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Lecture I

1.1 Density Matrix

Sometimes we have a pure system. That is, identically prepared particles or system of particle all in the same quantum state. We can make measurements on the system to learn about the state. If for example we have a system of spin 1/2 particles all in the state $\mid \alpha\rangle$, then

$$\mid \alpha\rangle = a\mid +\rangle + b\mid -\rangle.$$

We can determine a and b by measuring spin along various axis. Eventually we will find the polarization and our work is complete. Alternatively, we might have a mixture of states with fraction w_i in state α_i. The w_i sum to 1 and the $\mid \alpha_i\rangle$ may or may not be orthogonal. Suppose we want the ensemble of spin 1/2 particles that is unpolarized. Our linear combination is clearly not a candidate. It's spin is along some definite direction. Note that $|a|^2 + |b|^2 = 1$. We want the state that looks more like

$$w_+\mid +\rangle + w_-\mid -\rangle$$

where $w_- + w_+ = 1$ and both real so there is no relative phase information. If $w_+ = w_-$ then we get equal probablity for measuring $\mid +\rangle$ and $\mid -\rangle$ regardless of the orientation of our SG device. It could be a mixture of states that are not orhtogonal, like spin in x and y directions. Density operator formalism handy for dealing wth mixed and pure ensembles.

Suppose $\mid \alpha_i\rangle$ are normalized and in our mixture there is probability w_i to be in the pure state $\mid \alpha_i\rangle$. The average value of some observable

$$[A] = \sum_i w_i \langle\alpha_i \mid A \mid \alpha_i\rangle$$

In terms of a complete set of eigenstates $\mid a_i\rangle$ with eigenvalues a_i we write

$$\mid \alpha_i\rangle = \sum_j \langle a_j \mid \alpha_i\rangle \mid a_j\rangle$$

so that

$$[A] = \sum_j \sum_i w_i |\langle a_j \mid \alpha_i\rangle|^2 a_j$$

Or in terms of a complete set that is not an eigenbasis of A

$$[A] = \sum_j \sum_k \sum_i w_i \langle\alpha_i \mid b_j\rangle \langle b_j \mid A \mid b_k\rangle \langle b_k \mid \alpha_i\rangle$$

$$= \sum_j \sum_k \left[\sum_i w_i \langle b_k \mid \alpha_i\rangle\langle\alpha_i \mid b_j\rangle\right] \langle b_j \mid A \mid b_k\rangle$$

$$= \sum_k \langle b_k \mid \rho A \mid b_k\rangle = \mathrm{Tr}\,(\rho A)$$

Or

$$\rho = \sum_i w_i | \alpha_i\rangle\langle\alpha_i |$$

We see that ρ is Hermitian and

$$\mathrm{Tr}(\rho) = \sum_j \sum_i w_i \langle b_j \mid \alpha_i\rangle\langle\alpha_i \mid b_j\rangle = 1$$

In a pure ensemble, $w_i = 1$ for some i and $w_j, j \neq i = 0$. There is a single state. The density matrix

$$\rho = | \alpha_n\rangle\langle\alpha_n |$$

a projection operator and therefore $\rho^2 = \rho$ and $\mathrm{Tr}\rho^2 = 1$. The diagonalized density operator for a pure state has a single non-zero value on the diagonal.

1.1.1 Construction of the Density Matrix

Again, the spin 1/2 system. The density matrix for a pure $z = +\frac{1}{2}$ state

$$\rho = | +\rangle\langle+ | = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

Note that $\mathrm{Tr}\rho = 1$ and $\mathrm{Tr}\rho^2 = 1$ as this is a pure state. Also the expectation value of σ_z, $\mathrm{Tr}\rho\sigma_z = 1$ The density matrix for the pure state $S_x = \pm 1$ is

$$\rho = | S_x\rangle\langle S_x | = \frac{1}{\sqrt{2}} [| +\rangle \pm | -\rangle] \frac{1}{\sqrt{2}} [\langle+ | \pm \langle- |]$$

$$= \frac{1}{2} \begin{pmatrix} 1 \\ \pm 1 \end{pmatrix} \begin{pmatrix} 1 & \pm 1 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 & \pm 1 \\ \pm 1 & 1 \end{pmatrix}$$

Again $\mathrm{Tr}\rho = 1$,

$$\rho^2 = \frac{1}{4} \begin{pmatrix} 2 & \pm 2 \\ \mp 2 & 2 \end{pmatrix}$$

and $\mathrm{Tr}\rho^2 = 1$. A completely unpolarized state, with maximum disorder

$$\frac{1}{2} [| +\rangle\langle+ | + | -\rangle\langle- |] = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix}$$

now $\mathrm{Tr}\rho = 1$ but $\mathrm{Tr}p^2 = \frac{1}{2}$ and $\mathrm{Tr}(\sigma\rho) = 0$.

1.1.2 How many measurements

For a given ensemble, how many measurements are required to fully describe the system, which of course is fuly described by the density matrix. Consider again spin 1/2. If the system is in a pure state $| S_x\rangle\langle S_x |$ and we measure the z-component of spin, we get probability 1/2 of measuring $| \pm\rangle$. In a completely unpolarized state we measure the same. Clearly we need more observables to describe the state. In this case we need to measure S_x, S_y and S_z to learn all there is to know. The most general density matrix is Hermitian with spin 1. In an n dimensional space there are n^2 real parameters less one since $\mathrm{Tr}\rho = 1$. For spin 1/2 that leaves 3 real parameters. The most general density matrix can be constructed from σ as

$$\rho = \frac{1}{2}(1 + \mathbf{a}\cdot\sigma)$$

where $\mathbf{a}$ is a real vector. And we see as noted above that we need to measure 3 observables, namely the polarization, to determine the state of the ensemble. The polarization is

$$\langle\sigma_i\rangle = \mathrm{Tr}(\rho\sigma) = \mathrm{Tr}\left(\frac{1}{2}\mathbf{a}\cdot\sigma\sigma_i\right) = a_i$$

1.1.3 Spin 1

The density matrix for a spin 1 system has 8 independent parameters.

$$\rho = \frac{1}{3}\left(1 + \mathbf{P}\cdot\mathbf{J} + W_{ij}T_{ij}\right)$$

where

$$T_{ij} = \frac{1}{2}(J_iJ_j + J_jJ_i) - \frac{2}{3}\delta_{ij}$$

is symmetric with zero trace.

Note that the product operator is in general

$$\sum c_{ij}J_iJ_j = \frac{1}{2}\sum c_{ij}\left[(J_iJ_j - J_jJ_i) + (J_iJ_j + J_jJ_i)\right]$$

$$= \frac{1}{2}\sum c_{ij}\left[[J_i, J_j] + (J_iJ_j + J_jJ_i)\right] = \frac{1}{2}\sum c_{ij}\left[i\epsilon_{ijk}J_k + (J_iJ_j + J_jJ_i)\right]$$

The antisymmetric part is already included in the term linear in J. Of the symmetric piece, the $i = j$ component is the identity and already included. That leaves T_{ij}. As for higher orders, $J^3 \to J$ so there is no new information there.

What then characterizes the ensemble beyond polarization? Suppose the system is in the pure state

$$|\,\alpha\rangle = (i|\,1\rangle - |\,-1\rangle)$$

The density matrix

$$\rho = |\,\alpha\rangle\langle\alpha\,| = (i|\,1\rangle - |\,-1\rangle)\,(-i\langle 1\,| - \langle -1\,|)$$

$$= \frac{1}{2}\begin{pmatrix} 1 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 1 \end{pmatrix}$$

It is an eignestate of the operator

$$\left(\frac{1}{2}(J_1J_2 + J_2J_1)\right)$$

It is a pure state as $\mathrm{Tr}\rho = 1$ and $\rho^2 = \rho$. The expectation value of the spin

$$\langle\mathbf{J}\rangle = \mathrm{Tr}(\rho\mathbf{J}) = 0$$

There is zero polarization. But it is pure. Another observable, namely the quadrupole moment as represented by J_iJ_j identifies the ensemble.

1.1.4 Time Dependence

The density matrix

$$\rho(t_0) = \sum w_i | \alpha_i \rangle \langle \alpha_i |$$

As long as there are no external forces on the system, the w_i are constant. and

$$i\hbar \frac{\partial}{\partial t} \rho = \sum_i w_i [H | \alpha \rangle \langle \alpha | - | \alpha \rangle \langle \alpha | H] = [H, \rho]$$