Computing the Time Evolution Operator. Ch 4.1 (Townsend)

In general the state of a quantum system obeys the Schrödinger equation:

\[ i\hbar \frac{d}{dt} |\Psi(t)\rangle = \hat{H} |\Psi(t)\rangle \]

where we will usually be able to construct the Hamiltonian operator \( \hat{H} \) from physical considerations based on energies. Note that it is quite possible that the Hamiltonian operator depends on \( t \). Our aim is now to construct the relevant time evolution operator which will only depend on \( \hat{H} \). This is generally quite complicated. However, for the time independent Hamiltonian case it is relatively straightforward.

Time Independent Hamiltonian.

Note that Schrödinger's equation gives:

\[ \frac{d}{dt} |\Psi(t)\rangle = -\frac{i}{\hbar} \hat{H} |\Psi(t)\rangle \]

and this resembles the following equation for ordinary functions:

\[ \frac{dx}{dt} = \alpha x \]

which has solution:

\[ x(t) = e^{\alpha t} x(0) \]
Thus we propose:

$$|\Psi(t)\rangle = e^{-i\hat{H}t/\hbar} |\Psi(0)\rangle.$$ 

and you can easily show by differentiating the exponential of an operator that this works out. Thus

$$\frac{d}{dt} (e^{-i\hat{H}t/\hbar}) = \frac{d}{dt} \sum_{n=0}^{\infty} \frac{1}{n!} \left(-i\frac{\hat{H}}{\hbar}\right)^n = \frac{d}{dt} \sum_{n=0}^{\infty} \frac{1}{n!} \left(-i\frac{\hat{H}}{\hbar}\right)^n t^n$$

$$= \sum_{n=0}^{\infty} \frac{1}{n!} \left(-i\frac{\hat{H}}{\hbar}\right)^n t^{n-1}$$

$$= \sum_{n=1}^{\infty} \frac{1}{(n-1)!} \left(-i\frac{\hat{H}}{\hbar}\right)^{n-1} \left(-i\frac{\hat{H}}{\hbar}\right) t^{n-1}$$

$$= -i\frac{\hat{H}}{\hbar} \sum_{n=1}^{\infty} \frac{1}{(n-1)!} \left(-i\frac{\hat{H}}{\hbar}\right)^{n-1} t^{n-1} = -i\frac{\hat{H}}{\hbar} e^{-i\hat{H}t/\hbar}.$$ 

and substituting into the rewritten equation gives the result. Note that this only works if $\hat{A}$ is independent of $t$.

Thus the evolution operator is:

$$\hat{A} \text{ time independent } \Rightarrow \hat{U}(t) = e^{-i\hat{H}t/\hbar}$$
Consider a particle of mass \( m \) and charge \( q \), placed in a magnetic field

\[
\vec{B} = B_x \hat{\sigma}_x + B_y \hat{\sigma}_y + B_z \hat{\sigma}_z
\]

What should we use for the Hamiltonian? We will see how to guess a reasonable Hamiltonian by using the classical energy

\[
U = -\vec{p} \cdot \vec{B} = -\frac{q}{2m} \vec{S} \cdot \vec{B}
\]

where \( g \) is the gyromagnetic ratio and \( \vec{S} \) the particle's classical spin. We shall soon see that we can associate operators with the spin in the following way:

<table>
<thead>
<tr>
<th>classical</th>
<th>quantum</th>
</tr>
</thead>
<tbody>
<tr>
<td>( S_x )</td>
<td>( \frac{\hbar}{2} \hat{\sigma}_x )</td>
</tr>
<tr>
<td>( S_y )</td>
<td>( \frac{\hbar}{2} \hat{\sigma}_y )</td>
</tr>
<tr>
<td>( S_z )</td>
<td>( \frac{\hbar}{2} \hat{\sigma}_z )</td>
</tr>
</tbody>
</table>

This gives an energy operator or Hamiltonian:

\[
\hat{H} = -\frac{qq}{2m} \frac{\hbar}{2} \left( B_x \hat{\sigma}_x + B_y \hat{\sigma}_y + B_z \hat{\sigma}_z \right)
\]

This applies quite generally, even for time varying magnetic fields.
Particle in a constant magnetic field  Townsend 4.3

Suppose that the magnetic field is constant and that
\( \vec{B} = B_0 \hat{z} \)

Then:
\[
\hat{H} = -\frac{gq}{2m} \frac{\hbar}{2} B_0 \hat{\sigma}_z
\]

and the evolution operator is:
\[
\hat{U}(t) = e^{-i \left( -\frac{gq}{2m} \frac{\hbar}{2} B_0 \right) \hat{\sigma}_z t / \hbar}
\]
\[
= e^{-i \omega_0 t \hat{\sigma}_z}
\]

where
\[
\omega_0 = -\frac{gq}{2m} B_0 \quad \Rightarrow \quad \hat{H} = \frac{\hbar \omega_0}{2} \hat{\sigma}_z
\]

This describes a rotation through angle \( \omega_0 t \) about the \( \hat{z} \) axis.
Thus the rotation amounts to a precession at a constant frequency \( \omega_0 \). This is called the Larmor frequency.

The fact that this is reasonable is borne out by over 50 years of NMR experiments. The basic understanding for these comes from the choice of Hamiltonian used here.