Appendix A

Time Dependent Schrödinger Equation - Another Perspective

The time dependent Schrödinger equation given by Eq. 2.83 in the coordinate representation can be expressed in the state vector representation

$$i\hbar\frac{\partial|\psi(t)\rangle}{\partial t} = \hat{H}|\psi(t)\rangle \tag{A.1}$$

and for the corresponding adjoint state

$$-i\hbar\frac{\partial\langle\psi(t)|}{\partial t} = \langle\psi(t)|\hat{H} \tag{A.2}$$

This notation has already been used when the Dirac-Frenkel variational principle had been invoked, Eq. 2.86. Knowing the initial state of the system $|\psi_0\rangle$ at time t_0, the state vector at any time t can be obtained by applying the time-evolution operator $U(t, t_0)$ on the initial state vector

$$|\psi(t)\rangle = U(t, t_0)|\psi_0\rangle \tag{A.3}$$

and

$$\langle\psi(t)| = \langle\psi_0|U^\dagger(t, t_0) \tag{A.4}$$

It is obvious from the last two equations that $\lim\limits_{\tau\to 0} U(t_0 + \tau, t_0) = \lim\limits_{\tau\to 0} U^\dagger(t_0 + \tau, t_0) = \mathbf{I}$. Another important property of this operator is that its action can be split into different time intervals, $U(t, t_2) = U(t, t_1)U(t_1, t_2)$, assuming $0 \leq t_1 \leq t_2$. The time evolution operator is a unitary operator. Its equation of motion is obtained by inserting Eq. A.3 into Eq. A.1

$$i\hbar\frac{\partial U(t, t_0)}{\partial t} = \hat{H}U(t, t_0) \tag{A.5}$$

which for a time independent Hamiltonian leads to $U(t, t_0) = e^{-i\hat{H}(t-t_0)/\hbar}$. A formal solution of this partial differential equation for a general case when the

Hamiltonian is time dependent reads

$$U(t, t_0) = \mathbf{I} - \frac{i}{\hbar} \int_{t_0}^{t} d\tau \hat{H}(\tau) U(\tau, t_0) \tag{A.6}$$

An iterative solution of the last equation leads to [85]

$$U(t, t_0) = 1 + \sum_{n=1}^{\infty} \left(-\frac{i}{\hbar}\right)^n \int_{t_0}^{t} d\tau_n \int_{t_0}^{\tau_n} d\tau_{n-1} \ldots \int_{t_0}^{\tau_2} d\tau_1 \; \hat{H}(\tau_n)\hat{H}(\tau_{n-1}) \ldots \hat{H}(\tau_1) \tag{A.7}$$

and likewise for the Hermitian conjugate

$$U^{\dagger}(t, t_0) = 1 + \sum_{n=1}^{\infty} \left(\frac{i}{\hbar}\right)^n \int_{t_0}^{t} d\tau_n \int_{t_0}^{\tau_n} d\tau_{n-1} \ldots \int_{t_0}^{\tau_2} d\tau_1 \; \hat{H}(\tau_1)\hat{H}(\tau_2) \ldots \hat{H}(\tau_n) \tag{A.8}$$

Note the time ordering, i.e. $0 \leq \tau_1 \leq \tau_2 \ldots \leq \tau_n \leq t$. The disadvantage of the last two expressions is that they can easily, if truncated, break down, since the overall Hamiltonian is treated perturbatively. The solution would be to separate the total Hamiltonian into a part that can be solved exactly H_0, and a part which is treated in a perturbative manner $\hat{H}'$, $\hat{H} = \hat{H}_0 + \hat{H}'$. Usually, H_0 represents the Hamiltonian of the system alone (and is, thus, time independent), while $\hat{H}'$ is a perturbation, caused by an interaction with an external force. The state vector can be written as

$$|\psi(t)\rangle = U_0(t, t_0)|\psi^{(\mathrm{I})}(t)\rangle \tag{A.9}$$

with the time evolution operator

$$U_0(t, t_0) = e^{-i\hat{H}_0(t-t_0)/\hbar} \tag{A.10}$$

and $|\psi^{(\mathrm{I})}(t)\rangle$ being the state vector in the so - called *interaction representation* where the evolution of the state vector is obtained by a perturbative expansion of the ”interaction part”, and not the overall Hamiltonian, as will be shown in the following. Equation of motion of $|\psi^{(\mathrm{I})}(t)\rangle$ can be obtained by plugging the Eq. A.9 into Eq. A.1, making use of the fact that U_0 is a unitary operator

$$i\hbar\frac{\partial|\psi^{(\mathrm{I})}(t)\rangle}{\partial t} = \hat{H}'^{(\mathrm{I})}(t)|\psi^{(\mathrm{I})}(t)\rangle \tag{A.11}$$

where the operator $\hat{H}'$ in the interaction representation has been introduced

$$\hat{H}'^{(\mathrm{I})}(t) = U_0^{\dagger}(t, t_0)\hat{H}'U_0(t, t_0). \tag{A.12}$$

Recall how we solved a similar type of equation of motion for U_0 and obtained the exact expression A.7. The same reasoning leads to

$$|\psi^{(\mathrm{I})}(t)\rangle = \sum_{n=0}^{\infty} \left(-\frac{i}{\hbar}\right)^n \int_{t_0}^{t} d\tau_n \int_{t_0}^{\tau_n} d\tau_{n-1} \dots \int_{t_0}^{\tau_2} d\tau_1 \\ \hat{H}'^{(\mathrm{I})}(\tau_n)\hat{H}'^{(\mathrm{I})}(\tau_{n-1}) \dots \hat{H}'^{(\mathrm{I})}(\tau_1)|\psi(t_0)\rangle \tag{A.13}$$

The results obtained either using the last expression or Eq. A.7 would be identical, if one would be able to keep an infinite number of terms. However, it is necessary to truncate them at a certain point. Due to the fact that for the evolution of $|\psi^{(\mathrm{I})}(t)\rangle$ only the interaction part of the Hamiltonian is treated perturbatively, it is expected that the convergence of the last expression would be faster, i.e., it could be truncated at lower order. Concerning the numerical effort, this is a big advantage of the interaction over the Schrödinger representation. It is possible at any moment to switch between those two representations by employing Eq. A.9.

To summarize, the time dependent phenomena can be studied either by solving the Schrödinger equation A.1, or the equation of motion for the time evolution operator, Eq. A.5. In the later case, perturbative calculations can be performed using the interaction representation.