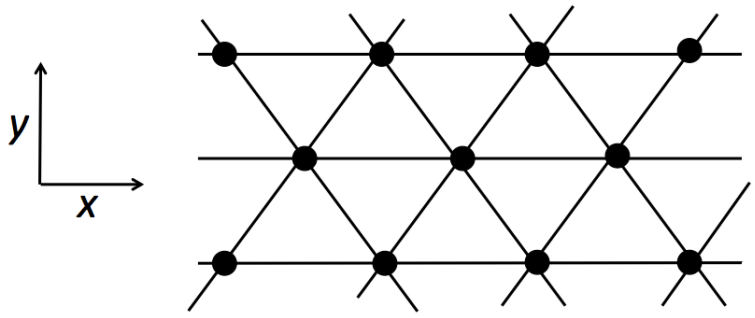
A. A two-dimensional periodic solid is defined by a unit cell containing a single H atom. Its electronic structure can be described by an orthogonal tight-binding model in which the generic basis set element, $|\mathbf{R}\rangle$, represents the H $1s$ orbital at the position $\mathbf{R}$. Use Bloch theorem to compute the expectation value of the following operator over a generic eigenstate of the system

$$\hat{O} = \sum_{\mathbf{R}} O_{\mathbf{R}} |\mathbf{R}\rangle\langle\mathbf{R}| \, .$$

Here $O_{\mathbf{R}}$ is a scalar number dependent on the atomic position $\mathbf{R}$ and the sum runs over all the atoms. What is the meaning of the operator, if $O_{\mathbf{R}} = 1$ for every $\mathbf{R}$? What is its expectation value?

B. Now consider the triangular lattice of H atoms shown in the figure. Each atom occupies the corner of equilateral triangles of side $a_0 = 1$.



Derive the band structure equation for such a system by using an orthogonal nearest neighbor tight-binding model in which every H atom is described by a single H $1s$ orbital. Take ϵ as on-site energy and t as hopping parameter.

C. Plot the band structure along the directions $\Gamma \to A \to B$, where $\Gamma = (0, 0)$, $A = (\pi, 0)$, $B = (\pi, \pi/\sqrt{3})$. For the plot use the values $\epsilon = 0$ eV and $t = -1$ eV.

D. Calculate and plot the two-dimensional Fermi surface for such lattice when the Fermi energy is $E_{\mathrm{F}} = -6 + \delta$ eV, with being δ a small positive quantity [use the same values for ϵ and t as those in C)].

Marking Scheme: A) 6 points, B) 6 points, C) 7 points, D) 6 points.