Physics 143a – Workshop 9

Two-Particle Systems and Schrödinger equation in $\mathbb{R}^3$

Week Summary

- **Separable Hamiltonians:** If we have a Hamiltonian $\hat{H}$ which can be written as

$$\hat{H} = \hat{H}_1 + \hat{H}_2, \tag{1}$$

where the degrees of freedom defining $\hat{H}_1$ do not appear in $\hat{H}_2$ and the degrees of freedom defining $\hat{H}_2$ do not appear in $\hat{H}_1$, then the energy eigenkets and eigenvalues of the system defined by Eq.(1) are, respectively,

$$|n_1, n_2, m_1, m_2, \ldots\rangle = |n_1, m_1, \ldots\rangle \otimes |n_2, m_2, \ldots\rangle, \qquad E_{n_1,n_2,m_1,m_2,\ldots} = E_{n_1,m_1,\ldots} + E_{n_2,m_2,\ldots}, \tag{2}$$

where $n_1, m_1, \ldots$ are the quantum numbers defining the eigenstates and eigenvalues of $\hat{H}_1$ and $n_2, m_2, \ldots$ are the quantum numbers defining the eigenstates and eigenvalues of $\hat{H}_2$.

- **Schrödinger equation in $\mathbb{R}^3$:** The time-independent Schrödinger equation in $\mathbb{R}^3$, for a particle of mass m in a potential V, can be written generally as

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})\right)\phi(\mathbf{r}) = E\phi(\mathbf{r}), \tag{3}$$

where ∇ is the gradient operator, and $\phi(\mathbf{r})$ and E are the wave function and energy eigenvalues of the relevant system with quantum numbers hidden. If our potential $V(\mathbf{r})$ is spherically symmetric (i.e., it is a function only of r), then Eq.(3) reduces to

$$\left[-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}\right) + \frac{\hat{\mathbf{L}}^2}{2mr^2} + V(r)\right]\phi(\mathbf{r}) = E\phi(\mathbf{r}), \tag{4}$$

where $\hat{\mathbf{L}}^2$ is the conserved angular-momentum-squared operator.

If the potential $V(\mathbf{r})$ is separable along the x, y, and z directions then Eq.(3) reduces to

$$\hat{H} = \hat{H}_x + \hat{H}_y + \hat{H}_z, \tag{5}$$

where $\hat{H}_q = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial q^2} + V(q)$.

- **Conservation and Commutation:** By Hamilton's equation of motion, the time evolution of an operator $\hat{A}$ is defined by

$$\frac{d}{dt}\langle A\rangle = \left\langle \frac{\partial \hat{A}}{\partial t}\right\rangle + \frac{i}{\hbar}\left\langle [\hat{H}, \hat{A}]\right\rangle. \tag{6}$$

Thus, an operator $\hat{A}$ without an explicit time dependence and which also commutes with the hamiltonian is conserved.

1 Problems

1. **Particle in a box**
Peter asks Cody a question about a quantum particle in a box. He states that the particle has mass m and potential energy

$$V(x) = \begin{cases} 0 & \text{for } 0 < x < a_x, \, 0 < y < a_y, \text{ and } 0 < z < a_z \\ \infty & \text{otherwise} \end{cases}, \tag{7}$$

where a_x, a_y, and a_z are the confines of the box. He then asks Cody what are the energy eigenfunctions and eigenvalues of this system. Using the one-dimensional problem as an analogy, Cody answers that the energy eigenfunctions and eigenvalues are, respectively,

$$\psi_{n_x,n_y,n_z}(x,y,z) = \sqrt{\frac{8}{a_x a_y a_z}} \sin\left[\pi\left(\frac{n_x}{a_x}x + \frac{n_y}{a_y}y + \frac{n_z}{a_z}z\right)\right], \quad E_{n_x,n_y,n_z} = \frac{\hbar^2\pi^2}{2m}\left(\frac{n_x}{a_x} + \frac{n_y}{a_y} + \frac{n_z}{a_z}\right)^2, \tag{8}$$

where n_x, n_y, and n_z are positive integers.

(a) Is Cody right? If not, then what are the correct energy eigenfunctions and energy eigenvalues?

(b) Peter is looking for more questions he can ask about this particle in a box system. What other questions could he ask?

2. **Degeneracy of Central Potentials**
In a previous assignment we found that if the operators $\hat{A}$, $\hat{B}$, and $\hat{C}$ obeyed the commutation relations

$$[\hat{A}, \hat{B}] = 0, \quad [\hat{A}, \hat{C}] = 0, \quad [\hat{B}, \hat{C}] \neq 0, \tag{9}$$

then $\hat{A}$ must have degenerate eigenvalues. For a particle in a central-force potential, the Hamiltonian is

$$\hat{H} = \frac{\hat{\mathbf{p}}^2}{2\mu} + V(|\hat{\mathbf{r}}|), \tag{10}$$

where μ is the reduced mass of the system and $\mathbf{r}$ is the radial vector. For such potentials, the z angular momentum, y angular momentum, and x angular momentum are all conserved. Using this fact, the properties of angular momentum operators, and Eq.(9), prove that Hamiltonians of the form Eq.(10) always have degenerate energy eigenvalues.

3. **Quantum Oscillator**
Say we have a coupled oscillator defined by the Hamiltonian

$$\hat{H} = \frac{\hat{p}_1^2}{2m} + \frac{\hat{p}_2^2}{2m} + \frac{1}{2}kx_1^2 + \frac{1}{2}kx_2^2 + \frac{1}{2}k(x_2 - x_1)^2. \tag{11}$$

From classical mechanics, we know we can express this Hamiltonian in the normal mode form

$$\hat{H} = \frac{\hat{p}_{q_1}^2}{4m} + \frac{\hat{p}_{q_2}^2}{4m} + kq_1^2 + 3kq_2^2, \tag{12}$$

where $q_1 = \frac{1}{2}(x_1 + x_2)$ and $q_2 = \frac{1}{2}(x_1 - x_2)$, and p_{q_1} and p_{q_2} are the conjugate momenta of q_1 and q_2 respectively.

(a) What are the energy eigenvalues of this coupled oscillator system? (Hint: The energy eigenvalues are defined by two quantum numbers.)

(b) Write the ground state wave function for this system in terms of x_1 and x_2.

2 Solutions

(a) i. Cody is not correct. Since the Hamiltonian for this system is separable, the energy eigenfunctions are a *product* of the energy eigenfunctions for each independent direction:

$$\psi_{n_x,n_y,n_z}(x,y,z) = \sqrt{\frac{8}{a_x a_y a_z}} \sin\left(\frac{n_x\pi}{a_x}x\right) \sin\left(\frac{n_y\pi}{a_y}y\right) \sin\left(\frac{n_z\pi}{a_z}z\right). \tag{13}$$

And the energy eigenvalues are a *sum* of the energy eigenvalues for each independent direction:

$$E_{n_x,n_y,n_z} = \frac{\hbar^2\pi^2}{2m}\left[\left(\frac{n_x}{a_x}\right)^2 + \left(\frac{n_y}{a_y}\right)^2 + \left(\frac{n_z}{a_z}\right)^2\right]. \tag{14}$$

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ii. By analogy to the one-dimensional case, we can ask a number of questions about this system:
- What is the uncertainty in position for each coordinate direction?
- What is the uncertainty in momentum for each coordinate direction?
- What is the time-dependent wave function presuming our system started with the factorizable wave function $\Psi(x,y,z;t=0) = f(x)g(y)h(z)$?

The final question is answered simply using the expansion of an arbitrary wave function in terms of the energy eigenfunctions. With this expansion we have

$$\Psi(x,y,z,t) = \sum_{n_x,n_y,n_z} c_{n_x}c_{n_y}c_{n_z}e^{-iE_{n_x,n_y,n_z}t/\hbar}\psi_{n_x,n_y,n_z}(x,y,z), \tag{15}$$

where the coefficients c_{n_x}, c_{n_y}, and c_{n_z} are given by

$$c_{n_x} = \sqrt{\frac{2}{a_x}}\int_0^{a_x} dx\, \sin\left(\frac{n_x\pi}{a_x}x\right) f(x), \tag{16}$$

$$c_{n_y} = \sqrt{\frac{2}{a_y}}\int_0^{a_y} dy\, \sin\left(\frac{n_y\pi}{a_y}y\right) g(y), \tag{17}$$

$$c_{n_z} = \sqrt{\frac{2}{a_z}}\int_0^{a_z} dz\, \sin\left(\frac{n_z\pi}{a_z}z\right) h(z). \tag{18}$$

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(b) For a particle in a central force potential the Hamiltonian

$$\hat{H} = \frac{\hat{\mathbf{p}}^2}{2\mu} + V(|\hat{\mathbf{r}}|), \tag{19}$$

conserves angular momentum. Thus, by the Heisenberg equations of motion for an operator, we have $[\hat{H},\hat{L}_x] = [\hat{H},\hat{L}_y] = [\hat{H},\hat{L}_z] = 0$. But we know that angular momentum operators defined along different directions do not commute. Namely, $[\hat{L}_x,\hat{L}_y] \neq 0$. Thus, given that $\hat{H}$ commutes with two operators which do not commute with each other, we can conclude that $\hat{H}$ has a degenerate spectrum of eigenvalues.

Choosing the **z** direction as the reference direction for our central force motion, this degenerate spectrum is the very same spectrum which defines the eigenstates of the $\hat{\mathbf{L}}^2$ and $\hat{L}_z$ operators. Specifically, the eigenstate $|\ell,m\rangle$ satisfying $\hat{\mathbf{L}}^2|\ell,m\rangle = \hbar^2\ell(\ell+1)|\ell,m\rangle$ and $\hat{L}_z|\ell,m\rangle = \hbar m|\ell,m\rangle$ are degenerate eigenstates of $\hat{H}$.

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(c) We can re-express Eq.(12) in a more transparent form by defining $m' = 2m$, $\omega_1 = \sqrt{k/m}$, $\omega_2 = \sqrt{3k/m}$. Doing so, gives us the new Hamiltonian

$$\hat{H} = \frac{\hat{p}_{q_1}^2}{2m'} + \frac{1}{2}m'\omega_1^2 q_1^2 + \frac{\hat{p}_{q_2}^2}{2m'} + \frac{1}{2}m'\omega_2^2 q_2^2 \equiv \hat{H}_{q_1} + \hat{H}_{q_2}, \tag{20}$$

where we defined the Hamiltonians containing q_1 and q_2 variables as $\hat{H}_{q_1}$ and $\hat{H}_{q_2}$, respectively. Having separated our Hamiltonian system, we can thus infer that the eigenvalues of the system are

$$\begin{aligned} E_{n_{q_1},n_{q_2}} &= \hbar\omega_1\left(n_{q_1} + \frac{1}{2}\right) + \hbar\omega_2\left(n_{q_2} + \frac{1}{2}\right) \\ &= \hbar\sqrt{\frac{k}{m}}\left[n_{q_1} + \frac{1}{2} + \sqrt{3}\left(n_{q_2} + \frac{1}{2}\right)\right]. \end{aligned} \tag{21}$$

Addendum: Contained in Eq.(21) is a hint of one of the problems in defining a quantum field theory. For a system of N coupled oscillators there are N independently oscillating modes. Quantizing such an N oscillator system, we would find N independent Hamiltonians, and thus a sum of N energy eigenvalues for each mode. In analogy to the first line of Eq.(21), the energy of the system would then be

$$E = \sum_{k=1}^{N} \hbar\omega_k\left(n_{q_k} + \frac{1}{2}\right). \tag{22}$$

The coupled oscillator system is of particular import to classical mechanics because taking $N \to \infty$ in the system produces a string which experiences longitudinal waves along its axis and is thus governed by a wave equation. However, if we were to try to study the quantum theory of this wave equation (which is really the quantum theory of the field for which the wave equation models the dynamics), then taking $N \to \infty$ in Eq.(22) presents some problems. Namely, considering the second term in Eq.(22) we find

$$\text{Ground state energy} = \lim_{N\to\infty}\sum_{k=1}^{N}\frac{\hbar\omega_k}{2} = \infty, \tag{23}$$

suggesting that a quantum mechanical continuous string has infinite energy[1] . This is one example of the infamous divergences which plague quantum field theory and which necessitated the development of renormalization theory to obtain sensible physical results.

(d) The ground state wave function for our coupled oscillator system is a product of the ground state wave functions for each normal mode of the system. Thus, this ground state wave function is

$$\begin{aligned} \psi_{0,0}(q_1, q_2) &= \left(\frac{m'\omega_1}{\pi\hbar}\right)^{1/4} e^{-m'\omega_1/2\hbar q_1^2}\left(\frac{m'\omega_2}{\pi\hbar}\right)^{1/4} e^{-m'\omega_2/2\hbar q_2^2} \\ &= \left(\frac{4m^2\omega_1\omega_2}{(\pi\hbar)^2}\right)^{1/4} \exp\left[-\frac{m}{4\hbar}\left(\omega_1(x_1+x_2)^2 + \omega_2(x_1-x_2)^2\right)\right], \end{aligned} \tag{24}$$

where we used $m' = 2m$ and $q_{1,2} = (x_1 \pm x_2)/2$ in the final line.

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[1]We know that ω_k doesn't go to zero in just the right way to obtain a finite result, because we label our modes so that higher-order modes have higher frequencies of oscillation.