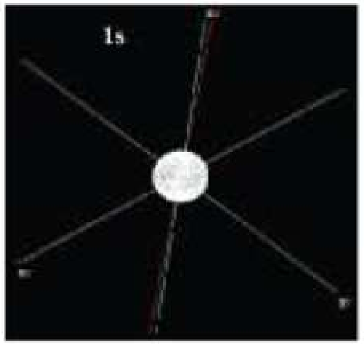
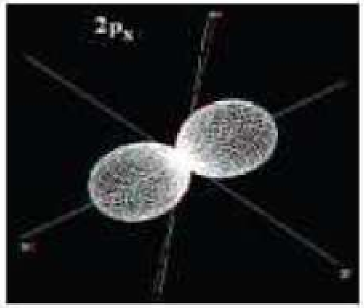
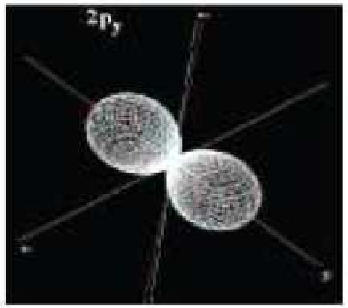
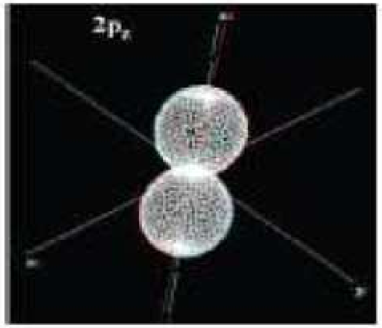
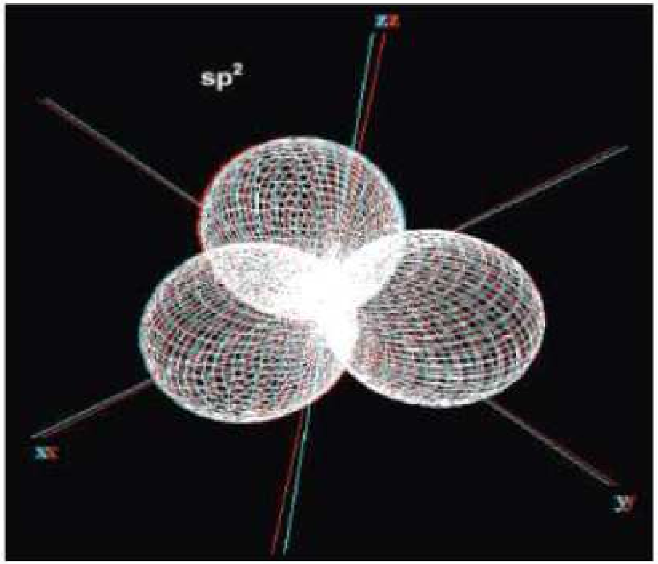
O básico do grafeno: hibridização sp^2



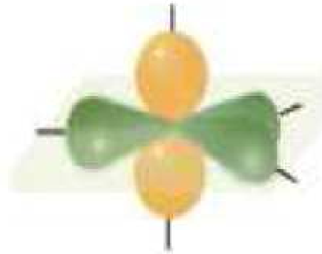


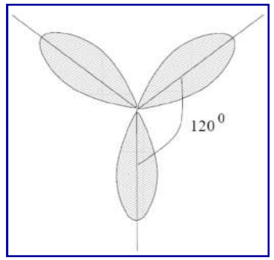






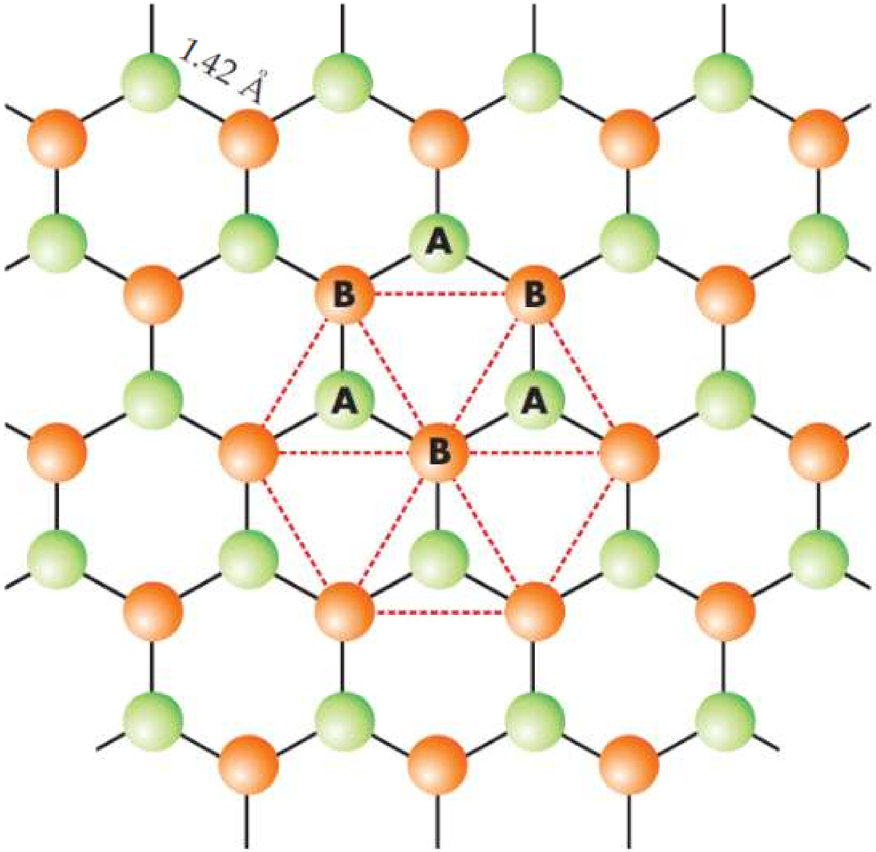
Geometria do orbital hibridizado:
trigonal plana
3 primeiros vizinhos

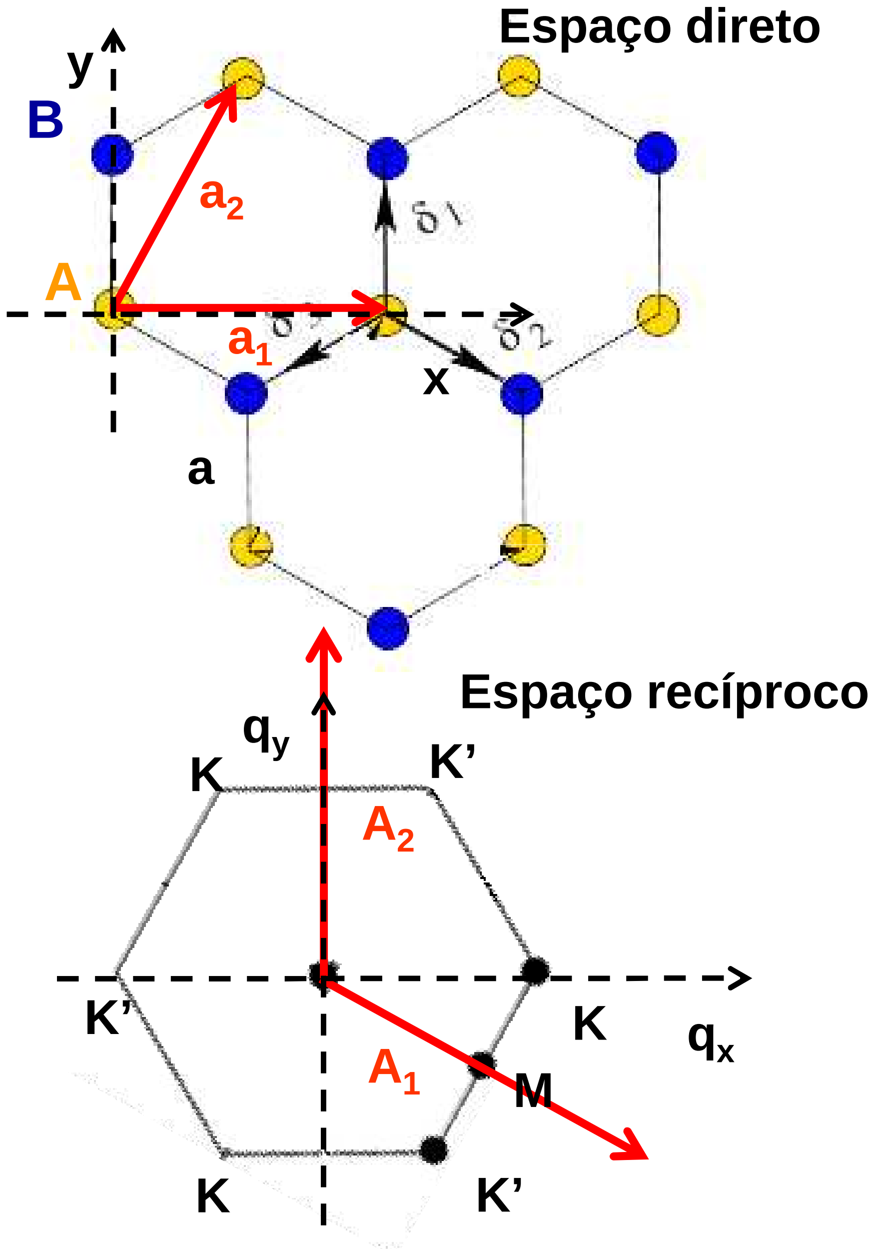




orbital p_z dá origem: orbital π

Grafeno: Rede triangular com base





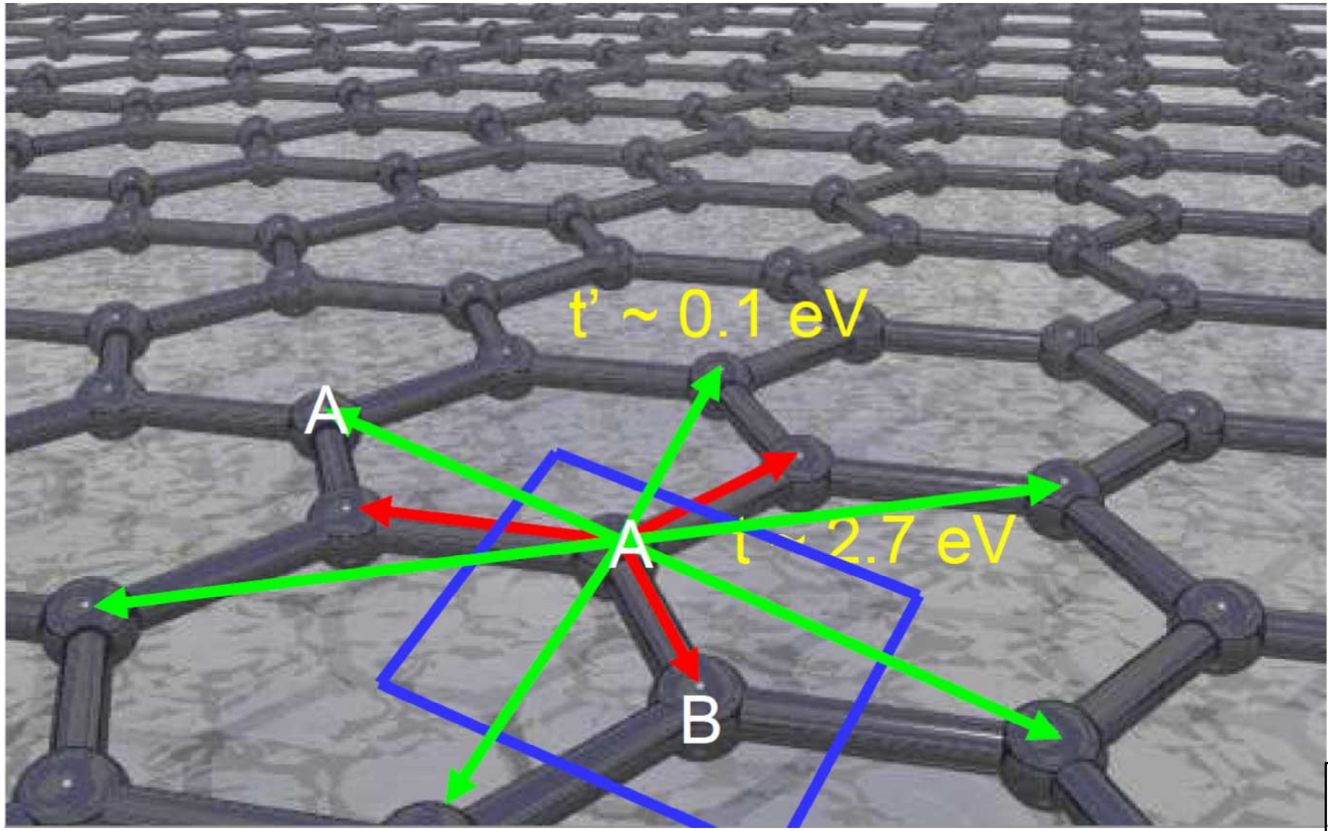
- **Tarefa 9 (hoje):**

1 - Escrever os vetores $\mathbf{a}_1$ e $\mathbf{a}_2$

2 – Calcular o módulo de:

$$\gamma_{\mathbf{q}} = 1 + e^{i\mathbf{q}\cdot\mathbf{a}_{\cancel{1}2}} + e^{i\mathbf{q}\cdot(\mathbf{a}_2-\mathbf{a}_1)}$$

Tight-binding para o grafeno: duas bandas.



Tight-binding de 1os…

$$H = -t \sum_{\langle i,j \rangle,\sigma} \left(a^{\dagger}_{\sigma,i} b_{\sigma,j} + \text{H.c.} \right)$$

$$- t' \sum_{\langle\langle i,j \rangle\rangle,\sigma} \left(a^{\dagger}_{\sigma,i} a_{\sigma,j} + b^{\dagger}_{\sigma,i} b_{\sigma,j} + \text{H.c.} \right)$$

…e 2os vizinhos

$$0.02t \leq t' \leq 0.2t$$

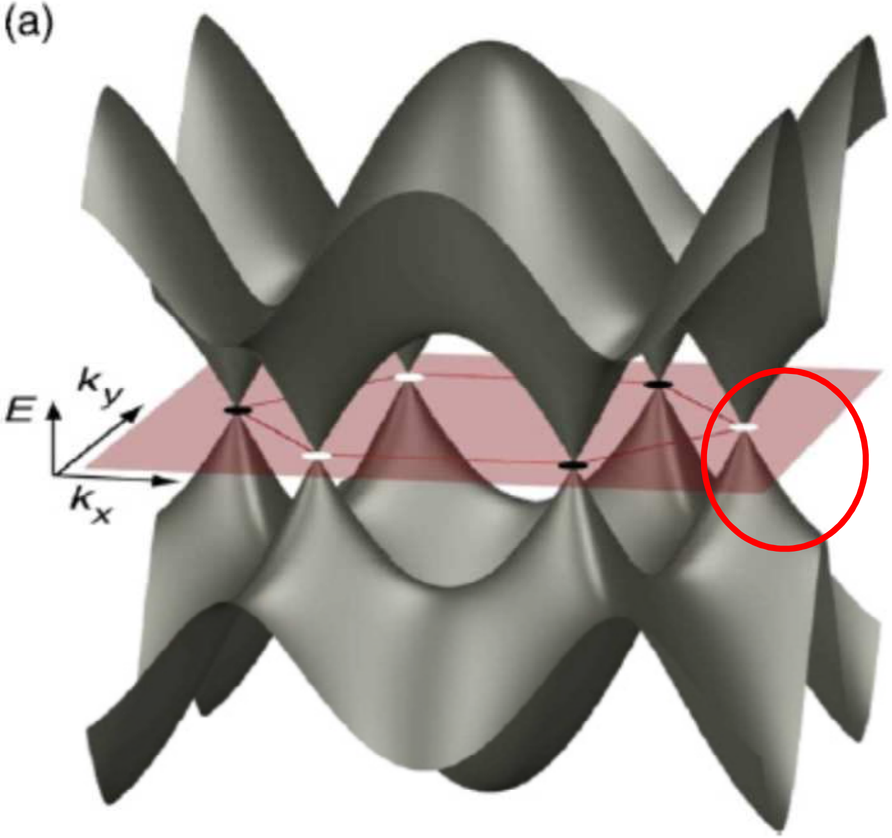
$$E_{\pm}(\mathbf{q}) = \pm t \sqrt{3 + f(\mathbf{q})} - t' f(\mathbf{q})$$

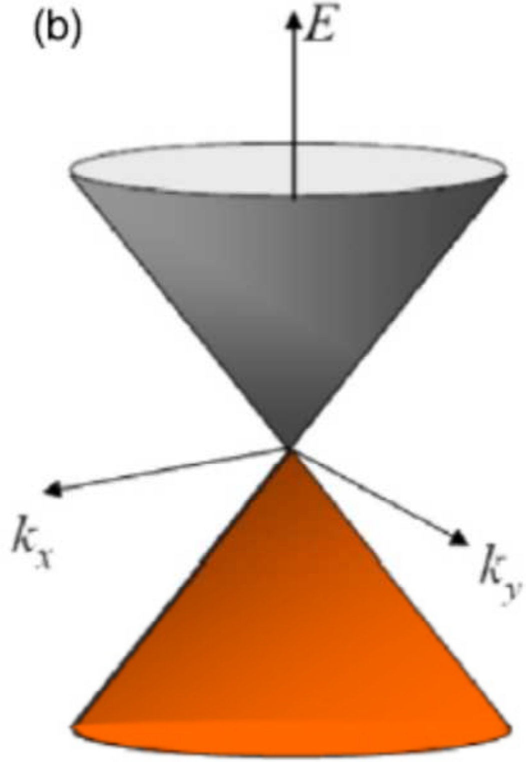
$$f(\mathbf{q}) = 2\cos\left(\sqrt{3} q_x a\right) + 4\cos\left(\frac{\sqrt{3}}{2} q_x a\right) \cos\left(\frac{3}{2} q_y a\right)$$

Resultado do final dos anos 40!

Wallace, P.R., *Phys. Rev.* 71 622 (1947)

Cones de Dirac.



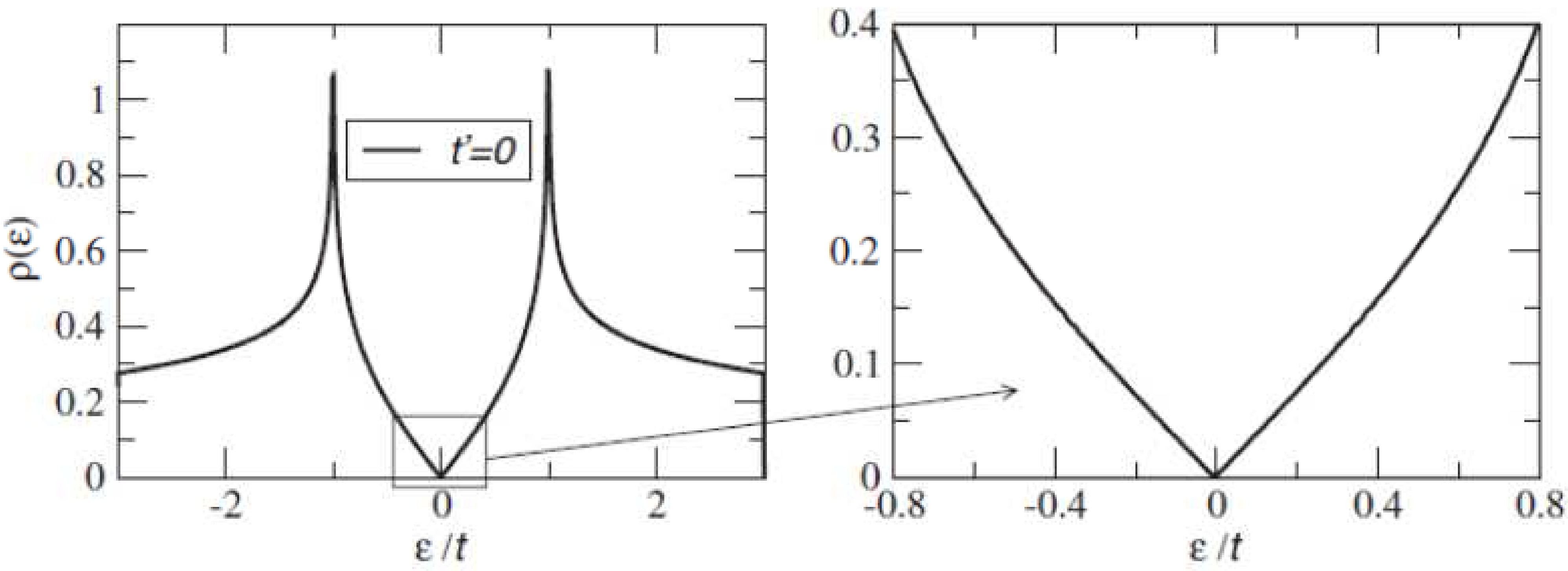


$$E_{\pm}(\mathbf{q}) \approx \pm t\sqrt{3 + f(\mathbf{q})}$$

$$E_{\pm}(\mathbf{q}) = \pm v_F|\mathbf{q}|$$

Analogia: dispersão de férmions “relativísticos sem massa” (“E=pc”)

Grafeno: densidade de estados



ρ(E) ∝ |E| (*linear*)
próximo ao ponto
de neutralidade de carga.

$$\rho(E) = \frac{2A_c}{\pi}\frac{|E|}{v_F^2}$$