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:

$|u|, |v|, (u \bullet v), \theta_{uv}$, where θ_{uv} is the angle between u and v.

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

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 $E = \langle H \rangle = \dfrac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle}$.

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?