Notes for the course in

QUANTUM MECHANICS

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By Prof. Dr.

By

Jun Wei Tan

Julius-Maximilians-Universität Würzburg

jun-wei.tan@stud-mail.uni-wuerzburg.de

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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

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

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 $\operatorname{Tr}\rho^2 = 1$.

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

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

Then, we differentiate Eq. (1.1) to get

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

□

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

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

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:

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

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

$$H = H_0 + H_1.$$

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 define the state in the interaction picture to be

$$|\psi_I(t)\rangle = U_0^\dagger(t)\,|\psi_S(t)\rangle$$

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.

1.4 The Lindblad Equation