Problem Set 12

Problem 1

In the lecture, you have seen the example of the infinite square well, that the number of nodes increases by one with every energetically higher lying state. In this problem, you will show that it is generally true that the number of nodes of the stationary states of a 1D potential increases with energy. Consider two (real, normalized) solutions ψ_n and ψ_m to the time-independent Schrödinger equation for a given potential $V(x)$. We denote the eigenenergies E_n and E_m and $E_n > E_m$.

1. Show that
$$\frac{d}{dx}\left(\frac{d\psi_m}{dx}\psi_n - \psi_m\frac{d\psi_n}{dx}\right) = \frac{2m}{\hbar^2}\left(E_n - E_m\right)\psi_m\psi_n \tag{1}$$

2. Let x_1 and x_2 be two adjacent nodes of the function $\psi_m(x)$. Show that

$$\psi'_m(x_2)\psi_n(x_2) - \psi'_m(x_1)\psi_n(x_1) = \frac{2m}{\hbar^2}\left(E_n - E_m\right)\int_{x_1}^{x_2} \psi_m \psi_n dx \tag{2}$$

3. If ψ_n has no nodes between x_1 and x_2, then it must have the same sign everywhere in the interval. Show that (2) then leads to a contradiction. Therefore between very pair of nodes of ψ_m, ψ_n must have at least one node and in particular the number of nodes increases with energy.

Problem 2

Consider the operator $\hat{A}$ and a state $|\Psi\rangle$. We can expand the state $|\Psi\rangle$ in some basis $\{|n\rangle\}$ as

$$|\Psi\rangle = \sum_n c_n |n\rangle \tag{3}$$

We can also represent $|\Psi\rangle$ as a vector in the basis of $\{|n\rangle\}$:

$$|\Psi\rangle = c_1 \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} + c_2 \begin{pmatrix} 0 \\ 1 \\ \vdots \\ 0 \end{pmatrix} + \ldots = \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_N \end{pmatrix} \tag{4}$$

where N is the dimensionality of the Hilbert Space (the number of basis states $|n\rangle$). Similarly, the operator $\hat{A}$ can be represented as a Matrix in the basis $\{|n\rangle\}$:

$$\hat{A} = \begin{pmatrix} A_{11} & A_{12} & A_{13} & \ldots & A_{1N} \\ A_{21} & A_{22} & A_{23} & \ldots & A_{2N} \\ \vdots & & \ddots & & \vdots \\ A_{N1} & A_{N2} & A_{N3} & \ldots & A_{NN} \end{pmatrix} \tag{5}$$

1. Show that the matrix element $A_{nn'}$ is found by

$$A_{nn'} = \langle n|\hat{A}n'\rangle \tag{6}$$

(Hint: Either insert the completeness relation of either side of $\hat{A}$, or try different values of n and n' and use the vector/matrix representation and see what the matrix multiplication gives for $A_{nn'}$. Note that the bra $\langle n|$ is a row vector!)

2. Write down the matrix representation of the Hamiltonian in the basis of energy eigenstates! (Hint: Replace $\hat{A}$ by $\hat{H}$ and take $\{|n\rangle\}$ to be energy eigenstates. Use orthonormality of the basis! No calculation is necessary in the exercise!)

3. Write down the matrix representation of the $\hat{L}_z$ operator in the basis of eigenstates to L_z with $\ell = 1$:

$$\{|\ell = 1; m_\ell = -1\rangle, |\ell = 1; m_\ell = 0\rangle, |\ell = 1; m_\ell = 1\rangle\} \tag{7}$$

and use

$$L\pm|\ell, m_\ell\rangle = \hbar\sqrt{\ell(\ell+1) - m_\ell(m_\ell \pm 1)}|\ell, m_\ell \pm 1\rangle \tag{8}$$

and

$$L_x = \frac{1}{2}(L_+ + L_-), \tag{9}$$

$$L_y = \frac{1}{2i}(L_+ - L_-), \tag{10}$$

to find the matrix elements of L_+, L_-, L_x and L_y in the basis $\{|\ell = 1; m_\ell = -1\rangle, |\ell = 1; m_\ell = 0\rangle, |\ell = 1; m_\ell = 1\rangle\}$.
(Hint: It may be convenient to define $|\ell = 1, m_\ell = p\rangle \equiv |p\rangle$.)

4. Show by matrix multiplication that $L_+|\ell = 1, m_\ell = -1\rangle = \hbar\sqrt{2}|\ell = 1, m_\ell = 0\rangle$.

Problem 3

The Feynman-Hellmann theorem relates the eigenvalues of a time-independent Hamiltonian to the parameters that it contains. According to the theorem, once the eigenfunctions of a system have been found by solving the Schrödinger equation, all forces in the system can be calculated. This you will see in the following exercise.

Suppose the Hamiltonian H for a particular quantum system, is a function of some parameter λ; let $E_n(\lambda)$ and $\psi_n(\lambda)$ be the eigenvalues and eigenfunctions of $H(\lambda)$. The Feynman-Hellmann theorem states that

$$\frac{\partial E_n}{\partial \lambda} = \langle \psi_n | \frac{\partial H}{\partial \lambda} \psi_n \rangle \tag{11}$$

(assuming either that E_n is nondegenerate, or - if degenerate - that the ψ_n are the "good" linear combinations of the degenerate eigenfunctions).

1. Prove the Feynman-Hellmann theorem. Hint: Use $E_n^{(1)} = \langle \psi_n^{(0)} | H' \psi_n^{(0)} \rangle$ where $E_n^{(1)}$ denotes the first-order energy correction and H' is the perturbation.

2. Apply it to the one-dimensional harmonic oscillator

   (a) using $\lambda = \omega$. This yields a formula for the expectation value of V.

   (b) using $\lambda = \hbar$. This yields $\langle T \rangle$.

   (c) using $\lambda = m$. This yields a relation between $\langle T \rangle$ and $\langle V \rangle$.

Problem 4

Two electrons with spin are located in an infinitely deep potential well of width L. As known from the lecture, the corresponding one-particle wavefunctions are, for a certain number n, given by:

$$\Psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right). \tag{12}$$

Hint: In this exercise we ignore the Coulomb interaction of the two electrons.

1. Assume that we prepared both electrons in the same spin state (spin-up), so that the total spin part of the two-particle wavefunction is given by $\chi_{s_1,s_2} = \chi_+\chi_+$. Write down the spatial part of the wavefunction for the two-particle system in the state with the lowest total energy permitted by symmetrization. What is the total wavefunction of the system (spatial and spin)?

2. Calculate the total energy in this case.
   Hint: In order to calculate the total energy you need to calculate the expectation value of the total Hamiltonian $\langle H \rangle = \langle H^{(1)} + H^{(2)} \rangle$, where $H^{(1)}(H^{(2)})$ only acts on the particle one (two).Ignore the Coulomb interaction part! Consider using the Dirac notation in order to simplify your calculations.

3. If we consider all the possibilities of the total spin part of the wavefunction, what would be the ground state of the system? Write down the total wavefunction and calculate the energy of the two-particle system for the ground state.