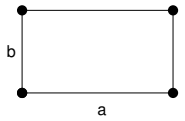
HW 3

Problem 1

Proof that $\psi_{n\mathbf{k}}(\mathbf{r})$ satisfies Bloch's theorem:

$$\psi_{n\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{N}} \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} \phi_n(\mathbf{r} - \mathbf{R}),$$

Problem 2:
a) Calculate band dispersion for a hydrogen like crystal in 2D:



For a = 10°A, b = 5°A, and γ(a) = 0.5 eV, γ(b) = 1 eV and ε_s = 2 eV.

b) Plot 1st BZ of the 2D crystal , e.g. E(k_x) and E(k_y)
c) Plot color surface plot of kx vs ky where E(k) is marked by color.
d) What is the bandwidth of the crystal?
e) What is the effect of overlap integral on band dispersion? Consider the case of γ(a) = 0.5 eV and γ(b) = 0.5 eV and γ(b) = 0 eV .

Problem 3:

Calculate band dispersion E(k) for a face-centered 3D cubic crystal of size *a* (12 nearest neighbors).