# Hilbert space and Operators 

2018 Oct 15

## orthnormal set

- quantum states in the configuration space are complex "wave" functions

$$
\varphi(q) \quad q=(x, y, z)
$$

- it can be specified uniquely in terms of a complete orthonormal set of functions.

$$
u_{a}(q) \quad a=1,2 \cdots
$$

basis index

## completeness

- complete means that any $\varphi$ can be expressed as a linear combination of the $u_{a}$

$$
\begin{gathered}
\varphi(q)=\sum_{a=1}^{\infty} c_{a} u_{a}(q) \\
c_{a}=\int(d q) u_{a}^{*}(q) \varphi(q)
\end{gathered}
$$

## Orthonormal

- the orthonormal means

$$
\int(d q) u_{a}^{*}(q) u_{a^{\prime}}(q)=\delta_{a a^{\prime}}
$$

- the completeness relation for the set $\left\{u_{a}\right\}$ :

$$
\sum_{a} u_{a}^{*}(q) u_{a}\left(q^{\prime}\right)=\delta^{3}\left(q-q^{\prime}\right)
$$

Dirac function $\delta^{3}\left(q-q^{\prime}\right)=\delta\left(x-x^{\prime}\right) \delta\left(y-y^{\prime}\right) \delta\left(z-z^{\prime}\right)$

$$
f\left(x^{\prime}\right)=\int_{-\infty}^{\infty} \delta\left(x-x^{\prime}\right) f(x) d x
$$

## Hilbert space

- The set of square integrable functions $\left\{u_{a}(q)\right\}$ constitute a basis in an infinite dimensional complex vector space, called a Hilbert space.
- The functions $u_{a}(q)$ on the configuration space do not form a unique description of this particular basis.


## Momentum basis

- the Fourier transform of $u_{a}$

$$
v_{a}(p)=\prod_{j} \int \frac{d q_{j}}{\sqrt{L}} e^{i p_{j} q_{j} / \hbar} u_{a}(q)
$$

- To satisfy the boundary condition

$$
\frac{p_{j}}{\hbar}=\frac{2 n_{j} \pi}{L}, \quad n_{j}=0, \pm 1, \pm 2 \cdots
$$



- the set of functions $\left\{v_{a}(p)\right\}$ in momentum space provides a "representation" of the same basis in H


## Plane wave basis

- the plane waves form a complete orthonormal basis

$$
\phi_{p_{1}, p_{2}, \ldots}(q)=\phi_{p}(q)=\frac{1}{\sqrt{L}} \prod_{j} e^{i_{p} q_{j} / \hbar}
$$

orthonormal

$$
\int(d q) \phi_{p}^{*}(q) \phi_{p^{\prime}}(q)=\prod_{j} \delta_{p_{j} p_{j}^{\prime}}
$$

completeness

$$
\sum_{p} \phi_{p}^{*}(q) \phi_{p}\left(q^{\prime}\right)=\delta^{3}\left(q-q^{\prime}\right)
$$

$$
v_{a}(p)=\int(d q) \phi_{p}^{*}(q) u_{a}(q) \longleftrightarrow u_{a}(p)=\sum_{\{p\}} \phi_{p}^{*}(p) v_{a}(p)
$$

## Dirac's notation

- In Dirac's nomenclature, the vectors in this space are called kets, and denoted by the symbol | >
- By the definition of a complex vector space, the product $\alpha|\xi\rangle$ is a vector in the space
- the sum is also a vector $|\zeta\rangle=\alpha|\xi\rangle+\beta|\eta\rangle$
$(\alpha, \beta, \gamma \cdots)$ are complex numbers


## scalar product

- to associate a dual vector to every ket in a one-to-one manner, called a bra, denoted by the <|
- scalar products are define between bras and kets.

$$
\langle\xi \mid \eta\rangle=\langle\eta \mid \xi\rangle^{*}
$$

- $\langle\xi \mid \xi\rangle$ of any ket is real, and by definition positive.


## scalar product

- The dual bra of $|\zeta\rangle=\alpha|\xi\rangle+\beta|\eta\rangle$

$$
\langle\zeta|=\alpha^{*}\langle\xi|+\beta^{*}\langle\eta|
$$

- the scalar product satisfies the linear relationship

$$
\langle\omega \mid \zeta\rangle=\alpha\langle\omega \mid \xi\rangle+\beta\langle\omega \mid \eta\rangle
$$

## Schwartz inequality

- similar in vector space

$$
|\vec{\omega} \cdot \vec{v}| \leq \omega v
$$

$$
|\langle\xi \mid \eta\rangle|^{2} \leq\langle\xi \mid \xi\rangle\langle\eta \mid \eta\rangle
$$

## orthonormal basis

- a set of basis, $\{|k\rangle\}$ satisfies

$$
\left\langle k \mid k^{\prime}\right\rangle=\delta_{k k^{\prime}}
$$

- any vector $|\omega\rangle$ can be expressed by linear combination

$$
\begin{aligned}
|\omega\rangle & =\sum_{k} c_{k}|k\rangle \\
& =\sum_{k}|k\rangle\langle k \mid \omega\rangle
\end{aligned}
$$

$$
c_{k}=\langle k \mid \omega\rangle
$$

## projection operator

- For Id subspace spanned by single basis $|k\rangle$ define projection operator

$$
\begin{aligned}
P_{k}|\omega\rangle & =c_{k}|k\rangle \\
& =|k\rangle\langle k \mid \omega\rangle \\
P_{k} & =|k\rangle\langle k|
\end{aligned}
$$

- summation of all independent projection operators gives the entire Hilbert space

$$
1=\sum_{k}|k\rangle\langle k|
$$

# product of projection operators <br> $$
\begin{array}{r} P_{k} P_{k^{\prime}}=|k\rangle\left\langle k \mid k^{\prime}\right\rangle\left\langle k^{\prime}\right|=\delta_{k k^{\prime}}|k\rangle\langle k|=\delta_{k k^{\prime}} P_{k} \\ P_{k}^{2}=P_{k} \end{array}
$$ 

- one can define a projection to multidimensional subspace that

$$
P_{\mathcal{K}}=\sum_{i=1}^{n}\left|k_{i}\right\rangle\left\langle k_{i}\right|
$$

again $\quad P_{\mathcal{K}}^{2}=P_{\mathcal{K}} \quad P_{\mathcal{K}} P_{\mathcal{K}^{\prime}}=0$ if K and $\mathrm{K}^{\prime}$ do not have common basis

## matrix element

- any operator A can be expressed in k representation

$$
A=\sum_{k k^{\prime}}\left|k^{\prime}\right\rangle\left\langle k^{\prime}\right| A|k\rangle\langle k|=\sum_{k k^{\prime}}\left\langle k^{\prime}\right| A|k\rangle\left|k^{\prime}\right\rangle\langle k|
$$

- $\left\langle k^{\prime}\right| A|k\rangle \quad$ is called matrix element
- for the product of operators

$$
\left\langle k^{\prime}\right| B A|k\rangle=\sum_{k^{\prime \prime}}\left\langle k^{\prime}\right| B\left|k^{\prime \prime}\right\rangle\left\langle k^{\prime \prime}\right| A|k\rangle
$$

# expectation value, trace and determinant 

- the diagonal matrix element $\langle k| A|k\rangle$ is called the expectation value in $|k\rangle$
- Global properties of an operator are

$$
\begin{aligned}
\operatorname{Tr} A & =\sum_{k}\langle k| A|k\rangle \\
\operatorname{det} A & =\operatorname{det}\left\{\left\langle k^{\prime}\right| A|k\rangle\right\}
\end{aligned}
$$

# transpose and complex conjugate 

- associate operator: transpose

$$
A^{T}=\sum_{k k^{\prime}}\left|k^{\prime}\right\rangle\left\langle k^{\prime}\right| A^{T}|k\rangle\langle k|=\sum_{k k^{\prime}}\langle k| A\left|k^{\prime}\right\rangle\left|k^{\prime}\right\rangle\langle k|
$$

- associate operator: complex conjugate

$$
A^{*}=\sum_{k k^{\prime}}\left|k^{\prime}\right\rangle\left\langle k^{\prime}\right| A^{*}|k\rangle\langle k|=\sum_{k k^{\prime}}\left\langle k^{\prime}\right| A|k\rangle^{*}\left|k^{\prime}\right\rangle\langle k|
$$

## Hermitian adjoint

- symmetric operator $A^{T}=A$
- Hermitian adjoint $\quad A^{\dagger}=\left(A^{T}\right)^{*} \quad(A B)^{\dagger}=B^{\dagger} A^{\dagger}$
- Self-adjoint (Hermitian) operator

$$
A^{\dagger}=A
$$

## commutator

- The commutator of two Hermitian operators is anti-Hermitian

$$
\begin{gathered}
{[A, B]=A B-B A} \\
{[A, B]^{\dagger}=(A B)^{\dagger}-(B A)^{\dagger}=B^{\dagger} A^{\dagger}-A^{\dagger} B^{\dagger}=-[A, B]}
\end{gathered}
$$

- The anti-commutator of two Hermitian operators is Hermitian

$$
\begin{gathered}
\{A, B\}=A B+B A \\
\{A, B\}^{\dagger}=(A B)^{\dagger}+(B A)^{\dagger}=B^{\dagger} A^{\dagger}+A^{\dagger} B^{\dagger}=\{A, B\}
\end{gathered}
$$

- Product of two Hermitian operators is Hermitian when they commute $[A, B]=0$


## decomposition

- any operator can be decomposed into Hermitian and anti-Hermitian parts

$$
\begin{aligned}
& A_{1}=\frac{1}{2}\left(A+A^{\dagger}\right) \\
& A_{2}=\frac{1}{2}\left(A-A^{\dagger}\right)
\end{aligned}
$$

- the products $A A^{\dagger}$ and $A^{\dagger} A$ are positive operators, namely the expectation values are real and positive

$$
A A^{\dagger}-A^{\dagger} A=\left[\left(A_{1}+A_{2}\right),\left(A_{1}-A_{2}\right)\right]=2\left[A_{2}, A_{1}\right]
$$

## unitary transformation

- An operator is unitary if $U U^{\dagger}=U^{\dagger} U=1$
- in terms of k-basis

$$
\begin{aligned}
& \sum_{k^{\prime \prime}}\langle k| U\left|k^{\prime \prime}\right\rangle\left\langle k^{\prime \prime}\right| U^{\dagger}\left|k^{\prime}\right\rangle=\delta_{k k^{\prime}} \\
& =\sum_{k^{\prime \prime}}\langle k| U\left|k^{\prime \prime}\right\rangle\left\langle k^{\prime}\right| U\left|k^{\prime \prime}\right\rangle^{*}
\end{aligned}
$$

## basis transformation

- consider a different orthonormal basis of the same Hilbert space $|r\rangle$
- they can be expressed by the basis $|k\rangle$

$$
|r\rangle=\sum_{k}\langle k \mid r\rangle|k\rangle
$$

$\langle k \mid r\rangle$ is transformation function
they are elements in a unitary matrix

$$
\sum_{k}\langle r \mid k\rangle\left\langle k \mid r^{\prime}\right\rangle=\delta_{r r^{\prime}}
$$

## unitary transformation

- unitary transformation of an operator is defined by $U^{\dagger} A U$
- We know that $\operatorname{Tr} A B=\operatorname{Tr} B A$

$$
\begin{gathered}
\operatorname{det}(A B)=\operatorname{det}(A) \operatorname{det}(B) \\
\operatorname{det}\left(U^{\dagger} U\right)=|\operatorname{det} U|^{2}=1 \\
\operatorname{Tr}\left(U^{\dagger} A U\right)=\operatorname{Tr}\left(U^{\dagger} U A\right)=\operatorname{Tr}(A) \\
\operatorname{det}\left(U^{\dagger} A U\right)=\operatorname{det}\left(U^{\star} U A\right)=\operatorname{det}(A)
\end{gathered}
$$

the trace and determinant of any operator are invariant under unitary transformations, or under a change of basis.

## Hermitian and unitary

- the common relation between Hermitian and unitary operators in QM is

$$
\begin{gathered}
U=e^{i Q}=\sum_{n} \frac{(i Q)^{n}}{n!} \\
U^{\dagger}=e^{-i Q}
\end{gathered}
$$

perturbation theory
continuous symmetries
another form $\quad U=\frac{1+i K}{1-i K}$

## q basis vs. p basis

- the product of plane waves is the unitary transformation from the $q$ to the $p$ basis:

$$
\begin{aligned}
& v_{a}(p)=\int(d q) \phi_{p}^{*}(q) u_{a}(q) \\
& |p\rangle=\sum_{q}\langle q \mid p\rangle|q\rangle \\
& \phi_{p}(q)=\frac{1}{\sqrt{L}} e^{i p q / \hbar}=\langle q \mid p\rangle \quad \text { discrete form }
\end{aligned}
$$

## discrete vs. continuous

- denumerable basis


## spatial continuum

$\longrightarrow$ discrete lattice
discrete momentum basis

$\longrightarrow$ continuum when $L \rightarrow \infty$

$$
\phi_{p}(q)=\frac{1}{\sqrt{L}} e^{i p q / \hbar} \quad \longrightarrow \quad \phi_{p}(q)=\frac{e^{i p q / \hbar}}{\sqrt{2 \pi \hbar}}
$$

## continuous limit

$$
\begin{gathered}
\phi_{p}(q)=\frac{e^{i p q / \hbar}}{\sqrt{2 \pi \hbar}} \\
\int d q \phi_{p}^{*}(q) \phi_{p^{\prime}}(q)=\delta\left(p-p^{\prime}\right) \\
\int d p \phi_{p}^{*}(q) \phi_{p}\left(q^{\prime}\right)=\delta\left(q-q^{\prime}\right) \\
\langle q \mid p\rangle_{\infty}=\varphi_{p}(q)=\frac{1}{\sqrt{2 \pi \hbar}} e^{i q q / \hbar}
\end{gathered}
$$

## eigenvalues

- Any single Hermitian operator A can be diagonalized by a unitary transformation.
- The elements of this diagonalized form are real and are called the eigenvalues
- The eigenvalues are the roots of the secular equation $\quad \operatorname{det}(A-a I)=0$


## eigenvectors

- The basis vectors that diagonalize A are called its eigenvectors or eigenkets

$$
A|n\rangle=a_{n}|n\rangle
$$

spectral decomposition $\quad A=\sum_{n} a_{n}|n\rangle\langle n|$

- Eigenvectors with different eigenvalues are orthogonal.


## commutator

- If $A_{i}$, where $i=I, \ldots, K$, is a set of $K$ commuting Hermitian operators, these operators can be diagonalized simultaneously

$$
A_{i}|n\rangle=a_{n}^{(i)}\left|a_{n}\right\rangle
$$

- If a pair of Hermitian matrices do not commute, they cannot be diagonalized simultaneously.
- If $|a\rangle_{\text {is an eigenket of } \mathrm{A}}$ with eigenvalue a , and $B$ is any operator (in general, not Hermitian) such that

$$
\begin{aligned}
& {[A, B]=\lambda B \quad \text { then }} \\
& B|a\rangle=\text { const }|a+\lambda\rangle
\end{aligned}
$$

## States and Probabilities

- the statistical character of quantum mechanics is irreducible - that there are no underlying "hidden variables" which behave in a deterministic manner, and that this statistical character is not an expression of ignorance about such hidden substructure.


## quantum states

- I.The most complete possible description of the state of any physical system $S$ at any instant is provided by some particular vector $|\phi\rangle$ in the Hilbert space appropriate to the system. Every linear combination of such state vectors represents a possible physical state of $S$.

When $S$ can be described by one vector, it is in a pure state. Should no single ket suffice, $S$ is in a mixed state, or mixture.

## observables

- 2.The physically meaningful entities of classical mechanics, such as momentum, energy, position and the like, are represented by Hermitian operators.

$$
A=\sum_{a}|a\rangle a\langle a|
$$

$\left(a, a^{\prime}, \ldots\right)$ are the real eigenvalues of $A$

## probability

- 3.A set of $N$ identically prepared replicas of a system $S$ described by the pure state $|\phi\rangle$, when subjected to a measurement designed to display the physical quantity represented by the observable A, will in each individual case display one of the values ( $\mathrm{a}, \mathrm{a}^{\prime}, \ldots$ ), and as $N \rightarrow \infty$ will do so with the probabilities $\mathrm{P}_{\varphi}(\mathrm{a}), \mathrm{P}^{\prime}{ }_{\varphi}\left(\mathrm{a}^{\prime}\right), \ldots$, where

$$
p_{\phi}(a)=|\langle a \mid \phi\rangle|^{2}
$$

## sum rule and mean value

- sum rule

$$
p_{\phi}(a) \geq 0 \quad \sum_{a} p_{\phi}(a)=1
$$

- mean value of $A$

$$
\begin{gathered}
\langle A\rangle_{\phi}=\sum_{a} a p_{\phi}(a) \\
\langle\phi| A|\phi\rangle=\sum_{a} a|\langle a \mid \phi\rangle|^{2}
\end{gathered}
$$

## projection operator <br> $$
p_{\phi}(a)=|\langle a \mid \phi\rangle|^{2}=\langle\phi| P_{a}|\phi\rangle
$$

- $\mathrm{P}_{\mathrm{a}}$ is the projection operator

$$
P_{a}=|a\rangle\langle a|
$$

in general the probability that a system $S$ in the state $|\phi\rangle$ will be found to be in the arbitrary state $|\psi\rangle$ is

$$
p_{\phi}(\psi)=|\langle\psi \mid \phi\rangle|^{2}
$$

## Hidden variables?

The common-sense inference that measurements reveal pre-existing values leads to implications that are contradicted by experiment, experiment, and are also incompatible with the Hilbert space structure of quantum mechanics.

Values cannot be ascribed to observables prior to measurement; such values are only the outcomes of measurement.

## measurement outcomes

example: polarization of a photon

```
photon state |\phi\rangle
```

circular polarization measurement

$$
M_{\text {circ }} \quad\left|k_{R}\right\rangle\left|k_{L}\right\rangle
$$

probabilities
$\left|\left\langle k_{R, L} \mid \phi\right\rangle\right|^{2}$
linear polarization measurement

$$
M_{\operatorname{lin}} \quad\left|k_{1}\right\rangle\left|k_{2}\right\rangle \quad\left|\left\langle k_{1,2} \mid \phi\right\rangle\right|^{2}
$$

## compatible observables

- compatible observables: observables that all commute with each other
- If $A$ and $B$ commute, there exist simultaneous eigenkets $\{|a b\rangle\}$ of A and B with eigenvalues ( $\mathrm{a}, \mathrm{a}^{\prime}, \ldots ., \mathrm{b}, \mathrm{b}^{\prime}, \ldots$...


## compatible observables

- the action of $f(A, B)$ on the simultaneous eigenkets is then

$$
f(A, B)|a b\rangle=f(a, b)|a b\rangle
$$

- the expectation value

$$
\langle\phi| f(A, B)|\phi\rangle=\sum_{a b} f(a, b)\langle a b \mid \phi\rangle
$$

- the joint probability

$$
p_{\phi}(a b)=|\langle a b \mid \phi\rangle|^{2}
$$

## Conditional probability

- the probability for the occurrence of $b$ given that a has definitely occurred.

$$
p_{\phi}(a \mid b)=\frac{p_{\phi}(a b)}{p_{\phi}(a)}
$$

some identities

$$
\sum_{b} p_{\phi}(a \mid b)=1 \quad \sum_{b} p_{\phi}(a b)=p_{\phi}(a)
$$

example: 2(or N )-particle wavefunction

## incompatible observables

- P and Q do not commute, simultaneous eigenkets of P and Q do not exist.

$$
P|p\rangle=p|p\rangle \quad Q|q\rangle=q|q\rangle
$$

- the probability distribution

$$
p_{\phi}(p)=|\langle p \mid \phi\rangle|^{2} \quad p_{\phi}(q)=|\langle q \mid \phi\rangle|^{2}
$$

- not possible to define a joint distribution
- first calculate the probability displaying eigenvalue $p$

$$
p_{\phi}(p)=|\langle p \mid \phi\rangle|^{2}
$$

- then calculate the probability displaying eigenvalue $q$

$$
p_{p}(q)=|\langle q \mid p\rangle|^{2}
$$

- sum over all possible p, we have

$$
\sum_{p} p_{p}(q) p_{\phi}(p)=\sum_{p}|\langle q \mid p\rangle\rangle^{2}|\langle p \mid \phi\rangle|^{2}
$$

- one can compare it to $p_{\phi}(q)=|\langle q \mid \phi\rangle|^{2}$


## physical interpretation

- first perform the measurement of $\mathrm{P} M_{P}$ as a consequence of which these individuals are known to be in the state $|p\rangle$
- then perform the measurement of $\mathrm{Q} M_{Q}$
- The sum on p only results a recoverable loss of knowledge.

$$
\sum_{p}|\langle q \mid p\rangle|^{2}|\langle p \mid \phi\rangle|^{2} \rightarrow\left|\sum_{p}\langle q \mid p\rangle\langle p \mid \phi\rangle\right|^{2}
$$

## Mixtures

- example : a collection of atoms in thermodynamic equilibrium.
- Hamiltonian H with energy eigenvalues $\{\mathrm{E}\}$. There will be other observables compatible with H, designated collectively by A, that together specify a basis $|E a\rangle$
- At temperature $T$ these states are populated in accordance with the Boltzmann probability distribution, $\quad p_{T}(E)=e^{-E / k T} / Z$
partition function $\quad Z=\sum_{E, a} \exp (-E / k T)$


## expectation value

- The expectation value of some observable Q, which need not be compatible with the the Hamiltonian,

$$
\begin{aligned}
& \langle Q\rangle_{T}=\sum_{E, a} p_{T}(E)\langle E a| Q|E a\rangle \\
& \langle Q\rangle_{T}=\left.\sum_{E, a} \sum_{q} q p_{T}(E)\langle Q| E a\right|^{2}
\end{aligned}
$$

the probability that such a pure state occurs in the thermal ensemble
statistical distribution of eigenvalues of Q in the pure states, $|E a\rangle$

## density matrix

- It is an operator
- The density matrix describing a thermal equilibrium ensemble is define as a sum of projection operators onto the basis $|E a\rangle$ weighted by the Boltzmann distribution.

$$
\rho_{T}=\sum_{E, a} p_{T}(E)|E a\rangle\langle E a|=\sum_{E, a} p_{T}(E) P(E a)
$$

- the trace of density matrix is $1 \operatorname{Tr} \rho_{T}=\sum_{E, a} p_{T}(E)=1$
- With the density matrix, the expectation value of Q can be written as

$$
\langle Q\rangle_{T}=\operatorname{Tr}\left(\rho_{T} Q\right)
$$

## Pure state

- Let $|\psi\rangle$ be some pure state, the density matrix is simply a projection operator

$$
\begin{gathered}
\rho_{\psi}=|\psi\rangle\langle\psi|=P_{\psi} \\
\langle Q\rangle_{\psi}=\sum_{q, q^{\prime}}\left\langle\psi \mid q^{\prime}\right\rangle\left\langle q^{\prime}\right| Q|q\rangle\langle q \mid \psi\rangle \\
=\sum_{q, q^{\prime}}\langle q \mid \psi\rangle\left\langle\psi \mid q^{\prime}\right\rangle\left\langle q^{\prime}\right| Q|q\rangle \\
=\sum_{q, q^{\prime}}\langle q| P_{\psi}\left|q^{\prime}\right\rangle\left\langle q^{\prime}\right| Q|q\rangle=\operatorname{Tr}\left(P_{\psi} Q\right)
\end{gathered}
$$

- the density matrix of a pure state is characterized by

$$
\rho_{\psi}^{2}=\rho_{\psi} \quad \operatorname{Tr}\left(\rho_{\psi}^{2}\right)=1
$$

- the square of the thermal density matrix
- the trace

$$
\operatorname{Tr}\left(\rho_{T}^{2}\right)=\sum_{E, a}\left[p_{T}(E)\right]^{2} \leq 1
$$

$$
\rho_{T}^{2}=\sum_{E, a}\left[p_{T}(E)\right]^{2} P(E a) \quad P^{2}(E a)=P(E a)
$$

$\operatorname{Tr}\left(\rho_{T}^{2}\right)=1 \quad$ only $\mathbf{T}=0$, a pure state of ground state
A state is pure if its density matrix P is a projection operator, and it is a mixture if it is not. The two cases are characterized by the invariant condition

$$
\operatorname{Tr}\left(\rho_{T}^{2}\right) \leq 1
$$

with the equality only holding if the state is pure.

- density matrix can be written in any basis, as an observable whose eigenvalues ( $\mathrm{p}, \mathrm{P} 2, \ldots$ ) satisfy

$$
0 \leq p_{i} \leq 1 \quad \sum_{i} p_{i}=1
$$

- Let $\left|a_{i}\right\rangle$ be the orthonormal basis that diagonalizes p , so that

$$
\rho=\sum_{i}\left|a_{i}\right\rangle p_{i}\left\langle a_{i}\right|
$$

- the expectation value of an observable Q in a state $p$, whether pure or mixed, can be written

$$
\langle Q\rangle=\operatorname{Tr}(\rho Q)
$$

- the probability of a finding a state $|\phi\rangle$ in a mixture

$$
p_{\phi}(\rho)=\operatorname{Tr}\left(\rho P_{\phi}\right)=\sum_{i} p_{i}\left|\left\langle a_{i} \mid \phi\right\rangle\right|^{2}
$$

## von Neumann entropy

- most important measure of the departure from purity

$$
S=-k \operatorname{Tr}(\rho \ln \rho) \quad \mathrm{k} \text { is Boltzmann's constant. }
$$

- When $p$ is the Boltzmann distribution, $S$ is the entropy of statistical thermodynamics

$$
S=-k \sum_{i} p_{i} \ln p_{i}
$$

- For a pure state, where only one $\mathrm{p}_{\mathrm{i}}=\mathrm{I}$ and the others vanish, $\mathrm{S}=\mathrm{O}$.


## maximal entropy

- The entropy has a maximal value

$$
\begin{aligned}
& \delta \sum_{i} p_{i}\left(\ln p_{i}+\lambda\right)=0 \quad \begin{array}{l}
\lambda \text { Lagrange mult } \\
\text { for constraint }
\end{array} \\
& \delta \sum_{i} p_{i}\left(\ln p_{i}+\lambda\right)=\sum_{i}\left(\ln p_{i}+\lambda\right) \delta p_{i}+p_{i} \delta \ln p_{i} \\
& =\sum_{i}\left(\ln p_{i}+1+\lambda\right) \delta p_{i} \\
& \rightarrow \quad \ln p_{i}+1+\lambda=0 \quad \text { or pi are equal }
\end{aligned}
$$

- if the Hilbert space has a finite dimension d

$$
p_{i}=1 / d
$$

- The entropy satisfies the inequalities

$$
0 \leq S \leq-k \ln d
$$

- the density matrix that maximizes $S$ is

$$
\rho_{\max }=\frac{1}{d} \sum_{i}\left|a_{i}\right\rangle\left\langle a_{i}\right|
$$

- The sum in is just the unit operator. the mixture in which the entropy is maximal is the one in which all states, in any basis, are populated with equal probability.

$$
\rho_{\text {max }}=\frac{1}{d}
$$

- The unknown density matrix (whether pure or mixed) is a d-dimensional Hermitian matrix of unit trace is specified by $\mathrm{d}^{2}-1$ real parameters.

$$
\rho=\sum_{i j}\left|a_{i}\right\rangle r_{i j}\left\langle a_{j}\right| \quad r_{j i}=r_{i j}^{*}
$$

- We need $\mathrm{d}^{2}-\mathrm{I}$ measurement to identify the density matrix

$$
\begin{gathered}
X_{i j}=\frac{1}{2}\left(\left|a_{i}\right\rangle\left\langle a_{j}\right|+\left|a_{j}\right\rangle\left\langle a_{i}\right|\right) \\
Y_{i j}=\frac{i}{2}\left(\left|a_{i}\right\rangle\left\langle a_{j}\right|-\left|a_{j}\right\rangle\left\langle a_{i}\right|\right) \\
\operatorname{Tr}\left(\rho X_{i j}\right)=\operatorname{Re} r_{i j} \quad \operatorname{Tr}\left(\rho Y_{i j}\right)=\operatorname{Im} r_{i j}
\end{gathered}
$$

## composite system

- mixtures do not only arise when pure states are "mixed" by the environment.
- If a composite system is in a pure state, its subsystems are in general in mixed states.
- consider a system composed of two subsystems with coordinates $\mathrm{q}_{1}$ and $\mathrm{q}_{2}$. Let $|\Psi\rangle$ be an arbitrary pure state of the system, with wave function $\Psi\left(q_{1} q_{2}\right)$, so that

$$
\left\langle q_{1}^{\prime} q_{2}^{\prime}\right| \rho\left|q_{1} q_{2}\right\rangle=\Psi\left(q_{1} q_{2}\right) \Psi^{*}\left(q_{1}^{\prime} q_{2}^{\prime}\right)
$$

- Let $A_{l}$ be an observable of the subsystem I;

$$
\left\langle q_{1}^{\prime} q_{2}^{\prime}\right| A_{1}\left|q_{1} q_{2}\right\rangle=\left\langle q_{1}^{\prime}\right| A_{1}\left|q_{1}\right\rangle \delta\left(q_{2}-q_{2}^{\prime}\right)
$$

- the expectation value of $A_{l}$ in $\Psi$ is

$$
\begin{aligned}
\langle A\rangle_{\Psi} & =\langle\Psi| A_{\mid}|\Psi\rangle \\
& =\int d q_{1} d q_{1}^{\prime} d q_{2} d q_{q^{\prime}}\left\langle q_{1}^{\prime}\right| A_{1}\left|q_{1}\right\rangle \Psi\left(q_{1} q_{2}\right) \Psi^{*}\left(q_{1}^{\prime} q_{2}^{\prime}\right) \delta\left(q_{2}-q_{2}^{\prime}\right) \\
& =\int d q_{1} d q_{1}^{\prime} d q_{2}\left\langle q_{1}^{\prime}\right| A_{1}\left|q_{1}\right\rangle \Psi\left(q_{1} q_{2}\right) \Psi^{*}\left(q_{1}^{\prime} q_{2}\right)
\end{aligned}
$$

- reduced density matrix

$$
\begin{aligned}
& \left\langle q_{1}^{\prime}\right| \rho_{1}\left|q_{1}\right\rangle=\int d q_{2}\left\langle q_{1}^{\prime} q_{2}\right| \rho\left|q_{1} q_{2}\right\rangle \\
& \begin{array}{l|}
\langle A\rangle_{\Psi}
\end{array}=\int d q_{1} d q_{1}^{\prime}\left\langle q_{1}^{\prime}\right| A_{1}\left|q_{1}\right\rangle\left\langle q_{1}\right| \rho_{1}\left|q_{1}^{\prime}\right\rangle \\
& \\
& =\operatorname{Tr}\left(\rho_{1} A_{1}\right)
\end{aligned}
$$

## entangled state

- entangled state is a pure state

$$
\begin{gathered}
\Psi=c_{1} u_{1}\left(q_{1}\right) v_{1}\left(q_{2}\right)+c_{2} u_{2}\left(q_{1}\right) v_{2}\left(q_{2}\right) \quad\left|c_{1}\right|^{2}+\left|c_{2}\right|^{2}=1 \\
\{\mathbf{u}\} \text { and }\{\mathbf{v}\} \text { are orthonormal, } \\
\int d q_{1} u_{i}^{*}\left(q_{1}\right) u_{j}\left(q_{1}\right)=\delta_{i j} \quad \int d q_{v_{2}} v_{i}^{*}\left(q_{2}\right) v_{j}\left(q_{2}\right)=\delta_{i j}
\end{gathered}
$$

- a state cannot be written as a simple product

$$
\Psi=\varphi\left(q_{1}\right) \chi\left(q_{2}\right)
$$

- the reduced density matrix of $\Psi$ is

$$
\begin{aligned}
\left\langle q_{1}^{\prime}\right| \rho_{1}\left|q_{1}\right\rangle & =\int d q_{2} \Psi^{*}\left(q_{1}^{\prime} q_{2}\right) \Psi\left(q_{1} q_{2}\right) \\
& =\left|c_{1}\right|^{2} u_{1}^{*}\left(q_{1}^{\prime}\right) u_{1}\left(q_{1}\right)+\left|c_{2}\right|^{2} u_{2}^{*}\left(q_{1}^{\prime}\right) u_{2}\left(q_{1}\right)
\end{aligned}
$$

- $\rho_{\mathrm{I}}$ does not describe a pure state of subsystem I

$$
\begin{gathered}
\left\langle q_{1}^{\prime}\right| \rho_{1}^{2}\left|q_{1}\right\rangle=\left|c_{1}\right|^{4} u_{1}^{*}\left(q_{1}^{\prime}\right) u_{1}\left(q_{1}\right)+\left|c_{2}\right|^{4} u_{2}^{*}\left(q_{1}^{\prime}\right) u_{2}\left(q_{1}\right) \\
\operatorname{Tr}\left(\rho_{1}^{2}\right)=\left|c_{1}\right|^{4}+\left|c_{2}\right|^{4}<1
\end{gathered}
$$

- Thus $\rho_{\mathrm{I}}$ is not pure, and cannot be represented by any single state in the Hilbert space of system
- the subsystem can only be pure if the density matrix of the whole system is of the form:

$$
\rho_{s} \otimes \rho_{R}
$$

pure subsystem Remainder

- The two-body probability distribution associated with the entangled state

$$
\begin{aligned}
p\left(q_{1} q_{2}\right) & =\left|c_{1} u_{1}\left(q_{1}\right) v_{1}\left(q_{2}\right)+c_{2} u_{2}\left(q_{1}\right) v_{2}\left(q_{2}\right)\right|^{2} \\
& =\left|c_{1}\right|^{2}\left|u_{1}\left(q_{1}\right)\right|^{2}\left|v_{1}\left(q_{2}\right)\right|^{2}+\left|c_{2}\right|^{2}\left|u_{2}\left(q_{1}\right)\right|^{2}\left|v_{2}\left(q_{2}\right)\right|^{2}+I_{2}
\end{aligned}
$$

the interference term

$$
I_{2}=2 \operatorname{Re}\left[c_{1} c_{2}^{*} u_{1}\left(q_{1}\right) u_{2}^{*}\left(q_{1}\right) v_{1}\left(q_{2}\right) v_{2}^{*}\left(q_{2}\right)\right]
$$

- the interference term describes correlations even though the particles do not interact and are far apart


## 2-particle interferometer

- An experimental setup allows two particles to traverse different paths
- It is possible to determine the path taken by one particle by some observation on the other.





# coincidence probability vs. I-particle probability <br> $$
P_{a b}=\left|\Psi\left(q_{a}, q_{b}, t\right)\right|
$$ <br> $$
P_{a}\left(q_{a}, t\right)=\int d q_{b} P_{a b}\left(q_{a}, q_{b}, t\right)
$$ 

- neither particle will display an interference pattern (in $\mathrm{P}_{\mathrm{a}}, \mathrm{P}_{\mathrm{b}}$ )
- there may be an interference pattern in the $a-b$ coincidence rate $P_{a b}$, in the correlation of positions for $a$ and $b$.


# 2-photon interference experiment 




- L. Mandel, Rev. Mod. Phys. 7I, S274 (1999).
- consider a pure entangled state for a twobody system

$$
\Phi=N\left[\varphi_{1}\left(q_{1}\right) \chi_{1}\left(q_{2}\right)+\varphi_{2}\left(q_{1}\right) \chi_{2}\left(q_{2}\right)\right]
$$

- The probability distribution associated with $\Phi$ has the two-body interference term

$$
I_{2}=2 N \operatorname{Re}\left[\varphi_{1}\left(q_{1}\right) \varphi_{2}^{*}\left(q_{1}\right) \chi_{1}\left(q_{2}\right) \chi_{2}^{*}\left(q_{2}\right)\right]
$$

- the probability distribution for a is that of a mixture, with the one-body interference term

$$
\begin{aligned}
I_{1} & =2 N^{2} \int \operatorname{Re}\left[\varphi_{1}\left(q_{1}\right) \varphi_{2}^{*}\left(q_{1}\right) \chi_{1}\left(q_{2}\right) \chi_{2}^{*}\left(q_{2}\right)\right] d q_{2} \\
& =2 N^{2} \operatorname{Re}\left[V \varphi_{1}\left(q_{1}\right) \varphi_{2}^{*}\left(q_{1}\right)\right]
\end{aligned}
$$

- a by itself will only show an interference pattern if the states $\mathrm{X}, 2$ of the other body $b$ are not orthogonal.
- the physical side, that the states of $b$ do not unambiguously determine the path of a.


The visibility $\mathrm{IVI}^{2}$ of the interference pattern displayed by a is a measure of the confidence with which an observation on $b$ determines the state of a.

