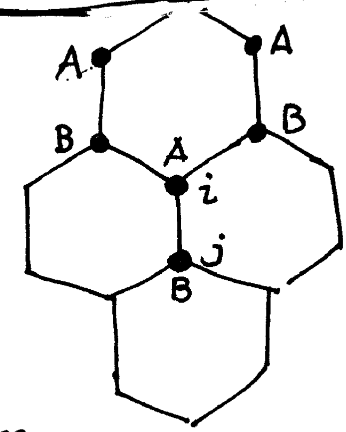
Mid term Phy 212C Quantum mechanics

1. Second quantization: the Dirac spectrum for Carbon system.



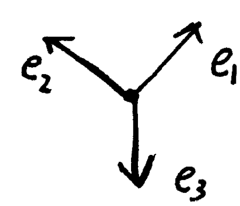
Graphene is a single layer of graphite, with a honeycomb lattice. Each unit cell contains two sites: A type and B type. On each site, the active electron is the one in Carbon's $2P_z$ orbit. These electrons hop from one site to another, and form an energy band.

The second quantized Hamiltonian is represented

$$H_0 = -t \sum_{i \in A, j=1,2,3} \left\{ C_i^\dagger C_{i+\hat{e}_j a} + C^\dagger_{i+\hat{e}_j a} C_i \right\},$$ where "i" is the index of site A,

and $e_1 = \frac{\sqrt{3}}{2} e_x + \frac{1}{2} e_y$; $e_2 = -\frac{\sqrt{3}}{2} e_x + \frac{1}{2} e_y$; $e_3 = -e_y$

are three unit vector. $i + \hat{e}_j a$ is the locations of three nearest neighbour sites to i, and they are B-sites; a is the nearest neighbour bond length.



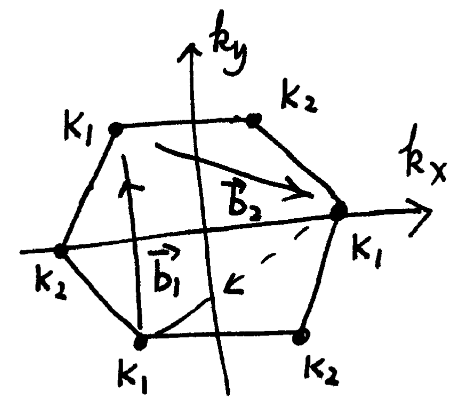
$C_i^\dagger$ C_i ; $C^\dagger_{i+\hat{e}_j a}$, $C_{i+\hat{e}_j a}$ are creation / annihilation operators for A and B type lattice site, respectively.

we introduce the Fourier transform for C_i, C_j $(i \in A, j \in B)$

$$C_{A,k} = \frac{1}{\sqrt{N_A}} \sum_{i \in A} e^{i \vec{k} \cdot \vec{R}_i} C_i$$

$$C_{B,k} = \frac{1}{\sqrt{N_B}} \sum_{j \in B} e^{i \vec{k} \cdot \vec{R}_j} C_j ,$$

where k is defined in a region called Brillouin Zone (BZ) in momentum space. The BZ is a regular hexagon with edge length $\frac{4\pi}{3\sqrt{3}a}$. The six vertices are classified into two classes K_1 and K_2.



The three K_1's are equivalent to each other up to a receiprocal lattice vecter of $\vec{b}_1$, $\vec{b}_2$ ~~and~~ or $(\vec{b}_1 + \vec{b}_2)$.

The reciprocal lattice vectors have the property that $\vec{b} \cdot \vec{R}_i = 2n\pi$.

① In the momentum space, find the expression for the Hamiltonian H_0, which should be

$$H_0 = \sum_{k \in BZ} (C^{\dagger}_{A,k}, C^{\dagger}_{B,k}) \, H(k) \begin{pmatrix} C_{A,k} \\ C_{B,k} \end{pmatrix}$$

where $H(k)$ is a 2×2 matrix. Define $\tau_1=\begin{pmatrix}0&1\\1&0\end{pmatrix}$ and $\tau_2=\begin{pmatrix}0&i\\-i&0\end{pmatrix}$, $\tau_3=\begin{pmatrix}1&0\\0&-1\end{pmatrix}$, prove $H(k)=a(k)\tau_1+b(k)\tau_2$ and find the expressions of $a(k)$ and $b(k)$.

② Diagonalize $H(k)$, prove that H_0 can be represented in the eigen-basis as

$$H_0=\sum_{k\in BZ}\varepsilon_k\alpha_k^{\dagger}\alpha_k-\varepsilon_k\beta_k^{\dagger}\beta_k,$$

where $\begin{pmatrix}C_{A,k}\\C_{B,k}\end{pmatrix}=U(k)\begin{pmatrix}\alpha_k\\\beta_k\end{pmatrix}$, and $\varepsilon_k=\sqrt{a^2(k)+b^2(k)}$.

$U(k)$ is unitary matrix diagonalizing $H(k)$. $U^{\dagger}(k)H(k)U(k)=\begin{pmatrix}\varepsilon_k&0\\0&-\varepsilon_k\end{pmatrix}$

③ Plot the spectrum of $\pm\varepsilon(k)$ in the entire BZ.

④ Prove at K_1 and K_2, $a(K_{1,2})=b(K_{1,2})=0$; thus $H(K_{1,2})=0$

Do linear expansion of $a(k)$ and $b(k)$ around K_1, K_2.

Prove around K_1, $H_{\vec{K}_1+\vec{q}}(\uparrow) \approx \frac{3t}{2} q_x \tau_1 - \frac{3t}{2} q_y \tau_2$ where $q_x = k_x - K_{1x}$
$q_y = k_y - K_{1y}$.

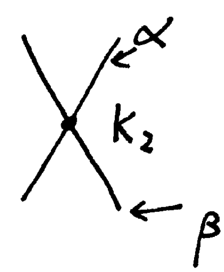
and around K_2 $H^{\vec{K}_2+\vec{q}\,'}(\downarrow) \approx \frac{-3}{2} t\, q'_x \tau_1 - \frac{3}{2} t\, q'_y \tau_y$

where $q'_x = k_x - K_{2,x}$ $q'_y = k_y - k_{2y}$.

Thus we have two Dirac cones around K_1 and K_2.

⑤ Let us look at the Dirac cone at K_2.

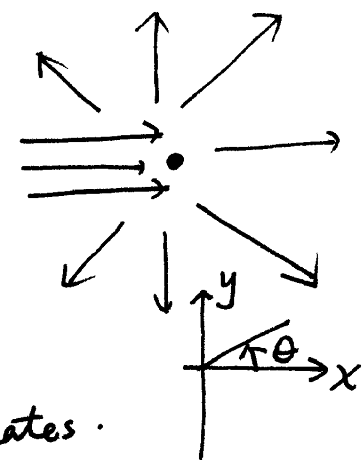
Solve the eigen-vectors for the positive energy solution α_K. Basically, you need to find the eigenstate for $H(\vec{k})$, where $\vec{k} = \vec{K}_2 + \vec{q}\,'$.



$$H(\vec{K}_2 + \vec{q}\,')\, \psi(\vec{K}_2 + \vec{q}\,') = \mathcal{E}(\vec{K}_2 + \vec{q}\,')\, \psi(\vec{K}_2 + \vec{q}\,')$$

where ψ is a two-row wave eigenvector with positive energy.

2. Partial wave for 2D scattering problem



The scattering boundary condition can be witten as

$$\psi(r,\theta) \xrightarrow[r\to\infty]{} e^{ikx} + f(\theta)\frac{e^{ikr}}{\sqrt{r}}$$

where r, θ are coordinate in the polar coordinates.

The incident wave can be expanded in terms of Bessel functions

$$e^{ikx} = e^{ikr\cos\theta} = \sum_{m=0}^{\infty} \epsilon_m i^m \cos m\theta \, J_m(kr)$$

where $\epsilon_m = 2$ for $m \neq 0$, and $\epsilon_0 = 1$.

① The Schrödinger equation for the scattering problem

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi,$$

By separating variables $\psi = R_m(r)\, T_m(\theta)$, where $T_m(\theta) = \frac{1}{\sqrt{\pi}}\cos m\theta$

Find the radial equation for $R(r)$.

(2) In the regim outsideo $V(r)$, prove than $R_m(kr)$ can be written as

$$R_m(kr) \xrightarrow{kr\to\infty} A_m \frac{1}{\sqrt{kr}} \cos\left(kr - \frac{\pi}{2}(m+1/2) + \delta_m\right)$$

where A_m is a coeffient, δ_m is the phase shift. You need to use the asymptotic form

$$J_m(kr) \xrightarrow{kr\to\infty} \sqrt{\frac{2}{\pi kr}} \cos\left(kr - \frac{\pi}{2}(m+1/2)\right)$$

$$N_m(kr) \xrightarrow{kr\to\infty} \sqrt{\frac{2}{\pi kr}} \sin\left(kr - \frac{\pi}{2}(m+1/2)\right),$$

where J_m, N_m are the m-th order Bessel and Neuman functions, respectively.

(3) Equating this with the scattering boundy condition

$$\psi(r,\theta) \xrightarrow[r\to\infty]{} e^{ikx} + f(\theta)\frac{e^{ikr}}{\sqrt{r}}.$$

we have $$\sum_{m=0}^{\infty} \epsilon_m i^m \cos m\theta \left(\frac{2}{\pi kr}\right)^{1/2} \cos\left(kr - \frac{\pi}{2}(m+\tfrac{1}{2})\right)$$

$$+ \frac{f(\theta)}{\sqrt{r}} e^{ikr} = \sum_{m=0}^{\infty} A_m (kr)^{-1/2} \cos\left[kr - \frac{\pi}{2}(m+\tfrac{1}{2}) + \delta_m\right] \cos m\theta$$

Show that A_m can be written as

$$A_m = 2\,\epsilon_m\, i^m\, (2\pi)^{-1/2}\, e^{i\delta_m}$$

and we have $f(\theta) = \left(\frac{1}{2\pi i k}\right)^{1/2} \sum_{m=0}^{\infty} \epsilon_m \cos(m\theta)\left[e^{2i\delta_m} - 1\right]$

(4) we can define "total scattering length"

$$\lambda = \int_0^{2\pi} \lambda(\theta)\, d\theta \,, \quad \text{where } \lambda(\theta) = |f(\theta)|^2$$

Show that $\lambda = \frac{4}{k} \sum_{m=0}^{\infty} \epsilon_m \sin^2 \delta_m \,.$