Condensed Matter Theory I WS 2022/2023

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Sheet 5
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Category A

1. Heisenberg equations of motion in graphene $(5 + 15 + 10 + 5 + 5 = 40$ Points)

The effective Hamiltonian operator in the vicinity of one of Dirac points in graphene reads

$$\hat{H} = v(\hat{p}_x\hat{\sigma}_x + \hat{p}_y\hat{\sigma}_y).$$

(a) The positive branch energy of the dispersion relation around this point is $\epsilon(\vec{k}) = \hbar v\sqrt{k_x^2 + k_y^2}$. Compute the corresponding group velocity.

Solution: The group velocity is $\vec{v}_g = \frac{1}{\hbar}\frac{\partial\epsilon}{\partial\vec{k}} = v\frac{\vec{k}}{\sqrt{k_x^2 + k_y^2}} = v\frac{\vec{k}}{|\vec{k}|}$

(b) Consider the case when an external electromagnetic field $(\phi(\vec{r}, t), \vec{A}(\vec{r}, t))$ is applied. Then,

$$\vec{p} \to \vec{p}_{kin} = \vec{p} - (e/c)\vec{A} \quad , \quad \hat{H} \to \hat{H} + e\phi \ .$$

For this case, derive the Heisenberg equations of motion for the operators $\vec{p}$, $\vec{p}_{kin}$, $\vec{r}$, $\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z$.

Solution: The hamiltonian operator submitted to an electromagnetic field can be rewritten such as:

$$H = v\left(\left[p_x - (e/c)A_x\right]\sigma_x + \left[p_y - (e/c)A_y\right]\sigma_y\right) + e\phi.$$

Fields $A_x(\boldsymbol{r}, t)$, $A_y(\boldsymbol{r}, t)$ and $\phi(\boldsymbol{r}, t)$ depends on $\boldsymbol{r}$ and t. For coordinates we have:

$$v_\alpha = \dot{r}_\alpha = (i/\hbar)[H, r_\alpha] = (i/\hbar)v\sigma_\alpha[p_\alpha, r_\alpha] = v\sigma_\alpha,$$

where $\alpha = x, y$.

For the momentum:

$$\begin{aligned}
\dot{p}_\alpha = (i/\hbar)[H, p_\alpha] &= (-iev/c\hbar)\sum_\beta \sigma_\beta[A_\beta, p_\alpha] + (ie/\hbar)[\phi, p_\alpha] \\
&= (ev/c)\sum_\beta \sigma_\beta\partial_\alpha A_\beta - e\partial_\alpha\phi \\
&= (e/c)\sum_\beta v_\beta\left(\partial_\alpha A_\beta - \partial_\beta A_\alpha + \partial_\beta A_\alpha\right) - e\partial_\alpha\phi \\
&= (e/c)\sum_\beta v_\beta\left(\partial_\alpha A_\beta - \partial_\beta A_\alpha\right) + (e/c)\sum_\beta v_\beta\partial_\beta A_\alpha - e\partial_\alpha\phi \ .
\end{aligned}$$

In order to compute $(d/dt)\boldsymbol{p}_{kin}$ we need $\dot{A}_\alpha$:

$$\begin{aligned}\dot{A}_\alpha &= (i/\hbar)[H, A_\alpha] + \partial_t A_\alpha = (iv/\hbar)\sum_\beta \sigma_\beta [p_\beta, A_\alpha] + \partial_t A_\alpha \\ &= v\sum_\beta \sigma_\beta \partial_\beta A_\alpha + \partial_t A_\alpha = \sum_\beta v_\beta \partial_\beta A_\alpha + \partial_t A_\alpha .\end{aligned}$$

We obtain:

$$\dot{p}_{kin,\alpha} = (e/c)\sum_\beta v_\beta \left(\partial_\alpha A_\beta - \partial_\beta A_\alpha\right) - (e/c)\partial_t A_\alpha - e\partial_\alpha \phi \ .$$

In vector-like form, this translates to

$$\frac{d}{dt}\boldsymbol{p}_{kin} = (e/c)\boldsymbol{v} \times \boldsymbol{B} + e\boldsymbol{E},$$

where $\boldsymbol{B}$ has only a non vanishing z component and we recover the usual classical equation of motion for a charged particle under an electromagnetic field.

Eventually, the acceleration is proportional to the time derivative of the Pauli matrices:

$$\begin{aligned}\dot{v}_x = v\dot{\sigma}_x = (iv/\hbar)[H, \sigma_x] &= (iv^2/\hbar)\left[p_y - (e/c)A_y\right][\sigma_y, \sigma_x] \\ &= (2v^2/\hbar)p_{kin,y}\sigma_z \ .\end{aligned}$$

$$\begin{aligned}\dot{v}_y = v\dot{\sigma}_y = (iv/\hbar)[H, \sigma_y] &= (iv^2/\hbar)\left[p_x - (e/c)A_x\right][\sigma_x, \sigma_y] \\ &= -(2v^2/\hbar)p_{kin,x}\sigma_z \ .\end{aligned}$$

and

$$\begin{aligned}\dot{\sigma}_z = (i/\hbar)[H, \sigma_z] &= (iv/\hbar)\left[p_x - (e/c)A_x\right][\sigma_x, \sigma_z] + (iv/\hbar)\left[p_y - (e/c)A_y\right][\sigma_y, \sigma_z] \\ &= (2v/\hbar)(p_{kin,x}\sigma_y - p_{kin,y}\sigma_x) \ .\end{aligned}$$

(c) Show that by taking the expectation value of the velocity operator, $\langle\psi|\,\vec{v}\,|\psi\rangle$ where ψ is a combination of eigenstate only in the positive energy branch, you recover the group velocity found from the classical approach (*Hint: First consider the expectation value of an eigenstate of the Hamiltonian*).

Solution: If $|\psi_q\rangle$ is an eigenstate of $\hat{H}$ in the positive energy branch we have

$$\begin{aligned}H\,|\psi_q\rangle &= v\vec{p}.\vec{\sigma}\,|\psi_q\rangle = \epsilon(\vec{q})\,|\psi_q\rangle = v\hbar|\vec{q}|\,|\psi_q\rangle \\ &\Leftrightarrow \langle\psi_{q'}|\,\vec{k}.\vec{\sigma}\,|\psi_q\rangle = |\vec{q}|\delta_{\vec{q},\vec{q}'} \\ &\Leftrightarrow \vec{q}'.\langle\psi_{q'}|\,\vec{\sigma}\,|\psi_q\rangle = |\vec{q}|\delta_{\vec{q},\vec{q}'}\end{aligned}$$

Here $\vec{k}$ denotes the operator while $\vec{q}$ is just a number and the operator $\vec{k}$ evaluates to $\vec{q}$ when applied to the eigenstate $|\psi_q\rangle$ $\vec{k}\,|\psi_q\rangle = \vec{q}\,|\psi_q\rangle$. The operator $\vec{\sigma}$ does not couple different plane wave vector $\vec{q}$ and $\vec{q}'$ i.e. $\langle\psi_{q'}|\,\vec{\sigma}\,|\psi_q\rangle = 0$ if $\vec{q} \neq \vec{q}'$. Moreover, $\vec{\sigma}$ is a unitary operator so $|\langle\psi_q|\,\vec{\sigma}\,|\psi_q\rangle| \leq 1$.We deduce from the above equation:

$$\langle\psi_{q'}|\,\vec{\sigma}\,|\psi_q\rangle = \frac{\vec{q}}{|\vec{q}|}\delta_{\vec{q},\vec{q}'} = \langle\psi_{q'}|\,\frac{\vec{k}}{|\vec{k}|}\,|\psi_q\rangle$$

Now, consider any state in the positive energy branch $|\psi\rangle = \sum_q \alpha_q |\psi_q\rangle$

$$\langle\psi|\,\vec{\sigma}\,|\psi\rangle = \sum_{q,q'} \alpha^*_{q'}\alpha_q \langle\psi_{q'}|\,\vec{\sigma}\,|\psi_q\rangle = \sum_{q,q'} \alpha^*_{q'}\alpha_q \langle\psi_{q'}|\,\frac{\vec{k}}{|\vec{k}|}\,|\psi_q\rangle = \langle\psi|\,\frac{\vec{k}}{|\vec{k}|}\,|\psi\rangle$$

We recover then:

$$\langle\psi|\,\vec{v}\,|\psi\rangle = v\,\langle\psi|\,\vec{\sigma}\,|\psi\rangle = v\,\langle\psi|\,\frac{\vec{k}}{|\vec{k}|}\,|\psi\rangle$$

(d) Calculate the cyclotron mass m_c in graphene as a function of energy ϵ using the relation $m_c = \frac{\hbar^2}{2\pi}\frac{\partial S}{\partial \epsilon}$. Here, $S(\epsilon)$ is an area of 2D orbit in k-space encircled by the particle of the energy $\epsilon(\mathbf{k}) = \hbar v\sqrt{k_x^2 + k_y^2}$.

Solution: The trajectory of a particle in k-space in graphene with constant energy ϵ is a circle of the radius $k_\epsilon = \frac{\epsilon}{\hbar v}$. The respective area in k-space is $S(\epsilon) = \pi k_\epsilon^2 = \pi\frac{\epsilon^2}{\hbar^2 v^2}$. Finally, the cyclotron mass is $m_c = \frac{\hbar^2}{2\pi}\frac{\partial S}{\partial \epsilon} = \frac{\epsilon}{v^2}$.

(e) Show that the energies of Landau levels in graphene scale as $E_n \propto \sqrt{n}$ in the limit $n \gg 1$. To show it, use the relation $S_n = \frac{A_n}{l_{\mathrm{B}}^4}$ between the areas in k- and r- spaces, S_n and A_n, respectively, where l_{B} is the magnetic length (see lecture). For A_n use semiclassical Bohr-Sommerfeld quantization condition.

Solution: The magnetic flux threading a closed orbit is $\Phi = \frac{hc}{|e|}(n+\gamma)$ according to Bohr-Sommerfeld quantization condition ($n \in \mathbb{Z}$). For the allowed areas in r-space we have $A_n = \Phi/B = \frac{hc}{|e|B}(n+\gamma)$. We use the relation between areas in k- and r-spaces, $S_n = \frac{A_n}{l_{\mathrm{B}}^4}$ with $l_B = \sqrt{\frac{\hbar c}{|eB|}}$, and find $S_n = \frac{2\pi|e|B}{\hbar c}(n+\gamma)$. From the previous subtask we know that the area in k-space for the particle with energy E in graphene is given by $S_E = \pi\frac{E^2}{\hbar^2 v^2}$. The equality $S_E = S_n$ provides the Landau levels as a function of discrete n: $E_n = v\sqrt{\frac{2\hbar|e|B}{c}(n+\gamma)}$. In the limit of large n we have $E_n \propto \sqrt{n}$.

Category B

2. Cyclotron mass of an anisotropic parabolic dispersion relation (10 points)

Let us consider such a dispersion relation:

$$\epsilon(\mathbf{k}) = \frac{\hbar^2}{2}\left(\frac{k_x^2}{m_x} + \frac{k_y^2}{m_y} + \frac{k_z^2}{m_z}\right)$$

Assume now there is a magnetic field along the z-direction $\vec{B} = B\vec{e_z}$. Compute the corresponding cyclotron mass.

Solution: First, because the magnetic field is along the z-direction, the motion is confined in the (x,y)-plane, k_z is a constant of motion. Therefore, in k-space the closed orbit formed by a particle of energy E and momentum along the z-direction k_z is an ellipse of equation

$$E - \frac{\hbar^2 k_z^2}{2m_z} = \frac{\hbar^2}{2}\left(\frac{k_x^2}{m_x} + \frac{k_y^2}{m_y}\right)$$

The length of the semi-axis of this ellipse are $a = \sqrt{\frac{2m_y}{\hbar^2}(E - \frac{\hbar^2 k_z^2}{2m_z})}$ and $b = \sqrt{\frac{2m_x}{\hbar^2}(E - \frac{\hbar^2 k_z^2}{2m_z})}$. To derive the cyclotron mass, we need first to compute the surface area of the closed orbit. The surface of an ellipse is given by $S = \pi ab$, we deduce:

$$S(E, k_z) = \frac{2\pi}{\hbar^2}\sqrt{m_x m_y}(E - \frac{\hbar^2 k_z^2}{2m_z})$$

The cyclotron mass is then

$$m_c = \frac{\hbar^2}{2\pi}\frac{\partial S}{\partial E} = \sqrt{m_x m_y}$$