

Problem 1. Band structure of graphite.

Consider a single sheet of graphite, composed of carbon atoms arranged on the sites of a honeycomb. The underlying Bravais lattice is triangular, with two sites per unit cell. The Basis vectors of the Bravais lattice are $\vec{a}_{\pm} = \frac{a}{2} (\pm 1, \sqrt{3})$ (see figure), where $a = d\sqrt{3}$, with d the near-neighbor carbon separation. Only one of the four outer shell electrons of each atom can tunnel between neighboring p_z orbitals.

a) Show that in the tight-binding approximation the Bloch states form two bands with energies

$$E_{\pm}(k) = E_0 \pm [|\xi(\vec{k})|^2]^{1/2}$$

$$\xi(\vec{k}) = 2t \cos\left(\frac{k_x a}{2}\right) e^{\frac{-ik_y a}{2\sqrt{3}}} + t e^{\frac{ik_y a}{\sqrt{3}}}$$

Hint: Consider overlaps between electron states on neighboring atoms only.

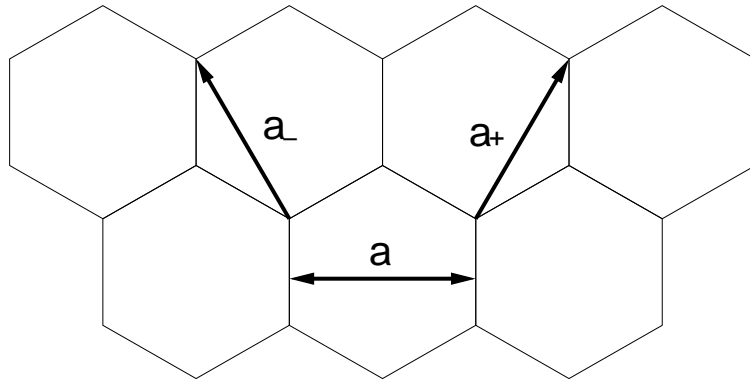


FIG. 1: A honeycomb lattice of C atoms in a sheet of graphite (Problem 1).

- b) Explain why an undoped graphite has a chemical potential $\mu = E_0$.
- c) Use results of parts a) and b) to explain why graphite is called a semimetal.

d*) (Extra credit problem). Single wall nanotubes consist of rolling the honeycomb sheet of carbon atoms into a cylinder. Each tube is characterized by two integers (N,M), which specify the super-lattice translation $T_{(N,M)} = N\vec{a}_+ + M\vec{a}_-$, which wraps around the waist of the cylinder. Discuss bandstructure of the nanotubes depending on N,M.

Problem 2** (Extra credit problem). Surface (Tamm) states in semiconductors. Electrical and optical properties of semiconductors depend on the quality of their surface and can change dramatically after polishing or chemical treatment. The origin of such sensitivity is the presence of electron states localized on crystal surfaces that coexist with the usual states in the bulk of a crystal. In this problem you will consider a simple one-dimensional model for such surface states (Tamm states).

Consider a one dimensional potential (see Fig. 2)

$$U(x) = \begin{cases} -G \sum_{n=1}^{\infty} \delta(x - na), & x > b \\ \infty, & x \leq b \end{cases} \quad (1)$$

with $\frac{a}{2} < b < a$, $\frac{2mGa}{\hbar^2} \gg 1$, and $\frac{2mG(a-b)}{\hbar^2} \gg 1$. Find the energy of the surface state.

Hint: In the spirit of the tight-binding approximation take

$$\psi(x) = \begin{cases} \sum_{n=0}^{\infty} e^{-\lambda n + ikn} \phi(x - an), & x > b \\ 0, & x \leq b \end{cases} \quad (2)$$

where $\phi(x - x_0)$ is the bound state wavefunction for $\tilde{U}(x) = -G\delta(x - x_0)$. Verify that when $\lambda \neq 0$, the condition that the energy is real requires $k = 0$ or π .

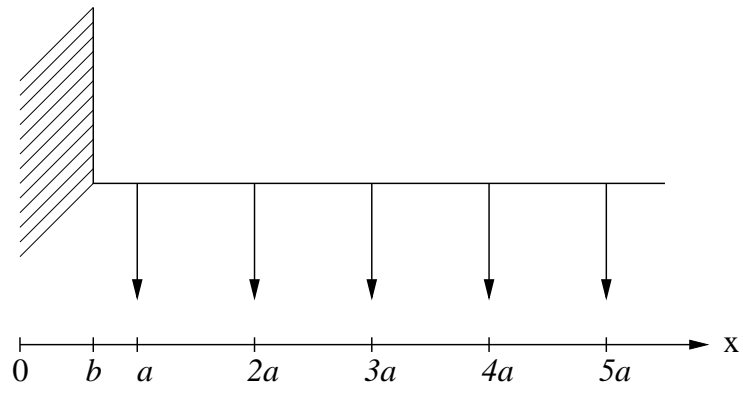


FIG. 2: One dimensional model for surface states in semiconductors (Problem 2).