1

The Harmonic Oscillator: Classical versus Quantum

> It seems to me that there are deep philosophical lessons to be learned in the way in which the practicing theoretical physicist thinks about the foundations of the subject, i.e., the manner in which he approaches the problems, the general criteria he brings to bear on what is a reasonable solution. So, the important thing then is to display the general world view, the world picture that the theoretical physicist has.
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> This is particularly significant in connection with the philosophical implications of quantum physics, because quantum physics or quantum mechanics – by which I think we mean finally the rational mode of understanding of microscopic or atomic phenomena – has perhaps had the greatest impact of any of the developments of physics upon the mode of thinking or the world picture of the physicist and thereby, indirectly, of the general citizen.
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> Julian Schwinger
> in the Prologue to *Quantum Mechanics: Symbolism of Atomic Measurement*, 2001

"Quantum mechanics – by which I think we mean finally the rational mode of understanding of microscopic or atomic phenomena," this, in a nutshell, is the topic of this book. We seek to present a calculus that encodes this rational understanding. This is not an easy task. It is in no way straightforward, and a cursory reading of the history of the development of the subject illustrates nothing if not how very difficult it was to discover the right calculus. It does not help that the right calculus is written in the language of some rather esoteric and sophisticated mathematics, and necessarily so, it seems, and that there are competing ways to interpret the resulting abstract formalism. Rather than repeat the history of the founding of the subject, which covers a period from roughly 1900 until the mid-1930s and involves the work of scores of physicists and even a few mathematicians, which involves many experiments and observations as well as many false starts and stops, we present the calculus as a *fait accompli* and then back track to fill in our understanding. The reader should understand at the outset, though, that there is a wealth of experimental justification for this calculus.

In this opening lecture, we present a contrast between classical mechanics and quantum mechanics through the lens of a single example. This example illustrates in stark relief the differences between the classical view of the world as articulated by Newton's laws and the modern view as articulated by the rules of quantum mechanics. The harmonic oscillator is the quintessential physical system and, as such, its analysis, whether classical or quantum, serves as an archetype of the discipline. In this lecture we review the classical treatment of the harmonic oscillator and outline the quantum treatment. The quantum treatment will seem ad hoc and unmotivated and should elicit some unease and, perhaps, even perplexity. The reader will see that the utter simplicity of both the methodology and results of the classical treatment stands in sharp contrast to the sophistication of the quantum treatment. Indeed, whereas both the application and meaning of the classical treatment are apparent from the mathematics itself, the methods and results of the quantum treatment cry out for explanation and interpretation. We present a standard interpretation of the quantum treatment here, but the reader should find our explanations, though internally coherent, nonetheless unmotivated. This interpretation was developed over a period of years concurrent with the development of the machinery of quantum mechanics itself, but the reader is warned that other interpretations are possible.

At the end of this lecture, we delve into some foundational issues surrounding the interpretation of quantum mechanics. This is something of a departure from our practice throughout the remainder of the book, where the development of the formalism takes precedence over philosophical issues.[1] Nonetheless, we want the reader to be aware at the outset that the quantum mechanical world view is a drastic departure from that of the classical and leaves open many deep philosophical issues.

Welcome to the world of the quantum!

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[1] The exception is Lecture 22, where a precise discussion of nonlocality in real systems is presented, along with its accommodation by the quantum formalism and its implications for hidden variables theories.

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More Information

1.1 The Classical Harmonic Oscillator

Consider a particle moving in a one-dimensional quadratic potential well $V(x) = \frac{1}{2}kx^2$, where the **spring constant** k is positive and x represents position along a line. The force experienced by the particle is $F = -\nabla V = -kx$, and serves to restore the particle to its equilibrium position $x = 0$. The force on the particle diminishes as it moves toward equilibrium but, since the particle has positive speed as it reaches the equilibrium point, it overshoots past equilibrium and begins to feel the restorative force again. Eventually the force slows the particle to rest at some maximum displacement from equilibrium, at which point the particle begins its journey back toward the equilibrium position, overshooting again, and reaching a maximum displacement opposite to that of its previous maximum displacement. And so it goes ad infinitum. This is the classical harmonic oscillator, the quintessential physical system of classical mechanics.

The newtonian analysis of the harmonic oscillator is straightforward. From Newton's second law, the equation of motion of the harmonic oscillator is

$$m\ddot{x} + kx = 0,$$

where m is the positive mass of the particle and $x = x(t)$ is position at time t. Here we are using Newton's notation, where the derivative of a function of the time variable is indicated by a dot above the function. The solution to the equation of motion, equally transparent, is

$$x(t) = a\cos\omega t + b\sin\omega t,$$

where the **natural** or **characteristic frequency** is

$$\omega = \sqrt{\frac{k}{m}}$$

and the initial conditions are $x(0) = a$ and $\dot{x}(0) = \omega b$. For simplicity, take $x(0) = X > 0$ and $\dot{x}(0) = 0$, so that $x(t) = X\cos\omega t$. Of course X is the magnitude of the maximum displacement. The kinetic energy of the system is $K = \frac{1}{2}m\dot{x}^2 = \frac{1}{2}m\omega^2X^2\sin^2\omega t$ and the potential energy is $V = \frac{1}{2}kx^2 = \frac{1}{2}kX^2\cos^2\omega t$, so that, using $k = m\omega^2$, the total energy $E = K + V$ is a constant of the motion:

$$E = \frac{1}{2}kX^2 = \frac{1}{2}m\omega^2X^2.$$

The picture presented by classical mechanics is clear and compelling.

The equation of motion involves the particle position $x = x(t)$ as a function of time and its solution provides a complete description of the location of the particle at all times. The motion, described precisely by sinusoidal terms, is periodic, oscillating between extremes $-X$ and X with a natural frequency determined by the mass of the particle and the spring constant, a characteristic of the potential well. The total energy is a constant of the motion with well-defined contributions at each instant in time, the kinetic energy from the particle's speed and the potential energy from the particle's position in the potential well. We now examine how the quantum mechanical rules treat the harmonic oscillator.

1.2 The Quantum Mechanical Treatment

The quantum mechanical analysis of the harmonic oscillator begins with the classical Hamiltonian $H(x,p)$ for the system, the total energy written in terms of the position x and its conjugate momentum $p = m\dot{x}$. The momentum conjugate to the position variable x is by definition $p = \partial L/\partial \dot{x}$, where the Lagrangian is $L(x,\dot{x}) = K - V = \frac{1}{2}m\dot{x}^2 - \frac{1}{2}kx^2$. The Lagrangian and Hamiltonian formulations of classical mechanics are reviewed in Lectures 6 and 7. The energy E of the system is given in Hamiltonian form by

$$H(x,p) = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 = E.$$

We now perform a surprising procedure that will yield the quantum mechanical equation of motion for the harmonic oscillator. To **quantize** the Hamiltonian equation, we replace the three dynamical variables, or **observables** – the position x, the momentum p, and the energy E – by differential operators according to the following prescription:

$$\begin{aligned} x &\rightsquigarrow \mathsf{X} \\ p &\rightsquigarrow \mathsf{P} = -\mathbf{i}\hbar\nabla = -\mathbf{i}\hbar\frac{\partial}{\partial x} \\ E &\rightsquigarrow \mathsf{E} = \mathbf{i}\hbar\frac{\partial}{\partial t}. \end{aligned}$$

Here X is the operator that multiplies by x, i.e., for a function f, $\mathsf{X}f(x) = xf(x)$ and $\hbar$ is the **reduced Planck constant**, the proportionality constant relating the energy of a photon to its angular frequency. These operators act linearly on a suitable class of functions. Upon replacing x,

p, and E in the Hamiltonian equation by these operators, we obtain the operator equation

$$H(\mathsf{X},\mathsf{P}) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2\mathsf{X}^2 = \mathbf{i}\hbar\frac{\partial}{\partial t} = \mathsf{E},$$

which operates on a suitable function $\Psi(x,t)$ to give the quantum mechanical equation of motion, the **Schrödinger equation**, for the harmonic oscillator:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + \frac{1}{2}m\omega^2x^2\Psi = \mathbf{i}\hbar\frac{\partial\Psi}{\partial t}.$$

At this point the novice might ask why we are transforming a classical Hamiltonian equation into an operator equation that then produces the Schrödinger equation. What does this have to do with the simple system of a particle in a quadratic potential well? It turns out to be quite a lot, but the way in which the Schrödinger equation encodes information about the physical oscillator is quite sophisticated. Some textbooks give plausibility arguments to “derive” the Schrödinger equation that, ultimately, in our opinion, offer little insight or comfort. Others proceed along the historical path, easing us into the quantum world view gently, and keeping the uncomfortable “why” questions at bay by recording the struggle to understand experimental results that, ultimately, led to the creation of the machinery. Still others report such results and then show how simple matrix manipulations can be used to predict the observed outcomes. This then is developed and generalized rapidly to arrive at the Schrödinger equation and the rest of the machinery. The real answer as to why we are performing this procedure is **that it works to give accurate statistical predictions and does so in the face of the failure of classical mechanics**. It is our view that there is no way to make quantum mechanics palatable to minds informed at every level of experience by the classical world. It is something we must get used to, and we must get used to it because it works. Our tactic then is to present the formalism for this simple physical system in this first lecture, without candy-coating, and then to jump into the formal mathematical structure immediately in the next lecture. So, read on and see this quantum mechanical calculation to its end, and then we will ask what happened and try to understand how to become comfortable with what we have done.

To solve the Schrödinger equation we separate variables by writing

$\Psi(x,t) = \psi(x)f(t)$, which gives the eigenvalue equations

$$\mathbf{i}\hbar\dot{f}(t) = Ef(t),$$
$$-\frac{\hbar^2}{2m}\psi''(x) + \frac{1}{2}m\omega^2x^2\psi(x) = E\psi(x),$$

where E is an unknown constant. Our use of the symbol E for the constant arising from the separation of variables anticipates its eventual interpretation as something to do with the energy of the system. The first equation has the solution

$$f(t) = C\exp\left(-\mathbf{i}\frac{E}{\hbar}t\right)$$

so that

$$\Psi(x,t) = Ce^{-\mathbf{i}Et/\hbar}\psi(x).$$

Here C may be taken to be an arbitrary complex constant, and the unimodular term $e^{-\mathbf{i}Et/\hbar}$ is called a **phase factor** of Ψ.

We are left with the second eigenvalue equation, known as the **time-independent Schrödinger equation**:

$$-\frac{\hbar^2}{2m}\psi''(x) + \frac{1}{2}m\omega^2x^2\psi(x) = E\psi(x).$$

This may be written succinctly as $\mathsf{H}\psi = E\psi$, where H is the linear differential operator given by

$$\mathsf{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2\mathsf{X}^2.$$

The boundary condition imposed on this equation is that ψ and its derivatives must decrease to 0 sufficiently rapidly as $x \to \pm\infty$, for example, by requiring that all the functional terms of the equation – ψ, $x^2\psi$, ψ'' – be functions in $L^2(\mathbb{R})$, the Hilbert space of square-integrable complex-valued functions on the real line. This requirement forces the eigenvalue E to take on only certain restricted values, namely, values in the discrete sequence

$$E_N = \left(N + \frac{1}{2}\right)\hbar\omega, \quad N = 0, 1, 2, \ldots$$

The eigenfunction ψ_N corresponding to the eigenvalue E_N, normalized to the unit L^2-norm, is

$$\psi_N(x) = \left(2^N N!\right)^{-1/2}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\exp\left(-\frac{m\omega x^2}{2\hbar}\right)H_N\left(\sqrt{\frac{m\omega}{\hbar}}x\right),$$

where H_N is the Nth Hermite polynomial. The family $\{\psi_N : N = 0, 1, 2, \dots\}$ forms a complete orthonormal (Schauder) basis of the Hilbert space $L^2(\mathbb{R})$. One can solve the time-independent Schrödinger equation and arrive at E_N and ψ_N via infinite series methods or via a beautifully elegant algebraic method using **annihilation** and **creation operators**. We present the details of the algebraic method in Lecture 11.

At this point we have applied the initial rules of quantum mechanics to the harmonic oscillator and have solved its quantum mechanical equation of motion, but we do not seem to have any information about the usual objects of interest for an understanding of the motion of the oscillator. We do not have a position function, we cannot calculate the momentum or the energy; we cannot even tell that the oscillator oscillates from the mathematics of this section. What we have done is to use rather unintuitive rules to quantize a classical Hamiltonian equation. This leads to the Schrödinger equation and, upon solving this resulting partial differential equation, a discrete sequence of numbers E_N with corresponding eigenfunctions ψ_N. The question before us serves as the title of the next section, where we present a standard, orthodox answer to the titled question.

1.3 What Does It All Mean?

The meaning given here of the calculations of the previous section is the result of a quantum world view that developed concurrently with the development of the machinery of quantum mechanics and was in place as the standard interpretation of quantum mechanics emerged by the nineteen thirties. The very fact that the machinery needed an interpretation, and that there are even today various competing interpretations, is part of what makes quantum mechanics a truly revolutionary break with the past. Indeed, the meaning or interpretation of classical mechanics is transparent in the mathematics of the discipline. After all, the primary physical attributes of a system are the particle positions. If appropriate initial or boundary conditions and the forces are known, then Newton's laws provide equations of motion from which the positions as functions of time can be derived, at least in principle. From these functions, various subsidiary physical attributes, like momentum and energy, can be calculated in a straightforward way. The classical world view provides a strongly intuitive mathematical model of the physical world where the correspondence between the mathematical objects and the physical attributes they represent is thought to accurately reflect the reality of the physical world. Nonetheless, as successful as classical mechanics is in its domain, it breaks down at the micro-level of the atom. The quantum world view offers a sophisticated calculus that works to describe the outcomes of experiments at the micro-level accurately. Indeed, it is primarily in the predictions of the outcomes of experiments that quantum mechanics derives its standard meaning.

We begin with an explanation of the eigenvalues E_N of the **energy equation** $\mathsf{H}\psi = E\psi$. These eigenvalues are, in fact, the possible values of the energy of the oscillator that are obtained upon measurement. This means that, if one performs an experiment to measure the energy of the oscillator, the value measured will, with certainty, be E_N for some value of $N = 0, 1, 2, \ldots$ Quantum mechanics thus predicts two surprising, nonclassical results: first, the energy of the system, rather than the continuously variable quantity $E = \frac{1}{2}m\omega^2 X^2$, $X \geq 0$, as derived in the classical analysis of the oscillator, is **quantized** into discrete units E_0, E_1, E_2, $\ldots$; second, the minimum possible energy of the oscillator is not zero, as in the classical case when the oscillator is at rest at equilibrium, but $E_0 = \frac{1}{2}\hbar\omega$, a positive quantity. This behavior is typical of micro-systems.

In the standard interpretation, the **energy eigenfunctions**, ψ_N, contain all the information that can be mined concerning the usual attributes we assign to physical systems, attributes such as the positions and momenta of particles and the energy of the system. We use these eigenfunctions to predict the outcomes of experimental measurements of these classical attributes by interpreting a general solution Ψ of the Schrödinger equation, expanded in terms of the eigenfunctions, as a **probability amplitude** that can be used to give probabilities for the various possible numerical values of these experimental measurements. A description of how these probabilities are determined from solutions to the Schrödinger equation will occupy the remainder of this section.

The full Schrödinger equation,

$$H\left(\mathsf{X}, \mathsf{P}\right)\Psi = \mathsf{E}\Psi,$$

is a linear homogeneous equation, so that the complex linear combination $a\Psi + b\Phi$ is a solution whenever Ψ and Φ are solutions. The most general solution to the Schrödinger equation for the quadratic potential well is

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the **wave function**

$$\Psi(x,t)=\sum_{N=0}^{\infty}c_N\psi_N(x)e^{-\mathbf{i}E_Nt/\hbar},$$

for complex constants c_N restricted only to ensure L^2-convergence of the infinite sum. The initial-value problem, solving the Schrödinger equation subject to $\Psi(x,0)=\psi(x)$, where $\psi\in L^2(\mathbb{R})$, has the solution $\Psi(x,t)$ given above when the coefficients are chosen so that $\psi=\sum c_N\psi_N$, which is possible since the family $\{\psi_N\}$ forms an orthonormal basis for $L^2(\mathbb{R})$. The immediate implication is that c_N is given by the Fourier coefficient

$$c_N=\int_{\mathbb{R}}\overline{\psi}_N\psi\,dx.$$

As the eigenfunctions ψ_N form an orthonormal collection, we may guarantee that the **state vector** $\psi_t=\Psi(-,t)$ is normalized in that, for each value of t,

$$\|\psi_t\|_2^2=\int_{\mathbb{R}}|\psi_t(x)|^2\,dx=1,$$

provided that the coefficients satisfy $\sum|c_N|^2=1$. Assuming this, the normalized state vector ψ_t is interpreted as a **probability amplitude** for the position of the oscillator at time t. This means precisely that, when the oscillator has initial state vector $\psi_{t=0}$, at time t its state vector is ψ_t and the squared modulus $|\psi_t|^2=\overline{\psi}_t\psi_t$ is the probability density for position measurements in the sense that, upon a position measurement of the oscillator at time t, the probability that the measured result is in the numerical range $[\alpha,\beta]$ is

$$\int_{\alpha}^{\beta}|\psi_t(x)|^2\,dx.$$

Another nonclassical result appears here. It turns out that no matter what values $\alpha<\beta$ are chosen, the probability expressed by this integral is nonzero and positive when the state vector is one of the energy eigenfunctions ψ_N, as these eigenfunctions are nonconstant on every nontrivial interval. In particular, when the state vector of the oscillator is ψ_N with energy E_N, there is a positive probability of measuring the position of the oscillator outside its classical range of motion, the interval $[-X_N,X_N]$ where $E_N=\frac{1}{2}m\omega^2X_N^2$. Of course, the expected value of the measured position is

$$\langle \mathsf{X}\rangle=\int_{\mathbb{R}}\overline{\psi_t(x)}\mathsf{X}\psi_t(x)\,dx=\int_{\mathbb{R}}\overline{\psi_t(x)}x\psi_t(x)\,dx$$

whenever the oscillator is in state ψ_t.

It is in this sense – that the state vector at time t gives probabilities for experimental measurements of position at that time – that the eigenfunctions contain information about the position of the oscillator at time t. But there is more, much more. The wave function contains not only information about the position, but, indeed, about any observable attribute of the system. For example, the expected value of a momentum measurement of the oscillator with state vector ψ_t is

$$\langle \mathsf{P} \rangle = \int_{\mathbb{R}} \overline{\psi_t(x)} \mathsf{P} \psi_t(x)\, dx = -\mathbf{i}\hbar \int_{\mathbb{R}} \overline{\psi_t(x)} \frac{\partial}{\partial x} \psi_t(x)\, dx,$$

and, it turns out, the probability amplitude for the momentum of the oscillator is the slightly modified Fourier transform

$$\widehat{\psi}_t(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{\mathbb{R}} \psi_t(x) e^{-\mathbf{i}px/\hbar}\, dx.$$

In particular, the probability that the result of a momentum measurement at time t is in the numerical range $[\alpha, \beta]$ is

$$\int_{\alpha}^{\beta} |\widehat{\psi}_t(p)|^2\, dp.$$

Why the interpretation articulated thus far should hold is still not in any way clear. Intrepidly, we continue. It is particularly enlightening to consider, in a bit more detail, energy measurements on the harmonic oscillator. The expected value of an energy measurement on the system with state vector ψ_t is

$$\langle \mathsf{E} \rangle = \int_{\mathbb{R}} \overline{\psi_t(x)} \mathsf{E} \psi_t(x)\, dx = \mathbf{i}\hbar \int_{\mathbb{R}} \overline{\psi_t(x)} \frac{\partial}{\partial t} \psi_t(x)\, dx.$$

A straightforward calculation using the orthonormality of the sequence of eigenfunctions ψ_N gives

$$\langle \mathsf{E} \rangle = \sum_{N=0}^{\infty} \bar{c}_N E_N c_N = \sum_{N=0}^{\infty} E_N |c_N|^2.$$

Now recall that an energy measurement of the system yields one of the eigenvalues E_N with certainty. In fact, if the state vector is the energy eigenfunction ψ_N, then the energy measurement returns the corresponding eigenvalue E_N with certainty. What happens in the general case with an arbitrary state vector ψ_t? Comparing the formula for the expected value $\langle \mathsf{E} \rangle$ with the usual formula for the expected value of a discrete