Chapter 3

Time Evolution (Part B)

3.1 Heisenberg Picture

We have seen that the expectation value of a given operator can be written as

$$\langle\psi(0)|\, e^{+\frac{i}{\hbar}\hat{H}\,t}\,\hat{A}\,e^{-\frac{i}{\hbar}\hat{H}\,t}\,|\psi(0)\rangle \;=\; \langle\psi(t)|\,\hat{A}\,|\psi(t)\rangle\,, \tag{3.1.1}$$

a view principally due to Schrödinger. An alternative approach, due to Dirac but most well-known as the Heisenberg picture, considers time-evolved operators

$$\hat{A}_h(t) \;\equiv\; e^{+\frac{i}{\hbar}\hat{H}\,t}\,\hat{A}\,e^{-\frac{i}{\hbar}\hat{H}\,t}, \tag{3.1.2}$$

and time-independent states. In this section, we denote Heisenberg operators by the subscript"h". Thus, in this picture, all quantum states are static, while operators carry the time dependence. This viewpoint is completely equivalent to Schrödinger's interpretation, but can sometimes be more convenient for certain calculations.
We can see this by obtaining the equations of motion for the Heisenberg operator $\hat{A}_h(t)$. Again assuming a time-independent Hamiltonian and no intrinsic time dependence for $\hat{A}$, we have

$$\begin{aligned}\hat{A}_h(t+\Delta t) &= \; e^{+\frac{i}{\hbar}\hat{H}\,(t+\Delta t)}\,\hat{A}\,e^{-\frac{i}{\hbar}\hat{H}\,(t+\Delta t)} \\ &= \; \hat{A}_h(t) \;+\; \frac{i\Delta t}{\hbar}\Big[\hat{H},\,\hat{A}_h(t)\Big] \;+\; \mathcal{O}\Big((\Delta t)^2\Big),\end{aligned} \tag{3.1.3}$$

so in the limit of small Δt,

$$\frac{d\,\hat{A}_h(t)}{dt} \;=\; \frac{i}{\hbar}\Big[\hat{H},\,\hat{A}_h(t)\Big]. \tag{3.1.4}$$

3.1.1 Conserved Quantities (Heisenberg Picture)

We already saw that if an operator commutes with the Hamiltonian, then its Bohr frequencies vanish and its expectation value is time-independent (Sec. **??**). This notion of conservation law being associated with the commutator $[\hat{H},\hat{A}]$ is particularly transparent in the Heisenberg picture. From Eq. (3.1.4), if $[\hat{H},\hat{A}] = 0$, the time derivative of $\hat{A}_h(t)$ vanishes, thus the operator is a constant of motion.

3.2 Example: Spin Precession

After having developed the machinery necessary to study quantum dynamics, it is instructive to look at an example. Here, we consider the case of a spin-$\frac{1}{2}$ particle (for example, an electron) inside a magnetic field. Classically, the potential energy of a magnetic dipole is

$$U \;=\; -\boldsymbol{\mu}\cdot\mathbf{B}, \tag{3.2.1}$$

where $\mathbf{B}$ is the magnetic field and $\boldsymbol{\mu}$ is the magnetic dipole moment. Inspired by this form and recalling that the Hamiltonian operator is related to measurements of the system's energy, we define the quantum Hamiltonian operator describing the interaction of the spin with the magnetic field:

$$\hat{H} \;=\; -\frac{e}{m}\,\hat{\mathbf{S}}\cdot\mathbf{B}, \tag{3.2.2}$$

considering the case in which the magnetic field is pointing in the z direction,

$$\hat{H} \;=\; -\frac{e}{m}\,\hat{S}_z\,B_z. \tag{3.2.3}$$

We see that since the Hamiltonian is proportional to $\hat{S}_z$, we have $[\hat{H}, \hat{S}_z] = 0$, and the eigenstates of $\hat{S}_z$ are also eigenstates of $\hat{H}$, such that

$$\hat{H}\,|S_z;\pm\rangle \;=\; \left(\pm\,\tfrac{\hbar}{2}\,\omega_B\right)|S_z;\pm\rangle\,, \tag{3.2.4}$$

where

$$\omega_B \;=\; \frac{|e|\,B_z}{m}. \tag{3.2.5}$$

Hence

$$\hat{U}(t) \;=\; \exp\!\left(-\,\tfrac{i}{\hbar}\,\hat{H}\,t\right) \;=\; \exp\!\left(-\,\tfrac{i}{\hbar}\,\omega_B\,\tfrac{\hat{S}_z}{2}\,t\right). \tag{3.2.6}$$

Thus, if at $t = 0$ the system is an arbitrary state

$$|\psi(0)\rangle \;=\; c_+\,|S_z;+\rangle \;+\; c_-\,|S_z;-\rangle\,, \tag{3.2.7}$$

then at time t, we simply find

$$|\psi(t)\rangle \;=\; c_+\,\exp\!\left(-\,i\,\tfrac{\omega_B}{2}\,t\right)|S_z;+\rangle \;+\; c_-\,\exp\!\left(+\,i\,\tfrac{\omega_B}{2}\,t\right)|S_z;-\rangle\,, \tag{3.2.8}$$

since the Hamiltonian is diagonal in the $\hat{S}_z$ basis.

3.2.1 Starting from an Eigenstate of S_z

Let us now analyze the specific case in which we start our time evolution from an eigenstate of $\hat{S}_z$, say $|S_z;+\rangle$, thus $c_+ = 1$ and $c_- = 0$. At time t, the state remains in the same state, differing only by a global (and physically irrelevant) phase:

$$|\psi(t)\rangle \;=\; \exp\!\left(-\,i\,\tfrac{\omega_B}{2}\,t\right)|S_z;+\rangle\,. \tag{3.2.9}$$

This is a stationary state for the dynamics, and since $\hat{S}_z$ commutes with the Hamiltonian, the expectation value of $\hat{S}_z$ does not change:

$$\langle S_z\rangle(t) \;=\; \langle S_z\rangle(0) \;=\; +\,\tfrac{\hbar}{2}. \tag{3.2.10}$$

3.2.2 Starting from an Eigenstate of S_x

The situation is more interesting if we start from an eigenstate of an operator that does not commute with the Hamiltonian. For example, let

$$|\psi(0)\rangle \;=\; |S_x;+\rangle \;=\; \frac{1}{\sqrt{2}}\Big(|S_z;+\rangle \;+\; |S_z;-\rangle\Big). \tag{3.2.11}$$

We can then compute the expectation value of $\hat{S}_x$ at later times. Denoting $|\psi(t)\rangle$ as in Eq. (3.2.8), one finds

$$\langle S_x\rangle(t) \;=\; \langle\psi(t)|\;\hat{S}_x\;|\psi(t)\rangle \;=\; \frac{\hbar}{2}\cos\!\Big(\omega_B\,t\Big), \tag{3.2.12}$$

$$\langle S_y\rangle(t) \;=\; \frac{\hbar}{2}\sin\!\Big(\omega_B\,t\Big), \qquad \langle S_z\rangle(t) \;=\; 0. \tag{3.2.13}$$

Hence the expectation value of the spin precesses with frequency ω_B around the z axis. This phenomenon is well known experimentally, and is the basis for very precise measurements of $\hbar$.

3.3 Time-Dependent Hamiltonians

We now generalize our discussion, and consider the case we have been so carefully avoiding until now, namely the case in which the time evolution operator depends not only on the time difference $t_1 - t_0$ but also on both t_1 and t_0. In this case, it is no longer true that the exponential form we have derived before is valid:

$$\hat{U}(t_0, t_1) \;\neq\; e^{-\frac{i}{\hbar}\hat{H}\,(t_1 - t_0)}. \tag{3.3.1}$$

This situation typically arises when the system interacts with an external degree of freedom that is explicitly time-dependent, and it is not isolated from the external environment[1]. To see why this is the case, let us consider the case we have analyzed so far, where we have identified the Hamiltonian operator $\hat{H}$ with the measurement of the energy of the system. We have seen that if an operator commutes with the Hamiltonian, then the Bohr frequencies are strictly vanishing, and the operator's expectation value is time independent. This corresponds precisely to an isolated system whose energy is conserved.

To go beyond this assumption, we allow $\hat{H}$ itself to carry an explicit time dependence (i.e. its matrix elements depend on t), meaning in general

$$\langle\psi(t)|\hat{H}(t)|\psi(t)\rangle \;\neq\; \langle\psi(0)|\hat{H}|\psi(0)\rangle.$$

Physically, the system can now exchange energy with its surroundings. Formally, the time evolution in such a case is still governed by the Schrödinger equation,

$$i\,\hbar\,\frac{\partial}{\partial t}\,|\psi(t)\rangle \;=\; \hat{H}(t)\,|\psi(t)\rangle, \tag{3.3.2}$$

but $\hat{H}(t)$ can change with time.

[1] In the previous discussion, the only allowed interaction with the environment was through the measurement process; otherwise, we assumed the system was perfectly isolated during its time evolution.

3.3.1 Time evolution operator

In order to derive an expression for the full time evolution operator $\hat{U}(t_0, t_1)$, it is useful to divide the interval $[t_0, t_1]$ into p small slices of duration Δt, such that $t_1 = t_0 + p\,\Delta t$. Within each small interval Δt, we approximate $\hat{H}(t)$ as constant (equal, for instance, to its value at the beginning of the interval). Then the time evolution over each small slice can be written as

$$\hat{U}_\epsilon(t) \;=\; \exp\!\Big[-\tfrac{i}{\hbar}\,\hat{H}(t)\,\Delta t\Big]. \tag{3.3.3}$$

By the composition property of time evolution (see Eq. (3.1.3)), the total evolution is the product of all these short evolutions:

$$\hat{U}(t_0, t_1) \;=\; \hat{U}_\epsilon\Big(t_0 + (p-1)\Delta t\Big)\;\ldots\;\hat{U}_\epsilon\Big(t_0 + \Delta t\Big)\,\hat{U}_\epsilon(t_0), \tag{3.3.4}$$

i.e.

$$\hat{U}(t_0, t_1) \;\approx\; \exp\!\Big[-\tfrac{i}{\hbar}\,\hat{H}\Big(t_0{+}(p{-}1)\Delta t\Big)\,\Delta t\Big]\;\ldots\;\exp\!\Big[-\tfrac{i}{\hbar}\,\hat{H}\Big(t_0{+}\Delta t\Big)\,\Delta t\Big]\;\exp\!\Big[-\tfrac{i}{\hbar}\,\hat{H}(t_0)\,\Delta t\Big]. \tag{3.3.5}$$

Taking $\Delta t \to 0$ (so $p \to \infty$) makes this expression exact.These kind of small-time expansions for the time evolution operators are of fundamental importance in a variety of applications of quantum mechanics, ranging from path integrals to quantum computing.

While the expression Eq. (3.3.5) is rather general, there are however some special cases in which it simplifies. Let us consider now two important sub-cases.

Hamiltonians at different times commute

A simpler expression arises if $\Big[\hat{H}(t_1),\,\hat{H}(t_2)\Big] = 0$ for all t_1, t_2. In that case, each exponential in Eq. (3.3.5) commutes with the others, so we can combine them into a single exponential:

$$\hat{U}(t_0, t_1) \;=\; \exp\!\Big[-\tfrac{i}{\hbar}\int_{t_0}^{t_1} dt'\,\hat{H}(t')\Big]. \tag{3.3.6}$$

This result follows from the property $e^A e^B = e^{A+B}$ if $[A, B] = 0$, and generalizes straightforwardly to multiple commuting operators.

Hamiltonians at different times do not commute

If instead $\Big[\hat{H}(t_1),\,\hat{H}(t_2)\Big] \neq 0$ for some $t_1 \neq t_2$, we cannot merge the exponentials in Eq. (3.3.5) into a single exponent. The expression

$$\hat{U}(t_0, t_1) \;=\; \lim_{p\to\infty}\prod_{k=0}^{p-1}\exp\!\Big[-\tfrac{i}{\hbar}\,\hat{H}\Big(t_0 + k\,\tfrac{t_1-t_0}{p}\Big)\,\tfrac{(t_1-t_0)}{p}\Big] \tag{3.3.7}$$

still holds, but it can no longer be simplified into a single exponential of the integral of $\hat{H}(t)$. Alternative expansions (Dyson series, Magnus expansions) exist but are more complicated.

In practice, for time-dependent Hamiltonians with non-commuting parts at different times, one often directly solves the Schrödinger equationby expanding $|\psi(t)\rangle$ in a fixed basis and integrating numerically. Concretely, if $|\psi(t)\rangle = \sum_k c_k(t)\, |A_k\rangle$ where $\hat{A}$ is a time-independent operator, then

$$i\,\hbar\,\dot{c}_k(t) \;=\; \sum_{k'} \langle A_k|\; \hat{H}(t)\; |A_{k'}\rangle\; c_{k'}(t), \tag{3.3.8}$$

is a system of linear ordinary differential equations, which can be tackled by standard methods once $\hat{H}(t)$ is specified.

3.4 Magnetic Resonance

Let us now analyze the dynamics of a spin in a magnetic field, extending our analysis to the case of time-dependent field.

Let us consider the situation in which a particle with spin 1/2 (for example an electron) is subjected to a time-dependent magnetic field. In the previous chapter, we have written the Hamiltonian in the case of a static magnetic field, and the situation is analogous also when $\mathbf{B}$ acquires a time dependence, with the notable exception that the Hamiltonian becomes time dependent:

$$\hat{H}(t) \;=\; -\frac{e}{m}\,\hat{\mathbf{S}}\cdot\mathbf{B}(t). \tag{3.4.1}$$

We imagine now that the magnetic field is such that

$$\mathbf{B}(t) \;=\; \mathbf{B}_0 \;+\; \mathbf{B}_1(t) \;=\; B_0\,\hat{z} \;+\; \Big[\hat{x}\,B_1\cos(\omega t) \;+\; \hat{y}\,B_1\sin(\omega t)\Big], \tag{3.4.2}$$

thus there is a static magnetic field in the z direction but also a time-dependent magnetic field in the xy plane oscillating with a frequency ω. The Hamiltonian then reads

$$\hat{H}(t) \;=\; \omega_0\,\hat{S}_z \;+\; \omega_1\Big[\cos(\omega t)\,\hat{S}_x \;+\; \sin(\omega t)\,\hat{S}_y\Big], \tag{3.4.3}$$

where we have defined

$$\omega_0 \;\equiv\; \frac{|e|\,B_0}{m}, \quad \omega_1 \;\equiv\; \frac{|e|\,B_1}{m}.$$

Using the expression for the Pauli operators, we can write the explicit matrix elements of the Hamiltonian in the basis of the eigen-kets of $\hat{S}_z$:

$$\hat{H}(t) \doteq \frac{\hbar}{2}\,\omega_0\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} \;+\; \frac{\hbar}{2}\,\omega_1\left[\cos(\omega t)\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} \;+\; i\,\sin(\omega t)\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}\right], \tag{3.4.4}$$

which, after combining terms, becomes

$$\hat{H}(t) \doteq \frac{\hbar}{2}\begin{pmatrix}\omega_0 & \omega_1\,e^{-i\,\omega t}\\ \omega_1\,e^{+i\,\omega t} & -\,\omega_0\end{pmatrix}. \tag{3.4.5}$$

We immediately notice that, in order to solve for the dynamics of the system, we cannot use the solution of the time evolution operator we found for time-independent Hamiltonians. Moreover, it is easy to prove (show this!) that

$$\left[\hat{H}(t_1),\, \hat{H}(t_2)\right] \;\neq\; 0 \quad \text{for } t_1 \neq t_2.$$

Since we cannot easily solve the time dependence for quantum states using the unitary evolution operator $\hat{U}$, we resort to the last method outlined in the previous Chapter, namely directly attacking the Schrödinger equation. We represent the state at time t as

$$|\psi(t)\rangle \;=\; c_+(t)\;|S_z;+\rangle \;+\; c_-(t)\;|S_z;-\rangle\,, \tag{3.4.6}$$

and, following Eq. (3.7.10), we write the Schrödinger equation in matrix form as

$$i\,\hbar \begin{pmatrix} \dot{c}_+(t) \\ \dot{c}_-(t) \end{pmatrix} \;=\; \frac{\hbar}{2} \begin{pmatrix} \omega_0 & \omega_1\, e^{-i\,\omega t} \\ \omega_1\, e^{+i\,\omega t} & -\,\omega_0 \end{pmatrix} \begin{pmatrix} c_+(t) \\ c_-(t) \end{pmatrix}, \tag{3.4.7}$$

thus the following system of coupled differential equations:

$$\begin{cases} i\,\partial_t\, c_+(t) \;=\; \dfrac{\omega_0}{2}\, c_+(t) \;+\; \dfrac{\omega_1}{2}\, e^{-i\,\omega t}\, c_-(t), \\[2ex] i\,\partial_t\, c_-(t) \;=\; \dfrac{\omega_1}{2}\, e^{+i\,\omega t}\, c_+(t) \;-\; \dfrac{\omega_0}{2}\, c_-(t). \end{cases} \tag{3.4.8}$$

3.4.1 Solving the Schrödinger Equation

Solving the previous differential equations can be easily done numerically; however, we focus here on finding an explicit analytic solution. For this purpose, we consider a change of variables:

$$a_+(t) \;=\; e^{+i\,\frac{\omega t}{2}}\; c_+(t), \quad a_-(t) \;=\; e^{-i\,\frac{\omega t}{2}}\; c_-(t). \tag{3.4.9}$$

Substituting into the original differential equations, the first one becomes:

$$i\, e^{-i\,\frac{\omega t}{2}} \left[\partial_t a_+(t) \;-\; i\,\tfrac{\omega}{2}\, a_+(t)\right] \;=\; \frac{\omega_0}{2}\, e^{-i\,\frac{\omega t}{2}}\; a_+(t) \;+\; \frac{\omega_1}{2}\, e^{-i\,\frac{\omega t}{2}}\; a_-(t).$$

Hence

$$i\,\partial_t a_+(t) \;=\; \left(\tfrac{\omega_0-\omega}{2}\right) a_+(t) \;+\; \left(\tfrac{\omega_1}{2}\right) a_-(t). \tag{3.4.10}$$

Similarly, the other equation transforms the same way, giving

$$\begin{cases} i\,\partial_t\, a_+(t) \;=\; \dfrac{\omega_0-\omega}{2}\, a_+(t) \;+\; \dfrac{\omega_1}{2}\, a_-(t), \\[2ex] i\,\partial_t\, a_-(t) \;=\; \dfrac{\omega_1}{2}\, a_+(t) \;-\; \dfrac{\omega_0-\omega}{2}\, a_-(t). \end{cases} \tag{3.4.11}$$

Another way of looking at the transformation (3.4.9) is that it defines a new state:

$$|\psi'(t)\rangle \;=\; \exp\!\left(+\,\tfrac{i}{\hbar}\,\tfrac{\hbar\omega}{2}\,\hat{S}_z\right)\;|\psi(t)\rangle\,, \tag{3.4.12}$$

which also leads to a transformed, <u>time-independent</u> Hamiltonian

$$\hat{H}' \doteq \frac{\hbar}{2} \begin{pmatrix} \omega_0-\omega & \omega_1 \\ \omega_1 & \omega-\omega_0 \end{pmatrix}, \tag{3.4.13}$$

so that it satisfies

$$i\,\hbar\,\partial_t\;|\psi'(t)\rangle \;=\; \hat{H}'\;|\psi'(t)\rangle\,. \tag{3.4.14}$$

Because the transformed Hamiltonian is time independent, we can easily solve this problem using the "standard" approach of diagonalizing $\hat{H}'$ and expanding the time-evolved states in its eigen-ket basis. The general solution is left as an exercise; here, we consider a few special cases (similarly to the static-field scenario).

At Resonance

At the resonance condition ($\omega_0 = \omega$), we have

$$\hat{H}' \doteq \frac{\hbar}{2}\begin{pmatrix} 0 & \omega_1 \\ \omega_1 & 0 \end{pmatrix} = \omega_1 \hat{S}_x. \tag{3.4.15}$$

Consider now the specific case in which we start our time evolution from an eigenstate of $\hat{S}_z$, say $|S_z;+\rangle$, so initially $c_+ = 1$ and $c_- = 0$. In terms of the transformed variables (3.4.9), we have $a_+ = 1$, $a_- = 0$. Hence

$$|\psi'(0)\rangle = |S_z;+\rangle\,, \tag{3.4.16}$$

and so

$$|\psi'(t)\rangle = \frac{1}{\sqrt{2}}\Big[e^{-i\frac{\omega_1 t}{2}}\,|S_x;+\rangle + e^{+i\frac{\omega_1 t}{2}}\,|S_x;-\rangle\Big]. \tag{3.4.17}$$

Rewriting $|S_x;\pm\rangle$ in terms of $|S_z;\pm\rangle$, one finds

$$|\psi'(t)\rangle = \cos\!\left(\frac{\omega_1 t}{2}\right)|S_z;+\rangle - i\,\sin\!\left(\frac{\omega_1 t}{2}\right)|S_z;-\rangle\,. \tag{3.4.18}$$

Inverting to get back to $|\psi(t)\rangle$, one obtains

$$|\psi(t)\rangle = e^{-\frac{i}{2}\omega t}\cos\!\left(\frac{\omega_1 t}{2}\right)|S_z;+\rangle - i\,e^{+\frac{i}{2}\omega t}\sin\!\left(\frac{\omega_1 t}{2}\right)|S_z;-\rangle\,. \tag{3.4.19}$$

Hence the probability of finding the state "flipped" (i.e. in $|S_z;-\rangle$) at time t is

$$P_-(t) = \Big|\langle S_z;-|\,\psi(t)\rangle\Big|^2 = \sin^2\!\left(\frac{\omega_1 t}{2}\right). \tag{3.4.20}$$

These oscillations (with frequency $\omega_1/2$) are at the heart of Magnetic Resonance Imaging (MRI), used to measure very small transverse magnetic fields B_1 (since $\omega_1 = |e|\,B_1/m$). The technique allows us to probe local chemical or physical composition (e.g. in biological tissues).

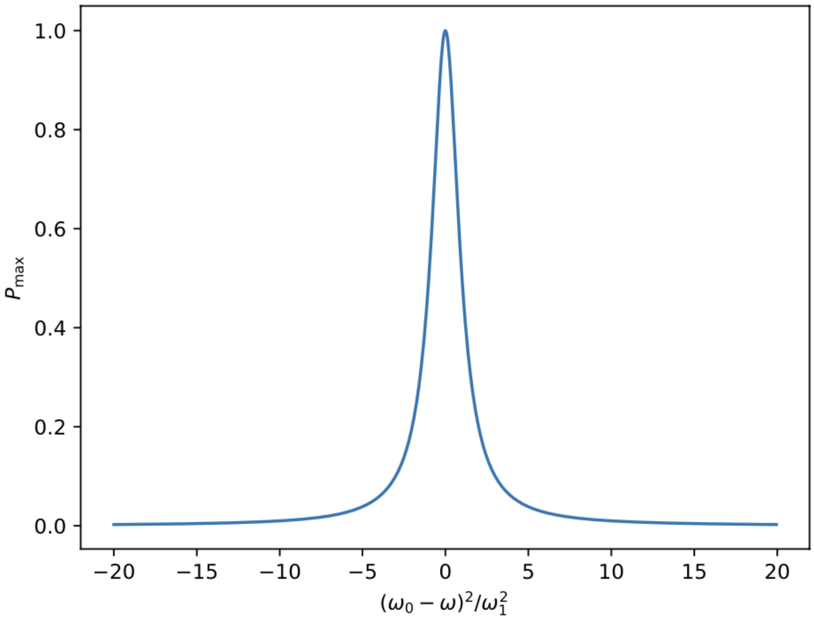

Figure 3.1: Maximum probability of flipping a spin using a time-dependent transverse field. At resonance, the maximum probability approaches unity.

Off Resonance

For the general (off-resonance $\omega \neq \omega_0$) case, the spin-flip probability at time t can be shown to be

$$P_-(t) \;=\; \frac{\omega_1^2}{\omega_1^2 + (\omega_0 - \omega)^2}\,\sin^2\!\Big(\tfrac{1}{2}\sqrt{\omega_1^2 + (\omega_0 - \omega)^2}\;t\Big). \tag{3.4.21}$$

This expression, first derived by Rabi, shows that unless we are spot-on the resonance ($\omega \simeq \omega_0$), the maximum probability of flipping the spin is small, given by a Lorentzian:

$$\max_t\, P_-(t) \;=\; \frac{\omega_1^2}{\omega_1^2 + (\omega_0 - \omega)^2}. \tag{3.4.22}$$

(See Fig. 3.1 for illustration.)