Notes for the course in

QUANTUM MECHANICS

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CHAPTER ONE

Quantum Postulates & Density Operators

1.1 Postulates Revision

Postulate 1.1 (Schrödinger Equation)**.** The time evolution of a state is given by

$$i\hbar\frac{\partial}{\partial t}\left|\psi\right\rangle = H\left|\psi\right\rangle.$$

Theorem 1.2 (Time Evolution)**.** The time evolution of a state can be given by the exponential of the Hamiltonian operator, if it is not explicitly time dependent

$$\left|\psi(t)\right\rangle = e^{-iHt/\hbar}\left|\psi(0)\right\rangle.$$

Theorem 1.3 (Time-Dependent Hamiltonians)**.** Where the Hamiltonian is time-dependent, the we must use the **time-ordering operator**

$$\left|\psi(t)\right\rangle = T_+ e^{iHt/\hbar}\left|\psi(0)\right\rangle.$$

The time ordering operator is given by

Definition 1.4. The time-ordering operator is a metaoperator acting on operators

$$T_+\{H(t_1)H(t_2)\} = \begin{cases} H(t_1)H(t_2) & t_1 < t_2 \\ H(t_2)H(t_1) & \text{otherwise.} \end{cases}$$

Postulate 1.5 (General Measurement)**.** A general measurement of a quantum state is defined by a set of measurement operators $\{M_k\}_{k=1}^n$ satisfying the normalisation condition

$$\sum_{k=1}^{n} M_k^\dagger M_k = 1.$$

After the measurement, the quantum state is given by

$$\left|\psi\right\rangle \to \frac{M_k\left|\psi\right\rangle}{\sqrt{p_k}}$$

with probability

$$p_k = \left\langle\psi\right| M_k^\dagger M_k \left|\psi\right\rangle.$$

Example 1.6 (Projection Valued Measurement)**.** In a projection valued measurement, we have a set of orthogonal projectors for the measurement operators.

Remark 1.7 (Positive Operator Valued Measurement)**.** Notice that the operator $E_k = M_k^\dagger M_k$ is a positive operator. Hence, the set of measurement operators is associated with a set of positive operators E_k. We call these operators the POVM elements.

1.2 Density Operator

The density operator describes "mixed states", or states where we are not entirely certain what quantum state the quantum system is in. For example, in quantum computing, we do not know the output of a measurement, only that it will be a few states with a certain probability.

Definition 1.8 (Density Operator)**.** A density operator is a positive trace 1 operator.

Remark 1.9 (Physical Construction)**.** Where a system can be in any of a set of states $\{|\psi_k\rangle\}$ with probability p_k, the density operator is given by

$$\rho = \sum_{k=1}^{n} p_k |\psi_k\rangle \langle\psi_k| . \tag{1.1}$$

We can show that it has trace 1, either by picking the states $|\psi_k\rangle$ as a basis and using the normalisation of probability, or by computing this in any other basis.

Definition 1.10 (Pure State)**.** A state is pure if there is only one state in the expansion Eq. (1.1). Equivalently, the density matrix is an orthogonal projector.

Remark 1.11. This means that we know what state the density operator is in. Note: This state could be entangled.

Corollary 1.12. A state is pure if and only if $\mathrm{Tr}\,\rho^2 = 1$.

Theorem 1.13 (Time Evolution)**.** The time evolution of a density matrix is given by

$$\rho(t) = U\rho U^\dagger$$

where U is the propagator.

Proof. This is done simply by considering the expansion Eq. (1.1). □

Theorem 1.14 (Liouville Equation)**.** The time evolution of a density matrix is given by

$$\frac{\mathrm{d}\rho(t)}{\mathrm{d}t} = -i\hbar[H,\rho].$$

Proof. We write the Schrödinger equation and its transpose

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle &= H|\psi(t)\rangle \\ -i\hbar\langle\psi(t)| &= \langle\psi(t)|\,H. \end{aligned}$$

Then, we differentiate Eq. (1.1) to get

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\sum_{k=1}^{n} p_k |\psi_k(t)\rangle\langle\psi_k(t)| &= \sum_{k=1}^{n} p_k \left[|\dot{\psi}(t)\rangle\langle\psi(t)| + |\psi(t)\rangle\;\langle\dot{\psi}(t)| \right] \\ &= \sum_{k=1}^{n} p_k \left[-i\hbar H|\psi_k(t)\rangle\langle\psi_k(t)| + i\hbar|\psi_k(t)\rangle\langle\psi_k(t)|\,H\right] \\ &= -i\hbar[H,\rho]. \end{aligned}$$

□

Theorem 1.15. A measurement of a density matrix ρ has outcomes with probability

$$\mathbb{P}(j) = \mathrm{Tr}\left(M_j^\dagger M_j \rho\right)$$

where we denote the probability as $\mathbb{P}(j)$ to distinguish this from the probabilities in Eq. (1.1) and the state after the measurement is

$$\rho \to \frac{M_k \rho M_K^\dagger}{p_k}.$$

Proof. Let us consider the expansion Eq. (1.1) of ρ in states $\{|\psi_k\rangle\}_{k=1}^n$ and a measurement defined by measurement operators $\{M_j\}_{j=1}^m$. The probability of a measurement outcome j is given by the sum of the probabilities over all states k:

$$\begin{aligned}\mathbb{P}(j) &= \sum_{k=1}^n p_k \langle\psi_k| M_j^\dagger M_j |\psi_k\rangle \\ &= \sum_{k=1}^n p_k \,\mathrm{Tr}\left(M_j^\dagger M_j |\psi_k\rangle\langle\psi_k|\right) \\ &= \mathrm{Tr}\left(M_k^\dagger M_k \rho\right),\end{aligned}$$

The density matrix after the measurement is given by

$$\begin{aligned}\rho &= \sum_{k=1}^n p_k |\psi_k\rangle\langle\psi_k| \\ &\to \sum_{k=1}^n p_k \frac{M_j|\psi_k\rangle}{\sqrt{\mathbb{P}(j)}} \frac{\langle\psi_k| M_j^\dagger}{\sqrt{\mathbb{P}(j)}}.\end{aligned}$$ □

We have used the following lemma in the above proof;

Lemma 1.16.

$$\mathrm{Tr}(A|\psi\rangle\langle\psi|) = \langle\psi|A|\psi\rangle.$$

Proof. We have

$$\begin{aligned}\mathrm{Tr}(A|\psi\rangle\langle\psi|) &= \sum_{k=1}^n \langle\varphi_k|A|\psi\rangle\langle\psi|\varphi_k\rangle \\ &= \langle\psi|\varphi_k\rangle\langle\varphi_k|A|\psi\rangle \\ &= \langle\psi|A|\psi\rangle.\end{aligned}$$ □

Proposition 1.17 (Composite Systems)**.** For composite systems, the tensor product basis is given by the tensor products of the basis elements $|i\rangle \otimes |j\rangle$. Hence, the density matrix can be expanded in its matrix elements

$$\rho = \sum_{ij\mu\nu} \lambda_{ij\mu\nu} |i\rangle\langle j| \otimes |\mu\rangle\langle\nu|.$$

Remark 1.18 (Separable Systems)**.** If there are no cross terms, i.e. $\lambda_{ij\mu\nu} = \lambda_{ij}^A \lambda_{\mu\nu}^B$, we can write the density matrix as

$$\rho = \rho_A \otimes \rho_B$$

where

$$\rho_A = \sum_{ij} \lambda_{ij}^A |i\rangle\langle j|, \qquad \rho_B = \sum_{\mu\nu} \lambda_{\mu\nu}^B |\mu\rangle\langle\nu|.$$

However, systems are not in general separable. The next question is how to deal with observables of one system

1.3 The Interaction Picture

The interaction picture describes evolution under a composite Hamiltonian

$$H = H_S^0 + H_S^1.$$

While this can in principle be done all the time, in general we will use this where H_0 is an easy Hamiltonian to solve while H_1 is difficult. We want to apply concepts like in the Heisenberg picture to eliminate the rotation of the state from H_0. Thus, we make the following definition for the state vector in the interaction picture:

Definition 1.19. The state vector in the interaction picture is given by

$$|\psi_I(t)\rangle = U_S^\dagger(t, t_0) |\psi_S(t)\rangle$$

where $|\psi_I\rangle$ and $|\psi_S\rangle$ are the state vectors in the interaction and schrödinger picture respectively and $U_0(t)$ is the propagator.

Now, we seek the Schrödinger equation

Theorem 1.20. The state vector in the interaction picture satisfies the equation

$$i\hbar \frac{\mathrm{d}}{\mathrm{d}t} |\psi_I(t)\rangle = H_I^1 |\psi_I(t)\rangle .$$

Alternatively, the propagator satisfies

$$i\hbar \frac{\mathrm{d}U_I}{\mathrm{d}t} = H_I^1 U_I(t, t_0).$$

Proof. We differentiate directly:

$$\begin{aligned} i\hbar \frac{\mathrm{d}}{\mathrm{d}t} |\psi_I(t)\rangle &= i\hbar \frac{\mathrm{d}U_S^{0\dagger}}{\mathrm{d}t} |\psi_S(t)\rangle + U_S^{0\dagger}(t, t_0) \frac{\mathrm{d}}{\mathrm{d}t} |\psi_S(t)\rangle \\ &= -U_S^{0\dagger} H_S^0 |\psi_S(t)\rangle + U_S^{0\dagger} (H_S^0 + H_S^1) |\psi_S(t)\rangle \\ &= U_S^{0\dagger} H_S^1 U_S^0 |\psi_I(t)\rangle \end{aligned}$$

Thus, if we identify

$$H_I^1 = H_S^{0\dagger} H_S^1 U_S^0$$

this gives us the desired result. We can also write this in terms of the propagator in the interaction picture

$$\begin{aligned} i\hbar \frac{\mathrm{d}U_I}{\mathrm{d}t} |\psi_I(t_0)\rangle &= U_S^{0\dagger} H_S^1 U_S^0 U_I(t, t_0) |\psi_I(t_0)\rangle \\ i\hbar \frac{\mathrm{d}U_I}{\mathrm{d}t} &= U_S^{0\dagger} H_S^1 U_S^0 U_I(t, t_0) \\ &= H_I^1 U_I(t, t_0). \end{aligned}$$

□

We also have the following result that relates the propagators in the interaction and Schrödinger pictures:

Theorem 1.21.

$$U_S(t, t_0) = U_S^0(t, t_0) U_I(t, t_0).$$

Proof. We can write the state vector in the Schrödinger picture by

$$|\psi_S(t)\rangle = U_S(t, t_0) |\psi_S(t_0)\rangle = U_S(t, t_0) |\psi_I(t_0)\rangle$$

because the two state vectors coincide at $t = t_0$. At the same time, we can perform the time evolution using

$$|\psi_S(t)\rangle = U_S^0(t, t_0) |\psi_I(t)\rangle = U_S^0(t, t_0) U_I(t, t_0) |\psi_I(t_0)\rangle .$$

Hence,

$$U_S(t, t_0) = U_S^0(t, t_0) U_I(t, t_0).$$

□

The Schrödinger equation in the interaction picture can be computed usin ga series that we call a Dyson series:

Theorem 1.22. The propagator in the interaction picture $U_I(t,t_0)$ satisfies the equation

$$U(t,t_0) = \sum_{n=0}^{\infty} U_n(t,t_0)$$

where

$$U_n = \frac{(-i)^n}{\hbar^n n!} \int_{t_0}^{1} \mathrm{d}t_1 \int_{t_0}^{t} \mathrm{d}t_2 \cdots \int_{t_0}^{t} \mathrm{d}t_n \, \mathcal{T} H^1(t_1) H^1(t_2) \ldots H^1(t_n).$$

Proof. We first write the Schrödinger equation in integral form

$$U_I(t,t_0) = 1 - \frac{i}{\hbar} \int_{t_0}^{t} H^1(t_1) U_I(t_1,t_0)\, \mathrm{d}t_1 \,.$$

Then, we just simply substitute U_I back in:

$$\begin{aligned} U_I(t,t_0) &= 1 - \frac{i}{\hbar} \int_{t_0}^{t} H^1(t_1) \left(1 - \frac{i}{\hbar} \int_{t_0}^{t_1} H^1(t_2) U_I(t_2,t_0)\, \mathrm{d}t_2 \right) \mathrm{d}t_1 \\ &= 1 - \frac{i}{\hbar} \int_{t_0}^{t_1} H^1(t_1)\, \mathrm{d}t_1 + \left(\frac{-i}{\hbar} \right)^2 \int_{t_0}^{t} \int_{t_0}^{t_1} H^1(t_1) H^1(t_2)\, \mathrm{d}t_2\, \mathrm{d}t_1 \,. \end{aligned}$$

The annoying part is the bounds of this iterated integral. Because t_2 only goes from 0 to t_1, this is difficult to deal with. Thus, we use the time ordering operator to define

$$\int_{t_0}^{t} \int_{t_0}^{t_1} \cdots \int_{t_0}^{t_n} \mathcal{T} H^1(t_1) H^1(t_2) \ldots H^1(t_n) = \frac{1}{n!} \int_{t_0}^{t} \cdots \int_{t_0}^{t} \mathcal{T} H^1(t_1) H^1(t_2) \ldots H^1(t_n)\, \mathrm{d}t_1\, \mathrm{d}t_2 \ldots \mathrm{d}t_n \,.$$

This is the desired series. □

1.4 Time-Dependent Perturbation Theory

In this section, we consider a time-dependent perturbation

$$H(t) = H^0 + H^1(t).$$

We seek to expand the state vector in terms of the eigenstates of H^0:

$$|\psi(t)\rangle = \sum_n c_n |n\rangle \,.$$

Since we know that $c_n(t) = e^{-iE_n t/\hbar}$, we expand

$$|\psi(t)\rangle = \sum_n d_n(t) e^{-iE_n t/\hbar} |n\rangle \,.$$

Then, we seek the Schrödinger equation

Theorem 1.23. The d_n s satisfy the Schrödinger equation

$$0 = \sum_n (i\hbar \dot{d}_n - d_n H_1) e^{-\frac{iE_n t}{\hbar}} |n\rangle \,.$$

Proof. We act with $i\hbar\frac{\partial}{\partial t} - H^0 - H^1$ on the state vector:

$$\begin{aligned}
0 &= \left(i\hbar\frac{\partial}{\partial t} - H^0 - H^1\right)|\psi(t)\rangle \\
&= \left(i\hbar\frac{\partial}{\partial t} - H^0 - H^1\right)\sum_n d_n(t)e^{-\frac{iE_nt}{\hbar}}|n\rangle \\
&= \sum_n \left(i\hbar\dot{d}_n e^{-\frac{iE_nt}{\hbar}} + d_nE_ne^{-\frac{iE_nt}{\hbar}} - d_nE_ne^{-\frac{iE_nt}{\hbar}} - d_ne^{-\frac{iE_nt}{\hbar}}H^1|n\rangle\right) \\
&= \sum_n \left(i\hbar\dot{d}_n - d_nH^1\right)e^{-\frac{iE_nt}{\hbar}}|n\rangle .
\end{aligned}$$

□

This leads us to the following differential equation

Theorem 1.24. The d_n satisfy the following differential equation

$$i\hbar\dot{d}_k = \sum_n d_n(t)\langle k|H^1|n\rangle e^{\frac{i(E_k-E_n)t}{\hbar}}.$$

Proof. We do this by dotting the previous equation with $\langle k| e^{\frac{iE_kt}{\hbar}}$:

$$\begin{aligned}
0 &= \langle k| e^{\frac{iE_kt}{\hbar}}\sum_n(i\hbar\dot{d}_n - d_nH^1)e^{-\frac{iE_nt}{\hbar}}|n\rangle \\
&= i\hbar\dot{d}_k - d_k\langle k|H^1|n\rangle e^{\frac{i(E_k-E_n)t}{\hbar}}.
\end{aligned}$$

□

We can then approximate the solutions using the method of successive approximations, which is equivalent to Picard iteration. First, the 0-th order solution is the constant solution, $d_k = \text{const}$. Then, the 1st order solution is

$$i\hbar\dot{d}_k = \sum_n d_n(0)\langle k|H^1|n\rangle e^{\frac{i(E_k-E_n)t}{\hbar}}.$$

1.4.1 Fermi's Golden Rule