Appendix A

Quantum mechanics of complex systems

This tutorial is using the single-photon polarization qubit as the model system. The Hilbert space of this system is spanned by the horizontal $|H\rangle$ and vertical $|V\rangle$ polarization states, which form the primary (*canonical*) basis of the Hilbert space. Other useful polarization states are

- $+45°$ polarization state: $|{+45°}\rangle = (|H\rangle + |V\rangle)/\sqrt{2}$;
- $-45°$ polarization state: $|{-45°}\rangle = (|H\rangle - |V\rangle)/\sqrt{2}$;
- right circular polarization state: $|R\rangle = (|H\rangle + i\,|V\rangle)/\sqrt{2}$;
- left circular polarization state: $|L\rangle = (|H\rangle - i\,|V\rangle)/\sqrt{2}$.

A.1 The density operator

Definition A.1 Suppose our knowledge of the state of a quantum system is incomplete. We know that a system can be in state $|\psi_1\rangle$ with a probability p_1, in state $|\psi_2\rangle$ with a probability p_2, etc., with $\sum_i p_i = 1$ and the $|\psi\rangle$'s being normalized, but not necessarily orthogonal; the number of $|\psi_i\rangle$'s does not have to be equal to the dimension of the Hilbert space. Such description of the system its called its *statistical ensemble.*

Problem A.1 Suppose an ensemble is measured in basis $\{|a_m\rangle\}$ $(1 \le m \le n)$. Show that the probability of detecting $|a_m\rangle$ is given by

$$\mathrm{pr}_m = \langle a_m|\,\hat{\rho}\,|a_m\rangle\,, \tag{A.1}$$

where

$$\hat{\rho} = \sum_i p_i\,|\psi_i\rangle\langle\psi_i|\,. \tag{A.2}$$

Definition A.2 The operator $\hat{\rho}$ in the equation above is called the *density operator* of the ensemble. The matrix of the density operator $\rho_{jk} = \langle a_j|\,\hat{\rho}\,|a_k\rangle$ in any orthonormal basis $\{|a_j\rangle\}$ is called the *density matrix.*

Note A.1 As follows from Eq. (A.1), the entire information about physical properties of an ensemble (i.e. the probabilities of any possible measurement results) is contained in its density matrix.

We can also see that the diagonal elements of the density matrix equal the probabilities of detecting the system in the corresponding basis states. This result implies that the diagonal elements of the density matrix cannot be negative and that their total is 1.

Note A.2 Frequently, the term "density matrix" is used to call the density operator.

Problem A.2 Write the density matrices (in the canonical basis) of the following ensembles in the photon polarization Hilbert stace:
a) $|H\rangle$;
b) $x|H\rangle + y|V\rangle$;
c) $|H\rangle$ with a probability 1/2, $|V\rangle$ with a probability 1/2;
c) $|+45°\rangle$ with a probability 1/2, $|-45°\rangle$ with a probability 1/2;
d) $(|H\rangle + |V\rangle)/\sqrt{2}$ with a probability 1/2, $|H\rangle$ with a probability 1/4, $|L\rangle$ with a probability 1/4.

Problem A.3 Show that the density operator is Hermitian but not necessarily unitary.

Note A.3 In a continuous-variable basis, the density matrix Eq. (A.2) becomes a two-variable function

$$\rho(x, x') = \langle x|\hat{\rho}|x'\rangle = \sum_i p_i \psi_i(x)\psi_i^*(x'), \tag{A.3}$$

where $\psi_i(x)$ are the wavefunctions of the components of the statistical ensemble.

Problem A.4 Find the representation of the density operator of the state $a|0\rangle + b|1\rangle$ of a harmonic oscillator

a) in the Fock basis;

b) in the position basis.

Definition A.3 An ensemble $\hat{\rho}$ is called *pure* if there exists a state $|\psi_0\rangle$ such that $\hat{\rho} = |\psi_0\rangle\langle\psi_0|$. Otherwise it is called *mixed*.

Problem A.5 Show that for a given density operator, there always exists a decomposition in the form (A.2), i.e. as a sum of pure state density operators. (**Hint:** If the states $|\psi_i\rangle$ in decomposition (A.2) are orthogonal, they are eigenstates of the density operators and diagonalize it).

Problem A.6 Show that such a decomposition is not always unique by using the result of Ex. A.2(d) as an example.

Note A.4 In other words, different non-pure ensembles can give rise to the same density operator. All these ensembles exhibit identical physical behavior, so by performing measurements, we cannot determine the history of how the ensemble was prepared.

Problem A.7 Show that for a pure state $|\psi_0\rangle$, there is no other pure state decomposition (A.2) of its density operator $\hat{\rho}$ aside from the trivial $\hat{\rho} = |\psi_0\rangle\langle\psi_0|$.

Problem A.8 Which of the states of Ex. A.2 are pure?

Problem A.9 Show that a diagonal density matrix with more than one non-zero element necessarily represents a non-pure ensemble.

Definition A.4 The ensemble with a density operator $\hat{\rho} = \hat{\mathbf{1}}/n$ (where n is the dimension of the Hilbert space) is called *fully mixed*. With the system described by such an ensemble, no information about the system is available.

Definition A.5 Show that the density matrix of a fully mixed state is basis independent. Interpret this result.

Problem A.10 Show that the evolution of the density matrix in the Schrödinger picture is governed by

$$\frac{d\hat{\rho}}{dt} = -\frac{i}{\hbar}[\hat{H}, \hat{\rho}]. \tag{A.4}$$

and thus

$$\hat{\rho}(t) = e^{-\frac{i}{\hbar}\hat{H}t}\hat{\rho}(0)e^{\frac{i}{\hbar}\hat{H}t} \tag{A.5}$$

Note the opposite sign in comparison with Eqs. (4.49) and (4.51).

A.2 Trace

Definition A.6 The *trace* of an operator $\hat{A}$ is the sum of its matrix's diagonal elements:

$$\mathrm{Tr}\hat{A} = \sum_{m=1}^{n} \langle a_m | \hat{A} | a_m \rangle , \tag{A.6}$$

where $\{|a_m\rangle\}$ is a basis of the Hilbert space.

Note A.5 A trace is a number.

Problem A.11 Show that the trace of an operator is basis independent (even though the matrix does depend on the basis!).

Problem A.12 Show that $\mathrm{Tr}(\hat{A}\hat{B}) = \mathrm{Tr}(\hat{B}\hat{A})$.

Note A.6 It follows that $\mathrm{Tr}(\hat{A}_1 \ldots \hat{A}_k) = \mathrm{Tr}(\hat{A}_k \hat{A}_1 \ldots \hat{A}_{k-1})$ (chain rule).

Problem A.13 Propose an example showing that, generally speaking, $\mathrm{Tr}(\hat{A}\hat{B}\hat{C}) \neq \mathrm{Tr}(\hat{B}\hat{A}\hat{C})$.

Problem A.14 Show that for a density operator $\hat{\rho}$, $\mathrm{Tr}(\hat{\rho}^2) \leq 1$ with equality if and only if $\hat{\rho}$ describes a pure state.

Note A.7 The quantity $\mathrm{Tr}(\hat{\rho}^2) \leq 1$ is often used as a purity measure of state $\hat{\rho}$.

Problem A.15 Suppose a non-destructive projection measurement in the basis $\{|a_m\rangle\}$ is performed on an ensemble $\hat{\rho}$ and yields the result $|a_m\rangle$. Show that:
a) the (unnormalized) ensemble after the measurement is given by

$$\hat{\rho}' = \Pi_m \hat{\rho} \hat{\Pi}_m, \tag{A.7}$$

where $\hat{\Pi}_m = |a_m\rangle\langle a_m|$ is the projection operator;
b) the probability of this event is

$$\mathrm{pr}_m = \mathrm{Tr}\hat{\rho}'. \tag{A.8}$$

Note A.8 Eqs. (A.7) and (A.8) also apply to partial measurements on a tensor product system. For example, if Alice and Bob share an ensemble $\hat{\rho}_{AB}$ and Alice performs a measurement in the basis $\{|a_m\rangle_A\}$ on her part of the ensemble, the resulting state is described by Eq. (A.7) with $\hat{\Pi}_m = |a_m\rangle_A \langle a_m|_A \otimes \hat{\mathbf{1}}_B$.

Problem A.16 Apply Eq. (A.7) to determine the probability of detecting a (+45°)-polarization in each of the ensembles of Ex. A.2.

Problem A.17 Show that the expectation value of an observable $\hat{X}$ in an ensemble $\hat{\rho}$ is $\mathrm{Tr}(\hat{\rho}\hat{X})$.

Problem A.18 Suppose an ensemble is subjected to a non-destructive projective measurement, and the measurement result is not known. Show that such a procedure will set all the off-diagonal elements from the ensemble's density matrix in the measurement basis to zero, while leaving the diagonal elements intact.

Definition A.7 A *partial trace* of a bipartite ensemble $\hat{\rho}_{AB}$ over subsystem A is the density operator in Hilbert space B is defined as

$$\mathrm{Tr}_A(\hat{\rho}_{AB}) = \sum_{m=1}^{n} \langle a_m | \hat{\rho}_{AB} | a_m \rangle . \tag{A.9}$$

It is also called the *reduced density operator*.

Problem A.19 Show that the partial trace is basis independent.

Problem A.20 Show that the reduced density operator describes the quantum state of Bob's subsystem if no information about Alice's subsystem is available.

Problem A.21 Show that if the original bipartite ensemble is in a pure, separable (non-entangled) state, then both Alice's and Bob's reduced density operators are also pure states.

Problem A.22 For each of the four Bell states, find the reduced density operator for each qubit.

Problem A.23 Find the reduced density operator for Alice's qubit of the state $|\Psi_{AB}\rangle = x|00\rangle + y|11\rangle + z|01\rangle + t|10\rangle$.

Problem A.24 Show that for an entangled state of two qubits $|\Psi_{AB}\rangle = x|00\rangle + y|11\rangle$, the reduced density matrix is

$$\hat{\rho}_A = \begin{pmatrix} |x|^2 & 0 \\ 0 & |y|^2 \end{pmatrix}. \tag{A.10}$$

Note A.9 Remarkably, a reduced density operator of a pure state can be a mixed state.

A.3 Measurement, entanglement, and decoherence

How a measurement apparatus works. We would like to perform a measurement associated with the $\{|0\rangle, |1\rangle\}$ basis on a system which is initially in a pure state $|\psi\rangle_s = x|0\rangle_s + y|1\rangle_s$. We employ an apparatus which is initially in the state $|\psi\rangle_A = |0\rangle_A$. Note that the apparatus is a complex entity, and its state is the simultaneous state of the many particles composing it. We bring the apparatus into interaction with the system and it *entangles* itself with it, producing a joint state $|\Psi_{sA}\rangle = x|0\rangle_s \otimes |0\rangle_A + y|1\rangle_s \otimes |1\rangle_A$. The apparatus is then removed, after which the system is in the state (A.10), which is consistent with Ex. A.18. If the apparatus is in the state $|0\rangle$, the system is also in the state $|0\rangle$, and the associated probability is $|x|^2$. The probability of the state $|1\rangle$ is $|y|^2$.

Definition A.8 A system may interact with the environment and entangle itself with it. Since the state of the environment cannot be controlled or measured, the system's density matrix (in the entanglement basis) will lose its off-diagonal elements as a result of such interaction (see Ex. A.18 and A.24). This undesired loss of quantum information caused by such "inadvertent" measurements is called *irreversible (homogeneous) dephasing* or *decoherence*.

Problem A.25 Consider an ensemble of electrons in an initial state $|\psi(t=0)\rangle = (|m_s = +1/2\rangle + |m_s = -1/2\rangle)/\sqrt{2}$. The electron is placed in a magnetic field $\vec{B}$ pointing in the z direction.
a) Find the density matrix in the $m_s = \pm 1/2$ basis and its evolution.
b) Suppose the ensemble experiences decoherence so, in addition to the precession in the field, the off-diagonal elements of the density matrix decay according to the factor $e^{-\gamma t}$ with $\gamma \ll \mu_B B/\hbar$. Find the expectation value of the x-component of the spin and plot it as a function of time.

Note A.10 Since most physical interactions have a highly local character, the position basis is particularly likely to become the basis in which the entanglement with the environment will take place. For example, a particle in a superposition state $|\psi\rangle = (|x_1\rangle + |x_2\rangle)/\sqrt{2}$ will entangle itself with the state of the environment ($|E\rangle$) in the following manner:

$$|\psi\rangle \otimes |E\rangle \to \frac{1}{\sqrt{2}} \left(|x_1\rangle \otimes |E_{x1}\rangle + |x_2\rangle \otimes |E_{x2}\rangle\right), \tag{A.11}$$

where $|E_{x1}\rangle$ and $|E_{x2}\rangle$ are two "incompatible" (i.e. orthogonal) states of the environment "having seen" the particle in positions x_1 and x_2, respectively. Because the environment cannot be measured, the state of the particle becomes a non-pure ensemble

$$\hat{\rho}_{\text{after}} = \frac{1}{2} \left(|x_1\rangle\langle x_1| + |x_2\rangle\langle x_2|\right), \tag{A.12}$$

i.e. localized *either* at x_1 *or* at x_2, but showing no coherence of these two states. For this reason, macroscopic coherent superpositions (i.e. the "Schrödinger cat" states) do not occur in nature.