Title: The Hamiltonian in Quantum Mechanics
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The Hamiltonian, like other observables, are differential operators in quantum mechanics. They act on a Hilbert function space, which contain what are known as wavefunctions (eigenfunctions) or state vectors (eigenvectors) that fully describe the observable state of the particle. Or something like that. What I'd like to focus on is the mathematical implications of the central equation describing the time evolution of the wavefunction interpretation that describes the particle - known as the time-dependent Schrodinger Equation:

$$\hat{H}\psi = i\hbar\frac{\partial\psi}{\partial t} \tag{1}$$

One popular idea presented in introductory courses is that for the time-independent, three spatial dimension Hamiltonian, Equation 1 can be solved by a separable ansatz - that:

$$\psi\left(\mathbf{r},t\right) = T\left(t\right)\rho\left(\mathbf{r}\right) = e^{-\frac{i\hat{H}t}{\hbar}}\rho\left(\mathbf{r}\right) \tag{2}$$

where $\hat{H}$ is purely dependent on $\mathbf{r}$ and its time derivatives. An implication of such a separability property of the wavefunction is the following eigenvalue-eigenfunction relation:

$$\hat{H}\psi = \lambda\psi \tag{3}$$

where λ is an eigenvalue of the Hamiltonian, commonly denoted by $\lambda = E$ - the energy eigenvalue. This notation choice aligns with the common definition of a Hamilonian as the total energy of the system. This theory aligns with the common emergence of eigenvalue problems in partial differential equations provided that boundary conditions specify the physical system. However, from a mathematical perspective, I plan to proceed with as few simplifications and assumptions as possible, until the analysis necessitates concession. However, this eigenvalue-eigenfunction relation is important, as it implies that the eigenvalue and eigenfunction are Hamiltonian dependent, as we'd intuitively expect. This means that given a different Hamiltonian, we will get different energies and different wavefunctions. Then, further, for time-dependent Hamiltonians, it is implied that for any specific instant in time, there will be corresponding eigenvalue-eigenfunction pairs. Thus, for time dependent Hamiltonians, we may write:

$$\hat{H}\left(t\right)\psi\left(\mathbf{r},t\right) = E\left(t\right)\psi\left(\mathbf{r},t\right) \tag{4}$$

Before delving into operator algebra, it is worth a brief description about linear operators, Hermitian linear operators, and how they are necessary to describe the physical system. First, we note the notion of the particle that is a wave - in quantum, the idea of a Lagrangian path in configuration space that a particle traverses is complicated by the idea that every observable point in this space is observable only probabilistically according to a purely real density function:

$$\Psi(\mathbf{r},t) = |\psi(\mathbf{r},t)|^2 = \psi(\mathbf{r},t)\,\psi^*(\mathbf{r},t) \tag{5}$$

where the density function is the absolute value of the wavefunction squared, which is the multiplication of the wavefunction and it's complex conjugate. Thus, while the wavefunction is a complex number at any specific point in the parameter space, the relevant physical quantity for determining the average of an observable is the integration of the norm of the wavefunction weighted by the Hermitian linear operator, consider $\hat{A}(t)$ in this case:

$$\langle \hat{A}(t) \rangle = \sum_{n}^{\infty} |c_n(t)|^2 \lambda_n(t) = \int_V \mathrm{d}\mathbf{r}\, \psi^*(\mathbf{r},t)\,\hat{A}(t)\,\psi(\mathbf{r},t) \tag{6}$$

where c_n is the probability amplitude of the nth instantaneous eigenstate, and the λ_n is the eigenvalue of the nth state. For any specific instant in time, $\sum_n |c_n(t)|^2 = 1$ as would be expected from the notion of a eigenstate probability amplitude as a part of the weighted average of $\lambda_n(t)$ eigenvalues in Equation 6. This discussion then leads to the following defining equalities:

$$\begin{aligned}
\langle \hat{A}(t) \rangle &= \sum_{n=-\infty}^{\infty} |c_n(t)|^2 \lambda_n(t) \text{ and } \langle \hat{A}(t) \rangle = \int_V \mathrm{d}\mathbf{r}\, \psi^*(\mathbf{r},t)\,\hat{A}(t)\,\psi(\mathbf{r},t) \\
\text{so}\, \psi(\mathbf{r},t) &= \sum_{n=-\infty}^{\infty} c_n(t)\,\rho_n(\mathbf{r},t)\, e^{-\frac{i\int_{t_0}^{t} \mathrm{d}t\, E_n(t)}{\hbar}} \\
\implies \hat{H}(t)\,\psi(\mathbf{r},t) &= i\hbar \sum_{n=-\infty}^{\infty} \left(\frac{\partial c_n}{\partial t} \rho_n(\mathbf{r},t) + \frac{E_n(t)\,c_n(t)}{i\hbar} \rho_n(\mathbf{r},t) + c_n(t) \frac{\partial \rho_n}{\partial t} \right) e^{-\frac{i\int_{t_0}^{t} \mathrm{d}t\, E_n(t)}{\hbar}} \\
\implies 0 &= i\hbar \sum_{n=-\infty}^{\infty} \left(\frac{\partial c_n(t)}{\partial t} \rho_n(\mathbf{r},t) + c_n(t) \frac{\partial \rho_n}{\partial t} \right) e^{-\frac{i\int_{t_0}^{t} \mathrm{d}t\, E_n(t)}{\hbar}}
\end{aligned} \tag{7}$$

where $\rho_n(\mathbf{r},t)$ is the energy eigenbasis, and where n sums over a superposition of all these eigenstates. We will return to this idea later, but first I must progress on other avenues. The general linear differential operator $\hat{A}(t)$ is needed to describe quantum phenomena since the concept of the observable must be generalized to the probabilistic wave, rather than a simpler localized point particle. For example, the (Hermitian) time-independent linear momentum operator is:

$$\hat{p} = -i\hbar\nabla_{\mathbf{r}}$$

which is an interesting perspective, as we see that prior to acting on a wavefunction, the general momentum is imaginary. However, the Hermitian conjugate of the partial derivative is the negative of the partial derivative, and thus the Hermitian conjugate of the momentum operator is unchanged from the original *due to* its imaginary nature. Furthermore, the general dynamics of a wave entail that momentum corresponds to a spatial gradient operator on the wavefunction. Now, we generally care about Hermitian operators because they produce purely real eigenvalues and purely orthogonal eigenvectors, thus making their probability amplitudes easy enough to solve for (orthogonal eigenvectors), and also their expectation values would be purely real (as their physically measurable eigenvalues are real). Proving these two properties is straightforward in Heisenberg's linear algebraic matrix interpretation of quantum mechanics. Strictly, the Hermitian operator exists when the operator and its complex adjoint are equal, indicated as:

$$\hat{H} = \hat{H}^\dagger \tag{8}$$

Then, the proofs follow for the eigenvalues:

$$\begin{aligned} \langle\psi|\hat{H}|\psi\rangle &= \lambda \\ \implies \langle\psi|\hat{H}^{\dagger}|\psi\rangle &= \lambda^* \\ \implies \langle\psi|\hat{H}|\psi\rangle &= \lambda^* \\ \implies \lambda &= \lambda^* \end{aligned} \tag{9}$$

And thus, λ must be real, as we would expect to measure. The proof of orthogonal eigenvectors then is:

$$\begin{aligned} \langle\psi_m|\hat{H}|\psi_n\rangle &= \lambda_n \langle\psi_m|\psi_n\rangle \\ \left(\langle\psi_n|\hat{H}|\psi_m\rangle\right)^{\dagger} = \left(\lambda_m \langle\psi_n|\psi_m\rangle\right)^{\dagger} &= \lambda_m \langle\psi_m|\psi_n\rangle \\ \implies (\lambda_n - \lambda_m)\langle\psi_m|\psi_n\rangle &= 0 \end{aligned} \tag{10}$$

where $\hat{H}$ is strictly right acting, and where $\langle\psi_m|\psi_n\rangle$ is the inner product of the Hilbert Space - the "bra" space is the complex transpose of the "ket" space - and thus, the inner product is a scalar, complex number. The Equation 10, therefore, states that for non-degenerate eigenstates n and m, we find that the state vectors (or eigenfunctions in the wavefunction interpretation) must be orthogonal. This brings us to an important philosophical point, since it is true that for degenerate eigenstates (where two different states have the same eigenvalue), it is not necessary for the degenerate states to be orthogonal (as given by the third line of Equation 10). Of course, using what is known as the Gram-Schmidt process, a finite number of non-orthogonal eigenstates can be made orthogonal. But more in that direction in the future. Where I will now give is the idea of the commutator, and how it allows for the definition of the time evolution of a quantum operator. First consider the commutator of the time-independent position and momentum function is:

$$[\hat{\mathbf{r}}, \hat{p}]|\psi_n\rangle = (\hat{\mathbf{r}}\hat{p} - \hat{p}\hat{\mathbf{r}})|\psi_n\rangle = (-\hat{\mathbf{r}}i\hbar\nabla_{\mathbf{r}} + i\hbar\nabla_{\mathbf{r}}\mathbf{r})|\psi_n\rangle = i\hbar|\psi_n\rangle$$

However, this result is more generally applicable than simply to time independent Hamiltonians. Since probability in quantum mechanics must be conserved (meaning the probability of measuring a particle in some state is always 1), it is thus true that the norm property of the state vector (the superposition of all states) must be conserved over time. This means that:

$$\langle\psi(\mathbf{r},t_0)|\psi(\mathbf{r},t_0)\rangle = \langle\psi(\mathbf{r},t)|\psi(\mathbf{r},t)\rangle = \langle\psi(\mathbf{r},t_0)|U^{\dagger}U|\psi(\mathbf{r},t_0)\rangle = \langle\psi(\mathbf{r},t_0)|\psi(\mathbf{r},t_0)\rangle$$

where the time evolution operator must be "unitary" ($U^{\dagger} = U^{-1}$). This computation means that due to the conservation of probability throughout quantum time evolution, the time evolution operator (defined as $U|\psi(\mathbf{r},t_0)\rangle = |\psi(\mathbf{r},t)\rangle$) is unitary by physical definition. For the commutator of position and momentum, this means:

$$\begin{aligned} \langle\psi_n(\mathbf{r},t)|[\hat{\mathbf{r}}(t),\hat{p}(t)]|\psi_n(\mathbf{r},t)\rangle &= \langle\psi_n(\mathbf{r},t_0)|U^{\dagger}(t,t_0)[\hat{\mathbf{r}}(t),\hat{p}(t)]U(t,t_0)|\psi_n(\mathbf{r},t_0)\rangle \\ &= \langle\psi_n(\mathbf{r},t_0)|U^{\dagger}U^{\dagger}[\hat{\mathbf{r}}(t_0),\hat{p}(t_0)]UU|\psi_n(\mathbf{r},t_0)\rangle \\ &= i\hbar\langle\psi_n(\mathbf{r},t_0)|\psi_n(\mathbf{r},t_0)\rangle \\ &= i\hbar \end{aligned} \tag{11}$$

where t_0 is a time where the commutator can be trivially calculated to be $[\hat{\mathbf{r}}(t_0), \hat{p}(t_0)] = i\hbar$, as we give above. Thus, the canonical relation $[\hat{\mathbf{r}}(t), \mathbf{p}(t)] = i\hbar$ always holds true at all times in quantum mechanics. Now we can prove that the Hamiltonian is deeply connected to time evolution through the following calculation. Consider the general time dependent operator $\hat{A}(t)$:

$$\begin{aligned}
\langle\psi(\mathbf{r},t)|\left[\hat{H}(t),\hat{A}(t)\right]|\psi(\mathbf{r},t)\rangle &= \langle\psi(\mathbf{r},t)|\hat{H}(t)\hat{A}(t)|\psi(\mathbf{r},t)\rangle - \langle\psi(\mathbf{r},t)|\hat{A}(t)\hat{H}(t)|\psi(\mathbf{r},t)\rangle \\
&= -i\hbar\frac{\partial\langle\psi(\mathbf{r},t)|}{\partial t}\hat{A}(t)|\psi(\mathbf{r},t)\rangle - i\hbar\langle\psi(\mathbf{r},t)|\hat{A}(t)\frac{\partial|\psi(\mathbf{r},t)\rangle}{\partial t} \\
&= -i\hbar\frac{\partial}{\partial t}\left(\langle\psi(\mathbf{r},t)|\hat{A}(t)|\psi(\mathbf{r},t)\rangle\right) + i\hbar\langle\psi(\mathbf{r},t)|\frac{\partial\hat{A}}{\partial t}|\psi(\mathbf{r},t)\rangle \\
\implies \frac{\partial\left\langle\hat{A}(t)\right\rangle}{\partial t} &= \frac{i}{\hbar}\langle[H,A]\rangle + \left\langle\frac{\partial\hat{A}}{\partial t}\right\rangle \\
\implies \frac{\mathrm{d}\left\langle\hat{A}(t)\right\rangle}{\mathrm{d}t} &= \frac{i}{\hbar}\langle[H,A]\rangle + \left\langle\frac{\partial\hat{A}}{\partial t}\right\rangle
\end{aligned} \tag{12}$$

Now, keeping with the idea that commutator relations hold just as well for the operators on their own as they do for the expectation value inner products (since they must hold for any arbitrary state $|\psi(\mathbf{r},t)\rangle$), we attain *Heisenberg's Equation of Motion*:

$$\implies \frac{\mathrm{d}\hat{A}(\mathbf{r},t)}{\mathrm{d}t} = \frac{i}{\hbar}\left[H(\mathbf{r},t),A(\mathbf{r},t)\right] + \frac{\partial\hat{A}(\mathbf{r},t)}{\partial t} \tag{13}$$

which is featuring a very innovative use of Schrodinger's Equation applied to the time evolution of the operator. Thus, the Hamiltonian is intricately connected to time evolution of the system, a central idea in quantum mechanics. The last line of Equation 12 is what is known as the exact solution analog for the simpler Ehrenfest's theorem of expectation values. Lastly, I will return to Equation 7, to discern just a bit more about the state-mixing for time-dependent Hamiltonian systems.

$$\begin{aligned}
0 &= \sum_{n=-\infty}^{\infty}\left(\frac{\partial c_n(t)}{\partial t}|\psi_n(\mathbf{r},t)\rangle + c_n(t)\frac{\partial\psi_n(\mathbf{r},t)}{\partial t}\right)e^{-\frac{i\int_{t_0}^{t}\mathrm{d}t\,E_n(t)}{\hbar}} \\
\frac{\mathrm{d}c_m(t)}{\mathrm{d}t} &= -\sum_{n=-\infty}^{\infty}c_n(t)\langle\psi_m(\mathbf{r},t)|\left(\frac{\partial}{\partial t}|\psi_n(\mathbf{r},t)\rangle\right)e^{-\frac{i\int_{t_0}^{t}\mathrm{d}t\,(E_n(t)-E_m(t))}{\hbar}}
\end{aligned} \tag{14}$$

I plan to start investigating this theory in the next post. This concludes this blog post.