**Final Examination**
**Physics 386 / Spring 1997**
**Professor Klaus Schulten**

## Problem 1: Two-State Quantum System (10 pts)

A two-state quantum system with states $|1\rangle$ and $|2\rangle$ is governed by the Hamiltonian

$$\hat{H} \; = \; \begin{pmatrix} \epsilon & v \\ v & \epsilon \end{pmatrix} \tag{1}$$

where $\epsilon, v \in \Re$.

(a) Determine the stationary states and corresponding energies of the system.

(b) The system is initially ($t = 0$) in state $|1\rangle$. Determine the probability to find the system in state $|2\rangle$ at time $t$.

## Problem 2: Harmonic Oscillator (15 pts)

At $t = 0$ a particle is in a state described by the following coherent superposition of harmonic oscillator stationary states

$$\psi(x,0) \; = \; \frac{1}{4}\phi_0(x) \; + \; \frac{i}{2}\phi_1(x) \; + \; \frac{\sqrt{11}}{4}\phi_2(x) \tag{2}$$

where $\phi_n(x)$ are the solutions of the time -independent Schrödinger equation

$$\left( -\frac{\hbar^2}{2m}\,\partial_x^2 \; + \; \frac{1}{2}m\omega^2 x^2 \right) \; \phi_n(x) \; = \; \hbar\omega(n + \frac{1}{2})\,\phi_n(x) \tag{3}$$

(a) Determine the wave function at time $t$.

(b) Determine the probability to measure the energy $\frac{3}{2}\hbar\omega$ at time $t$.

(c) Argue why the functions $\phi_n(x)$ are orthonormal. (Hint: Consider the energy eigenvalues.)

(d) Evalute the expectation value of the position operator $\hat{x}$. For this purpose express $\hat{x}$ in terms of the creation and annihilation operators defined in class, use the action of these operators on the functions $\phi_n(x)$, e.g., $a^+\phi_n(x) \;=\; \sqrt{n+1}\,\phi_n(x)$ and use the orthonormality of the functions $\phi_n(x)$.

**Problem 3: Cyclobutadiene (10pts)**

The so-called $\pi$-electrons in the molecule cyclobutadiene are described by linear combinations (molecular orbitals) of atomic orbital states $|j\rangle$, $j = 1, 2, 3, 4$ and are governed by the Hamiltonian

$$\hat{H} = \begin{pmatrix} \epsilon & v & 0 & v \\ v & \epsilon & v & 0 \\ 0 & v & \epsilon & v \\ v & 0 & v & \epsilon \end{pmatrix} \tag{4}$$

where $\epsilon, v \in \Re$.

Determine the stationary states and energies eigenvalues for this system.

**Problem 4: Electron in a Box (20 pts)**

An electron is in the ground state of a box with sides at $x = 0$ and $x = a$. Suddenly, a wall is moved from $x = a$ to $x = 2a$. What is the probability that the electron will be found (a) in the ground state and (b) in the first excited state of the new box. (c) For which states will the corresponding probability be zero?

**Problem 5: Three-dimensional harmonic oscillator (15 pts)**

The Hamiltonian for a three-dimensional simple harmonic oscillator is

$$\hat{H} = -\frac{\hbar^2}{2m}\left(\partial_x^2 + \partial_y^2 + \partial_z^2\right) + \frac{1}{2}m\omega^2\left(x^2 + y^2 + z^2\right) \tag{5}$$

(a) By expressing the Hamilonian (5) as a sum of three operators

$$\hat{H} = \hat{H}_x + \hat{H}_y + \hat{H}_z \tag{6}$$

where $\hat{H}_x$ is the Hamiltonian of the one-dimensional oscillator in x and $\hat{H}_y$ and $\hat{H}_z$ are similarly defined, show that the wave functions

$$\psi(x, y, z) = \phi_j(x)\,\phi_k(y)\,\phi_\ell(z) \tag{7}$$

are eigenstates of (5), i.e., $\hat{H}\,\psi = E\,\psi$, when the functions $\phi_m$ are the energy eigenfunctions of the one-dimensional oscillator.

(b) Find the energy eigenvalues $E$ of the Hamiltonian (5).

(c) Using a result derived in class demonstrate that the ground state (lowest energy stationary state) wave function for the three-dimensional oscillator defined through (5) is spherically symmetric.

**Problem 6: Two state system in a magnetic field (15 pts)**

A certain type of particle can exist in one of two states, $|1\rangle$ and $|2\rangle$. An ensemble of these particles is prepared and shot out in a beam, all with velocity $v_o$ and all in state $|1\rangle$. The beam passes through a region of uniform magnetic field of length $l_o$. In this region, the Hamiltonian governing the system is

$$H_1 = \hbar\omega_o \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} . \tag{8}$$

In terms of $v_o$ and $w_o$, find the *shortest* length $l_o$ of the magnetic field region, such that the probability of finding a particle in $|2\rangle$ after it has passed through the field is $1/4$.