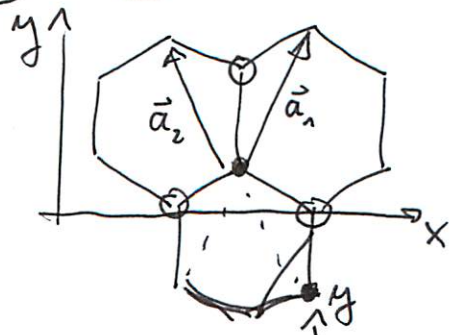
6.1 a

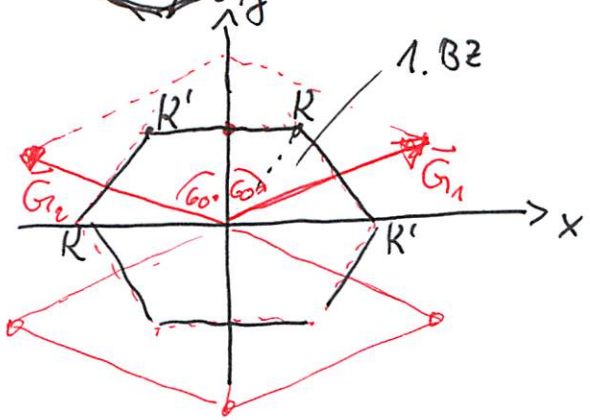


$$\vec{a}_1 = \frac{a}{2}(1, \sqrt{3})$$

$$\vec{a}_2 = \frac{a}{2}(-1, \sqrt{3})$$

$$\Rightarrow \vec{G}_i \cdot \vec{a}_j = \delta_{ij} \cdot 2\pi \; , \; A = \frac{a}{2}\begin{pmatrix} 1 & -1 \\ \sqrt{3} & \sqrt{3} \end{pmatrix}$$

$$\Rightarrow \begin{pmatrix} - \vec{G}_1 - \\ - \vec{G}_2 - \end{pmatrix} = 2\pi \begin{pmatrix} | & | \\ \vec{a}_1 & \vec{a}_2 \\ | & | \end{pmatrix}^{-1} = A^{-1} \cdot 2\pi$$



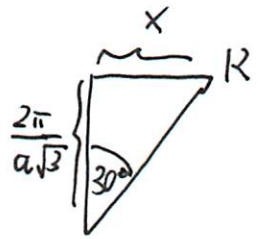
$$\Rightarrow A^{-1} = \frac{\frac{a}{2}}{\left(\frac{a}{2}\right)^2 (2\sqrt{3})} \begin{pmatrix} \sqrt{3} & 1 \\ -\sqrt{3} & 1 \end{pmatrix} = \frac{1}{\sqrt{3}\, a} \begin{pmatrix} \sqrt{3} & 1 \\ -\sqrt{3} & 1 \end{pmatrix} =$$

$$\Rightarrow \begin{pmatrix} - \vec{G}_1 - \\ - \vec{G}_2 - \end{pmatrix} = \frac{2\pi}{a} \begin{pmatrix} 1 & 1/\sqrt{3} \\ -1 & 1/\sqrt{3} \end{pmatrix} =$$

$$= \frac{4\pi}{\sqrt{3}\, a} \begin{pmatrix} \sqrt{3}/2 & 1/2 \\ -\sqrt{3}/2 & 1/2 \end{pmatrix} = \frac{4\pi}{\sqrt{3}\, a} \begin{pmatrix} \sin 60° & \cos 60° \\ \sin 60° & \cos 60° \end{pmatrix}$$

$$\Rightarrow \boxed{\begin{aligned} \vec{G}_1 &= \frac{2\pi}{a}\left(1, 1/\sqrt{3}\right) \\ \vec{G}_2 &= \frac{2\pi}{a}\left(-1, 1/\sqrt{3}\right) \end{aligned}}$$

$$\boxed{K = \left(\frac{2\pi}{a\sqrt{3}}, \frac{2\pi}{a\sqrt{3}}\right) = \frac{2\pi}{a\sqrt{3}}\left(1, \frac{1}{\sqrt{3}}\right) \; ; \; K' = \frac{2\pi}{a\sqrt{3}}\left(-\frac{1}{\sqrt{3}}, 1\right)}$$



$$\tan(30°) = \frac{x}{\frac{2\pi}{a\sqrt{3}}} \Rightarrow x = \frac{2\pi}{a\sqrt{3}} \tan(30°) = \frac{2\pi}{a3}$$

Bandstruktur von Graphen: $H = \sum_{\sigma=\pm} H_\sigma$ (no mixing of spins)

$$H = -t \sum_{\langle i,j \rangle} \left(c_i^\dagger c_j + h.c. \right) =$$

i is a composite index: $i = (\mu, \alpha) = (R_\mu, \alpha)$.

Bravais unit cell — Basis sites A,B

Bravais lattice vectors

$$H = -t \sum_{R_\mu} \sum_{\{\delta_{AB}\}} \left(c^\dagger_{R_\mu + \delta_{AB}, B} \, c_{R_\mu, A} + h.c. \right) \; ; \; \delta_{AB} = \{(0,0), -\vec{a}_2, -\vec{a}_1\}.$$

$$c_{R_\mu, A} \equiv a_{R_\mu} = \frac{1}{\sqrt{N_L}} \sum_{k \in 1.BZ} e^{i\vec{k}(\vec{R}_\mu + \vec{b}_A)} \underbrace{c_{k,A}}_{= a_k} \; ; \; b_A = (0,0)$$

$$c_{R_\mu, B} = b_{R_\mu} = \frac{1}{\sqrt{N_L}} \sum_{k} e^{i\vec{k}(\vec{R}_\mu + \vec{b}_B)} \underbrace{c_{k,B}}_{b_k} \; ; \; \vec{b}_B = (0, a/\sqrt{3}).$$

$$\frac{1}{\sqrt{2}}\left[|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle\right]$$

$$\sqrt{N}$$

$$\frac{1+\sqrt{N}}{N} \longrightarrow \frac{1}{\sqrt{N}}$$

$$\Rightarrow H = -t \sum_{R_\mu} \sum_{\{\delta_{AB}\}} \sum_{k,q} \frac{1}{N_L} \left(b_k^+ a_q \, e^{i[(q-k)R_\mu + q(\vec{b}_A - k(b_B + \delta_{AB})]} + h.c. \right) =$$

$$= -t \sum_{\{\delta_{AB}\}} \sum_{k} \left(b_k^+ a_k \, e^{i[\vec{k}(\vec{b}_A - \vec{b}_B - \vec{\delta}_{AB})]} + h.c. \right) =$$

$$\sum_{R_\mu} e^{i(q-k)R_\mu} = N_L \delta_{k,q}$$

$$= -t \sum_{k} \left(f(k) \, b_k^+ a_k + h.c. \right),$$

where $f(k) = \sum_{\{\vec{\delta}_{AB}\}} e^{-ik(\vec{b}_B + \vec{\delta}_{AB})} =$ ~~$\cos(\frac{k_x}{2})\cos(\frac{k_y}{2\sqrt{3}}) + \cos(\frac{k_y}{\sqrt{3}})$~~ .

$\vec{b}_A = (0,0)$

$$\boxed{= e^{-\frac{ik_y}{\sqrt{3}}} + (1 + e^{ik_x}) e^{-\frac{i}{6}(3k_x - \sqrt{3}k_y)} = f(k)}$$

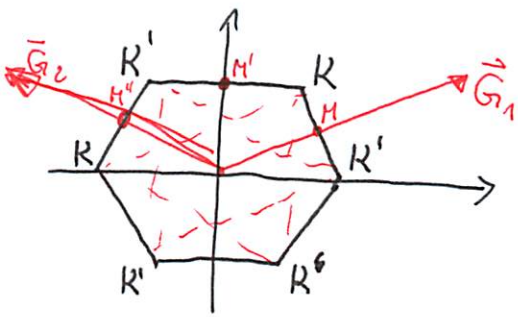
$$\Rightarrow H = -t \sum_{k} (a_k^+, b_k^+) \begin{pmatrix} 0 & f(k)^* \\ f(k) & 0 \end{pmatrix} \begin{pmatrix} a_k \\ b_k \end{pmatrix}$$

Diagonalizing the bandstructure yields:

$$\lambda^2 = \pm\sqrt{|f(k)|^2} \Rightarrow \boxed{\pm|f(k)| = \varepsilon(k)/t} \quad \boxed{\Rightarrow \varepsilon(k) = \sqrt{3 + 2\cos(k_x) + 4\cos\left(\frac{k_x}{2}\right)\cos\left(\frac{\sqrt{3}k_y}{2}\right)}}.$$

$\Rightarrow$ [illegible] .

(1b) $K = \frac{2\pi}{\sqrt{3}a}\left(\frac{1}{\sqrt{3}}, 1\right)$; $K' = \frac{2\pi}{\sqrt{3}a}\left(-\frac{1}{\sqrt{3}}, 1\right)$



2 of the corners of the BZ are non-equivalent.

$\Rightarrow$ K, K' valley pseudo-spin degree of freedom.

$\varepsilon(K) = 0$, $\varepsilon(K') = 0$; $\boxed{\varepsilon(K + \vec{q}) = \pm\frac{\sqrt{3}t}{2}\sqrt{q_x^2 + q_y^2} = \pm v_F|\vec{q}| \quad \text{with } v_F = \frac{\sqrt{3}t}{2}.}$

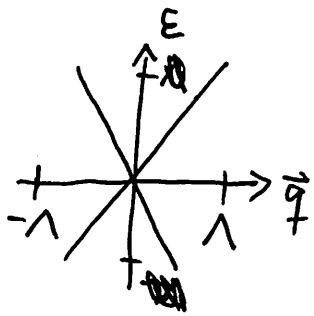
(6.1) (c)

Density of states close to the <u>Dirac point</u> (4x degeneracy due to spin & valley degree of freedom)

$$\rho(\varepsilon_0) = \frac{L^d}{(2\pi)^d}\int d^d k\, \delta(\varepsilon_0 - \varepsilon(k)) \quad , \text{ here } d=2, \quad \varepsilon(K+q) = \pm v_F |\vec{q}| .$$

spin & valley

$$\Rightarrow \rho(\varepsilon_0) = \frac{4L^2}{(2\pi)^2}\int_0^{\Lambda} dq\, q \int_0^{2\pi} d\varphi \left[\delta(\varepsilon_0 - v_F q) + \delta(\varepsilon_0 + v_F q)\right] =$$



$$= \frac{4L^2}{2\pi}\frac{1}{v_F}\cdot\frac{|\varepsilon_0|}{v_F} = \boxed{\frac{4L^2}{2\pi v_F^2}|\varepsilon_0| = \rho(\varepsilon_0)}$$

$$[v_F] = \frac{\text{Energy}}{\text{mom.}} = \text{Energy}\cdot\text{length}$$

(d) general conditions for van-Hove singularity: $\nabla_k \varepsilon(k) = 0$, i.e., minima, maxima, saddle-points.

$$\rho(\varepsilon_0) \sim \int d^d k \frac{\delta(k-k_0)}{|\nabla_k \varepsilon(k)|_{k_0}} \quad \text{with } \varepsilon(k_0) = \varepsilon_0 .$$

$\varepsilon(k_0) = \varepsilon_0$

close to such a 'critical point' will

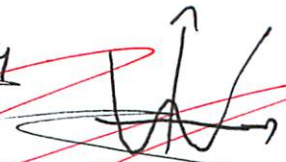
$$\nabla_k \varepsilon(k) = 0 \Rightarrow \varepsilon(k) \approx \varepsilon_0 \pm C|k|^2$$

in the direction of integration

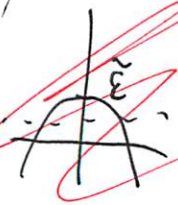
$$\Leftrightarrow \boxed{\rho(\varepsilon_0) = \frac{L^d}{(2\pi)^d} \int_{S_{\varepsilon_0}} d\Omega \cdot \frac{1}{\left|\nabla_k \varepsilon(k)\right|_{\varepsilon(k)=\varepsilon_0}}}$$

Surface integral over surface of constant energy ε_0.

~~Example in 3D: for band structure: $\varepsilon(k) = -r k^2 + u k^4$~~



~~$\varepsilon(k) = \tilde{\varepsilon} - r k^2 \Rightarrow |\nabla_k \varepsilon| = r k$ ε_0 ~~ be positive~~



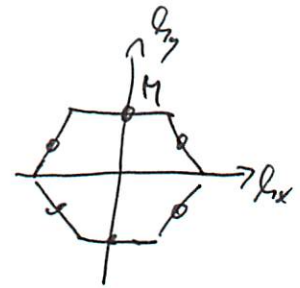
~~$\Rightarrow \rho(\varepsilon_0) = \frac{L^3}{(2\pi)^3}$~~

For graphene:

$$\nabla_k \varepsilon(k) = 0 \Rightarrow \begin{pmatrix} \partial_{k_x} \varepsilon(k) \\ \partial_{k_y} \varepsilon(k) \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

$$\Leftrightarrow \boxed{k_x = \pm\pi, \; k_y = \pm\frac{\pi}{\sqrt{3}} \Rightarrow \varepsilon\left(\pm\pi, \pm\frac{\pi}{\sqrt{3}}\right) = \pm 1.}$$

these are the so-called M-points.



Expand energy around <u>M point</u>. (ε in units of t)

$$\varepsilon(M+\vec{q}) = 1 + \frac{1}{2}\left(q_x^2 - \sqrt{3}\, q_x q_y\right) \underset{p}{=}$$

change variables:

$$(q_x\ q_y)\begin{pmatrix} 1 & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & 0 \end{pmatrix}\begin{pmatrix} q_x \\ q_y \end{pmatrix} \Rightarrow \lambda^2 - \lambda - \frac{3}{4} = 0 \Rightarrow \lambda_{1,2} = \frac{1}{2} \pm \sqrt{\frac{1}{4}+\frac{3}{4}} = \frac{1}{2} \pm 1$$

$$\Rightarrow \lambda_1 = \frac{3}{2}\ ;\ \lambda_2 = -\frac{1}{2}.$$

(saddle-point!)

<u>Eigenvectors</u>.

$\lambda_1 = \frac{3}{2}$; $\vec{v}_1 = (-\sqrt{3}, 1)$

$\lambda_2 = -\frac{1}{2}$; $\vec{v}_2 = (\frac{1}{\sqrt{3}}, 1)$ $\Rightarrow$ $\varepsilon(M+\vec{q}) = 1 + \frac{1}{2}\left[\frac{3}{2} q_1^2 - \frac{1}{2} q_2^2\right]$

direction of $\vec{v}_1$. direction of $\vec{v}_2$.

Calculate DoS:

$$\varepsilon_0 - (q_1^2 + q_2^2) = 0 \Rightarrow \boxed{q_2^2 = +\varepsilon_0 - q_1^2}$$

$$q_1^2 + q_2^2 = 0 \Rightarrow q_2^2 = -q_1^2.$$

$$\Rightarrow q_2^{(0)} = \pm\sqrt{q_1^2}$$

$$\rho(\varepsilon_0) = \frac{6L^2}{(2\pi)^2}\int d^2k\ \delta(\varepsilon_0 - \varepsilon(M+k)) =$$

spin $\times$ (3-M points)

$$= \frac{6L^2}{(2\pi)^2}\int_{-\Lambda_M}^{\Lambda_M} dq_1\, dq_2\ \delta\left(\varepsilon_0 - 1 - \frac{1}{4}\left[3q_1^2 - q_2^2\right]\right)$$

use eigenbasis directions q_1 & q_2

Perform integration over q_1:

$$\rho(\varepsilon_0) = \frac{6L^2}{(2\pi)^2}\int_{-\Lambda_M}^{\Lambda_M} dq_1\, dq_2\, \frac{\delta(q_1 - q_1^{(0)})}{\left|\frac{3}{2}q_1^{(0)}\right|}$$

$$q_1^{(0)} = \pm\frac{1}{\sqrt{3}}\sqrt{2(\varepsilon_0-1)+q_2^2} = \pm a\sqrt{b+q_2^2}.$$

$$\varepsilon_0 - 1 = \frac{1}{4}(3q_1^2 - q_2^2) \quad ; \quad \boxed{b = 2(\varepsilon_0-1)}$$

$$\Leftrightarrow 4(\varepsilon_0-1) + q_2^2 = 3q_1^2$$

$$\Leftrightarrow q_1^{(0)} = \pm\frac{1}{\sqrt{3}}\sqrt{2(\varepsilon_0-1)+q_2^2}.$$

$$\Leftrightarrow \rho(\varepsilon_0) = \frac{6L^2}{(2\pi)^2}\int_{-\Lambda_M}^{\Lambda_M} dq_2\, \frac{1}{\frac{3a}{2}\sqrt{b+q_2^2}} =$$

$$= \frac{12L^2\, 2}{3a(2\pi)^2}\cdot\underbrace{\int_0^{\Lambda_M}\frac{dq_2}{\sqrt{b+q_2^2}}}$$

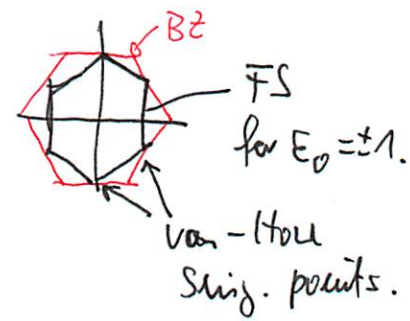
$$\boxed{\Lambda_M \sim t}$$

b acts as lower cutoff of infrared divergens of the integral

$$\boxed{\Rightarrow \int_{\sqrt{b}}^{\Lambda_M} dx\, \frac{dx}{|x|} = \log\left(\frac{\Lambda_M}{\sqrt{b}}\right) \approx \left|\log\left|\frac{t}{\varepsilon_0-1}\right|\right|.}$$

$$\rho(\varepsilon_0) \sim \left|\log\left|\frac{t}{\varepsilon_0-1}\right|\right|.$$

parametrize Fermi surface



logarithmic accuracy.

$$\int_0^{\Lambda_M}\frac{dq}{\sqrt{q^2+b}} \approx \underbrace{\int_0^b \frac{dq}{\sqrt{b}}}_{\text{finite!}} + \int_b^{\Lambda_M}\frac{dq}{|q|}$$