SCHRÖDINGER EQUATION AND PROPAGATORS

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One of the postulates of quantum mechanics states that in non-relativistic quantum mechanics, a state satisfies the Schrödinger equation:

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

where H is the Hamiltonian, which is obtained from the classical Hamiltonian by means of the other postulates of quantum mechanics, namely that we replace all references to the position x by the quantum position operator X with matrix elements (in the x basis in one dimension) of

$$\left\langle x'\left|X\right|x\right\rangle = \delta\left(x-x'\right) \tag{2}$$

and all references to classical momentum p by the momentum operator $P = -i\hbar\frac{\partial}{\partial x}$ with matrix elements

$$\left\langle x'\left|P\right|x\right\rangle = -i\hbar\delta'\left(x-x'\right) \tag{3}$$

One approach to solving the Schrödinger equation 1 is to begin with an initial state $|\psi(0)\rangle$ at $t=0$ and then to find an operator $U(t)$ known as a *propagator* which, when applied to the initial state, determines the state at some later time. That is, we want to find a solution of the form:

$$|\psi(t)\rangle = U(t)|\psi(0)\rangle \tag{4}$$

For the case of a time-independent Hamiltonian, we can actually construct $U(t)$ in terms of the eigenvectors of H. To begin, we'll consider the case where all the eigenvalues of H are non-degenerate, which means there is only one eigenvector for each eigenvalue. Further, the set of eigenvectors can be chosen to form an orthonormal basis for the Hilbert space in which the solution states $|\psi(t)\rangle$ reside.

The eigenvalue equation is

$$H|E\rangle = E|E\rangle \tag{5}$$

where E is an eigenvalue of H and $|E\rangle$ is its corresponding eigenvector. Since the eigenvectors form a vector space, we can expand the wave function in terms of them in the usual way

$$\begin{aligned} |\psi(t)\rangle &= \sum |E\rangle \langle E|\psi(t)\rangle & (6)\\ &\equiv \sum a_E(t)|E\rangle & (7)\end{aligned}$$

The coefficient $a_E(t)$ is the component of $|\psi(t)\rangle$ along the $|E\rangle$ vector as a function of time. We can now apply the Schrödinger equation 1 to get (a dot over a symbol indicates a time derivative):

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle &= i\hbar\sum \dot{a}_E(t)|E\rangle & (8)\\ &= H|\psi(t)\rangle & (9)\\ &= \sum a_E(t)H|E\rangle & (10)\\ &= \sum a_E(t)E|E\rangle & (11)\end{aligned}$$

Since the eigenvectors $|E\rangle$ are linearly independent, each term in the sum in the first line must be equal to the corresponding term in the sum in the last line, so we have

$$i\hbar\dot{a}_E(t) = a_E(t)E \tag{12}$$

The solution is

$$\begin{aligned} a_E(t) &= a_E(0)e^{-iEt/\hbar} & (13)\\ &= e^{-iEt/\hbar}\langle E|\psi(0)\rangle & (14)\end{aligned}$$

The general solution 7 is therefore

$$|\psi(t)\rangle = \sum e^{-iEt/\hbar}|E\rangle\langle E|\psi(0)\rangle \tag{15}$$

from which we can read off the propagator:

$$U(t) = \sum e^{-iEt/\hbar}|E\rangle\langle E| \tag{16}$$

Thus if we can determine the eigenvalues and eigenvectors of H, we can write the propagator in terms of them and get the general solution. We can see from this that $U(t)$ is unitary:

$$U^{\dagger}U = \sum_{E'}\sum_{E} e^{-i(E-E')t/\hbar}\,|E\rangle\,\langle E\,|E'\rangle\,\langle E'| \tag{17}$$

$$= \sum_{E'}\sum_{E} e^{-i(E-E')t/\hbar}\,|E\rangle\,\delta_{EE'}\,\langle E'| \tag{18}$$

$$= \sum_{E} |E\rangle\,\langle E| \tag{19}$$

$$= 1 \tag{20}$$

This derivation uses the fact that the eigenvectors are orthonormal and form a complete set, so that $\langle E\,|E'\rangle = \delta_{EE'}$ and $\sum_E |E\rangle\,\langle E| = 1$. Since a unitary operator doesn't change the norm of a vector, we see from 4 that if $|\psi(0)\rangle$ is normalized, then so is $|\psi(t)\rangle$ for all times t. Further, the probability that the state will be measured to be in eigenstate $|E\rangle$ is constant over time, since, from 14, this probability is given by

$$|a_E(t)|^2 = \left|e^{-iEt/\hbar}\,\langle E\,|\psi(0)\rangle\right|^2 = |\langle E\,|\psi(0)\rangle|^2 \tag{21}$$

This derivation assumed that the spectrum of H was discrete and non-degenerate. If the possible eigenvalues E are continuous, then the sum is replaced by an integral

$$U(t) = \int e^{-iEt/\hbar}\,|E\rangle\,\langle E|\,dE \tag{22}$$

If the spectrum is discrete and degenerate, then we need to find an orthonormal set of eigenvectors that spans each degenerate subspace, and sum over these sets. For example, if E_1 is degenerate, then we find a set of eigenvectors $\left|E_1,\alpha_{(1)}\right\rangle$ that spans the subspace for which E_1 is the eigenvalue. The index $\alpha_{(1)}$ runs from 1 up to the degree of degeneracy of E_1, and the propagator is then

$$U(t) = \sum_{\alpha_{(i)}}\sum_{E_i} e^{-iE_it/\hbar}\,\left|E_i,\alpha_{(i)}\right\rangle\,\left\langle E_i,\alpha_{(i)}\right| \tag{23}$$

where $\alpha_{(i)}$ covers the numbers from 1 up to the degeneracy of E_i. The sum over E_i runs over all the distinct eigenvalues, and the sum over $\alpha_{(i)}$ runs over the eigenvectors for each different E_i.

Another form of the propagator can be written directly in terms of the time-independent Hamiltonian H as

$$U(t) = e^{-iHt/\hbar} \tag{24}$$

This relies on the concept of the function of an operator, so that $e^{-iHt/\hbar}$ is a matrix whose elements are power series of the exponent $-\frac{iHt}{\hbar}$. The power series must, of course, converge for this solution to be valid. Since H is Hermitian, $U(t)$ is unitary. We can verify that the solution using this form of $U(t)$ satisfies the Schrödinger equation:

$$\begin{aligned}
|\psi(t)\rangle &= U(t)\,|\psi(0)\rangle && (25)\\
&= e^{-iHt/\hbar}\,|\psi(0)\rangle && (26)\\
i\hbar\,\left|\dot{\psi}(t)\right\rangle &= i\hbar\frac{d}{dt}\left(e^{-iHt/\hbar}\right)|\psi(0)\rangle && (27)\\
&= i\hbar\left(-\frac{i}{\hbar}\right)He^{-iHt/\hbar}\,|\psi(0)\rangle && (28)\\
&= He^{-iHt/\hbar}\,|\psi(0)\rangle && (29)\\
&= H\,|\psi(t)\rangle && (30)
\end{aligned}$$

The derivative of $U(t)$ can be calculated from the derivatives of its matrix elements, which are all power series.

The form 24 is frequently used in quantum mechanics and in quantum field theory.

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