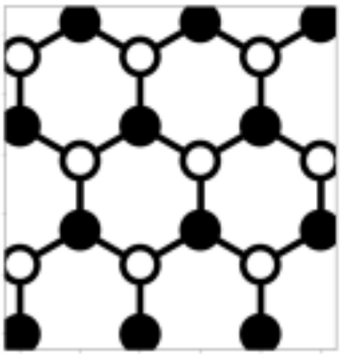
Solid state physics 2019 Minitest 3

29 March 2019

Good luck!

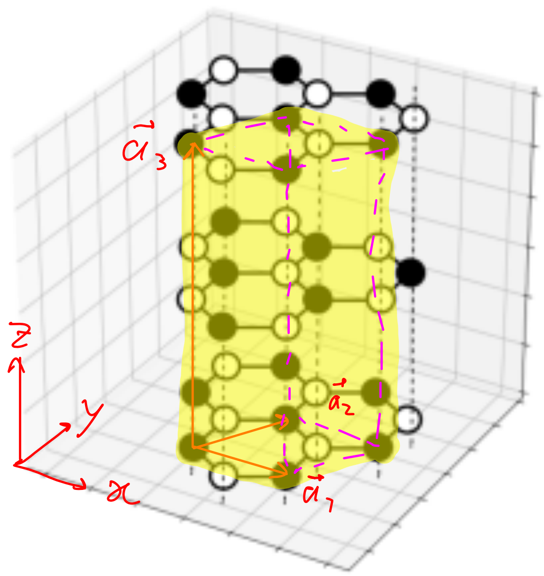
- You may not use textbooks, notes, or calculators.
- When plotting, label the axes and mark the important values.
- If you need extra answer space: ask for an extra exam copy, fill in your name and continue writing the solution.

1. (50 points) Consider hexagonal boron nitride - a crystal that consists of atomic layers that have a honeycomb crystal structure, with half the atoms being boron (B, filled circles) and half nitrogen (N, empty circles) shown here:



The layers are stacked such that on top of each boron atom there is a nitrogen atom in the next layer and vice versa, as shown in the plot below. The distance between neighboring B and N atoms within each layer is a, the distance between the layers is h.

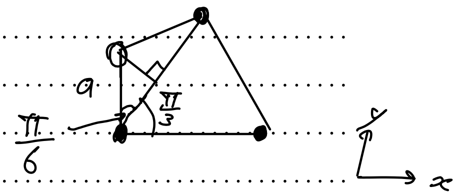
(a) (10 points) Draw the primitive lattice vectors, and a primitive unit cell of hexagonal boron nitride in the plot below. Does this unit cell stay primitive if we make all atoms the same? Explain your answer.



If all atoms are the same, the unit cell will be smaller. The height will be halved.

(b) (10 points) Write down the lattice vectors in Cartesian coordinates. Write down the basis.

B to B distane:



$2 \cdot a \cdot \cos\left(\frac{\pi}{6}\right) = \sqrt{3} \cdot a$

Thus $\vec{a}_1 = \sqrt{3} \cdot a\, \hat{x}$

$$\vec{a}_2 = \cos\left(\frac{\pi}{3}\right)\sqrt{3}\, a\, \hat{x} + \sin\left(\frac{\pi}{3}\right)\sqrt{3}\, a\, \hat{y}$$

$$= \frac{1}{2}\sqrt{3}\, a\, \hat{x} + \frac{3}{2}\, a\, \hat{y}$$

$\vec{a}_3 = 2h\,\hat{z}$

Basis: Boron at $(0,0,0)$ and $(\sqrt{3}a, a, h)$

Nitrogen at $(\sqrt{3}a, a, 0)$ and $(0, 0, h)$

(c) (10 points) Compute the reciprocal lattice vectors.

Usefull: volume unit cell

$$V = \sqrt{3} \cdot a \cdot \frac{3}{2} \cdot a \cdot 2h = 3\sqrt{3}\, a^2 h$$

$$\vec{b}_1 = \frac{2\pi}{V}(\vec{a}_2 \times \vec{a}_3) = \frac{2\pi}{3\sqrt{3}\, a} \cdot (3\hat{x} - \sqrt{3}\,\hat{y})$$

$$\vec{b}_2 = \frac{2\pi}{V}(\vec{a}_3 \times \vec{a}_1) = \frac{4\pi}{3a}\,\hat{y}$$

$$\vec{b}_3 = \frac{2\pi}{V}(\vec{a}_1 \times \vec{a}_2) = \frac{\pi}{h}\,\hat{z}$$

(d) (10 points) Compute the structure factor using the form factors f_B and f_N of boron and nitrogen.

$$S = \sum_j f_j \exp(i \vec{G} \cdot \vec{r}_j) \quad \text{with} \quad \vec{G} = m_1 \vec{b}_1 + m_2 \vec{b}_2 + m_3 \vec{b}_3$$

$$= f_B + f_N \exp\left(i \vec{G} \cdot a[\sqrt{3}\hat{x} + \hat{y}]\right) + f_N \exp\left(i \vec{G} \cdot h\hat{z}\right)$$

$$+ f_B \exp\left(i \vec{G} \cdot [a(\sqrt{3}\hat{x} + \hat{y}) + h\hat{z}]\right)$$

$$= f_B \left(1 + \exp\left(i\left[\frac{4\pi}{3} m_1 + \frac{4\pi}{3} m_2 + \pi m_3\right]\right)\right) +$$

$$f_N \left(\exp\left(i\left[\frac{4\pi}{3} m_1 + \frac{4\pi}{3} m_2\right]\right) + \exp(i \pi m_3)\right)$$

(e) (10 points) For which reciprocal lattice vectors $\mathbf{G} = m_1\mathbf{b}_1 + m_2\mathbf{b}_2 + m_3\mathbf{b}_3$ do diffraction peaks disappear when $f_B = f_N$?

From d, $S = 0$ for $f_B = f_N$ if m_3 is odd

and $\frac{4\pi}{3}(m_1 + m_2) = 2\pi n$ with $n \in \mathbb{Z}$

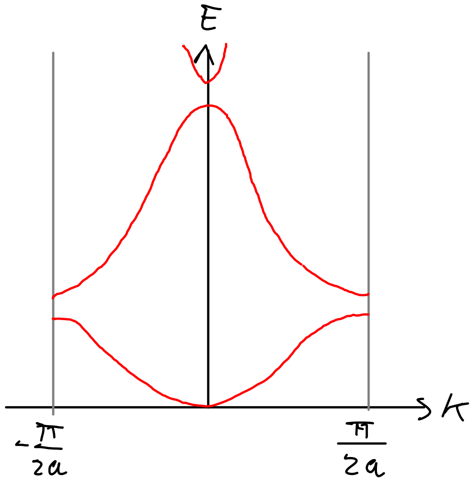
$\Rightarrow \frac{2}{3}(m_1 + m_2) = n \Rightarrow m_1 + m_2 = 3n$

2. (50 points) Consider 1D electrons in a potential

$$V(x) = \sum_{n=-\infty}^{\infty} [A\delta(x - 2na) + B\delta(x - (2n+1)a)].$$

Here $\delta(x)$ is the Dirac delta-function.

(a) (10 points) Sketch the nearly free electron model band structure for this potential (you do not have to compute the sizes of the gaps between different bands). Use the *reduced* Brillouin zone scheme.



Note that the period of potential is $2a$ so period in reciprocal space is $\frac{2\pi}{2a}$.

(b) (10 points) Compute the size of the gap between the first and the second band, and the gap between second and the third band.

Let $|\phi_k\rangle$ be a free electron with wave number k

between 1st and 2nd:

$$2\left|\langle \phi_{\frac{\pi}{2a}} | \hat{V} | \phi_{-\frac{\pi}{2a}} \rangle\right| = \frac{2}{2a}\int_{-a+\varepsilon}^{a+\varepsilon} \exp\left(-i\frac{\pi}{a}x\right) V(x)\, dx$$

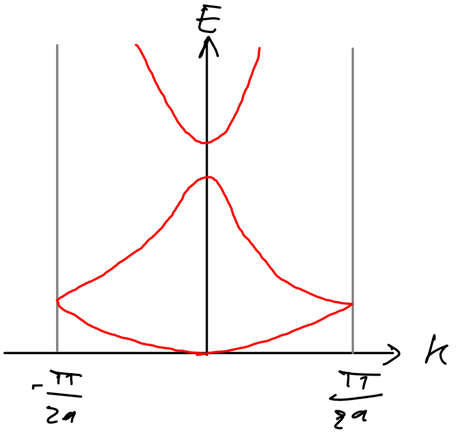
$$= \frac{1}{a}(A - B)$$

between 2nd and 3rd:

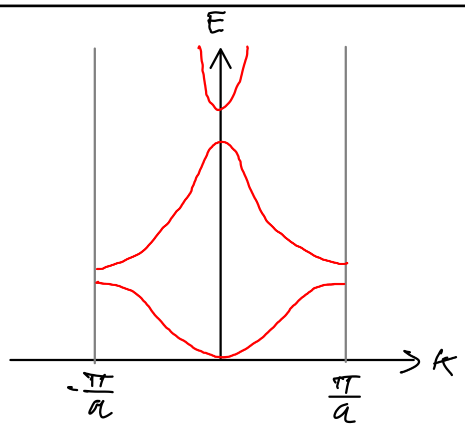
$$2\left|\langle \phi_{\frac{\pi}{a}} | \hat{V} | \phi_{-\frac{\pi}{a}} \rangle\right| = \frac{2}{2a}\int_{-a+\varepsilon}^{a+\varepsilon} \exp\left(-i\frac{2\pi}{a}x\right) V(x)\, dx$$

$$= \frac{1}{a}(A + B)$$

(c) (10 points) Sketch the band structure in the case $A = B$. How is it related to the case $A \neq B$?

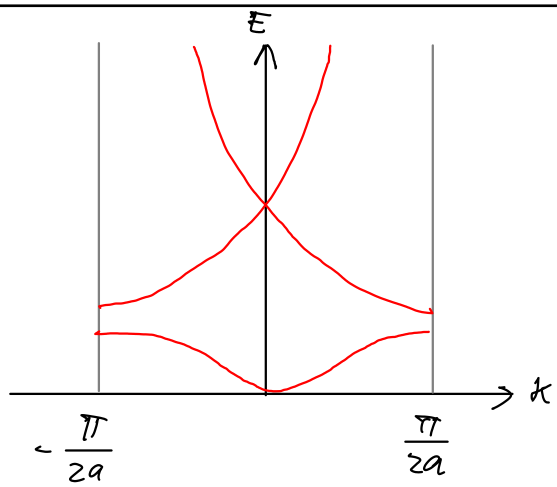


or



The period of the potential will become $2a \to a$ if $A = B$. Which means that the BZ will increase in size $\frac{\pi}{a} \to \frac{2\pi}{a}$. This also explains why the gap between 1st and 2nd band have to become 0 if $A = B$.

(d) (10 points) Sketch the band structure for $A = -B$. Which band gaps are equal to 0?



All band gaps that are at k point equivalent to $k = 0$ will become zero.

(e) (10 points) Compute the effective electron mass for the first band at $k = 0$. Write down the dispersion relation near $k = \pi/2a$ for $A \neq B$. Would you expect the effective mass at $k = \pi/2a$ to be lower or higher than at $k = 0$? Explain your answer.

At the lowest band at $k=0$, we have more or less free electron model so the effective mass here is just the electron mass m_e.

At $k = \frac{\pi}{2a}$;

$$\hat{H} = \begin{pmatrix} \frac{\hbar^2}{2m}\left(\frac{\pi}{2a}\right)^2 + V_0 + \hbar v \delta k & V_1 \\ V_1^* & \frac{\hbar^2}{2m}\left(\frac{\pi}{2a}\right)^2 + V_0 - \hbar v \delta k \end{pmatrix}$$

$$\rightarrow \quad E = \frac{\hbar^2}{2m}\left(\frac{\pi}{2a}\right)^2 + V_0 \pm \sqrt{(\hbar v \delta k)^2 + |V_1|^2}$$

where $v = \frac{\hbar \pi}{2ma}$ $\quad V_0 = \frac{1}{2a}(A + B)$ $\quad V_1 = \frac{1}{2a}(A - B)$

It's expected that the effective mass at $k = \frac{\pi}{2a}$ is much lower as $|V_1|$ should not be very large in the nearly free electron model.

so that the slope of the upper band will quickly go from 0 to $\hbar v$.