Physics 492 - Quantum II

Lecture 14: Composite Quantum Systems

Last semester we began to study quantum mechanics associated with "multiple degrees of freedom", e.g. the hydrogen atom. In classical physics each degree of freedom is described by a pair of canonical coordinates (x,p) for each point particle and each spatial dimension. In quantum physics we generalize the "degrees of freedom" to include non-motion related quantities such as spin.

Such composite quantum systems are important for understanding

- Condensed matter, e.g. multielectron atoms, molecules, liquids solids

- Entangled States

The former is obvious - complex systems involve many degrees of freedom, so we must understand the subtle feature associate with quantum many-body systems.

The latter involves the bizzare essense of quantum mechanics - nonlocal correlations. It is at the heart of quantum measurement and is proving to be a useful technological resource for information processing. The new field of "quantum information" ~~puts those~~ explores this.

Review: Wave mechanics description for multiple d'o'f

Consider a system with two motional degrees of freedom. This could be a single particle moving in 2D or two particles confined to move in 1D. The wave function describing the (pure) state of the system is a complex function of

$$\Psi(x_1, x_2) \quad \text{where } x_1, x_2$$

describe the two motional positions.

Joint probability density $P(x_1, x_2) = |\Psi(x_1, x_2)|^2$.
The Hilbert space is the set of "square integrable functions", i.e. normalizable probability distributions

$$\int dx_1\, dx_2\, |\Psi(x_1, x_2)|^2 < \infty$$

We define this space as $\underbrace{\mathcal{L}_2}_{\text{square normalizable}} (\overbrace{\mathbb{R}^2}^{\text{plane } \mathbb{R}^2})$

The inner product is defined

$$\langle \Psi | \Phi \rangle = \int dx_1\, dx_2\, \Psi^*(x_1, x_2)\, \Phi(x_1, x_2)$$

Then $\|\Psi\|^2 = \langle \Psi | \Psi \rangle$

<u>Basis:</u> A basis for $\mathcal{L}_2(\mathbb{R}^2)$ can be formed from the product of all basis functions for $\mathcal{L}_2(\mathbb{R}^1)$ (Hilbert space on 1D)

e.g. Harmonic oscillator energy eigenfunctions

$$\{ u_n(x) = A_n H_n(x) e^{-x^2} \}$$

Span $\mathcal{L}_2(\mathbb{R}^1)$

$$\Rightarrow \{ U_{n_1 n_2}(x_1, x_2) = u_{n_1}(x_1)\, u_{n_2}(x_2) \mid n_1, n_2 = 0, 1, 2 \ldots \infty \}$$

Span $\mathcal{L}_2(\mathbb{R}^2)$

So

$$\Psi(x_1, x_2) = \sum_{n_1, n_2 = 0}^{\infty} C_{n_1 n_2} U_{n_1 n_2}(x_1, x_2)$$

$$= \sum_{n_1 n_2}' \underbrace{C_{n_1 n_2}}_{\text{expansion coefficient}} \underbrace{u_{n_1}(x_1)\, u_{n_2}(x_2)}_{\text{product basis}}$$

where

$$C_{n_1 n_2} = \langle U_{n_1, n_2} | \Psi \rangle$$

$$C_{n_1 n_2} = \int dx_1 dx_2\, u^*_{n_1}(x_1)\, u^*_{n_2}(x_2)\, \Psi(x_1, x_2)$$

The fact that a basis for $\mathcal{L}_2(\mathbb{R}^2)$ can be formed from products of the basis elements of $\mathcal{L}_2(\mathbb{R}^1)$ means that the composite Hilbert space has a structure known in mathematics as the "tensor product"

$$\mathcal{L}_2(\mathbb{R}^2) = \mathcal{L}_2(\mathbb{R}^1) \underset{\uparrow}{\otimes} \mathcal{L}_2(\mathbb{R}^1)$$

"tensor product"

Wave functions in $\mathcal{L}_2(\mathbb{R}^2)$ can be constructed from products of functions in $\mathcal{L}_2(\mathbb{R}^1)$

e.g. $$\left.\begin{aligned} \Psi(x_1, x_2) &= \psi_1(x_1)\,\psi_2(x_2) \\ \Phi(x_1, x_2) &= \phi_1(x_1)\,\phi_2(x_2) \end{aligned}\right\} \text{"product states"}$$

Note: for two product states above

$$\langle \Psi | \Phi \rangle = \int dx_1\, dx_2\, \psi_1^*(x_1)\psi_2^*(x_2)\,\phi_1(x_1)\,\phi_2(x_2)$$

$$= \underbrace{\int dx_1\, \psi_1^*(x_1)\,\phi_1(x_1)}_{\langle \psi_1 | \phi_1 \rangle}\ \underbrace{\int dx_2\, \psi_2^*(x_2)\,\phi_2(x_2)}_{\langle \psi_2 | \phi_2 \rangle}$$

Thus, the inner product of the joint states is the product of inner-products for the individual subsystems

Marginals: Last semester we discussed the idea of a "marginal" probability distribution. Given a joint density $P(x_1, x_2)$ we ask, what is the probability distribution for x_1 irrespective of the value of x_2.

Thus the "marginal"

$$P(x_1) = \int dx_2 \; P(x_1, x_2) \quad \left(\begin{array}{c}\text{Add up all}\\ \text{possible values}\\ \text{of } x_2\end{array}\right)$$

Note: For a product state

$$\Psi(x_1, x_2) = \psi_1(x_1)\,\psi_2(x_2)$$

$$P(x_1, x_2) = |\psi_1(x_1)|^2 \; |\psi_2(x_2)|^2$$

$$= P_1(x_1)\, P_2(x_2)$$

$\Rightarrow$ The joint probability distribution factorizes into its marginals. Each d'o'f is described by its own wave function and the statistics of x_1 and x_2 are uncorrected.

If $\Psi(x_1, x_2) \neq \psi_1(x_1)\,\psi_2(x_2)$ the wave function is said to be entangled.

These correlations are the heart of quantum mech

Tensor products: Dirac Notation

We generalize the notion of product wave functions to "product kets" using Dirac notation. Some new unnoticed features appear when we include finite dimensional Hilbert spaces such as those that appear for spin degrees of freedom.

Define h_1 and h_2 be Hilbert space for two degrees of freedom. The composite Hilbert space is then the tensor product space

$$\mathcal{H}_{12} = h_1 \otimes h_2$$

If $|\psi_1\rangle \in h_1$ and $|\psi_2\rangle \in h_2$ then

$$|\Psi_{12}\rangle \equiv |\psi_1\rangle \otimes |\psi_2\rangle \in \mathcal{H}_{12}$$

Given another product state $|\Phi_{12}\rangle \equiv |\phi_1\rangle \otimes |\phi_2\rangle$

the $\langle \Psi_{12} | \Phi_{12} \rangle \equiv \langle \psi_1 | \phi_1 \rangle \langle \psi_2 | \phi_2 \rangle$

Basis: If $\{|e_i\rangle \,|\, i = 1, 2, \ldots, d_1\}$ is a bases for h_1 and

$$\{|f_j\rangle \,|\, j = 1, 2, 3, \ldots d_2\}$$ is a

basis for h_2 then (next page)

then $\{ |u_{ij}\rangle = |e_i\rangle \otimes |f_j\rangle \}$ is a basis for $\mathcal{H}_{12}$

$$|\Phi_{12}\rangle = \sum_{i=1}^{d_1} \sum_{j=1}^{d_2} c_{ij} \, |u_{ij}\rangle$$

$$= \sum_{ij} c_{ij} \, |e_i\rangle \otimes |f_j\rangle$$

Note: If d_1 = dim of h_1, d_2 = dim of h_2

then the dimension of $\mathcal{H}_{12} = d_1 d_2$

This is a fantastic fact. Suppose we have n degrees of freedom, each described by a Hibert space of dimension d, then the composite Hilbert space

$$\mathcal{H}_n = \underbrace{h \otimes h \otimes \cdots \otimes h}_{n \text{ times}} \equiv h^{\otimes n}$$

has dimension $\underline{\underline{d^n}}$. This is an exponential growth in complexity, making the many-body problem in quantum mechanics extremely difficult.

<u>Representations:</u> Suppose we consider a product-state

$$|\Psi_{12}\rangle = |\psi_1\rangle \otimes |\psi_2\rangle$$

Let $|\psi_1\rangle = \sum_{i=1}^{d_1} a_i |e_i\rangle$ where $a_i = \langle e_i|\psi_1\rangle$

$$\Rightarrow \quad |\psi_1\rangle \doteq \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_{d_1} \end{bmatrix} \text{ in basis } \{|e_i\rangle\}$$

$|\psi_2\rangle = \sum_{j=1}^{d_2} b_j |f_j\rangle$ where $b_j = \langle f_j|\psi_2\rangle$

$$\Rightarrow \quad |\psi_2\rangle \doteq \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_{d_2} \end{bmatrix} \text{ in basis } \{|f_j\rangle\}$$

Then $|\Psi_{12}\rangle = \sum_{i,j}' c_{ij} \; |e_i\rangle \otimes |f_j\rangle$

where $c_{ij} = \left(\langle e_i| \otimes \langle f_j|\right) |\Psi_{12}\rangle$

$$= \langle e_i|\psi_1\rangle \langle f_j|\psi_2\rangle = a_i b_j$$

$$\Rightarrow |\Psi_{12}\rangle \doteq \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_{d_1} \end{bmatrix} \otimes \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_{d_2} \end{bmatrix} = \begin{bmatrix} a_1 b_1 \\ a_1 b_2 \\ \vdots \\ a_1 b_{d_2} \\ a_2 b_1 \\ \vdots \\ a_{d_1} b_{d_2} \end{bmatrix}$$

Example: Two spin-1/2 particles

Each particle's spin d'o'f is described by a 2D Hilbert space spanned by the standard basis

$$\{|\uparrow\rangle, |\downarrow\rangle\}$$ up and down along z-axis

The joint Hilbert space is spanned by

$$\{|\uparrow\rangle, |\downarrow\rangle\} \otimes \{|\uparrow\rangle, |\downarrow\rangle\}$$

$$= \{|\uparrow\rangle\otimes|\uparrow\rangle, |\uparrow\rangle\otimes|\downarrow\rangle, |\downarrow\rangle\otimes|\uparrow\rangle, |\downarrow\rangle\otimes|\downarrow\rangle\}$$

Note: We alternatively abreviate the tensor product

$$|\uparrow\rangle\otimes|\uparrow\rangle = |\uparrow\rangle|\uparrow\rangle = |\uparrow,\uparrow\rangle = |\uparrow\uparrow\rangle$$

Consider the product state

$$|\Psi_{12}\rangle = |\uparrow_z\rangle \otimes |\uparrow_x\rangle$$

Recall $|\uparrow_x\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow_z\rangle + |\downarrow_z\rangle\right)$

$$\Rightarrow |\Psi_{12}\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\uparrow\rangle + |\uparrow\downarrow\rangle\right)$$

(note without subscript, z implied)

In the standard "product basis"

$$|\Psi_{12}\rangle = \frac{1}{\sqrt{2}} \begin{array}{c c} \begin{bmatrix} 1 \\ 1 \\ 0 \\ 0 \end{bmatrix} & \begin{array}{c} \langle\uparrow\uparrow| \\ \langle\uparrow\downarrow| \\ \langle\downarrow\uparrow| \\ \langle\downarrow\downarrow| \end{array} \end{array}$$

Note

$$|\Psi_{12}\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \otimes \begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix} = \begin{bmatrix} 1 \begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix} \\ 0 \begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix} \end{bmatrix}$$

$$= \begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \\ 0 \\ 0 \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \\ 0 \\ 0 \end{bmatrix}$$ by rules of tensor product

In contrast: Consider

$$|\Phi_{12}\rangle \equiv \frac{1}{\sqrt{2}} \left(|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle \right)$$

$$= \frac{1}{\sqrt{2}} \begin{array}{c c} \begin{bmatrix} 1 \\ 0 \\ 0 \\ 1 \end{bmatrix} & \begin{array}{c} \langle\uparrow\uparrow| \\ \langle\uparrow\downarrow| \\ \langle\downarrow\uparrow| \\ \langle\downarrow\downarrow| \end{array} \end{array}$$

Though ~~these~~ $|\Psi_{12}\rangle$ and $|\Phi_{12}\rangle$ look very similar as column vectors they are very different in nature. $|\Phi_{12}\rangle$ is entangled. It is <u>not a product state</u>.

Marginals:

Consider the (discrete) joint probability distrution

$$P_{ij} = |\langle e_i, f_j | \Psi \rangle|^2$$

As before, we define the marginals

$$P_i = \sum_j{}' P_{ij} \qquad P_j = \sum_i{}' P_{ij}$$

If $|\Psi\rangle = |\psi_1\rangle \otimes |\psi_2\rangle$ (product state)

Then $P_{ij} = P_i P_j$ (uncorrelated factorization of marginals)

However, suppose $|\Psi\rangle$ is <u>entangled</u> ?

Consider 2 spin-½ particles

Let $P_{n_1 n_2} = |\langle n_1 n_2 | \Psi \rangle|^2$

where $n = \pm 1$ is the spin eigenvalue along an arbitrary direction

Marginal $P_{n_1} = \sum_{n_2 = \pm 1} P_{n_1 n_2}$

Let $|\Psi\rangle = \frac{1}{\sqrt{2}} (|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle)$

$$\Rightarrow P_{n_1 n_2} = \frac{1}{2} \left| \langle n_1 n_2 | \uparrow\uparrow\rangle + \langle n_1 n_2 | \downarrow\downarrow\rangle \right|^2$$

$$= \frac{1}{2} |\langle n_1 n_2 | \uparrow\uparrow\rangle|^2 + \frac{1}{2} |\langle n_1 n_2 | \downarrow\downarrow\rangle|^2$$

$$+ \frac{1}{2} \langle \uparrow\uparrow | n_1 n_2\rangle \langle n_1 n_2 | \downarrow\downarrow\rangle$$

$$+ \frac{1}{2} \langle \downarrow\downarrow | n_1 n_2\rangle \langle n_1 n_2 | \uparrow\uparrow\rangle$$

$$= \frac{1}{2} |\langle n_1 | \uparrow\rangle|^2 |\langle n_2 | \uparrow\rangle|^2$$

$$+ \frac{1}{2} |\langle n_1 | \downarrow\rangle|^2 |\langle n_2 | \downarrow\rangle|^2$$

$$+ \frac{1}{2} \left(\langle \uparrow | n_1\rangle \langle n_1 | \downarrow\rangle\right) \left(\langle \uparrow | n_2\rangle \langle n_2 | \downarrow\rangle\right)$$

$$+ \frac{1}{2} \left(\langle \downarrow | n_1\rangle \langle n_1 | \uparrow\rangle\right) \left(\langle \downarrow | n_2\rangle \langle n_2 | \uparrow\rangle\right)$$

Thus $P_{n_1} = \sum_{n_2} P_{n_1 n_2}$

Aside: $\sum_{n_2} |\langle n_2 | \uparrow\rangle|^2 = \sum_{n_2} |\langle n_2 | \downarrow\rangle|^2 = 1$

since $|\uparrow\rangle$ and $|\downarrow\rangle$ normalized

But $\sum_{n_2} \langle \downarrow | n_2\rangle \langle n_2 | \uparrow\rangle = \langle \downarrow | \uparrow\rangle = 0$

$$\sum_{n_2} \langle \uparrow | n_2\rangle \langle n_2 | \downarrow\rangle = \langle \uparrow | \downarrow\rangle = 0$$

thus $P_{n_1} = \frac{1}{2}|\langle n_1|\uparrow\rangle|^2 + \frac{1}{2}|\langle n_1|\downarrow\rangle|^2$

$$= \langle n_1|\hat{\rho}_1|n_1\rangle$$

where $\hat{\rho}_1 = \frac{1}{2}|\uparrow\rangle\langle\uparrow| + \frac{1}{2}|\downarrow\rangle\langle\downarrow|$

$\Rightarrow$ Particle 1 is described by a completely mixed state

This is a remarkable properties of joint quantum systems. If the joint state is entangled, the marginals are mixed states.

Even though we have a pure state for the joint system, and ~~thus~~ maximal possible information, we have minimal information about the subsystem. All information is in the correlations.