2018 Explorer Competition

November 11, 2018

Guidelines

Student teams will have a total of **two weeks** to work on each section of the 2018 Explorer Competition. It consists of two separate sections: one section on **quantum mechanics** and another on **statistical mechanics**. Teams may complete both sections or choose to complete only one, as is specified in the grading section below. For successful completion of both sections, we recommend that teams set aside at least 20 hours of time. Please refer to the submission explanation below for details on both formatting and the submission process.

Scoring

Students are encouraged to work on as much of both sections of the exam as possible. However, teams **may choose to submit solutions for only one of the two sections** if they desire. The two **sections will be graded separately** and may not necessarily be worth the same amount of points. The award structure will be as follows:

1. Awards will be given to the four teams with the **highest score in each section**. There will be an award for first place, second place, and third place. One team can win an award for both sections, such as second place in quantum mechanics and third place in statistical mechanics. Teams are therefore encouraged to attempt solutions for both sections of the competition.

2. We will additionally award one **overall award to the highest scoring team** on the entire competition. A team which wins this overall award can still receive one of the top three awards for each individual section. The team that wins this overall award will most likely have completed both sections of the exam. It will be at the judges' discretion to choose the overall award for the best submission.

Collaboration Policy and External Resources

Students participating in the competition **may only correspond with members of their team**. Absolutely and unequivocally, **no other form of human correspondence is allowed**. This includes any form of correspondence with mentors, teachers, professors, and other students. Participating students are barred from posting content or asking questions related to the exam on the internet (except where specified below), and moreover, they are unequivocally barred from seeking the solution to any of the exams' parts from the internet or another resource. Students are allowed, however, to use the following resources for purposes of reference and computation:

- **Internet:** Teams may use the internet for purposes of reference with appropriate citation. Again, teams are in no way allowed to seek the solution to any of the exams' parts from the internet. For information about appropriate citation, see below.

- **Books and Other Literature:** Teams may use books or other literature, in print or online, for purposes of reference with appropriate citation. As with the use of the internet, teams are in no way allowed to seek the solution to any of the exams' parts from books or other literature.

- **Computational Software:** Teams may use computational software, e.g. Mathematica, Matlab, Python, whenever they deem it appropriate. Of course, teams must clearly indiciate that they have used such software. Additionally, the judges reserve to right to deduct points for the use of computational software where the solution may be obtained simply otherwise.

- **Piazza:** We have created a Piazza page for competitors to ask any clarifying questions about the exam as they work through it. Questions will be answered by the person who wrote the exam. Competitors should again not interact with each other. The sign up link is piazza.com/princeton_university_physics_competition/fall2018/phy101 . You will need to enter the access code putigers.

Citation

All student submissions that include outside material must include numbered citations. We do not prefer any style of citation in particular.

Submission

All submissions, regardless of formatting, **should include a cover page listing the title of the work, the date, and signatures of all team participants**. The work must be submitted as a single **PDF document** with the ".pdf." extension. All other formatting decisions are delegated to the teams themselves. No one style is favored over another. That being said, we recommend that teams use a typesetting language (e.g. LaTeX) or a word-processing program (e.g. Microsoft Word, Pages). **Handwritten solutions are allowed**, but we reserve the right **to refuse grading of any portion of a team's submission in the case that the writing or solution is illegible.**

Teams must submit their solutions to the quantum mechanics portion of the Explorer Competition by **e-mailing directors@physicsu.org by 11:59 am (noon) Eastern Time (UTC-5) on Sunday, November 25, 2018**. Teams will not be able to submit their solutions to this section of the Explorer Competition at any later time. Any team member may send the submission. **The title of the submission e-mail should be formatted as "SUBMISSION - Team Name"**. All teams may make multiple submissions. However, we will **only grade the most recent submission submitted before the deadline**. Teams will receive confirmation once their submission has been received within at most two days. **In the case of extraordinary circumstances, please contact us as soon as possible.**

Sponsors

Quantum Mechanics Section

To get a good sense of what's going on in quantum mechanics, or for that matter to even try to understand what exactly quantum mechanics is, problem solving is our best tool. After all, physics is no spectator sport, and though we could dwell at length on the more philosophical aspects of the subject, it is best to hold off on asking "Why?" before we have even seen the obligatory "What?" and "How?". Indeed, though quantum mechanics will seem quite unnatural at first, it is our hope that as your study of physics progresses, you will see it more and more as *the* theory that underpins the workings of Universe. Let's take the first step.

Contents

Learning Goals

This exam is meant more as an exercise in learning than as an exercise in solving problems or external research. The goal of this competition is for the readers, who have not necessarily seen any quantum mechanics in the course of their education so far, to walk away with a set of examples and ideas that will be helpful in shaping their thinking long into the future.

Topic Format and Grading

This document consists of two sections of expository material with exercises and questions interspersed along with a final section that asks for students to conduct a small independent investigation on a topic of their choosing. Exercises will typically ask students to mathematically derive or demonstrate a result useful to the discussion. Questions will ask students to, in their own words, interpret stated results. We are looking to see how well you understand the subject, so to receive full credit, all work shown must be complete and properly justified.

Expected Amount of Work

Do not expect to understand the concepts in this document after only one read through; these concepts take time to absorb. While it may feel like you are not getting much accomplished as you try to understand the reading, persevere. It may be necessary to read some passages several times in a row before understanding them completely. Because there are not too many questions in this document, you should have time to complete the readings. We have made every attempt to be rigorous in our presentation, but simplifications have been made when appropriate. Students are welcome to investigate the subject in more detail outside of this document.

1 Wave Functions, Observables, and the Schrödinger Equation

Here, we introduce the fundamental notion of the wave function, the time evolution of which is determined by Schrödinger's equation. Observables, which in everyday life we encounter in such forms as momentum, energy, and position, will turn out to be nothing more than operators on wave functions.

1.1 The Wave Function

Whereas in classical mechanics, the state of a particle, that is to say all information about its current and subsequent motion, is determined entirely by its position $x(t)$ and momentum $v(t)$ as functions of time, in quantum mechanics, it is *taken as a postulate* that the state of the particle is determined entirely by an abstract ket vector $|\Psi(t)\rangle$ belonging to an infinite-dimensional Hilbert space. For present purposes, it is sufficient to think of the Hilbert space as a vector space containing square-integrable complex-valued functions $\Psi(x,t)$, $\Phi(x,t)$ called wave functions with the inner product

$$\langle\phi|\psi\rangle = \int_{-\infty}^{\infty} \Phi(x,t)^* \Psi(x,t) dx \tag{1}$$

where $\Phi(x,t)^*$ represents the complex conjugate of $\Phi(x,t)$. Operating with the assumption that Born's statistical interpretation of the wave function, that $|\Psi(x,t)|^2 dx$ represents the probability of finding the particle between x and $x + dx$ at a time t, is valid, we impose the **normalization condition**

$$\int_{-\infty}^{\infty} |\Psi(x,t)|^2 dx = 1 \tag{2}$$

for wave-functions corresponding to physical realizable states.

Question: To check your own understanding, provide an interpretation of condition (1).

Of course, we are free to make a measurement of the particle's position at some time t, and as we expect, doing so will yield a perfectly definite answer. Importantly, however, and in contrast with classical mechanics, we are unable to say anything at all about where the particle was just before the measurement was made. Indeed, provided one accepts the validity of **Born's statistical interpretation** of the wave function, which for the record has strong experimental backing, the particle never has a well-defined position to begin with; its "position" being nothing more than a probability distribution that evolves in time according to the Schrödinger equation, which will be introduced shortly. One could argue that the particle does in fact always have some definite position and it is only our ignorance that forces us to fall back upon a probabilistic interpretation, but such *hidden variables* theories are heavily constrained by Bell's theorem, a fascinating topic that we will not develop further here.

Equipped with this probabilistic interpretation of the wave function, it readily follows that the **expectation value** of the particle's position x (in 1D), is given by

$$\langle x\rangle = \int_{-\infty}^{\infty} x|\Psi(x,t)|^2 dx. \tag{3}$$

Exercise: Suppose that at a time $t = 0$, a particle's state is described by the wave function $\Psi(x,0) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-m\omega x^2/2\hbar}$. Find $\langle x\rangle$.

Similar calculations follow for such things as $\langle x^2\rangle$ or $\langle x^4\rangle$, but at this point, we need to introduce more material if we are to talk about anything interesting.

1.2 Schrödinger's Equation

To that end, we now introduce the famous, or perhaps infamous, **Schrödinger equation**:

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V(x)\Psi. \tag{4}$$

A priori, there is no clear reason why this equation must hold, seeing as though it somehow relates the time derivative of some strange thing called a wave function to its spatial derivatives and the potential energy $V(x)$ via the introduction of the imaginary unit i and the **reduced Planck constant** $\hbar = 1.05 \times 10^{-34} J \cdot s$. If you are interested, you can observe that Schrödinger's equation has the form of a wave equation wherein time t has been taken to imaginary time $i\tau$ via a *Wick rotation*, but it is better for now to simply think of the equation's validity as another postulate of theory that has been back by a century's worth of experimentation.

Through the presence of the time derivative on the left side of (4), we are now able to add the momentum p, and subsequently the kinetic energy $\frac{p^2}{2m}$ to our repertoire of observable quantities. Though a formal proof will have to wait until Section 2, we now present the assertion

$$\langle p \rangle = m\frac{d\langle x \rangle}{dt}. \tag{5}$$

Question: Provide a comparison of (5) with classical mechanics, offering an explanation of how the presence of expectation values, that is to say averages, in (5) is rectifiable with day-to-day experience.

Earlier, we claimed that observables could be represented as operators on wave functions, so it is now worth showing it.

Exercise: Using (5) and the Schrödinger equation, derive both sides of (5) with respect to time to find $\langle p \rangle$, deducing p in terms of a derivative operator, $\hbar$, and i.

Exercise: Based on the result of the previous exercise, and rewriting (3) as $\langle x \rangle = \int_{-\infty}^{\infty} \Psi(x,t)^* x \Psi(x,t) dx$, deduce a similar expression for the expectation value of any dynamical variable $F(x,p)$. Can you express this in terms of the inner product (1)?

Exercise: The Schrödinger equation (4) describes how the wave function evolves in time. In (2), I claimed that physical realizable states must satisfy a certain normalization condition consistent with the Born interpretation of the wave function. If a wave function is normalized at some time t, in the sense that it satisfies (2), it ought to remain normalized at all subsequent times. Prove it.

2 Mathematical Formalism and Quantum Quirks

Here, we develop mathematical formalism that is necessary for a full understanding of the quantum theory. In the process, a picture of physics will emerge that differs radically from common understanding and observation.

2.1 Solving Schrödinger's Equation

It is wonderful to have the result that the wave function $\Psi(x,t)$ must satisfy the second order linear differential equation

$$i\hbar\frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + V(x)\Psi, \tag{6}$$

but how do we go about solving this equation for $\Psi(x,t)$? Certainly, we are always capable of doing so in principle, but in practice, our progress will depend heavily on the exact form of the potential energy term $V(x)$. Fortunately, many situations can be modeled with potentials that allow us to solve for $\Psi(x,t)$ without too much trouble, and we will turn shortly to doing exactly that over the course of a few examples.

As a first step towards solving the Schrödinger equation, it is useful to learn a common trick in solving partial different equations called the technique of **separation of variables**. In this procedure, we *assume* that a solution $\Psi(x,t)$ of (6) may be written as

$$\Psi(x,t) = \psi(x)\phi(t), \tag{7}$$

the product of two separate functions of x and t.

Exercise: Plug the expression (7) into (6) to show that $\psi(x)$ and $\phi(t)$ must respectively satisfy the ordinary differential equations

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi = E\psi \tag{8}$$

and

$$\frac{d\phi}{dt} = -\frac{iE}{\hbar}\phi \tag{9}$$

where E is an arbitrary constant that has been suggestively labeled.

Equation (9) can be directly integrated to yield $\phi(t) = \exp[\frac{-iEt}{\hbar}]$ (we'll add the constant of integration back in later), and equation (8) is known simply as the **time-independent Schrödinger equation**. The whole business of solving the Schrödinger equation, then, really boils down to solving the time-independent Schrödinger equation for some given potential energy $V(x)$. Once we have found $\psi(x)$ for some value E, we may simply write $\Psi(x,t) = \psi(x)\exp[\frac{-iEt}{\hbar}]$. Noting that any linear combination of solutions $\Psi_n(x,t)$ to (6) is itelf a solution to (6), we have most generally

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \psi_n(x) e^{-iE_n t/\hbar} \tag{10}$$

for constants c_n we will soon see how to determine.

Up to this point, we have not done much besides determining the form that a solution to (6) must take from a purely mathematical sense; it is about time we introduced some physics.

2.2 The Hamiltonian and Hermitian Operators

In the language of operators acting on elements of a Hilbert space, (8) can be cast in an extraordinarily suggestive and familiar form to those acquainted with basic linear algebra. As discussed in Section 1, observable quantities, for instance linear momentum p, position x, or some function thereof, can be expressed as operators equipped to act on complex-valued wave functions. Assuming the completion of Exercise 2 from that section, we may write

$$\hat{p} = \frac{\hbar}{i}\frac{\partial}{\partial x} \tag{11}$$

where the hat is written over p to emphasize that it is to be treated as an operator, that is as a rule that assigns one element of our Hilbert space to another. Similarly taking position as the operator $\hat{x}$, we have the potential energy operator $\hat{V}(\hat{x})$, allowing us to recast (8) in the form

$$\hat{H}\psi = E\psi \tag{12}$$

where

$$\hat{H} \equiv \frac{\hat{p}^2}{2m}\frac{\partial}{\partial x} + \hat{V}(\hat{x}) \tag{13}$$

is the **Hamiltonian operator**.

Equation (12) is nothing more than an eigenvalue problem whence we see that an energy E is nothing more than an eigenvalue of the Hamiltonian $\hat{H}$. In contrast with the linear algebra of finite matrices, there exist situations wherein E can take on a continuum of possible values in addition to those cases where E belongs to some discrete set, but the startling point remains that any old value of E does not satisfy (12). The *only* permissible values for the energy E are those that are eigenvalues of the Hamiltonian $\hat{H}$.

Delving temporarily into a little more linear algebra, say that an operator $\hat{O}$ is **hermitian** if

$$\hat{O} = \hat{O}^\dagger, \text{ i.e. } \langle\phi|\hat{O}\psi\rangle = \langle\hat{O}\phi|\psi\rangle, \tag{14}$$

for all ϕ, ψ in our Hilbert space where $\hat{O}^\dagger$ represents the conjugate transpose of $\hat{O}$.

Exercise: Prove that $\hat{H}, \hat{x},$ and $\hat{p}$ are hermitian operators.

Exercise: Prove that hermitian operators have real eigenvalues.

Exercise: Prove that eigenfunctions ϕ, ψ corresponding to distinct eigenvalues of a hermitian operator are orthogonal in the sense that $\langle\phi|\psi\rangle = 0$.

As can be surmised from the result of the exercise at the bottom of page 6, it is *taken as a postulate* of the quantum theory that *any* observable quantity can be represented as a hermitian operator acting on the given

Hilbert space of wave functions. Moreover, given the further result that the orthonormal eigenfunctions ψ_n of a hermitian operator $\hat{O}$ form a complete set in the sense that any wave function ψ may be expressed as a linear combination $\psi = \sum_n c_n \psi_n$, we may write

$$c_n = \langle \psi_n(x) | \psi(x,0) \rangle \tag{15}$$

for a given initial state $\psi(x,0)$ that has been normalized per (2). (We assume here that the eigenvalues have a discrete spectrum. The natural generalization for eigenvalues with a continuous spectrum is not particularly enlightening or relevant.)

Question: Provide an interpretation of (15) in the language of linear algebra.

Exercise: Verify the validity of writing (15), a result known as Fourier's trick.

Having determined the c_n that appear in (10), we recall the imposition of (2) to arrive at the condition

$$\sum_n |c_n|^2 = 1. \tag{16}$$

Exercise: Show that (16) holds.

We now are in a position to truly drive home the statistical nature of quantum mechanics.

Given some normalized initial state $\psi(x,0)$, we determine $\Psi(x,t)$ for all future times $t > 0$ by writing $\psi(x,0)$ as a linear combination $\psi(x,0) = \sum_n c_n \psi_n$ of normalized eigenfunctions ψ_n of the Hamiltonian operator $\hat{H}$ where the c_n are given by (15) and then tacking on the time-dependent terms $e^{-iE_n t/h}$ to reach (10).

Now, if we were to take a measurement at time $t = 0$ of a particle's energy in a state $\psi(x,0) = \sum_n c_n \psi_n$, it is apparent that the only possible outcomes would be the eigenvalues E_n of the Hamiltonian with respective probabilities

$$P_n = |c_n|^2 = |\langle \psi_n(x) | \psi(x,0) \rangle|^2 \text{ such that } \langle E \rangle = \sum_n P_n E_n, \tag{17}$$

which is nothing more than the expression for an average we are all familiar with.

More generally, for any arbitrary hermitian operator $\hat{O}$ with normalized eigenfunctions $\psi_n(x)$ and associated eigenvalues λ_n, we run through this same procedure. If we were to take a measurement of O at some time t on a particle in the normalized state $\Psi(x,t)$, the only possible outcomes would be the eigenvalues λ_n of $\hat{O}$ with respective probabilities

$$P_n(t) = |c_n(t)|^2 = |\langle \psi_n(x) | \Psi(x,t) \rangle|^2 \text{ such that } \langle O \rangle = \sum_n P_n \lambda_n. \tag{18}$$

From the above, it is tempting to say that a particle in a state $\psi(x,0) = \sum_n c_n \psi_n$ is in the state ψ_i with probability $|c_i|^2$, the state ψ_j with probability $|c_j|^2$, and so on, but this is interpretation is simply incorrect. The particle *is in one definite state*, $\psi(x,0)$, that is the superposition of other states with some weight determined by the c_n. Upon performing a measurement, which, despite the complex-valued nature of the wave function, is guaranteed to yield a real number due to the fact that hermitian operators have real eigenvalues, there is a $|c_i|^2$ chance the result is λ_i, in which case we conclude that the particle *is in the state* ψ_i *after* the measurement. *Before* the measurement, the particle *is in the state* $\psi(x,0)$ certainly.

Exercise: Suppose a particle is found in a state $\psi(x,0) = N(\frac{2}{i}\psi_1 + e^{\frac{\pi i}{2}}\psi_2)$ where ψ_1, ψ_2 are normalized eigenfunctions of the Hamiltonian with respective eigenenergies E_1, E_2. Determine N. Additionally, find $\langle H \rangle$ at this time $t = 0$.

Exercise: Solve the eigenvalue problem (12) in the case where $V(x) = \begin{cases} 0, & 0 < x < L \\ \infty, & \text{elsewhere} \end{cases}$. What are the normalized eigenfunctions and associated eigenenergies?

Exercise: Subject to the above potential, a particle is known to have the wave function $\Psi(x,0) = \aleph \sin^3(\pi x/L)$ for $0 \le x \le L$. Normalize $\Psi(x,0)$, find $\Psi(x,t)$, and find $\langle x \rangle$ and $\langle E \rangle$ for all times t.

Exercise and Question: Solve the Schrödinger equation (6) for a free particle, i.e. in the case where $V(x)$=0 for all x. You will find that the solution is not normalizable in the sense of equation (2) and thus cannot correspond to a physical state. There is nothing wrong with having a free particle, so something must have gone wrong with one of your initial assumptions about the particle and its "energy." Identify the problem.

2.3 The Harmonic Oscillator

The motion of the classical harmonic oscillator is determined by the solution to the equation

$$\frac{d^2x}{dt^2} + \frac{k}{m}x = 0 \tag{19}$$

for $x(t)$ where the potential energy $V(x) = \frac{1}{2}kx^2$. In quantum mechanics, we may treat the same potential in terms of the angular frequency $\omega = \sqrt{\frac{k}{m}}$, writing

$$V(x) = \frac{1}{2}m\omega^2x^2 \tag{20}$$

such that the time-independent Schrödinger equation takes the form

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2}m\omega^2x^2\psi = E\psi. \tag{21}$$

If you have the patience, you are welcome to try to solve (21) for ψ by brute force, which involves expressing ψ in terms of an infinite power series, substituting this series into (21), and then solving an ugly recurrence relation that determines the coefficients of the power series expansion and ultimately ψ. However, physicists are significantly more clever than engineers, and we will solve (21) by introducing operators known as the **raising and lowering operators**, or in the context of quantum field theory, **creation and annihilation operators**. Respectively, such operators are defined by

$$a_{\pm} \equiv \frac{1}{\sqrt{2hm\omega}}(\mp ip + m\omega x) \tag{22}$$

where we have dropped the hat over the operators p, x since we are doing quantum mechanics. As ugly as this expression seems now, it will make our lives significantly easier moving forward. Along the way, we will additionally see the seemingly innocent but immensely important concept of a commutator for the first time. To get to that point, we simply compute the product

$$a_-a_+ = \frac{1}{2\hbar m\omega}\left[p^2 + (m\omega x)^2 - im\omega(xp - px)\right]. \tag{23}$$

Defining the **commutator** of two operators $\hat{O}_1, \hat{O}_2$ by the expression

$$[\hat{O}_1, \hat{O}_2] \equiv \hat{O}_1\hat{O}_2 - \hat{O}_2\hat{O}_1. \tag{24}$$

Clearly, if the two operators commute, their commutator is simply 0, so the commutator may be interpreted as a measure of the extent to which two operators commute. In quantum mechanics, we know that observable quantities are represented by hermitian operators, and it may be thus deduced that the *commutator of two such hermitian operators is an indication of whether or not these two quantities may be measured simultaneously.* We will return to this point later.

Exercise: Verify that $[x, p] = i\hbar$.

With this result in hand, we may solve (23) for the Hamiltonian H, writing

$$H = \hbar\omega\left(a_-a_+ - \frac{1}{2}\right). \tag{25}$$

This is useful to know in and of itself, but we can extract another result from it.

Exercise: Show that we may write $H = \hbar\omega\left(a_+a_- + \frac{1}{2}\right)$, i.e compute the commutator $[a_-, a_+]$.

With these two results in hand, we may now express the time-independent Schrödinger equation in the form

$$\hbar\omega\left(a_{\pm}a_{\mp} \pm \frac{1}{2}\right)\psi = E\psi. \tag{26}$$

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If ψ is a solution to (26) with associated eigenenergy E, it can be confirmed by a straightforward computation that

$$H(a_{+}\psi) = (E + \hbar\omega)(a_{+}\psi), \tag{27}$$

i.e. the raising operator a_{+} takes a state with energy level E and "raises" it to another state with energy level $E + \hbar\omega$. (*In quantum field theory, you can also think of an electromagnetic field as set of harmonic oscillators such that the raising operator corresponds to the creation a photon with energy $\hbar\omega$, the smallest possible excitation of the field*).

Exercise: Verify (27).

A similar statement can be said about the lowering operator a_{-}, which takes a state with energy level E and "lowers" it to another state with energy level $E - \hbar\omega$. If we denote the ground state, that is to say the state with the lowest energy, by ψ_0, it follows by definition that we must have

$$a_{-}\psi_0 = \frac{1}{\sqrt{2\hbar m\omega}}\left(\hbar\frac{d}{dx} + m\omega x\right)\psi_0 = 0, \tag{28}$$

which is readily solved to yield, after normalizing,

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2}. \tag{29}$$

From the expression $H = \hbar\omega\left(a_{+}a_{-} + \frac{1}{2}\right)$ and the fact that $a_{-}\psi_0 = 0$, it readily follows that the energy of the ground state E_0 satisfies

$$E_0 = \frac{1}{2}\hbar\omega \neq 0. \tag{30}$$

Question: How does (30) compare to what occurs in classical mechanics?

To build up all the possible states of the quantum harmonic oscillator, all we need to do is act on ψ_0 with the raising operator a_{+} and normalize the resulting wave function. From (27), we have the result

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega, \tag{31}$$

and after the appropriate normalization, which of course you will be asked to prove, we have

$$\psi_n = \frac{1}{\sqrt{n!}}\left(a_{+}\right)^n\psi_0, \tag{32}$$

completing our goal to determine the eigenenergies and eigenfunctions of the quantum harmonic oscillator.

Exercise: Prove (32).

Exercise: Find $\langle x^4 \rangle$ of a particle in the state ψ_{75}. As a hint, find $\langle x^4 \rangle$ of a particle in the general state ψ_n first.

Exercise: Calculate the expectation values of the kinetic and potential energy of a particle in the state ψ_n. Compare the result to the classical virial theorem.

2.4 The Commutator

Although at first glance commutators may seem like nothing more than mathematical constructions that have no bearing on the physical world, their introduction into our present discussion will soon be seen to speak to the observed spookiness of quantum mechanics.

In (5), I made the assertion that $\langle p\rangle = m\frac{d\langle x\rangle}{dt}$ without proof. Having built up a sizable tool box of problem solving skills, we are now in a position to fill that void. Given that the wave function evolves in time, it is perfectly reasonable to ask how the expectation value $\langle O\rangle$ of a given operator $\hat{O}$ evolves in time. Applying the definition presented in (3), we have

$$\frac{d}{dt}\langle Q\rangle = \left\langle \frac{\partial\Psi}{\partial t}|\hat{O}\Psi\right\rangle + \langle\Psi|\frac{\partial\hat{O}}{\partial t}\Psi\rangle + \langle\Psi|\hat{O}\frac{\partial\Psi}{\partial t}\rangle \tag{33}$$

from the product rule. The Schrödinger equation (6) gives $\frac{\partial\Psi}{\partial t}$ explicitly in terms of the Hamiltonian $\hat{H}$, so again applying (3) to rewrite the last term, we have

$$\frac{d}{dt}\langle O\rangle = -\frac{1}{i\hbar}\langle\hat{H}\Psi|\hat{O}\Psi\rangle + \frac{1}{i\hbar}\langle\Psi|\hat{O}\hat{H}\Psi\rangle + \left\langle\frac{\partial\hat{O}}{\partial t}\right\rangle = -\frac{1}{i\hbar}\langle\Psi|\hat{H}\hat{O}\Psi\rangle + \frac{1}{i\hbar}\langle\Psi|\hat{O}\hat{H}\Psi\rangle + \left\langle\frac{\partial\hat{O}}{\partial t}\right\rangle. \tag{34}$$

The first two terms can be combined using the definition of the commutator $[\hat{H},\hat{O}] = \hat{H}\hat{O} - \hat{O}\hat{H}$, leading to the result

$$\frac{d}{dt}\langle O\rangle = \frac{i}{\hbar}\langle[\hat{H},\hat{O}]\rangle + \left\langle\frac{\partial\hat{O}}{\partial t}\right\rangle. \tag{35}$$

Question: Why is the second equality in (34) justified?

Exercise: Take $\hat{O} = x$ and show that one recovers the assertion of (5). Additionally, take $\hat{O} = p$ and show that one recovers Newton's Second Law in the form $\frac{d}{dt}\langle p\rangle = -\langle V'(x)\rangle$. This result, known as **Ehrenfest's theorem**, says that the expectation values $\langle x\rangle, \langle p\rangle$ obey classical dynamics, though (35) is even more general.

Presumably, the well-informed student will be a familiar with a result known as the **Heisenberg uncertainty principle**, which maintains

$$\sigma_x\sigma_p \geq \frac{\hbar}{2} \tag{36}$$

where

$$\sigma_O^2 = \left\langle(\hat{O} - \langle O\rangle)^2\right\rangle \tag{37}$$

is the variance of the observable $\hat{O}$.

Exercise: Prove the **general uncertainty principle**

$$\sigma_{O_1}^2\sigma_{O_2}^2 \geq \left(\frac{1}{2i}\langle[\hat{O}_1,\hat{O}_2]\rangle\right)^2, \tag{38}$$

taking care to justify all steps clearly. As a hint, first write $\sigma_{O_1}^2 = \langle(\hat{O} - \langle O\rangle)\Psi|(\hat{O} - \langle O\rangle)\Psi\rangle$, justifying why this follows from (37). Do the same for $\sigma_{O_2}^2$. Write the product of the two, apply the Cauchy-Schwarz inequality, observe $|z|^2 \geq [\mathrm{Im}(z)]^2 = \left[\frac{1}{2i}(z - z^*)\right]^2$ for any complex number z by the triangle inequality, and apply the definition of the commutator $[\hat{O}_1,\hat{O}_2]$.

Stating what is now obvious, we take $\hat{O}_1 = x, \hat{O}_2 = p$ to conclude $\sigma_x^2\sigma_p^2 \geq \left(\frac{\hbar}{2}\right)^2$, having used the fact $[x,p] = i\hbar$. Taking the square root of both sides, we have, beautifully,

$$\sigma_x\sigma_p \geq \frac{\hbar}{2}. \tag{39}$$

In words, (39) tells us that it simply does not make sense to speak of a particle as having a well-defined position and a well-defined momentum simultaneously. To draw a rough analogy, consider this: If we take a photograph of a pitcher throwing a baseball at 90 mph, we have a clear image of the ball's position but no clue how fast it is moving. Likewise, we can sit back and watch the ball speed through the air, but we then have no clue where it is exactly. Of course, the presence of the commutator in (38) means that there is a similar uncertainty principle between any two observables that do not commute, and indeed, some students may be familiar with the **energy-time uncertainty principle**

$$\sigma_E\sigma_t \geq \frac{\hbar}{2} \tag{40}$$

that underpins quantum tunnelling and Gamow's theory of alpha decay. Importantly, we made no additional assumptions in deriving the uncertainty principle beyond the postulates of the quantum theory previously discussed. Uncertainty is a natural consequence of a probabilistic theory that, as quirky as it is, has held up in the face of a century's worth of experimental tests and philosophical challenges from the likes of Einstein himself.

3 Experimental Foundations

To reward your patience in sticking with us to the end of this document, we invite you to explore the topic of quantum mechanics according to your own desires. We've spoken much about the experimental basis that supports an objectively outlandish theory on the surface, so it is natural that we include some discussion of these experiments in this competition. To that end, we ask you now to research an experiment conducted to support the validity of the quantum theory and write a short report that clearly elucidates its motivation and goals, accurately depicts and describes the experimental setup, and comments upon the results of the experiment in regard to how exactly they support the validity of the quantum theory. Grading will be based on the clarity and accuracy of the report. Keep in mind, we simply want to see that you understand the subject well.