

**1) Measurements:** A hermitean operator  $\Lambda$  has orthonormal eigenkets  $|\lambda_1\rangle$ ,  $|\lambda_2\rangle$ ,  $|\lambda_3\rangle$  and  $|\lambda_4\rangle$ . The corresponding eigenvalues are  $\lambda_1 = 3$ , and  $\lambda_2 = \lambda_3 = \lambda_4 = 1$ . In terms of the  $\{|\lambda_i\rangle\}$ -basis, a certain state,  $|\psi\rangle$ , is given by

$$|\psi\rangle = i|\lambda_1\rangle + |\lambda_2\rangle - i|\lambda_3\rangle - |\lambda_4\rangle.$$

- a) Calculate the probability of obtaining the result  $\lambda = 1$  upon measurement of the physical quantity which the operator  $\Lambda$  represents.
- b) Calculate the probability of obtaining  $\lambda = 2$ . Why do you get this result?
- c) Calculate the probability of obtaining  $\lambda = 3$ .
- d) Suppose that the observation is made a large number of times on an identically prepared state  $|\psi\rangle$ . Calculate the mean of the values obtained for  $\lambda$ .
- e) Calculate the mean-square value.
- f) Is the mean-square value equal to the square of the mean value?
- g) In the light of your answer to part (f), would you say that this quantum mechanical system has fluctuations?
- h) Do classical systems fluctuate?
- i) Suppose  $\lambda$  is measured and the result  $\lambda = 1$  is obtained. Calculate the state vector immediately after the measurement is made.
- j)  $\{|\lambda_i\rangle\}$  are simultaneously eigenkets of the operator  $\Omega$  corresponding to the observable  $\omega$ . Their  $\omega$ -eigenvalues are  $\omega_1 = \omega_2 = \omega_3 = 7$ , and  $\omega_4 = 5$ . Suppose  $\Omega$  is measured immediately after the result  $\lambda = 1$  is obtained. Calculate the possible outcomes, and their probabilities.
- k) Suppose the result  $\omega = 7$  is obtained. Calculate the state vector immediately thereafter? What are the possible results if an immediate measurement of  $\lambda$  is now made?

**2) Angular momentum (after Shankar, 4.2.1):** Consider the following matrices representing operators on the Hilbert space  $\mathcal{V}^3(\mathcal{C})$ :

$$L_x \leftrightarrow \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad L_y \leftrightarrow \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \quad L_z \leftrightarrow \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

- If  $L_z$  is measured, determine the possible values one can obtain.
- Take the state in which  $L_z = 1$ . In this state, determine the values of  $\langle L_x \rangle$ ,  $\langle L_x^2 \rangle$  and  $\Delta L_x$ .
- Find the eigenvalues and normalised eigenstates of  $L_x$  in the  $L_z$  basis.
- If the system is in the state with  $L_z = -1$  and  $L_x$  is measured, state the possible outcomes, together with their probabilities.
- Consider the state  $|\psi\rangle \propto |1\rangle + |0\rangle + \sqrt{2}|-1\rangle$  (where  $\{|0, \pm 1\rangle\}$  is the  $L_z$  basis). If  $L_z^2$  is measured and the result  $+1$  is obtained, give the state after the measurement. Determine how probable this result was. If, subsequently,  $L_z$  is measured, determine the possible outcomes and their respective probabilities.
- The system is in a state for which the probabilities  $P(\ell)$  of obtaining the result  $\ell$  for  $L_z$  are  $\{P(1), P(0), P(-1)\} = \{1/4, 1/2, 1/4\}$ . Determine the most general normalized state consistent with this information. Specify how many independent phases characterise this state. Is the physical content of the state sensitive to these phases? Justify your answer by considering the probability to find zero upon measuring  $L_x$ .

**3) Mean positions and momenta:** A particle moving in one dimension is in a state described by the wave function

$$\psi(x) = \frac{N e^{iqx}}{\sqrt{x^2 + a^2}}.$$

- Calculate the value of  $N$  that normalises  $\psi$ .
- Calculate the normalised probability density for finding the particle at position  $x$ .
- Calculate the mean particle position.
- Is the root mean square particle position finite?
- Calculate the probability of finding the particle in the interval  $-a \leq \sqrt{3}x \leq a$ .
- Calculate the mean value of the momentum of the particle.
- Calculate the root mean square value of the momentum.

[Hint: Use the substitution  $x = a \tan \theta$ .]

**4) Ehrenfest's theorem:** Consider a one-dimensional particle of mass  $m$  moving in an external potential  $V(x)$ . The particle is in the state  $|\psi\rangle$ . Use the following steps to prove Ehrenfest's theorem, which says that

$$\frac{d}{dt}\langle\psi(t)|P|\psi(t)\rangle = -\langle\psi(t)|V'(X)|\psi(t)\rangle$$

where  $V'(X)$  is the operator  $\partial V(x)/\partial x|_{x=X}$ .

- a) By recognising that  $\langle\psi(t)|P|\psi(t)\rangle$  depends on  $t$  through both the bra and the ket, write down an expression for  $\frac{d}{dt}\langle\psi(t)|P|\psi(t)\rangle$ .
- b) By using the time-dependent Schrödinger equation, eliminate the time-derivative terms in favour of the hamiltonian operator acting on a bra or a ket.
- c) Rewrite your answer to part (b) in terms of the commutator between the operators  $P$  and  $H$ .
- d) Establish that if  $H = (P^2/2m) + V(X)$  then  $[P, H] = -i\hbar V'(X)$ . Use this result to prove Ehrenfest's theorem.
- e) Briefly discuss the time-evolution of momentum expectation values, as described by Ehrenfest's theorem, in relation to the classical time-evolution of momentum as described by Hamilton's equations.

Now follow these alternative steps to prove Ehrenfest's theorem, using the Heisenberg picture rather than the Schrödinger picture. (Of course, the result is picture-independent.)

- f) For an arbitrary operator  $F$  define the Heisenberg operator  $F(t)$  through  $F(t) = e^{iHt/\hbar} F e^{-iHt/\hbar}$ . Use this definition to establish an equation of motion for  $P(t)$ .
- g) If the commutator between two arbitrary operators  $A$  and  $B$ , is the operator  $C$ , i.e.,  $[A, B] = C$ , evaluate the commutator  $[A(t), B(t)]$  in terms of  $C(t)$ ? Use this result to prove that

$$i\hbar \frac{d}{dt} P(t) = [P(t), H] = -i\hbar V'(X(t)).$$

- h) By taking the expectation value of this operator equation in the state  $|\psi\rangle$ , establish Ehrenfest's theorem.

**5) Density matrices – optional but strongly recommended:** In class, we considered ensembles of identical systems, prepared in identical quantum states. Practically, this might be achieved by measuring some observable and retaining *only* cases for which some specified non-degenerate eigenvalue is obtained. Often, particularly in statistical mechanics, it is useful to consider more general ensembles. Instead of retaining a single state, we retain a variety of states, each with a certain statistical frequency. To be more precise, our ensemble contains systems in a variety of distinct states  $\{|\psi_i\rangle\}$ . The ensemble is defined by giving the probability  $p_i$  of finding each of the possible states  $|\psi_i\rangle$ . Notice that there is no requirement

for  $\{|\psi_i\rangle\}$  to be orthogonal, or for them to be complete. We shall, however, require them to be normalised, so that  $\langle\psi_i|\psi_i\rangle = 1$  for each  $i$ . As the  $\{p_i\}$  are probabilities,

$$0 \leq p_i \leq 1 \quad \text{for each } i, \quad \text{and} \quad \sum_i p_i = 1.$$

An ensemble, such as this, is described by an operator,  $\rho$ , usually called *the density matrix*, and defined by

$$\rho \equiv \sum_i p_i |\psi_i\rangle\langle\psi_i|.$$

For any operator  $\Omega$  the quantity  $\text{Tr } \Omega$  is known as the *trace* of  $\Omega$  and is defined by

$$\text{Tr } \Omega \equiv \sum_n \langle u_n | \Omega | u_n \rangle,$$

where  $\{|u_n\rangle\}$  is some complete orthonormal basis.

a) Show that

$$\text{Tr } \Omega \rho = \text{Tr } \rho \Omega = \sum_i p_i \langle \psi_i | \Omega | \psi_i \rangle.$$

- b) Discuss why  $\text{Tr } \rho \Omega$  is the mean value of the results of observations of the quantity  $\Omega$ , when observations of  $\Omega$  are made on systems drawn from the the ensemble specified by  $\rho$ .
- c) Demonstrate the following statements:
- c-i)  $\text{Tr } \rho = 1$ ;
  - c-ii)  $\text{Tr } \rho^2 \leq 1$ ;
  - c-iii) If  $\text{Tr } \rho^2 = 1$  then all but one of the probabilities  $\{p_i\}$  vanish.
  - c-iv) An ensemble for which  $\text{Tr } \rho^2 = 1$  is called a *pure state*, because it is defined by a single quantum state. Which state is this? Note that if  $\text{Tr } \rho^2 \leq 1$  then the ensemble is defined by more than one state, and is called a *mixed state*;
  - c-v) The operator  $\rho$  is hermitean;
  - c-vi)  $\rho^2 = \rho$  for a pure state only.
- d) Suppose the observable  $\Lambda$  is measured in the ensemble defined by  $\rho$ . The eigenvalues of  $\Lambda$  are  $\{\lambda_a\}$ . Show that the probability of obtaining the result  $\lambda$  is given by  $\text{Tr } \mathcal{P}(\lambda)\rho$ , where  $\mathcal{P}(\lambda)$  is the projection operator on to the  $\lambda$ -subspace (*i.e.*, the subset of states with eigenvalue  $\lambda$ ).
- e) To describe a system in thermal equilibrium at temperature  $T$ , we often use an ensemble called the *canonical ensemble*, which is defined by the density matrix

$$\rho = Z^{-1} \exp(-H/k_B T).$$

Here,  $k_B$  is Boltzmann's constant,  $H$  is the hamiltonian operator, and the partition function  $Z \equiv \text{Tr } \exp(-H/k_B T)$  provides the normalisation. The Helmholtz free energy  $F$  is given by  $F = -k_B T \ln Z$ ; the internal energy  $U$  is given by  $U = \text{Tr } \rho H$ ; and the entropy  $S$  is given by  $S = -k_B \text{Tr } \rho \ln \rho$ . Show that  $F = U - TS$ .

**6) General projection operators – optional:** Consider the normalised kets  $|u\rangle$  and  $|w\rangle$ .

- a) Show that  $P_u \equiv |u\rangle\langle u|$  is a projection operator.
- b) On to what subspace does  $P_u$  project?
- c) Now also consider  $P_w \equiv |w\rangle\langle w|$ . Under what condition is the operator  $(P_u + P_w)$  also projection operator?

**7) Symmetrisation of operators – optional:** Consider the classical variable  $\omega = x^2p$  built from the position,  $x$ , and momentum,  $p$ , of a one-dimensional classical particle. Suppose we *quantise* by promoting the classical variables  $x$  and  $p$  to hermitean operators  $X$  and  $P$ .

- a) Is the operator  $X^2P$  hermitean?
- b) Form the fully symmetrised operator,  $\Omega$ , corresponding to the classical variable  $\omega$ .
- c) Show that this symmetrised operator is hermitean.

**8) Uncertainty principle – optional:** Shankar, 9.4.2, page 244.