

Lecture Notes: 22/01/2013

Density Matrix:

If N_i particles are in the state $|\psi_i\rangle$ then the density matrix for such mixed state is,

$$\hat{\rho} = \sum p_i |\psi_i\rangle \langle \psi_i|$$

and $p_i = \frac{N_i}{N}$, $\sum_i p_i = 1$

The polarization is defined as,

$P_j = \sum_i p_i \langle \psi_i | \sigma_j | \psi_i \rangle$, $j = 0, 1, 2, 3$. We always have $P_0 = 1$ and $0 \leq |\vec{P}| \leq 1$. If \hat{O} is any observable then average of expectation value of \hat{O} is,

$$\langle \bar{O} \rangle = \frac{1}{2} \sum_j \text{tr}(\hat{O} \sigma_j) P_j$$

Again, $\{\frac{1}{\sqrt{2}}\sigma_j\}$ forms a basis for operators. We can write $\hat{\rho}$ as,

$$\hat{\rho} = \frac{1}{2} \sum_j \text{tr}(\rho \sigma_j) \sigma_j$$

Also,

$$\begin{aligned} \text{tr}(\rho \sigma_j) &= \sum_k \langle k | \sum_i p_i |\psi_i\rangle \langle \psi_i | \sigma_j | k \rangle \\ &= \sum_i p_i \langle \psi_i | \sigma_j | \left(\sum_k |k\rangle \langle k| \right) | \psi_i \rangle \\ &= \sum_i p_i \langle \psi_i | \sigma_j | \psi_i \rangle \\ &= P_j \end{aligned}$$

Therefore, $\hat{\rho} = \frac{1}{2} \sum_j P_j \sigma_j$

Multi Particle System:

If we want to describe N particles then we need $V^{R^{3N}}$ dimensional vector space. the most general basis for this space will be,

$|x_1, y_1, z_1, x_2, y_2, z_2, \dots, x_N, y_N, z_N\rangle$

the wave function will look like,

$\int \dots \int dx_1 dx_2 \dots dx_N dy_1 \dots dy_N dz_1 \dots dz_N \psi(x_1, y_1, z_1, \dots, x_N, y_N, z_N) |x_1, y_1, z_1, \dots, x_N, y_N, z_N\rangle$

But there is always possibility that physical condition may reduce the dimension of this vector space.

Operators:

In case of two spin half particles, for instance, we can introduce z-component of spin of 1st particle as $S_{z1} = S_z \otimes 1$. This acts only on the first basis. Similarly, we can introduce operator for second particle which will be $S_{z2} = 1 \otimes S_z$.

In the same way, consider a three dimensional N particle vector space. If we let all particle move around and ask: what is x-component of position of 2^{nd} particle (not caring anything else)?

Ans: Obviously the answer has to be a real number because it has to be somewhere. $x_2 = -\infty \dots + \infty$. The corresponding operator that describes this observable is $X_2 = \mathbf{1} \otimes \mathbf{1} \otimes \mathbf{1} \otimes X \otimes \mathbf{1} \otimes \dots \otimes \mathbf{1}$.

To calculate the probability we have to find a projection operator, which would be,

$\hat{P}_{x_2} = \int \dots \int dx_1 dx_3 \dots dx_N dy_1 \dots dy_N dz_1 \dots dz_N \cdot |x_1, y_1, z_1 \dots x_N, y_N, z_N\rangle \langle x_1, y_1, z_1 \dots x_N, y_N, z_N|$
 x_2 is fixed and integration is carried over all other variables.

The probability to measure x_2 is ,

$$\delta P(x_2, x_2 + \delta x) = [\langle \psi | \hat{P}_{x_2} | \psi \rangle] \delta x =$$

$$\left[\int \dots \int dx_1 dx_3 \dots dx_N dy_1 \dots dy_N dz_1 \dots dz_N \psi^*(x_1, y_1, z_1 \dots x_N, y_N, z_N) \psi(x_1, y_1, z_1 \dots x_N, y_N, z_N) \right] \delta x$$

Time Evolution:

The time evolution is governed by Schrodinger Equation,

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

Here H should be expressed in terms of all degrees of freedom.

Two Particle Hilbert Space:

Each particle is described by the vector space C. Two particle live in $C_1 \otimes C_2$ dimensional vector space.

We can take $(|k_1\rangle \otimes |k_2\rangle)$ a basis for $C_1 \otimes C_2$. Then the most general state will

be,

$$|\psi\rangle = \sum_{k_1} \sum_{k_2} C_{k_1} C_{k_2} |k_1\rangle \otimes |k_2\rangle$$

If we take two spin $\frac{1}{2}$ particles. Then,

Basis for C_1 , $|k_1\rangle = \{|\uparrow\rangle_1, |\downarrow\rangle_1\}$

Basis for C_2 , $|k_2\rangle = \{|\uparrow\rangle_2, |\downarrow\rangle_2\}$

The most general state in this vector space will be,

$$|\psi\rangle = \sum_{k_1} \sum_{k_2} C_{k_1} C_{k_2} |k_1\rangle \otimes |k_2\rangle$$

If $S = 0$ then

$$|\psi\rangle = \frac{1}{\sqrt{2}} (|\uparrow\rangle_1 \otimes |\downarrow\rangle_2 - |\downarrow\rangle_1 \otimes |\uparrow\rangle_2)$$

It is not eigenstate for S_{z1} and S_{z2} as well but it is eigenstate for $S_{ztotal} = S_{z1} + S_{z2}$

Case of two Non-Interacting Particles:

The Hamiltonian can be defined as,

$$H = \frac{p_1^2}{2m_1} + V_1(x_1) + \frac{p_2^2}{2m_2} + V_2(x_2)$$

We want to solve for $H|\psi\rangle = E|\psi\rangle$

In position space, we can write,

$$\left[\frac{-\hbar^2}{2m_1} \frac{\partial^2}{\partial x_1^2} + V_1(x_1, x_2) \right] \psi(x_1, x_2) + \left[\frac{-\hbar^2}{2m_2} \frac{\partial^2}{\partial x_2^2} + V_2(x_2) \right] \psi(x_1, x_2) = E\psi(x_1, x_2)$$

In case of non-interacting particles, we can write $\psi(x_1, x_2) = \psi(x_1)\psi(x_2)$

With the assumption that

$$H_1\psi(x_1) = E_1\psi(x_1)$$

$$H_2\psi(x_2) = E_2\psi(x_2)$$

Then we will have,

$$E_1\psi(x_1)\psi(x_2) + \psi(x_1)E_2\psi(x_2) = E\psi(x_1)\psi(x_2); E = E_1 + E_2.$$

Now, method of separation of variable could be used to solve this equation.

Case of two interacting particle:

The Hamiltonian can be defined as,

$$H = \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} + V(x_1 - x_2)$$

In this case method of separation of variable will not work so we employ a trick to get rid of this difficulty. We describe the system in new coordinates , $X = X_{cm} = (m_1x_1 + m_2x_2)/M$ and $x = x_{rel} = x_1 - x_2$; then we can write our hamiltonian as

$$H = \frac{p_{total}^2}{2M} + \frac{p_{rel}^2}{2\mu} + V(x_{rel})$$

In such case the wave function can be written as,

$$\psi = \psi_{cm}(X_{cm})\psi_{rel}(x_{rel})$$

where ψ_{cm} is a solution for free particle motion with constant momentum $P_{cm} = p_{total}$ and ψ_{rel} is an eigenfunction for the 1-particle Hamiltonian $\frac{p_{rel}^2}{2\mu} + V(x_{rel})$.