GRADUATE QUANTUM MECHANICS: 502 Spring 2002

Assignment 1: due Mon, Feb 3rd.

Read: Sakurai Chapter 4 266-282.

1. A particle can move on a three-dimensional square lattice at positions $\mathbf{r} = l\hat{\mathbf{x}} + m\hat{\mathbf{y}} + n\hat{\mathbf{z}}$, where $(\hat{\mathbf{x}}, \hat{\mathbf{y}}, \hat{\mathbf{z}})$ is a set of three orthogonal unit vectors. Suppose the Hamiltonian has a tight binding form, with diagonal elements

$$\langle \mathbf{r}|H|\mathbf{r}\rangle = E_o \tag{1}$$

and where the only non-zero off-diagonal matrix elements are

$$\langle \mathbf{r} + \mathbf{a}|H|\mathbf{r}\rangle = \langle \mathbf{r}|H|\mathbf{r} + \mathbf{a}\rangle = -\Delta \tag{2}$$

where $\hat{a} = (\pm\hat{\mathbf{x}}, \pm\hat{\mathbf{y}}, \pm\hat{\mathbf{z}})$ denotes the vector from one site to any one of its six nearest neighbors.

   (a) The translation operator has the following action: $\tau(\hat{\mathbf{a}})|\mathbf{r}\rangle = |\mathbf{r}+\mathbf{a}\rangle$. Construct an eigenket of this operator.

   (b) Show that the eigenket of the translation operator is an energy eigenstate and calculate the energy spectrum.

2. Sakurai problem 4.2.

3. Sakurai, Problem 4.9.

4. Sakurai problem 4.12.

5. Sakurai problem 4.6. *Hint: Don't try to do this problem exactly, rather calculate the mixing between the states in the left-hand and right-hand wells. First consider the problem when the separation between the two wells is infinite and calculate the energy eigenstates $|\psi_L\rangle$ and $|\psi_R\rangle$ for the two seperate wells. Now suppose that when you bring the two wells together, the first and second excited states can be written as a linear combination of these two states. Use the two states that you have constructed as a basis set for constructing an "effective" 2×2 Hamiltonian. For consistency, you need to first orthogonalize the states, writing $|\tilde{\psi}_R\rangle = |\psi_R\rangle$, $|\tilde{\psi}_L\rangle = (|\psi_L\rangle - |\psi_R\rangle\langle\psi_R|\psi_L\rangle)/\sqrt{1 - |\langle\psi_R|\psi_L\rangle|^2}$. Then, working to leading exponential accuracy, calculate the 2×2 Hamiltonian for this basis set. Show that it is the off-diagonal elements $|\langle\tilde{\psi}_L|H\tilde{\psi}_R\rangle| = \Delta$ that give the splitting $E \pm \Delta$, and calculate these elements to leading exponential accuracy.*