ?

Solution:

The massive Dirac Hamiltonian at K_+ is

$$H_{K_+} = \begin{pmatrix} m & \hbar\omega_c a \\ \hbar\omega_c a^\dagger & -m \end{pmatrix}$$

$$H_{K_+}^2 = \begin{pmatrix} m^2 + \hbar^2\omega_c^2 aa^\dagger & 0 \\ 0 & \hbar^2\omega_c^2 a^\dagger a + m^2 \end{pmatrix} = \begin{pmatrix} m^2 + \hbar^2\omega_c^2 (N+1) & 0 \\ 0 & \hbar^2\omega_c^2 N + m^2 \end{pmatrix}$$

The eigenenergies are

$$\epsilon_{\lambda,n} = \lambda\sqrt{\omega_c^2 n + m^2}\,, \quad n = 1, 2, \dots . \qquad \text{with } \lambda = \pm 1.$$

For $n = 0$,

$$H_{K_+}\frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ |0\rangle \end{pmatrix} = -m\frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ |0\rangle \end{pmatrix}$$

The energy is $\epsilon_0^{K_+} = -m$. For the valley K_-, we obtain the same spectrum for Landau levels $n \neq 0$ but the energy of the first Landau level is at $\epsilon_0^{K_-} = +m$.

Category B

2. Berry-connection for spin-1/2: (20 Points)

In the lecture you introduced the time-dependent unitary matrix $R(t)$, which gives the basis change to the instantaneous eigenbasis results.

Now calculate the so-called Berry connection

$$i\dot{R}R^{-1},$$

in the case

$$R^{-1}(t) = e^{-i\varphi(t)\sigma_z/2}e^{-i\theta(t)\sigma_y/2}e^{-i\psi(t)\sigma_z/2}.$$

Solution: First we write R^{-1} in 2×2 matrix form:

$$R^{-1} = e^{-i\varphi\sigma_z/2}e^{-i\vartheta\sigma_y/2}e^{-i\psi\sigma_z/2} = \begin{pmatrix} \cos(\vartheta/2)e^{-i(\varphi+\psi)/2} & -\sin(\vartheta/2)e^{-i(\varphi-\psi)/2} \\ \sin(\vartheta/2)e^{i(\varphi-\psi)/2} & \cos(\vartheta/2)e^{i(\varphi+\psi)/2} \end{pmatrix}$$

The inverse matrix is then:

$$R = \begin{pmatrix} \cos(\vartheta/2)e^{i(\varphi+\psi)/2} & \sin(\vartheta/2)e^{-i(\varphi-\psi)/2} \\ -\sin(\vartheta/2)e^{i(\varphi-\psi)/2} & \cos(\vartheta/2)e^{-i(\varphi+\psi)/2} \end{pmatrix} = e^{i\psi\sigma_z/2}e^{i\vartheta\sigma_y/2}e^{i\varphi\sigma_z/2}$$

To calculate the derivative, we can use both forms. In matrix form we get

$$\dot{R} = \frac{\dot{\vartheta}}{2}\begin{pmatrix} -\sin(\vartheta/2)e^{i(\varphi+\psi)/2} & \cos(\vartheta/2)e^{-i(\varphi-\psi)/2} \\ -\cos(\vartheta/2)e^{i(\varphi-\psi)/2} & -\sin(\vartheta/2)e^{-i(\varphi+\psi)/2} \end{pmatrix}$$

$$+\frac{i}{2}\begin{pmatrix} (\dot{\varphi}+\dot{\psi})\cos(\vartheta/2)e^{i(\varphi+\psi)/2} & -(\dot{\varphi}-\dot{\psi})\sin(\vartheta/2)e^{-i(\varphi-\psi)/2} \\ -(\dot{\varphi}-\dot{\psi})\sin(\vartheta/2)e^{i(\varphi-\psi)/2} & -(\dot{\varphi}+\dot{\psi})\cos(\vartheta/2)e^{-i(\varphi+\psi)/2} \end{pmatrix}$$

Finally, we find

$$i\dot{R}R^{-1} = \frac{1}{2}\begin{pmatrix} -(\dot{\psi}+\dot{\varphi}\cos\vartheta) & (i\dot{\vartheta}+\dot{\varphi}\sin\vartheta)e^{i\psi} \\ -(i\dot{\vartheta}-\dot{\varphi}\sin\vartheta)e^{-i\psi} & \dot{\psi}+\dot{\varphi}\cos\vartheta \end{pmatrix}$$

Diagonal elements represent the Berry phase.