ASSIGNMENT 1
Reading: Kittel, Chapter 3
Problems

1. Given two vectors u and v in an orthogonal system with \( u = \begin{bmatrix} 3 \\ 7 \\ 2 \end{bmatrix} \) and \( v = \begin{bmatrix} 2 \\ 0 \\ 1 \end{bmatrix} \) find:
\[ |u|, |v|, (u \cdot v), \theta_{uv}, \text{ where } \theta_{uv} \text{ is the angle between } u \text{ and } v. \]

2. Given the 3 x 3 matrix \( A = \begin{bmatrix} 1 & 0 & 2 \\ 1 & 1 & 1 \\ 0 & 2 & 1 \end{bmatrix} \) calculate \( A^{-1} \). Verify that \( AA^{-1} = I \)

3. Let \( \Psi(x) \) be a 1-dimensional wave function. If \( \Psi_1(x) = Ae^{-ax^2}, \Psi_2(x) = Bxe^{-ax^2}, \) and \( P = ex \), calculate \( I_{11}, I_{12}, \) and \( I_{22} \) where \( I_{ij} = \int_{-\infty}^{\infty} \Psi_i^*(x)P\Psi_j(x)dx. \)

4. Consider an periodic, infinite 1-dimensional square wave of amplitude A and period a, whose value is \(-A/2\) in the region between \(x = -a/2\) and \(x = 0\) and \(A/2\) between \(x = 0\) and \(x = a/2\). Calculate the first 3 terms in its Fourier expansion.

5. Find the new energy eigenstates created by forming a linear combination of two identical s-wave functions so that \( \Psi(r) = u_1 \Psi_1(r) + u_2 \Psi_2(r). \)

The energy \( E = \langle H \rangle = \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle} \).

Find an expression for \( E \) in terms of the coefficients \( u_i \) and matrix elements \( H_{ij} \). Assume that the wavefunctions are orthonormal. Apply the variational principle by differentiating with respect to \( u_1^* \) and \( u_2^* \) independently. Find the eigenvalue equation and solve for the energies in terms of \( H_{11} (= H_{22}) \) and \( H_{12} (= H_{21}) \). How does this relate to the existence of bonding and antibonding electron states?