

# Physics 241: Final Report

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## 1 Linear vector spaces and operators. Wavefunctions and state vectors.

- (a) **Obtain the spectral decomposition of a state vector or wave function with respect to an arbitrary basis set: discretely and continuously labelled elements.**

The principle of spectral decomposition states that an arbitrary state of a system can be expressed as a superposition of states in a basis. A basis is a set of linearly independent vectors that completely span the considered state space. Thus, given a state vector  $|\psi\rangle$  in Hilbert space that forms a discrete basis  $|\phi_i\rangle$ , the state vector can be expressed as

$$|\psi\rangle = \sum_i b_i |\phi_i\rangle = \sum_i \langle\phi_i|\psi\rangle |\phi_i\rangle \quad (1)$$

For a continuous basis, we have continuously indexed vectors  $|\phi_\alpha\rangle$  where

$$|\psi\rangle = \int d\alpha \zeta(\alpha) |\phi_\alpha\rangle = \int d\alpha \left[ \int dV \langle\phi_\alpha|\psi\rangle \right] |\phi_\alpha\rangle \quad (2)$$

- (b) **Use inner products to perform basis transformations.**

Recall that the inner product of state kets  $|a\rangle$  and  $|b\rangle$  is denoted as  $\langle a|b\rangle$ . Let us now consider a transformation  $S$  between one orthonormal basis  $\{\phi_i\}$  to another orthonormal basis  $\{\chi_k\}$ . The elements of this transformation matrix is given by

$$S_{ik} = \langle\phi_i|\chi_k\rangle \quad (3)$$

while the elements of the said matrix's Hermitian conjugate  $S^\dagger$  is given by

$$((S_{ik})^T)^* = \langle\chi_k|\phi_i\rangle = S_{ki}^\dagger \quad (4)$$

Note that we can also use closure relations:

$$\sum_i |\phi_i\rangle \langle\phi_i| = 1 \quad (5)$$

$$\sum_k |\chi_k\rangle \langle\chi_k| = 1 \quad (6)$$

and orthogonalization conditions:

$$\langle\phi_i|\phi_j\rangle = \delta_{ij} \quad (7)$$

$$\langle\chi_k|\chi_l\rangle = \delta_{kl} \quad (8)$$

to perform a change of basis from  $\{\phi_i\}$  to  $\{\chi_k\}$  for...

- ... the components of a state ket  $|\psi\rangle$ . Substituting Eq. (5), we have

$$\begin{aligned}\langle\chi_k|\psi\rangle &= \langle\chi_k|1|\psi\rangle \\ &= \sum_i \langle\chi_k|\phi_i\rangle \langle\phi_i|\psi\rangle \\ \langle\chi_k|\psi\rangle &= \sum_i S_{ki}^\dagger \langle\phi_i|\psi\rangle\end{aligned}\tag{9}$$

after applying Eq. (4).

- ... the components of a state bra  $\langle\psi|$ . Substituting Eq. (5), we have

$$\begin{aligned}\langle\psi|\chi_k\rangle &= \langle\psi|1|\chi_k\rangle \\ &= \sum_i \langle\psi|\phi_i\rangle \langle\phi_i|\chi_k\rangle \\ \langle\psi|\chi_k\rangle &= \sum_i \langle\psi|\phi_i\rangle S_{ik}\end{aligned}\tag{10}$$

after applying Eq. (3).

- ... the elements of an operator  $A$ . Substituting Eq. (5), we have

$$\begin{aligned}\langle\chi_k|A|\chi_l\rangle &= \langle\chi_k|1 \cdot A \cdot 1|\chi_l\rangle \\ &= \sum_i \sum_j \langle\chi_k|\phi_i\rangle \langle\phi_i|A|\phi_j\rangle \langle\phi_j|\chi_l\rangle \\ A_{kl} &= \sum_{i,j} S_{ki}^\dagger A_{ij} S_{jl}\end{aligned}\tag{11}$$

after applying Eqs. (3) and (4).

- (c) **Explain how commuting observables can be used to generate additional quantum numbers to label degenerate states.**

A set of commuting operators in quantum mechanics is called a complete set of commuting observables (CSCO) if the eigenvalues of these operators completely specify the state of a system. Now, consider an operator  $\hat{A}$  with eigenvalues  $\{a_n\}$  that corresponds to an observable  $\alpha$ . If some of these eigenvalues are degenerate, we have to differentiate the eigenfunctions corresponding to the same eigenvalue. To do so, we must introduce a second observable  $\beta$  (corresponding to an operator  $\hat{B}$ ), which is compatible with  $\alpha$ . Using the compatibility theorem which states that  $\hat{A}$  and  $\hat{B}$  have a common eigenbasis and are commuting if  $\alpha$  and  $\beta$  are compatible, we can obtain eigenvalue pairs  $\{(a_n, b_n)\}$ . If a pair uniquely specifies a state of this basis, then we have formed a CSCO and the degeneracy in  $\hat{A}$  vanishes. If it is still degenerate, we can look for another observable compatible with  $\alpha$  and perform the same process until a CSCO is obtained. Since quantum numbers correspond to the eigenvalues of operators, we see here that commuting observables can be used to generate additional quantum numbers to label degenerate states.

- (d) **Establish the link between quantum states and elements of a Hilbert space; observables and Hermitian operators.**

- The Hilbert space is a vector space that is also a complete inner product since it has a natural inner product (dot product) that gives a sense of distance. It was proven that square integrable functions can be elements of a complete inner product space, or effectively, a Hilbert space. Note that square integrable functions are functions that give a finite value when integrating the square of its absolute value.

On the other hand, wavefunctions that mathematically describe quantum states must be square integrable because their probabilistic interpretation should be finite. To better understand this concept, let us consider the wavefunction  $\psi(\mathbf{r}, t)$  of a particle. The probability

of finding the particle in a volume  $d^3r$  at time  $t$  is represented by  $|\psi(\mathbf{r}, t)|^2 d^3r$  and the total probability of finding this particle is given by integrating the probability over all space:

$$\int |\psi(\mathbf{r}, t)|^2 d^3r = 1 \quad (12)$$

Note here that the integral does not diverge. Thus, we return to the earlier point that wavefunctions in quantum mechanics are square integrable. Therefore, quantum states can essentially be elements to a Hilbert space.

- Operators are mathematical rules that transform one function to another. Hermitian operators are operators that are self-adjoint and satisfy certain boundary conditions. One of their properties is that they have real eigenvalues. On the other hand, observables like position, momentum, charge, etc. can be mathematically described in quantum mechanics by operators. However, these operators must have real eigenvalues to correspond to physical quantities so they must be self-adjoint. This means that observables are described specifically by Hermitian operators

## 2 Postulates of quantum mechanics. Position and translation (generators). Momentum.

### (a) Review the core postulates of quantum mechanics.

1. The dynamical state of a quantum mechanical system is at each instant of time associated with a state vector  $|\psi\rangle$ . Possible state vectors are elements of a complex linear vector space  $S$ , referred to as state space or Hilbert space.
2. Every observable  $\mathcal{A}$  of a quantum mechanical system is associated with a linear Hermitian operator  $A$  whose eigenstates form a complete orthonormal basis for the quantum mechanical state space
3. (a) The only value which can be obtained as a result of an attempt to measure an observable  $\mathcal{A}$  of a quantum mechanical system in a normalized state  $|\psi\rangle$  is one of the eigenvalue in the spectrum of the Hermitian operator  $A$  associated with it. Exactly which eigenvalue will be measured cannot generally be predicted. It is possible however to predict the probability for obtaining each eigenvalue.  
 (b) Immediately after a measurement of an observable  $\mathcal{A}$  performed on a system in the state  $|\psi\rangle$  that yields the value  $a$ , the state of the system is the normalized projection of  $|\psi\rangle$  onto the eigensubspace  $S_a$  associated with the eigenvalue measured.
4. Between measurements, the state vector  $|\psi(t)\rangle$  of a quantum system evolves deterministically according to Schrödinger's equation of motion

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = H |\psi(t)\rangle \quad (13)$$

in which the Hamiltonian operator  $H$  is the observable associated with the total energy of the system at time  $t$ .

### (b) Use an infinitesimal translation operator and its postulated properties to identify momentum as a generator of translations.

An infinitesimal translation operator that describes an infinitesimal translation by  $d\mathbf{x}'$  is denoted by  $\mathcal{T}(d\mathbf{x}')$ . It has four properties:

1. Unitarity:  $\mathcal{T}^\dagger(d\mathbf{x}') \mathcal{T}(d\mathbf{x}') = 1$
2. An infinitesimal translation by  $d\mathbf{x}'$  followed another by  $d\mathbf{x}''$  can be thought as an infinitesimal translation by the vector sum of the two:  $\mathcal{T}(d\mathbf{x}'') \mathcal{T}(d\mathbf{x}') = \mathcal{T}(d\mathbf{x}' + d\mathbf{x}'')$

3. A translation in the opposite direction is equivalent to the inverse of the original translation:  
 $\mathcal{T}(-d\mathbf{x}') = \mathcal{T}^{-1}(d\mathbf{x}')$
4. The operator reduces to the identity as  $d\mathbf{x}' \rightarrow 0$ :  $\lim_{d\mathbf{x}' \rightarrow 0} \mathcal{T}(d\mathbf{x}') = 1$

We let the infinitesimal translation operator to be of the form

$$\mathcal{T}(d\mathbf{x}') = 1 - i\mathbf{K} \cdot d\mathbf{x}' \quad (14)$$

where the components of  $\mathbf{K}$  -  $K_x$ ,  $K_y$ ,  $K_z$  - are Hermitian operators, since all of the postulated properties can be satisfied with this form as shown:

1. Ignoring second order terms of  $d\mathbf{x}'$ , we get

$$\begin{aligned} \mathcal{T}^\dagger(d\mathbf{x}') \mathcal{T}(d\mathbf{x}') &= (1 + i\mathbf{K}^\dagger \cdot d\mathbf{x}') (1 - i\mathbf{K} \cdot d\mathbf{x}') \\ &= 1 - i(\mathbf{K} - \mathbf{K}^\dagger) \cdot d\mathbf{x}' + \mathcal{O}[(d\mathbf{x}')^2] \\ \mathcal{T}^\dagger(d\mathbf{x}') \mathcal{T}(d\mathbf{x}') &\simeq 1 \end{aligned} \quad (15)$$

- 2.

$$\begin{aligned} \mathcal{T}(d\mathbf{x}'') \mathcal{T}(d\mathbf{x}') &= (1 - i\mathbf{K} \cdot d\mathbf{x}'') (1 - i\mathbf{K} \cdot d\mathbf{x}') \\ &\simeq 1 - i\mathbf{K} \cdot (d\mathbf{x}' + d\mathbf{x}'') \\ \mathcal{T}(d\mathbf{x}'') \mathcal{T}(d\mathbf{x}') &= \mathcal{T}(d\mathbf{x}' + d\mathbf{x}'') \end{aligned} \quad (16)$$

- 3.

$$\mathcal{T}(-d\mathbf{x}') = 1 + i\mathbf{K} \cdot d\mathbf{x}' = \mathcal{T}^{-1}(d\mathbf{x}') \quad (17)$$

- 4.

$$\lim_{d\mathbf{x}' \rightarrow 0} \mathcal{T}(d\mathbf{x}') = \lim_{d\mathbf{x}' \rightarrow 0} (1 - i\mathbf{K} \cdot d\mathbf{x}') = 1 \quad (18)$$

Moving on, we note that an infinitesimal translation in classical mechanics can be performed using a generating function:

$$F(\mathbf{x}, \mathbf{P}) = \mathbf{x} \cdot \mathbf{P} + \mathbf{p} \cdot d\mathbf{x} \quad (19)$$

where  $\mathbf{p}$  and  $\mathbf{P}$  are the old and new momenta respectively and are related by  $\mathbf{p} = \mathbf{P}$ . Notice the similarity between Eqs. (14) and (19) (especially when we also note that the generating function for the identity transformation is  $\mathbf{x} \cdot \mathbf{P}$ ). We can infer that

$$\mathbf{K} = \frac{\mathbf{p}}{(\text{a universal constant with the dimensions of work or energy})} \quad (20)$$

as  $\mathbf{K}$  must be in dimensions of  $\text{length}^{-1}$  with  $\mathbf{K} \cdot d\mathbf{x}'$  being dimensionless. It turns out that this universal constant is the same as  $\hbar$ . Thus, the infinitesimal translation can be written as

$$\mathcal{T}(d\mathbf{x}') = 1 - i\frac{\mathbf{P}}{\hbar} \cdot d\mathbf{x}' \quad (21)$$

which shows momentum as a generator of translations.

- (c) **Perform a change of basis (Fourier transformation) to relate the coordinate space wavefunction  $\langle \mathbf{x} | \psi \rangle$  and the momentum space wavefunctions  $\langle \mathbf{p} | \psi \rangle$ .**

For simplicity, let's first consider one-dimensional spaces in performing this change of basis. Recall that

$$\langle x | \hat{p} | p \rangle = p \langle x | p \rangle = -i\hbar \frac{d}{dx} \langle x | p \rangle \quad (22)$$

Solving this differential equation,

$$\langle x | p \rangle = N \exp\left(\frac{ipx}{\hbar}\right) \quad (23)$$

where  $N$  is the normalization constant which we can take from

$$\begin{aligned}
\langle x|x' \rangle &= \int \langle x|p \rangle \langle p|x' \rangle dp \\
\delta(x-x') &= \int \left( N \exp\left(\frac{ipx}{\hbar}\right) \right) \left( N^* \exp\left(\frac{-ipx'}{\hbar}\right) \right) dp \\
&= |N|^2 \int \exp\left[\frac{ip(x-x')}{\hbar}\right] dp \\
\delta(x-x') &= |N|^2 2\pi\hbar \delta(x-x')
\end{aligned} \tag{24}$$

after using the orthogonality condition  $\langle x|x' \rangle = \delta(x-x')$ . With  $|N|^2 = 1/(2\pi\hbar)$  and choosing  $N$  as positive in value, Eq. (23) becomes

$$\langle x|p \rangle = \frac{1}{\sqrt{2\pi\hbar}} \exp\left(\frac{ipx}{\hbar}\right) \tag{25}$$

Thus, a change of basis from position space to momentum space yields

$$\langle x|\psi \rangle = \int \langle x|p \rangle \langle p|\psi \rangle dp = \frac{1}{\sqrt{2\pi\hbar}} \int \exp\left(\frac{ipx}{\hbar}\right) \langle p|\psi \rangle dp \tag{26}$$

while the change vice versa yields

$$\langle p|\psi \rangle = \int \langle p|x \rangle \langle x|\psi \rangle dx = \frac{1}{\sqrt{2\pi\hbar}} \int \exp\left(\frac{-ipx}{\hbar}\right) \langle x|\psi \rangle dx \tag{27}$$

Extending these results to three dimensions, we have

$$\langle \mathbf{x}|\psi \rangle = \left(\frac{1}{2\pi\hbar}\right)^{3/2} \int \exp\left(\frac{i\mathbf{p} \cdot \mathbf{x}}{\hbar}\right) \langle \mathbf{p}|\psi \rangle d^3p \tag{28}$$

and

$$\langle \mathbf{p}|\psi \rangle = \left(\frac{1}{2\pi\hbar}\right)^{3/2} \int \exp\left(\frac{-i\mathbf{p} \cdot \mathbf{x}}{\hbar}\right) \langle \mathbf{x}|\psi \rangle d^3x \tag{29}$$

### 3 Time evolution. Heisenberg picture. Coherent states.

#### (a) Determine the time development of states in the Schrodinger picture.

States evolve with the use of a time evolution operator  $\mathcal{U}(t, t_0)$ :

$$|\psi(t)\rangle = \mathcal{U}(t, t_0) |\psi(t_0)\rangle \tag{30}$$

Let's consider an infinitesimal time evolution operator  $\mathcal{U}(t_0 + dt, t_0)$ . In the same manner as constructing an infinitesimal translation operator in terms of momentum as a generator of translations, we can construct  $\mathcal{U}(t_0 + dt, t_0)$  in terms of the Hamiltonian  $H$  as a generator of time evolution:

$$\mathcal{U}(t_0 + dt, t_0) = 1 - i\frac{H}{\hbar}dt \tag{31}$$

Using the composition property of the time evolution operator

$$\mathcal{U}(t_2, t_1)\mathcal{U}(t_1, t_0) = \mathcal{U}(t_2, t_0), \tag{32}$$

we have

$$\mathcal{U}(t + dt, t_0) = \mathcal{U}(t + dt, t)\mathcal{U}(t, t_0) = \left(1 - \frac{iHdt}{\hbar}\right) \mathcal{U}(t, t_0) \tag{33}$$

which we can rearrange into

$$\begin{aligned}\mathcal{U}(t+dt, t_0) - \mathcal{U}(t, t_0) &= -\frac{iH}{\hbar} dt \mathcal{U}(t, t_0) \\ d\mathcal{U}(t, t_0) &= \frac{H}{i\hbar} dt \mathcal{U}(t, t_0) \\ i\hbar \frac{d}{dt} \mathcal{U}(t, t_0) &= H \mathcal{U}(t, t_0)\end{aligned}\tag{34}$$

Multiplying both sides by  $|\psi(t_0)\rangle$  and applying Eq. (30), we get

$$\begin{aligned}i\hbar \frac{d}{dt} \mathcal{U}(t, t_0) |\psi(t_0)\rangle &= H \mathcal{U}(t, t_0) |\psi(t_0)\rangle \\ i\hbar \frac{d}{dt} |\psi(t)\rangle &= H |\psi(t)\rangle\end{aligned}\tag{35}$$

which we notice to be the Schrödinger equation.

- (b) **Determine the time development of operators in the Heisenberg picture.** Let  $t_0 = 0$ . We can define the time evolution of operators to be

$$A^{(H)}(t) \equiv \mathcal{U}^\dagger(t) A^{(S)} \mathcal{U}(t)\tag{36}$$

where  $H$  and  $S$  represents the observable in the Heisenberg and Schrödinger picture respectively. Taking the derivative of this with respect to time, we get

$$\begin{aligned}\frac{dA^{(H)}}{dt} &= \frac{\partial \mathcal{U}^\dagger}{\partial t} A^{(S)} \mathcal{U} + \mathcal{U}^\dagger A^{(S)} \frac{\partial \mathcal{U}}{\partial t} \\ &= -\frac{1}{i\hbar} \mathcal{U}^\dagger H \mathcal{U} \mathcal{U}^\dagger A^{(S)} \mathcal{U} + \frac{1}{i\hbar} \mathcal{U}^\dagger A^{(S)} \mathcal{U} \mathcal{U}^\dagger H \mathcal{U} \\ &= \frac{1}{i\hbar} A^{(H)} \mathcal{U}^\dagger H \mathcal{U} - \frac{1}{i\hbar} \mathcal{U}^\dagger H \mathcal{U} A^{(H)} \\ \frac{dA^{(H)}}{dt} &= \frac{1}{i\hbar} [A^{(H)}, \mathcal{U}^\dagger H \mathcal{U}]\end{aligned}\tag{37}$$

by substituting in

$$\frac{\partial \mathcal{U}}{\partial t} = \frac{1}{i\hbar} H \mathcal{U}, \quad \frac{\partial \mathcal{U}^\dagger}{\partial t} = -\frac{1}{i\hbar} \mathcal{U}^\dagger H\tag{38}$$

and applying the definition of a commutator

$$[A, B] \equiv AB - BA\tag{39}$$

Since the Hamiltonian is Hermitian and the time evolution operator is unitary,

$$\mathcal{U}^\dagger H \mathcal{U} = \mathcal{U}^\dagger \mathcal{U} \overset{1}{H}\tag{40}$$

Thus, we obtain

$$\frac{dA^{(H)}}{dt} = \frac{1}{i\hbar} [A^{(H)}, H]\tag{41}$$

which is known as the Heisenberg equation of motion.

- (c) **Construct coherent (Glauber) states. Calculate the expectation values of position and momentum in these states.**

We can construct a coherent state  $|\lambda\rangle$  that satisfies  $a|\lambda\rangle = \lambda|\lambda\rangle$  by translating the oscillator ground state  $|0\rangle$  by some finite distance:

$$|\lambda\rangle = \mathcal{T}(l) |0\rangle = e^{-i\hat{p}l/\hbar} |0\rangle\tag{42}$$

By solving the Heisenberg equations of motion for a harmonic oscillator, we know that  $\hat{x}(t)$  and  $\hat{p}(t)$  are given by

$$\hat{x}(t) = \hat{x}(0) \cos \omega t + \frac{\hat{p}(0)}{m\omega} \sin \omega t \quad (43)$$

$$\hat{p}(t) = -m\omega \hat{x}(0) \sin \omega t + \hat{p}(0) \cos \omega t \quad (44)$$

Recall the state in Eq. (42). Then,  $\langle \hat{x}(t) \rangle$  is calculated as

$$\begin{aligned} \langle \hat{x}(t) \rangle &= \langle \lambda | \hat{x}(t) | \lambda \rangle \\ &= \langle 0 | e^{i\hat{p}l/\hbar} \hat{x}(t) e^{-i\hat{p}l/\hbar} | 0 \rangle \\ &= \langle 0 | e^{i\hat{p}l/\hbar} \left( \hat{x}(0) \cos \omega t + \frac{\hat{p}(0)}{m\omega} \sin \omega t \right) e^{-i\hat{p}l/\hbar} | 0 \rangle \\ \langle \hat{x}(t) \rangle &= \langle 0 | e^{i\hat{p}l/\hbar} \hat{x}(0) e^{-i\hat{p}l/\hbar} | 0 \rangle \cos \omega t + \frac{1}{m\omega} \langle 0 | e^{i\hat{p}l/\hbar} \hat{p}(0) e^{-i\hat{p}l/\hbar} | 0 \rangle \sin \omega t \end{aligned} \quad (45)$$

In a one-dimensional space, the effect of the finite translation operator on  $\langle \hat{x} \rangle$  and  $\langle \hat{p} \rangle$  results to the following relations:

$$e^{i\hat{p}l/\hbar} \hat{x}(0) e^{-i\hat{p}l/\hbar} = \hat{x}(0) + l, \quad e^{i\hat{p}l/\hbar} \hat{p}(0) e^{-i\hat{p}l/\hbar} = \hat{p}(0) \quad (46)$$

Applying these on  $\langle \hat{x}(t) \rangle$ , we get

$$\begin{aligned} \langle \hat{x}(t) \rangle &= \langle 0 | (\hat{x}(0) + l) | 0 \rangle \cos \omega t + \frac{1}{m\omega} \langle 0 | \hat{p}(0) | 0 \rangle \sin \omega t \\ &= \cancel{\langle 0 | \hat{x}(0) | 0 \rangle}^0 \cos \omega t + l \cancel{\langle 0 | 0 \rangle}^1 \cos \omega t + \frac{1}{m\omega} \cancel{\langle 0 | \hat{p}(0) | 0 \rangle}^0 \sin \omega t \\ \langle \hat{x}(t) \rangle &= l \cos \omega t \end{aligned} \quad (47)$$

In the same manner for  $\langle \hat{p}(t) \rangle$ , we have

$$\begin{aligned} \langle \hat{p}(t) \rangle &= \langle \lambda | \hat{p}(t) | \lambda \rangle \\ &= \langle 0 | e^{i\hat{p}l/\hbar} \hat{p}(t) e^{-i\hat{p}l/\hbar} | 0 \rangle \\ &= \langle 0 | e^{i\hat{p}l/\hbar} (-m\omega \hat{x}(0) \sin \omega t + \hat{p}(0) \cos \omega t) e^{-i\hat{p}l/\hbar} | 0 \rangle \\ &= -m\omega \langle 0 | e^{i\hat{p}l/\hbar} \hat{x}(0) e^{-i\hat{p}l/\hbar} | 0 \rangle \sin \omega t + \langle 0 | e^{i\hat{p}l/\hbar} \hat{p}(0) e^{-i\hat{p}l/\hbar} | 0 \rangle \cos \omega t \\ &= -m\omega \langle 0 | (\hat{x}(0) + l) | 0 \rangle \sin \omega t + \langle 0 | \hat{p}(0) | 0 \rangle \cos \omega t \\ &= -m\omega \cancel{\langle 0 | \hat{x}(0) | 0 \rangle}^0 \sin \omega t - m\omega l \cancel{\langle 0 | 0 \rangle}^1 \sin \omega t + \cancel{\langle 0 | \hat{p}(0) | 0 \rangle}^0 \cos \omega t \\ \langle \hat{p}(t) \rangle &= -m\omega l \sin \omega t \end{aligned} \quad (48)$$

In addition, with the calculated form of  $\langle \hat{x}(t) \rangle$  and  $\langle \hat{p}(t) \rangle$ , we can see that they have the same time development as a classical oscillator.

## 4 Schrodinger's wave equation, Hamilton-Jacobi formulation. WKB approximation.

- (a) **Identify the classical analogs of the amplitude and phase of a wavefunction in a Hamilton-Jacobi formulation.**

The wavefunction in a Hamilton-Jacobi formulation can be written as

$$\psi(\mathbf{x}, t) = \sqrt{\rho(\mathbf{x}, t)} \exp \left[ \frac{iS(\mathbf{x}, t)}{\hbar} \right] \quad (49)$$

Its amplitude given by  $\sqrt{\rho(\mathbf{x}, t)}$  corresponds to the probability density of the particle that the wavefunction pertains. Then, we can think of this as the variable that gives the position

of the particle in classical mechanics. As for the phase which is given by  $S$ , the relation of its gradient to the probability flux  $j$  given by

$$\mathbf{j} = \frac{\rho \nabla S}{m} \quad (50)$$

implies that the phase can be classically analogous to the rate of motion the particle has since the probability flux is related to the momentum when integrated over all space.

- (b) **Set up the WKB connection formulas to be able to approximate the energy eigenvalues in (spatially) slowly-varying potentials.**

In the classical region ( $E > V(x)$ ), the wavefunction in the semiclassical limit is

$$\psi(x) \cong c_+ \frac{1}{\sqrt{p(x)}} \exp \left[ \frac{i}{\hbar} \int^x dx' p(x') \right] + c_- \frac{1}{\sqrt{p(x)}} \exp \left[ -\frac{i}{\hbar} \int^x dx' p(x') \right] \quad (51)$$

where  $p(x) = \sqrt{2m(E - V(x))}$ . On the other hand, the wavefunction in the said limit for the forbidden region ( $E < V(x)$ ) is

$$\psi(x) \cong d_+ \frac{1}{\sqrt{\kappa(x)}} \exp \left[ \frac{1}{\hbar} \int^x dx' \kappa(x') \right] + d_- \frac{1}{\sqrt{\kappa(x)}} \exp \left[ -\frac{1}{\hbar} \int^x dx' \kappa(x') \right] \quad (52)$$

where  $\kappa(x) = \sqrt{2m(V(x) - E)}$ . Note that  $c_{\pm}$  and  $d_{\pm}$  are constants. We need connection formulas to connect these two regions that are separated by a classical turning point  $x_0$  ( $E = V(x_0)$ ). If the forbidden region is to the right of the classical region, then the connection formula is

$$\frac{1}{\sqrt{\kappa(x)}} \exp \left[ -\frac{1}{\hbar} \int_a^x \kappa(x') dx' \right] \Rightarrow \frac{2}{\sqrt{p(x)}} \cos \left[ \frac{1}{\hbar} \int_x^a p(x') dx' - \frac{\pi}{4} \right] \quad (53)$$

if the given wavefunction is known to be exponentially falling in the forbidden region. On the other hand, if the given wavefunction is  $90^\circ$  out of phase in the allowed region and grows exponentially in the forbidden region, then the connection formula is

$$\frac{1}{\sqrt{p(x)}} \cos \left[ \frac{1}{\hbar} \int_x^a p(x') dx' + \frac{\pi}{4} \right] \Rightarrow \frac{1}{\sqrt{\kappa(x)}} \exp \left[ \frac{1}{\hbar} \int_a^x \kappa(x') dx' \right] \quad (54)$$

## 5 Propagators, Feynman path integrals.

- (a) **Recognize the propagator as a Green's function and integral kernel.**

We start with the time evolution of states is given by

$$|\psi(t)\rangle = \exp \left[ -\frac{iH(t-t_0)}{\hbar} \right] |\psi(t_0)\rangle = \sum_{a'} |a'\rangle \langle a'|\psi(t_0)\rangle \exp \left[ -\frac{iE_{a'}(t-t_0)}{\hbar} \right] \quad (55)$$

where  $|a'\rangle$  form an energy eigenbasis. Multiplying both sides by  $\langle \mathbf{x}'|$ ,

$$\langle \mathbf{x}'|\psi(t)\rangle = \sum_{a'} \langle \mathbf{x}'|a'\rangle \langle a'|\psi(t_0)\rangle \exp \left[ -\frac{iE_{a'}(t-t_0)}{\hbar} \right] \quad (56)$$

Defining

$$u_{a'}(\mathbf{x}') = \langle \mathbf{x}'|a'\rangle \quad (57)$$

to be energy eigenfunctions, we can write  $\langle \mathbf{x}'|\psi(t)\rangle$  as

$$\psi(\mathbf{x}', t) = \sum_{a'} C_{a'}(t_0) u_{a'}(\mathbf{x}') \exp \left[ -\frac{iE_{a'}(t-t_0)}{\hbar} \right] \quad (58)$$



where also noted that

$$\langle a' | \psi(t_0) \rangle = \int \langle a' | \mathbf{x}' \rangle \langle \mathbf{x}' | \psi(t_0) \rangle d^3x \quad (59)$$

which is the rule in wave mechanics for getting the the initial state's expansion coefficients

$$C_{a'}(t_0) = \int u_{a'}^*(\mathbf{x}') \psi(\mathbf{x}', t) d^3x \quad (60)$$

With Eqs. (56) and (59), it seems that we have some kind of integral operator acting on the initial wave function to produce the final wave function

$$\psi(\mathbf{x}'', t) = \int d^3x' K(\mathbf{x}'', t; \mathbf{x}', t_0) \psi(\mathbf{x}', t_0) \quad (61)$$

where the integral kernel  $K(\mathbf{x}'', t; \mathbf{x}', t_0)$  is the propagator in wave mechanics given by

$$K(\mathbf{x}'', t; \mathbf{x}', t_0) = \sum_{a'} \langle \mathbf{x}'' | a' \rangle \langle a' | \mathbf{x}' \rangle \exp \left[ \frac{-iE_{a'}(t - t_0)}{\hbar} \right] \quad (62)$$

This propagator has two properties:

1. It satisfies the time-dependent Schrödinger equation at  $t > t_0$  with fixed  $\mathbf{x}'$  and  $t_0$ .
2.  $\lim_{t \rightarrow t_0} K(\mathbf{x}'', t; \mathbf{x}', t_0) = \delta^3(\mathbf{x}'' - \mathbf{x}')$

Now, recall that Green's functions satisfy

$$\mathcal{L}G(x, y) = \delta(x - y) \quad (63)$$

and are solutions to differential equations with a forcing term given by a point source (the Dirac delta term). With this and the properties of the propagator in mind, we can say that  $K(\mathbf{x}'', t; \mathbf{x}', t_0)$  is a Green's function for time-dependent Schrödinger equation that satisfies

$$\left[ -\left( \frac{\hbar^2}{2m} \right) \nabla''^2 + V(\mathbf{x}'') - i\hbar \frac{\partial}{\partial t} \right] K(\mathbf{x}'', t; \mathbf{x}', t_0) = -i\hbar \delta^3(\mathbf{x}'' - \mathbf{x}') \delta(t - t_0) \quad (64)$$

**(b) Write down the propagator as a Feynman path integral.**

The propagator as a Feynman path integral can be written as

$$K(x_N, t_N; x_1, t_1) = \int_{x_1}^{x_N} \mathcal{D}[x(t)] e^{iS[x(t)]/\hbar} \quad (65)$$

where the multi-dimensional integral operator is defined to be

$$\int_{x_1}^{x_N} \mathcal{D}[x(t)] \equiv \lim_{N \rightarrow \infty} \left( \frac{m}{2\pi i \hbar \Delta t} \right)^{(N-1)/2} \int dx_{N-1} \int dx_{N-2} \cdots \int dx_2 \quad (66)$$

and  $S[x(t)]$  is the action defined as

$$S[x(t)] \equiv \int_{t_1}^{t_N} L_{\text{classical}}(x, \dot{x}) dt \quad (67)$$

in which  $L_{\text{classical}}(x, \dot{x})$  is the Lagrangian in classical mechanics.

**(c) Provide examples where a path integral formulation is convenient.**

The path integral formulation provides an elegant way of solving statistical mechanics problems since the partition function can be written as a path integral. This formulation has also been used in problems involving the Aharonov-Bohm effect, magnetic monopoles and the quantization of electric charge as we can infer interesting effect in path integrals on situations where there are holes in the configuration space and two paths between the same initial and final point are not necessarily deformable into one another.

## 6 Potentials and gauge transformations.

- (a) **Describe how the scalar and vector potentials enter the Schrödinger equation for quantum systems in the presence of electromagnetic fields.**

We first consider the Lagrangian of a charged particle in an EM field which is expressed as

$$L = \frac{1}{2}m\dot{\mathbf{x}}^2 + \frac{e}{c}\mathbf{A} \cdot \dot{\mathbf{x}} - e\phi \quad (68)$$

where  $e$  is the charge,  $\mathbf{A}$  is vector potential and  $\phi$  is the scalar potential. Taking the canonical momentum evaluated as

$$\mathbf{p} \equiv \frac{\partial L}{\partial \dot{\mathbf{x}}} = m\dot{\mathbf{x}} + \frac{e}{c}\mathbf{A}, \quad (69)$$

we can obtain the Hamiltonian for this system:

$$H = \mathbf{p} \cdot \dot{\mathbf{x}} - L = \frac{1}{2}m\dot{\mathbf{x}}^2 + e\phi = \frac{(\mathbf{p} - \frac{e}{c}\mathbf{A})^2}{2m} + e\phi = \frac{(-i\hbar\nabla - \frac{e}{c}\mathbf{A})^2}{2m} + e\phi \quad (70)$$

in which we used  $\mathbf{p} = -i\hbar\nabla$ . In the context of quantum mechanics, we can see that the scalar and vector potentials appear in the Schrödinger equation by substituting the Hamiltonian into the said equation as follows:

$$\begin{aligned} i\hbar \frac{\partial \psi}{\partial t} &= H\psi \\ &= \left[ \frac{(-i\hbar\nabla - \frac{e}{c}\mathbf{A})^2}{2m} + e\phi \right] \psi \end{aligned} \quad (71)$$

- (b) **Explain how the Aharonov-Bohm effect can distinguish situations in which a quantum particle confined to an annular cylinder is subject to the vector potential of a magnetic field within the hollow or not.**

For context, the given scenario is the bound-state version of the Aharonov-Bohm effect. As a recap, this effect is a phenomenon where a charged particle is quantum mechanically affected by EM potentials in a region with non-existent electric and magnetic fields. If the vector potential of a magnetic field within the hollow affects the particle confined to the annular cylinder through the Aharonov-Bohm effect, we should be able to observe a change in the energy spectrum (which we mathematically see from the Hamiltonian in Eq. (70) with the replacement of the gradient  $\nabla$  to  $\nabla - ie/(\hbar c)\mathbf{A}$ ).

## 7 Angular momentum and tensor operators.

- (a) **Identify advanced experimental situations that utilize angular momentum eigenstates.**

There are experiments in molecular, atomic, and nuclear spectroscopy that utilize angular momentum eigenstates since they can be used to obtain the selection rules that describes all the possible transitions from one quantum state to another. They are also used in scattering and collision experiments in particle physics as they can shed light on the nature of particles involved in these experiments.

- (b) **Construct angular momentum operators as generators of rotations.**

We must define the angular momentum operator  $J$ , along with the property of it being Hermitian, so that the infinitesimal operator for rotation about the direction characterized by a unit vector  $\hat{\mathbf{n}}$  by an infinitesimal angle  $d\phi$  is in the form

$$\mathcal{D}(\hat{\mathbf{n}}, d\phi) = 1 - i \left( \frac{\mathbf{J} \cdot \hat{\mathbf{n}}}{\hbar} \right) d\phi \quad (72)$$

which shows that the angular momentum is a generator of rotations.

- (c) **Familiarize oneself with the notation used for vector and tensor operators. Use the formalism to write angular momentum operators as spherical tensor operators.**

From the formalism of vector and tensor operators, we define a spherical tensor operator of rank  $k$  with  $(2k + 1)$  components as

$$\mathcal{D}(R)T_q^{(k)}\mathcal{D}^\dagger(R) = \sum_{q'=-k}^k \mathcal{D}_{q'q}^{(k)}(R)T_{q'}^{(k)} \quad (73)$$

Expressing Eq. (72) as

$$\mathcal{D}(R) = 1 - \frac{i\varepsilon \mathbf{J} \cdot \hat{\mathbf{n}}}{\hbar}, \quad (74)$$

Eq. (73) becomes

$$\left(1 + \frac{i\mathbf{J} \cdot \hat{\mathbf{n}}\varepsilon}{\hbar}\right) T_q^{(k)} \left(1 - \frac{i\mathbf{J} \cdot \hat{\mathbf{n}}\varepsilon}{\hbar}\right) = \sum_{q'=-k}^k T_{q'}^{(k)} \left\langle kq' \left| \left(1 + \frac{i\mathbf{J} \cdot \hat{\mathbf{n}}\varepsilon}{\hbar}\right) \right| kq \right\rangle \quad (75)$$

which can be written as

$$\left[\mathbf{J} \cdot \hat{\mathbf{n}}, T_q^{(k)}\right] = \sum_{q'} T_{q'}^{(k)} \langle kq' | \mathbf{J} \cdot \hat{\mathbf{n}} | kq \rangle \quad (76)$$

By taking  $\hat{\mathbf{n}}$  in the direction of  $\hat{\mathbf{z}}$  and  $(\hat{\mathbf{x}} + i\hat{\mathbf{y}})$  and considering only the non-vanishing elements of  $J_z$  and  $J_\pm$ , we get

$$\left[J_z, T_q^{(k)}\right] = \hbar q T_q^{(k)} \quad (77)$$

and

$$\left[J_\pm, T_q^{(k)}\right] = \hbar \sqrt{(k \mp q)(k \pm q + 1)} T_{q\pm 1}^{(k)} \quad (78)$$

from Eq. (76). These relations shows angular momentum operators expressed as spherical tensor operators.

- (d) **Illustrate use cases for the projection formula**

The projection formula (or projection theorem), a special case of the Wigner-Eckart theorem which states that it is possible to factor the matrix element into a reduced matrix element, is given by

$$\langle \alpha', jm' | V_q | \alpha, jm \rangle = \frac{\langle \alpha', jm | \mathbf{J} \cdot \mathbf{V} | \alpha, jm \rangle}{\hbar^2 j(j+1)} \langle jm' | J_q | jm \rangle \quad (79)$$

where  $\mathbf{V}$  is an arbitrary vector observable. The fraction term here is the reduced matrix element.

As an example of using the projection formula, let us consider the 2p orbitals of a Hydrogen atom when an external magnetic field is applied. The Hamiltonian for this scenario has a contribution from

$$W = \frac{eB}{2m_e c} (L_z + 2S_z) \quad (80)$$

Although this operator is not proportional to  $J_z$ , the projection theorem states that matrix elements in a subspace given by fixed  $j$  are proportional to the matrix elements of  $J_z$ . Note that

$$\mathbf{L} \cdot \mathbf{J} = \mathbf{L} \cdot (\mathbf{L} + \mathbf{S}) = \mathbf{L}^2 + \mathbf{L} \cdot \mathbf{S} = \mathbf{L}^2 + \frac{1}{2}(\mathbf{J}^2 - \mathbf{L}^2 - \mathbf{S}^2) \quad (81)$$

by applying  $\mathbf{L} \cdot \mathbf{S} = \frac{1}{2}(\mathbf{J}^2 - \mathbf{L}^2 - \mathbf{S}^2)$ . In the same manner, we have

$$\mathbf{S} \cdot \mathbf{J} = \mathbf{S}^2 + \frac{1}{2}(\mathbf{J}^2 - \mathbf{L}^2 - \mathbf{S}^2) \quad (82)$$

The expectation values for these relations are

$$\begin{aligned} \langle j, m | \mathbf{L} \cdot \mathbf{J} | j, m \rangle &= \frac{\hbar^2}{2} [j(j+1) + l(l+1) - s(s+1)] \\ \langle j, m | \mathbf{S} \cdot \mathbf{J} | j, m \rangle &= \frac{\hbar^2}{2} [j(j+1) + s(s+1) - l(l+1)] \end{aligned} \quad (83)$$

Applying the projection theorem and recalling that the matrix elements of  $J_z$  are  $\langle j, m' | J_z | j, m \rangle = m\hbar\delta_{m'm}$ , we have

$$\begin{aligned}\langle j, m | L_z | j, m \rangle &= \frac{\langle j, m | \mathbf{J} \cdot \mathbf{L} | j, m \rangle}{\hbar^2 j(j+1)} \langle j, m | J_z | j, m \rangle \\ &= \frac{\hbar^2}{2\hbar^2 j(j+1)} [j(j+1) + l(l+1) - s(s+1)] m\hbar = \frac{\hbar m}{2j(j+1)} [j(j+1) + l(l+1) - s(s+1)]\end{aligned}\quad (84)$$

In the same manner, we obtain

$$\langle j, m | S_z | j, m \rangle = \frac{\hbar m}{2j(j+1)} [j(j+1) + s(s+1) - l(l+1)] \quad (85)$$

Since the energy correction that corresponds to Eq. (80) is  $E_W = \langle W \rangle$  for any  $j$ , we get

$$\begin{aligned}E_W &= \frac{eB}{2m_e c} \langle (L_z + 2S_z) \rangle \\ &= \frac{eB}{2m_e c} m\hbar \left( \frac{1}{2} - \frac{s(s+1) - l(l+1)}{2j(j+1)} + 1 + 2 \frac{s(s+1) - l(l+1)}{2j(j+1)} \right) \\ &= \left( \frac{3}{2} + \frac{s(s+1) - l(l+1)}{2j(j+1)} \right) \frac{qB}{2m_e c} m\hbar \\ E_W &= g_j \frac{qB}{2m_e c} m\hbar\end{aligned}\quad (86)$$

where  $g_j$  is the Lande g-factor.

## 8 Potentials and gauge transformations.

**Construct AM eigenkets and derive the corresponding eigenvalues using ladder operators.**

We define a new operator given by

$$\mathbf{J}^2 \equiv J_x J_x + J_y J_y + J_z J_z \quad (87)$$

which commutes with the components of  $\mathbf{J}$  ( $J_x$ ,  $J_y$ ,  $J_z$ ). By convention, we pick  $J_z$  among the three components to be diagonalized simultaneously with  $\mathbf{J}^2$  since the said components do not commute with each other. Denoting the eigenvalues of  $\mathbf{J}^2$  and  $J_z$  as  $a$  and  $b$  respectively, we can construct the eigenkets of these two operators as

$$\begin{aligned}\mathbf{J}^2 |a, b\rangle &= a |a, b\rangle \\ J_z |a, b\rangle &= b |a, b\rangle\end{aligned}\quad (88)$$

To determine the values of the eigenvalues, it would be better to define the ladder operators

$$J_{\pm} \equiv J_x \pm iJ_y \quad (89)$$

which are non-Hermitian and satisfy the commutation relations

$$[J_+, J_-] = 2\hbar J_z, \quad [J_z, J_{\pm}] = \pm\hbar J_{\pm}, \quad [\mathbf{J}^2, J_{\pm}] = 0 \quad (90)$$

Note that  $J_{\pm}$  changes the eigenvalue of  $J_z$  by one unit of  $\hbar$  but it does not affect the eigenvalues of  $\mathbf{J}^2$  as follows:

$$\begin{aligned}J_z (J_{\pm} |a, b\rangle) &= (J_z, J_{\pm} - J_{\pm} J_z + J_{\pm} J_z) |a, b\rangle \\ &= ([J_z, J_{\pm}] + J_{\pm} J_z) |a, b\rangle \\ &= (b \pm \hbar) (J_{\pm} |a, b\rangle)\end{aligned}\quad (91)$$

$$\begin{aligned}\mathbf{J}^2 (J_{\pm} |a, b\rangle) &= (\mathbf{J}^2, J_{\pm} - J_{\pm} \mathbf{J}^2 + J_{\pm} \mathbf{J}^2) |a, b\rangle \\ &= ([\mathbf{J}^2, J_{\pm}] + J_{\pm} \mathbf{J}^2) |a, b\rangle \\ &= a (J_{\pm} |a, b\rangle)\end{aligned}\quad (92)$$

where we used some of the relations in Eq. (90).

Now, suppose we let  $J_+$  to act on a simultaneous eigenket of  $\mathbf{J}^2$  and  $J_z$  by  $n$  time. This results to another eigenket of  $\mathbf{J}^2$  and  $J_z$  in which  $b$  (the  $J_z$  eigenvalue) is increased by  $n\hbar$  and  $a$  (the  $\mathbf{J}^2$  eigenvalue) remains unchanged. However, we will find out that the given value of  $a$  imposes an upper limit to  $b$ . To do this, note that

$$\begin{aligned}\mathbf{J}^2 - J_z^2 &= \frac{1}{2} (J_+ J_- + J_- J_+) \\ &= \frac{1}{2} (J_+ J_+^\dagger + J_+^\dagger J_+)\end{aligned}\tag{93}$$

We expect  $J_+ J_+^\dagger$  and  $J_+^\dagger J_+$  to have non-negative expectation values since

$$J_+^\dagger |a, b\rangle \xleftrightarrow{\text{DC}} \langle a, b | J_+, \quad J_+ |a, b\rangle \xleftrightarrow{\text{DC}} \langle a, b | J_+^\dagger\tag{94}$$

So, we have

$$\langle a, b | (\mathbf{J}^2 - J_z^2) | a, b \rangle \geq 0\tag{95}$$

which implies the condition

$$a \geq b^2\tag{96}$$

It follows that  $b$  must have a maximum value such that

$$J_+ |a, b_{\text{max}}\rangle = 0\tag{97}$$

This also implies

$$J_- J_+ |a, b_{\text{max}}\rangle = 0\tag{98}$$

which becomes

$$(\mathbf{J}^2 - J_z^2 - \hbar J_z) |a, b_{\text{max}}\rangle = 0\tag{99}$$

with

$$\begin{aligned}J_- J_+ &= J_x^2 + J_y^2 - i (J_y J_x - J_x J_y) \\ &= J_x^2 + J_y^2 - i [J_y J_x] \\ &= \mathbf{J}^2 - J_z^2 - \hbar J_z\end{aligned}\tag{100}$$

Since  $|a, b_{\text{max}}\rangle$  is not a null ket, the relation in Eq. (99) is true only if

$$a - b_{\text{max}}^2 - b_{\text{max}}\hbar = 0\tag{101}$$

which can be written as

$$a = b_{\text{max}}(b_{\text{max}} + \hbar)\tag{102}$$

In the same manner, we can say that there should exist a minimum value of  $b$  such that

$$J_- |a, b_{\text{min}}\rangle = 0\tag{103}$$

From

$$\begin{aligned}J_+ J_- &= J_x^2 + J_y^2 + i (J_y J_x - J_x J_y) \\ &= J_x^2 + J_y^2 + i [J_y J_x] \\ &= \mathbf{J}^2 - J_z^2 + \hbar J_z\end{aligned}\tag{104}$$

we can infer that

$$a = b_{\text{min}}(b_{\text{min}} + \hbar)\tag{105}$$

as previously done to get Eq. (102). Comparing Eqs. (102) and (105), we have

$$b_{\text{max}} = -b_{\text{min}}\tag{106}$$

Thus, with  $b_{\max}$  being positive, values of  $b$  must lie within

$$-b_{\max} \leq b \leq b_{\max} \quad (107)$$

Notice that we can obtain the state of  $|a, b_{\max}\rangle$  by letting  $J_+$  successively act on  $|a, b_{\min}\rangle$  a finite number of times. So, we get

$$b_{\max} = b_{\min} + n\hbar \quad (108)$$

with  $n$  as some integer which results to

$$b_{\max} = \frac{n\hbar}{2} \quad (109)$$

after applying Eq. (107). By convention, we define  $j = b_{\max}/\hbar$  and work with this variable instead of  $b_{\max}$  so that

$$j = \frac{n}{2} \quad (110)$$

From this, we see that the maximum value of the  $J_z$  eigenvalue is  $j\hbar$  where  $j$  can either be an integer or a half-integer. Recall Eq. (102). Substituting in Eq. (109), we have

$$a = \hbar^2 j(j+1) \quad (111)$$

as the eigenvalue of  $\mathbf{J}^2$ . We also define an  $m$  such that

$$b = m\hbar \quad (112)$$

Since it would be more convenient to denote  $|a, b\rangle$  as  $|j, m\rangle$ , Eq. (88) is now expressed as

$$\begin{aligned} \mathbf{J}^2|j, m\rangle &= \hbar^2 j(j+1)|j, m\rangle \\ J_z|j, m\rangle &= m\hbar|j, m\rangle \end{aligned} \quad (113)$$

## 9 Pure and mixed states.

### Use the density operator formulation to distinguish pure from mixed states.

Pure states are quantum states that cannot no longer be decomposed into more fundamental states. On the other hand, mixed states are generally written as a linear combination of pure states. To distinguish the two in terms of the density operator, note that the operator is defined as

$$\rho \equiv \sum_k^N p_k |\psi_k\rangle \langle \psi_k| \quad (114)$$

where  $\{|\psi_k\rangle\}$  is a set of pure states,  $p_k$  are weights that satisfy  $0 < p_k \leq 1$  and the normalization condition

$$\sum_k^N p_k = 1 \quad (115)$$

For a pure state,  $p_k = 1$  for some  $|\psi_k\rangle$  with  $k = n$  and  $p_k = 0$  for other possible state kets (when  $k \neq n$ ). Thus, we have

$$\rho = |\psi_n\rangle \langle \psi_n| \quad (116)$$

as the density operator for a pure state. In addition, 0 and 1 are the only eigenvalues of  $\rho$  and  $\text{Tr}(\rho^2) = 1$  for a pure state. When diagonalized, the density matrix for a pure state looks like

$$\rho = \begin{pmatrix} 0 & \dots & \dots & 0 \\ \vdots & 1 & & \vdots \\ \vdots & & \ddots & \vdots \\ 0 & \dots & \dots & 0 \end{pmatrix} \quad (117)$$

If the given density operator do not have these characteristics, then it must pertain to a mixed state.

## 10 Quantum correlations.

**Explain how quantum correlations are measured in simple entangled systems.**

In measuring simple entangled systems, we first assign observers that would specialize in a certain particle in the system. One observer would then measure a certain variable with his/her particle, after which the other observer (or observers) would follow who may or may not measure the same variable with his/her own assigned particle. This is repeated for many trials. As shown for a two-electron system in spin-singlet states, the kind of measurement by the first observer will affect the outcome of the next observer's measurement. Tabulating the results would let the experimenters see how measurements affect each other.