

## Quantum Mechanics of Multiple Degrees of Freedom

Consider the simplest classical system with two degrees of freedom - two point particles moving on a line:



The quantum mechanical wave function for the joint probability amplitude

$$\Psi(x_A, x_B) \Rightarrow P(x_A, x_B) = |\Psi(x_A, x_B)|^2$$

We define the marginal probability distributions

$$P(x_A) = \int_{-\infty}^{\infty} dx_B P(x_A, x_B), \quad P(x_B) = \int_{-\infty}^{\infty} dx_A P(x_A, x_B)$$

Question: Does  $P(x_A) = |\psi_A(x_A)|^2$ ,  $P(x_B) = |\psi_B(x_B)|^2$  for some  $\psi_A$  and  $\psi_B$ ?

Answer: Iff  $\Psi(x_A, x_B) = \psi_A(x_A)\psi_B(x_B) \Rightarrow P(x_A, x_B) = P(x_A)P(x_B)$

$\Rightarrow x_A$  &  $x_B$  are uncorrelated  $\rightarrow \Psi$  is a "product state": separable

If  $\Psi(x_A, x_B) \neq \psi_A(x_A)\psi_B(x_B)$  for some  $\psi_A$  &  $\psi_B$  the state is said to be entangled

Note we assumed the joint state of  $A+B$  was pure. If the state of joint state of  $A+B$  is mixed, the definition and quantification of entanglement becomes much more complicated. We will not treat that problem here.

## Tensor product

The formal structure of Hilbert space for multiple degrees of freedom is the tensor product. Consider two degrees of freedom (two parts = bipartite).

$$\mathcal{H}_{AB} = \mathcal{H}_A \otimes \mathcal{H}_B \quad \text{tensor (Kronecker) product}$$

Joint Hilbert space of the joint system  
Hilbert spaces of the two "subsystems"

$$\text{if } |\psi\rangle_A \in \mathcal{H}_A \quad |\phi\rangle_B \in \mathcal{H}_B \quad \text{Define } |\Psi_{AB}\rangle \equiv |\psi\rangle_A \otimes |\phi\rangle_B \in \mathcal{H}_{AB}$$

product state

$$\text{Basis } \{|e_i\rangle_A \mid i=1,2,\dots,d_A\} \text{ for } \mathcal{H}_A \quad \{|f_j\rangle_B \mid j=1,2,\dots,d_B\}$$

↑ dimension of  $\mathcal{H}_A$ ,  $\mathcal{H}_B$  respectively

$$\text{Basis for } \mathcal{H}_{AB} : |i,j\rangle \equiv |e_i\rangle_A \otimes |f_j\rangle_B : \text{Dim}(\mathcal{H}_{AB}) = d_A d_B$$

$$\text{Representation: } \alpha_i \equiv \langle e_i | \psi \rangle_A = \begin{bmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \\ \alpha_{d_A} \end{bmatrix} \quad \beta_j \equiv \langle f_j | \phi \rangle_B = \begin{bmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \beta_{d_B} \end{bmatrix}$$

$$\Rightarrow \gamma_{ij}^{AB} \equiv \langle i,j | \Psi \rangle_{AB} = \left( \langle e_i | \otimes \langle f_j | \right) \left( |\psi\rangle_A \otimes |\phi\rangle_B \right) = \langle e_i | \psi \rangle_A \langle f_j | \phi \rangle_B$$

$$\Rightarrow \gamma_{ij}^{AB} = \alpha_i \beta_j : \text{tensor product, outer product, Kronecker product}$$

$$\gamma_{ij}^{AB} = \begin{bmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \\ \alpha_{d_A} \end{bmatrix}_A \otimes \begin{bmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \beta_{d_B} \end{bmatrix}_B = \begin{bmatrix} \alpha_1 \begin{bmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \beta_{d_B} \end{bmatrix} \\ \alpha_2 \begin{bmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \beta_{d_B} \end{bmatrix} \\ \vdots \\ \alpha_{d_A} \begin{bmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \beta_{d_B} \end{bmatrix} \end{bmatrix} = \begin{bmatrix} \alpha_1 \beta_1 \\ \alpha_1 \beta_2 \\ \vdots \\ \alpha_1 \beta_{d_B} \\ \alpha_2 \beta_1 \\ \alpha_2 \beta_2 \\ \vdots \\ \alpha_2 \beta_{d_B} \\ \vdots \\ \alpha_{d_A} \beta_1 \\ \alpha_{d_A} \beta_2 \\ \vdots \\ \alpha_{d_A} \beta_{d_B} \end{bmatrix}_{AB}$$

## Tensor product of operators

If  $\hat{M}^{(A)}$  is an operator on  $\mathcal{H}_A$  and  $\hat{N}^{(B)}$  is an operator on  $\mathcal{H}_B$ .

Define  $\hat{O}^{(AB)} = \hat{M}^{(A)} \otimes \hat{N}^{(B)}$  on  $\mathcal{H}_{AB}$  s.t.  $\hat{O}^{(AB)} |\psi\rangle_A \otimes |\phi\rangle_B = \hat{M}^{(A)} |\psi\rangle_A \otimes \hat{N}^{(B)} |\phi\rangle_B$

Matrix representation:  $O_{(ij)(i'j')}^{AB} = \langle ij | \hat{O}^{(AB)} | i'j' \rangle = N_{i'j'}^{(B)} M_{ij}^{(A)}$

Example: Two qubits  $d_A = d_B = 2$

$\hat{O}^{AB} = \hat{\sigma}_x^A \otimes \hat{\sigma}_z^B$  Standard basis:  $|ij\rangle$   $|0\rangle = |\uparrow\rangle$ ,  $|1\rangle = |\downarrow\rangle$   
binary for 1,2,3,4

$$\hat{O}^{AB} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \otimes \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} = \begin{bmatrix} 0 \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} & 1 \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \\ 1 \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} & 0 \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \end{bmatrix} = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{bmatrix}$$

## Marginal State (reduced density operator)

Joint probability distribution:  $p_{ij}^{AB} = |\langle ij | \Psi \rangle_{AB}|^2 = \langle ij | \hat{\rho}^{AB} | ij \rangle$

$$\hat{\rho}_{AB} = |\Psi\rangle_{AB} \langle \Psi| \quad (\text{pure state})$$

Marginal  $p_i^A = \sum_j p_{ij}^{AB} = \sum_j \langle i | \otimes \langle j | \hat{\rho}^{AB} | j \rangle \otimes | i \rangle = \langle i | \hat{\rho}^A | i \rangle$

where  $\hat{\rho}^A = \text{Tr}_B (\hat{\rho}^{AB}) = \underbrace{\sum_j \langle j | \hat{\rho}^{AB} | j \rangle_B}_{\text{partial trace}} =$  marginal density operator  
(often the "reduced" density op)

Partial trace:  $\hat{\rho}^{AB} = \sum_{ij i'j'} \rho_{(ij)(i'j')} |ij\rangle \langle i'j'| = \sum_{ij i'j'} \rho_{(ij)(i'j')} |i\rangle_A \langle i'|_A \otimes |j\rangle_B \langle j'|_B$

$$\Rightarrow \hat{\rho}^A = \text{Tr}_B (\hat{\rho}^{AB}) = \sum_j \rho_{(ij)(ij)} |j\rangle_B \langle j|_B \\ = \text{Tr}_B (\rho_{(ij)(i'j')})$$

## Entangled States

- A pure state in  $\mathcal{H}_{AB}$  is separable if a product state:  $|\Psi\rangle_{AB} = |\psi\rangle_A \otimes |\phi\rangle_B$  for some  $|\psi\rangle_A \in \mathcal{H}_A$ ,  $|\phi\rangle_B \in \mathcal{H}_B$ . Otherwise  $|\Psi\rangle_{AB}$  is entangled.

Example: Two qubits. Consider the state

$$|\Psi\rangle_{AB} = \frac{1}{2} (|\uparrow\uparrow\rangle + i|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle + i|\downarrow\downarrow\rangle)$$

Though at first glance this looks entangled, in fact it is not.

$$|\Psi\rangle_{AB} = |\uparrow_x\rangle_A \otimes |\uparrow_y\rangle_B : \quad |\uparrow_x\rangle = \frac{1}{\sqrt{2}} (|\uparrow\rangle + |\downarrow\rangle), \quad |\uparrow_y\rangle = \frac{1}{\sqrt{2}} (|\uparrow\rangle + i|\downarrow\rangle)$$

While it might be possible to see this by eye for two qubits, for higher dimensional systems this becomes increasingly more difficult. We thus seek a more systematic method for determining the entanglement and, moreover, to quantify the degree of entanglement.

## Classical vs. Quantum Correlations

How is entanglement different from classical correlations? Consider the singlet state

$$|\Psi\rangle_{AB} = \frac{1}{\sqrt{2}} |\uparrow_z\rangle_A \otimes |\downarrow_z\rangle_B - \frac{1}{\sqrt{2}} |\downarrow_z\rangle_A \otimes |\uparrow_z\rangle_B$$

The measure outcomes on spin-A and spin-B are correlated. Suppose Alice measures has access to spin-A. Her marginal state  $\hat{\rho}_A = \frac{1}{2} \hat{1}$ , the completely mixed state. Thus no matter what she measures, she gets a random result:  $\frac{1}{2}$  probability of outcome. Suppose she measures  $\hat{\sigma}_z^A$ , and finds  $|\uparrow_z\rangle_A$  (with probability  $\frac{1}{2}$ ). If she knows the joint state, then she can assign a state to Bob (who has access to spin-B), after her

measurement  $|\psi\rangle_B |_{|\uparrow_z\rangle_A} = \frac{\langle \uparrow_z^A | \Psi_{AB} \rangle}{\| \langle \uparrow_z^A | \Psi_{AB} \rangle \|} = |\downarrow_z\rangle_B \Rightarrow$  If Bob measures his spin along z, he certainly finds  $|\downarrow_z\rangle_B$

Similarly, if Alice finds  $|\downarrow\rangle_A$ , Bob's Post measurement state is  $|\uparrow\rangle_B$ . The spins of Alice and Bob are anticorrelated along z. But now consider the following state

$$\hat{\rho}_{AB} = \frac{1}{2} |\uparrow\rangle_A \langle\uparrow| \otimes |\downarrow\rangle_B \langle\downarrow| + \frac{1}{2} |\downarrow\rangle_A \langle\downarrow| \otimes |\uparrow\rangle_B \langle\uparrow|$$

Here too, the marginals are completely mixed  $\hat{\rho}_A = \hat{\rho}_B = \frac{1}{2} \hat{1}$ , so the individual outcomes are random, but the measurement outcomes are correlated

$$P_{AB}(\uparrow_z, \downarrow_z) = P_A(\downarrow_z, \uparrow_z) = \frac{1}{2}, \quad P_{AB}(\uparrow_z, \uparrow_z) = P_{AB}(\downarrow_z, \downarrow_z) = 0 \Rightarrow \text{Measurement outcomes are anticorrelated along } z$$

Moreover Alice can predict Bob's spin measurement along-z, based on her measurement.

$$\hat{\rho}_B |_{\uparrow_z^A} = \frac{\langle\uparrow_z| \hat{\rho}_{AB} | \uparrow_z\rangle_A}{P_{\uparrow_z}^A} = |\downarrow\rangle_B \langle\downarrow|, \quad \hat{\rho}_B |_{\downarrow_z^A} = \frac{\langle\downarrow_z| \hat{\rho}_{AB} | \downarrow_z\rangle_A}{P_{\downarrow_z}^A} = |\uparrow\rangle_B \langle\uparrow|$$

So, what's different about the entangled state? This state is classically correlated,

it is a statistical mixture of possible correlations. The entangled state is a coherent superposition of possible correlations. Thus, for example, suppose

Alice measures the spin along any other axis  $\vec{n}$ .  $|\uparrow_{\vec{n}}\rangle = \cos\frac{\theta}{2} |\uparrow_z\rangle + e^{i\phi} \sin\frac{\theta}{2} |\downarrow_z\rangle$ ,  
 $|\downarrow_{\vec{n}}\rangle = \cos\frac{\theta}{2} |\downarrow_z\rangle - e^{i\phi} \sin\frac{\theta}{2} |\uparrow_z\rangle$ . For the singlet  $|\Psi\rangle = \frac{1}{\sqrt{2}} (|\uparrow_{\vec{n}}\rangle |\downarrow_{\vec{n}}\rangle - |\downarrow_{\vec{n}}\rangle |\uparrow_{\vec{n}}\rangle)$

thus, if Alice measures  $\vec{n} \cdot \hat{\sigma}$  and finds  $|\uparrow_{\vec{n}}\rangle_A$  Bob's state is projected to  $|\downarrow_{\vec{n}}\rangle$  and vice versa. The measurement outcomes are perfectly anti-correlated along any axis.

This is a special feature of entanglement, impossible with classical correlations.

## Schmidt Decomposition

How do we determine if a state is entangled and quantify the amount of entanglement?

In the case of bipartite pure states, the complete description is given in terms of:

Theorem: Given a bipartite pure state on a tensor product space  $|\Psi\rangle \in \mathcal{H}_{AB} = \mathcal{h}_A \otimes \mathcal{h}_B$

then  $|\Psi\rangle_{AB} = \sum_{\mu=1}^X \lambda_{\mu} |u_{\mu}\rangle_A \otimes |v_{\mu}\rangle_B$  (Schmidt decomposition)

•  $1 \leq X \leq \min(d_A, d_B)$  : Schmidt Rank  $X > 1 \Rightarrow |\Psi\rangle_{AB}$  entangled

•  $\lambda_{\mu} > 0$  (Schmidt numbers)

•  $\langle u_{\mu} | u_{\mu'} \rangle_A = \langle v_{\mu} | v_{\mu'} \rangle_B = \delta_{\mu\mu'}$  : Schmidt vectors

- The Schmidt decomposition differs from the expansion in arbitrary basis in that it involves the sum over one index.

- The bases  $\{|u_\mu\rangle_A\}$  and  $\{|v_\mu\rangle_B\}$  are known as the Schmidt bases. They are functions of the state  $|\Psi\rangle_{AB}$ .

- If the Schmidt rank = 1, the state is separable

$$|\Psi\rangle_{AB} = |u_1\rangle_A \otimes |v_1\rangle_B$$

Before proving this theorem, let's look at its implications.

- Unitarily equivalent marginals

$$\hat{\rho}_{AB} = |\Psi\rangle_{AB} \langle\Psi|_{AB} = \sum_{\mu, \mu'} \lambda_\mu \lambda_{\mu'}^* |u_\mu\rangle_A \langle u_{\mu'}|_A \otimes |v_\mu\rangle_B \langle v_{\mu'}|_B$$

$$\Rightarrow \hat{\rho}_A = \text{Tr}_B(\hat{\rho}_{AB}) = \sum_{\mu=1}^x p_\mu |u_\mu\rangle_A \langle u_\mu|_A, \quad \hat{\rho}_B = \text{Tr}_A(\hat{\rho}_{AB}) = \sum_{\mu=1}^x p_\mu |v_\mu\rangle_B \langle v_\mu|_B, \quad p_\mu \equiv \lambda_\mu^2$$

The marginal (reduced) density operators for the two subsystems have the same spectrum (eigenvalues). The Schmidt numbers are the (positive) square root of the eigenvalues. The Schmidt vectors are the eigenvectors of the marginals (up to an overall phase). The (relative phase) of  $|u_\mu\rangle_A$  and  $|v_\mu\rangle_B$  are important to the average state  $|\Psi\rangle_{AB}$ . We cannot reconstruct  $|\Psi\rangle_{AB}$  from the marginals.

- Quantifying entanglement

Note the purity of the marginals are equal  $\text{Tr}(\hat{\rho}_A^2) = \text{Tr}(\hat{\rho}_B^2) = \sum_{\mu=1}^x \lambda_\mu^4$

This is one measure of entanglement. The more entangled is  $|\Psi\rangle_{AB}$  the more mixed are  $\hat{\rho}_A$  and  $\hat{\rho}_B$ . A standard measure of entanglement is the von Neumann entropy of the marginals. This is a measure of the "information content" of the marginals.

von Neumann entropy  $S_A(\hat{\rho}_A) = S_B(\hat{\rho}_B) = -\text{tr}(\hat{\rho}_A \log \hat{\rho}_A) = \sum_{\mu=1}^{\chi} -P_{\mu} \log P_{\mu}$

$$0 \leq S \leq \log d_L \quad d_L = \min(d_A, d_B)$$

$\uparrow$  separable  $|\psi_{AB}\rangle$        $\uparrow$  maximally entangled  $|\underline{\Psi}\rangle = \frac{1}{\sqrt{d_L}} \sum_{\mu=1}^{d_L} |u_{\mu}\rangle_A \otimes |v_{\mu}\rangle_B$

We typically measure the log in base-2 so entropy in "bits"

$$0 \leq E \leq \log_2 d \quad (d = \min(d_A, d_B))$$

$\uparrow$  separable       $\uparrow$  maximally entangled

Eg. Two qubits  $|\underline{\Psi}\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) \Rightarrow$  Schmid decomposition

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

$$\lambda^2 = \left(\frac{1}{2}, \frac{1}{2}\right) \text{ max entropy } E = 1 \text{ bit}$$

- The Von-Neumann entropy of the marginals  $\hat{\rho}^A$  and  $\hat{\rho}^B$  are equal and determined the entanglement of  $|\Psi\rangle_{AB}$

$$E_{|\Psi\rangle_{AB}} = S(\hat{\rho}_A) = S(\hat{\rho}_B) = -\text{Tr}(\hat{\rho}_A \log_2 \hat{\rho}_A)$$

This is one of the most profound results of quantum theory. Even though we have maximal information about the joint system, it is in a pure state,  $|\Psi\rangle_{AB}$ , if it is entangled we have an incomplete description of the parts taken alone; they are in mixed state  $\hat{\rho}^A, \hat{\rho}^B$ . The missing information is in the quantum correlations between A + B. The entropy of the state represents our the missing information about the state. When the state is pure, its entropy is zero. When it is maximally mixed, its entropy is  $\log d$ . If  $|\Psi\rangle_{AB}$  is maximally entangled, and  $d_A = d_B = d$ , then  $\hat{\rho}_A$  and  $\hat{\rho}_B$  are maximally mixed.

### Proof of the Schmidt Decomposition

Let  $|\Psi_{AB}\rangle \in \mathcal{H}_{AB} = \mathcal{H}_A \otimes \mathcal{H}_B$      $\dim(\mathcal{H}_A) = d_A$      $\dim(\mathcal{H}_B) = d_B$   
 Basis for  $\mathcal{H}_{AB}$      $\{|i, j\rangle\} = \{|e_i\rangle_A \otimes |f_j\rangle_B\}$      $i=1, \dots, d_A$  ;  $j=1, \dots, d_B$

$$\Rightarrow |\Psi_{AB}\rangle = \sum_{i,j} \gamma_{ij} |e_i\rangle_A \otimes |f_j\rangle_B, \quad \gamma_{ij} = \langle i, j | \Psi_{AB} \rangle$$

The expansion coefficients form a  $d_A \times d_B$  rectangular matrix. The Schmidt decomposition follows from the singular value decomposition (SVD), which is a generalization of diagonalization of Hermitian matrices.



## Aside: Spectral Theorem and the Diagonalization of Hermitian Operators

Consider  $\hat{A}: \mathcal{H} \rightarrow \mathcal{H}$  a (Hermitian) linear operator on  $\mathcal{H} \{ |e_i\rangle \mid i=1, \dots, d \}$  basis

$$\Rightarrow \hat{A} = \sum_{ij} A_{ij} |e_i\rangle \langle e_j| \quad A_{ij} = \langle e_i | \hat{A} | e_j \rangle = d \times d \text{ matrix representation}$$

Spectral theorem  $\hat{A} = \sum_{\mu, \nu=1}^d D_{\mu\nu} |a_\mu\rangle \langle a_\nu|$

where  $\hat{A} |a_\mu\rangle = a_\mu |a_\mu\rangle$ ,  $\{ |a_\mu\rangle \mid \mu=1 \dots d \}$  orthonormal basis  $\langle a_\mu | a_{\mu'} \rangle = \delta_{\mu\mu'}$   
 $a_\mu$  eigenvalues,  $|a_\mu\rangle$  eigenvectors

$$D_{\mu\nu} = \langle a_\mu | \hat{A} | a_\nu \rangle = a_\mu \delta_{\mu\nu} \text{ diagonal matrix}$$

Similarity transformation:  $A_{ij} = \sum_{\mu, \mu'} \underbrace{\langle e_i | a_\mu \rangle}_{\text{Change of basis}} D_{\mu\mu'} \underbrace{\langle a_{\mu'} | e_j \rangle}_{(U^\dagger)_{\mu'j}} = U_{i\mu} D_{\mu\mu'} (U^\dagger)_{\mu'j}$   
Change of basis  $\rightarrow U_{i\mu}$  basis matrix

## Aside: Singular value decomposition

Let us define  $\hat{\gamma} = \sum_{ij} \gamma_{ij} |e_i\rangle_A \langle f_j|_B$ . This is a linear operator

that maps  $\mathcal{H}_B \rightarrow \mathcal{H}_A$  and  $\mathcal{H}_B^\dagger \rightarrow \mathcal{H}_A^\dagger$

$$\begin{cases} \hat{\gamma} | \psi \rangle_B = | \phi \rangle_A \\ \langle \tilde{\psi} |_A | \hat{\gamma} = \langle \tilde{\phi} |_B \end{cases}$$

$\gamma_{ij}$  is the (rectangular) representation in the bases of  $\mathcal{H}_A + \mathcal{H}_B$

SVD  $\hat{\gamma} = \sum_{\mu=1}^n \lambda_\mu |u_\mu\rangle_A \langle v_\mu|_B$   
 $\lambda_\mu$  singular values,  $|u_\mu\rangle_A$  left eigenvectors,  $\langle v_\mu|_B$  right eigenvectors,  $\lambda_\mu \geq 0$  (including zero)

$$\hat{\gamma} |v_\mu\rangle_B = |u_\mu\rangle_A \quad \langle u_\mu|_A \hat{\gamma} = \langle v_\mu|_B, \quad (\text{Relative phase of } |u_\mu\rangle_A + |v_\mu\rangle_B \text{ set by } \hat{\gamma})$$

$$\hat{\gamma} \hat{\gamma}^\dagger: \mathcal{H}_A \rightarrow \mathcal{H}_A \quad \hat{\gamma}^\dagger \hat{\gamma}: \mathcal{H}_B \rightarrow \mathcal{H}_B. \quad \text{Both are Hermitian } \geq 0: \text{ Diagonalizable}$$

SVD  $\Rightarrow$  they have the same eigenvalues

$$\hat{\gamma} \hat{\gamma}^\dagger = \sum_{\mu=1}^{d_L} \lambda_\mu^2 |u_\mu\rangle_A \langle u_\mu|, \quad \hat{\gamma}^\dagger \hat{\gamma} = \sum_{\mu=1}^{d_L} \lambda_\mu^2 |v_\mu\rangle_B \langle v_\mu|$$

If some  $\lambda_\mu = 0$  they don't contribute  $\chi \leq d_L$

$$\gamma_{ij} = \langle e_i | \hat{\gamma} | f_j \rangle = \sum_{\mu} \lambda_{\mu} \underbrace{\langle e_i | u_{\mu} \rangle}_U \underbrace{\langle v_{\mu} | f_j \rangle}_{(V^\dagger)_{\mu j}} = \sum_{\mu, \mu'} \underbrace{U_{i\mu}}_{d_A \times d_A} \underbrace{D_{\mu\mu'}}_{d_A \times d_B} \underbrace{(V^\dagger)_{\mu'j}}_{d_B \times d_B}$$

As a matrix  $\gamma = \begin{bmatrix} U \\ d_A \times d_A \end{bmatrix} \begin{bmatrix} D \\ d_A \times d_B \end{bmatrix} \begin{bmatrix} V^\dagger \\ d_B \times d_B \end{bmatrix}$

$$\text{Given } \gamma_{ij} = \sum_{\mu} \lambda_{\mu} U_{i\mu} V_{\mu j}^\dagger = \sum_{\mu} \lambda_{\mu} \langle e_i | u_{\mu} \rangle \langle f_j | v_{\mu} \rangle^* \Rightarrow |\Psi_{AB}\rangle = \sum_{\mu} \lambda_{\mu} \sum_i |e_i\rangle \langle e_i | u_{\mu} \rangle \otimes \sum_j |f_j\rangle \langle f_j | v_{\mu} \rangle^*$$

$$\Rightarrow |\Psi_{AB}\rangle = \sum_{\mu} \lambda_{\mu} |u_{\mu}\rangle_A \otimes |v_{\mu}^*\rangle_B$$

(Note: Here the  $|v_{\mu}^*\rangle_B$  arose because we considered  $\hat{\gamma} = \sum \gamma_{ij} |e_i\rangle_A \langle f_j|_B$  (bra))  
The standard Schmidt decomposition would take  $\gamma_{ij} = U_{i\mu} D_{\mu\mu'} V_{\mu'j}^\dagger$  as in Nielsen & Chuang).

## The generation of entanglement

Entanglement corresponds to the quantum correlation between degrees of freedom. Thus, to create entanglement, one must have interactions between these degrees of freedom. A Hamiltonian which acts separately on the two degrees of freedom is said to be "separable"

$$\hat{H}_{BA} = \hat{H}_A \otimes \hat{1}_B + \hat{1}_A \otimes \hat{H}_B$$

Such as Hamiltonian has separable (product-state) eigenstates,  $|\Psi_{nm}\rangle_{AB} = |e_n\rangle_A |f_m\rangle_B$ .  
The unitary evolution acts "locally" on each subsystem

$$\hat{U}_{AB} = e^{-i\hat{H}_{AB}t} = e^{-i(\hat{H}_A \otimes \hat{1}_B + \hat{1}_A \otimes \hat{H}_B)t} = \underbrace{e^{-i\hat{H}_A t}}_{\hat{U}_A} \otimes \underbrace{e^{-i\hat{H}_B t}}_{\hat{U}_B}$$

When there are interactions between the subsystems, the Hamiltonian is not separable

$$\hat{H}_{AB} \neq \hat{H}_A \otimes \hat{1}_B + \hat{1}_A \otimes \hat{H}_B \quad \text{e.g.} \quad \hat{H}_{AB} = \hat{H}_A \otimes \hat{1}_B + \hat{1}_A \otimes \hat{H}_B + \hat{H}_A^{\text{int}} \otimes \hat{H}_B^{\text{int}}$$

$$\Rightarrow \hat{U}_{AB} = e^{-i\hat{H}_{AB}t} \neq \hat{U}_A \otimes \hat{U}_B$$

Such a unitary map is said to be an "entangling unitary" in that

$$\hat{U}_{AB} |\psi\rangle_A \otimes |\phi\rangle_B \text{ is an entangled state}$$

The eigenstates of the interacting Hamiltonian are entangled

$$|\Psi_{nm}\rangle_{AB} \neq |e_n\rangle_A \otimes |f_m\rangle_B$$

### Entanglement and the choice of subsystem "coordinates."

In classical physics, we know that the choice of coordinate is critical in simplifying the problem to allow for a solution. For example, for a coupled set of oscillators, we can write the solution instantly in terms of "normal mode" coordinates. A famous example is "two-body" problem, e.g. the Hydrogen atom. We can consider two subsystems, the electron and the nucleus (proton)

$$\hat{H}_{\text{Hyd}} = \hat{H}_{eN} = \frac{\vec{p}_e^2}{2m_e} + \frac{\vec{p}_N^2}{2m_N} - \frac{e^2}{|\vec{r}_e - \vec{r}_N|} \neq \hat{H}_e \otimes \hat{1}_N + \hat{1}_e \otimes \hat{H}_N$$

This Hamiltonian is not separable in electron and proton degrees of freedom. However, we know that we can separate center-of-mass and relative coords.

$$\hat{H}_{\text{Hyd}} = \hat{H}_{\text{cm}} = \frac{\vec{p}_c^2}{2M} + \frac{\vec{p}_r^2}{2\mu} - \frac{e}{r} = \hat{H}_c \otimes \hat{1}_r + \hat{1}_c \otimes \hat{H}_r$$

The eigenfunctions of the hydrogen atom are product states in center of mass and relative coordinates

$$|\Psi\rangle_{\text{hydrogen}} = |\vec{k}\rangle_c \otimes |n, l, m\rangle_{\text{rel}} \neq |\psi\rangle_e \otimes |\phi\rangle_p$$

$\uparrow$   
 center of mass  
 free particle plane wave

$\mathbb{R}$  Hydrogenic wave function  
 for the relative motion

Thus, we see that the choice of subsystem can determine whether or not the system is entangled or not.

The Hydrogen Hamiltonian is entangling in electron+proton coordinates but separable in relative and center-of-mass coordinates.

### Note on change of basis/coordinates and entanglement

There are two different notions of a "basis change" that can be confusing, but are relevant to the question of entanglement.

- Change of "local basis" Given a multipartite system, e.g. bipartite, with Hilbert space  $\mathcal{H}_{AB} = \mathcal{H}_A \otimes \mathcal{H}_B$ , the entanglement of the state is unchanged by a local change of basis on  $\mathcal{H}_A$  and  $\mathcal{H}_B$ .

$$\text{Given } |\Psi\rangle_{AB} = \sum \gamma_{ij} |e_i\rangle_A \otimes |f_j\rangle_B = \sum \delta_{ij} |d_i\rangle_A \otimes |g_j\rangle_B$$

$$\text{where } |d_i\rangle_A = \hat{U}_A |e_i\rangle_A, \quad |g_j\rangle_B = \hat{U}_B |f_j\rangle_B \quad (\text{local basis change})$$

$$\gamma_{ij} = \langle e_i |_A \otimes \langle f_j |_B | \Psi \rangle_{AB} \quad \& \quad \delta_{ij} = \langle d_i |_A \otimes \langle g_j |_B | \Psi \rangle_{AB} \quad \text{have the same Schmidt decomposition}$$

- Change of subsystem decomposition

The change of coordinates  $(x_A, x_B) \Rightarrow \left( \frac{x_A - x_B}{\sqrt{2}}, \frac{x_A + x_B}{\sqrt{2}} \right)$  is a basis change of the classical degrees of freedom. This is not a local basis change on the subsystem describing the motion of particle A+B.