## Many-particle systems



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## many particle wavefunction

- many particle wavefunction

$$
\psi_{T}\left(x_{1}, x_{2}, x_{3}, \cdots, x_{N}\right)
$$

- normalization condition

$$
\iint \cdots \int d x_{1} d x_{2} \cdots d x_{N}\left|\psi_{T}\left(x_{1}, x_{2}, x_{3}, \cdots, x_{N}\right)\right|^{2}=1
$$

- time evolution

$$
i \hbar \frac{\partial}{\partial t} \psi_{T}\left(x_{1}, x_{2}, x_{3}, \cdots, x_{N}\right)=H \psi_{T}\left(x_{1}, x_{2}, x_{3}, \cdots, x_{N}\right)
$$

## N -noninteracting particles

- For non-interacting particles

$$
V\left(x_{1}, x_{2}, x_{3}, \cdots, x_{N}\right)=V\left(x_{1}\right)+V\left(x_{2}\right)+\cdots V\left(x_{N}\right)
$$

- Hamiltonian is separable

$$
\begin{aligned}
H & =\sum_{j} H_{j} \\
H_{j} & =\frac{p_{j}^{2}}{2 m}+V\left(x_{j}\right)
\end{aligned}
$$

## 2-particle wavefunction

- wavefunctions are separable

$$
H \psi_{\alpha}(1,2, \cdots, N)=E_{\alpha} \psi_{\alpha}(1,2, \cdots, N)
$$

- for 2-particles, the following are the solutions to the Schrodinger equations

$$
\psi_{E}(1,2)=\psi_{\alpha}\left(x_{1}\right) \psi_{\beta}\left(x_{2}\right) \quad \psi_{E}(1,2)=\psi_{\alpha}\left(x_{2}\right) \psi_{\beta}\left(x_{1}\right)
$$

- energy is additive

$$
E=E_{\alpha}+E_{\beta}
$$

## identical particles

- the particles are indistinguishable
- Probability density should be invariant under index interchange

$$
\begin{gathered}
\psi_{E}^{*}(1,2) \psi_{E}(1,2)=\psi_{E}^{*}(2,1) \psi_{E}(2,1) \\
\psi_{\alpha}\left(x_{1}\right) \psi_{\beta}\left(x_{2}\right) \leftrightarrow \psi_{\alpha}\left(x_{2}\right) \psi_{\beta}\left(x_{1}\right)
\end{gathered}
$$

- The possible choices of 2-particle wave functions are

$$
\begin{aligned}
& \psi_{S}=\frac{1}{\sqrt{2}}\left[\psi_{\alpha}\left(x_{1}\right) \psi_{\beta}\left(x_{2}\right)+\psi_{\beta}\left(x_{1}\right) \psi_{\alpha}\left(x_{2}\right)\right] \\
& \psi_{A}=\frac{1}{\sqrt{2}}\left[\psi_{\alpha}\left(x_{1}\right) \psi_{\beta}\left(x_{2}\right)-\psi_{\beta}\left(x_{1}\right) \psi_{\alpha}\left(x_{2}\right)\right]
\end{aligned}
$$

## index exchange

- For symmetric wavefunction

$$
\begin{aligned}
\psi_{s} \xrightarrow[1 \leftrightarrow 2]{\longrightarrow} & \frac{1}{\sqrt{2}}\left[\psi_{\alpha}\left(x_{1}\right) \psi_{\beta}\left(x_{2}\right)+\psi_{\beta}\left(x_{1}\right) \psi_{\alpha}\left(x_{2}\right)\right]=\psi_{s} \\
& \psi_{s}^{*} \psi_{s} \xrightarrow[1 \leftrightarrow 2]{\longrightarrow} \psi_{s}^{*} \psi_{s}
\end{aligned}
$$

- For anti-symmetric wavefunction

$$
\begin{aligned}
& \psi_{A} \xrightarrow[1 \leftrightarrow 2]{\longrightarrow} \frac{1}{\sqrt{2}}\left[\psi_{\alpha}\left(x_{2}\right) \psi_{\beta}\left(x_{1}\right)-\psi_{\beta}\left(x_{2}\right) \psi_{\alpha}\left(x_{1}\right)\right]=-\psi_{A} \\
& \psi_{A}^{*} \psi_{A} \xrightarrow{1 \leftrightarrow 2} \longrightarrow(-1)^{2} \psi_{A}^{*} \psi_{A}
\end{aligned}
$$

## Pauli principle

- Fermions: systems consisting identical particles of half-odd-integral spin are described by anti-symmetric wave functions
- Bosons: systems consisting identical particles of integral spin are described by symmetric wave functions
- Anyons

$$
\psi_{\alpha}\left(x_{1}\right) \psi_{\beta}\left(x_{2}\right) \xrightarrow[1 \leftrightarrow 2]{\longrightarrow} e^{i \theta} \psi_{\beta}\left(x_{1}\right) \psi_{\alpha}\left(x_{2}\right)
$$

## Pauli principle

- Fermions: no more than one fermion can be in the same quantum state.
- Why?

$$
\psi_{A}=\frac{1}{\sqrt{2}}\left[\psi_{\alpha}\left(x_{1}\right) \psi_{\alpha}\left(x_{2}\right)-\psi_{\alpha}\left(x_{1}\right) \psi_{\alpha}\left(x_{2}\right)\right]=0
$$

## Slater determinant

- For many particles, we can express the answer using the determinant
change state
change position

$$
\psi_{A}(1,2, \cdots, N)=\frac{1}{\sqrt{N!}}\left|\begin{array}{cccc}
\psi_{\alpha}\left(x_{1}\right) & \psi_{\alpha}\left(x_{2}\right) & \cdots & \psi_{\alpha}\left(x_{N}\right) \\
\psi_{\beta}\left(x_{1}\right) & \psi_{\beta}\left(x_{2}\right) & & \\
\vdots & & \ddots & \\
\psi_{\rho}\left(x_{1}\right) & & & \psi_{\rho}\left(x_{N}\right)
\end{array}\right| \downarrow
$$

## antisymmetrized wavefunction

- For Fermions, the 2-particle wavefunction has to be anti-symmetrized

$$
u_{A}(1,2)=\frac{1}{\sqrt{2}}\left[u_{E_{1}}\left(x_{1}\right) u_{E_{2}}\left(x_{2}\right)-u_{E_{1}}\left(x_{2}\right) u_{E_{2}}\left(x_{1}\right)\right]
$$

example: 2 particles in a infinite well

$$
\frac{1}{\sqrt{2}}\left[\sin \left(\frac{\pi x_{1}}{a}\right) \sin \left(\frac{2 \pi x_{2}}{a}\right)-\sin \left(\frac{\pi x_{2}}{a}\right) \sin \left(\frac{2 \pi x_{1}}{a}\right)\right]
$$

- 3-particle case

$$
\begin{aligned}
\psi_{A}(1,2,3) & =\frac{1}{\sqrt{3!}}[\psi(1,2,3)-\psi(2,1,3)+\psi(2,3,1) \\
& -\psi(3,2,1)+\psi(3,1,2)-\psi(1,3,2)]
\end{aligned}
$$

## the necessity for

## (anti-)symmertization

$$
\psi_{S, A}\left(x_{1}, x_{2}\right)=\frac{1}{\sqrt{2}}\left[\psi_{a}\left(x_{1}\right) \psi_{b}\left(x_{2}\right) \pm \psi_{a}\left(x_{2}\right) \psi_{b}\left(x_{1}\right)\right]
$$

- When two particles are close.
- How close? calculate the overlapping probability

$$
\int \psi_{a}^{*}(x) \psi_{b}(x) d x
$$

- If it is very small, we can treat them separably


## Probability property

- Consider the probability for the particles are close $\mathrm{x}_{1} \sim \mathrm{x}_{2}$

$$
\begin{aligned}
\psi_{A} & =\frac{1}{\sqrt{2}}\left[\psi_{\alpha}\left(x_{1}\right) \psi_{\beta}\left(x_{2}\right)-\psi_{\beta}\left(x_{1}\right) \psi_{\alpha}\left(x_{2}\right)\right] \\
& \sim \frac{1}{\sqrt{2}}\left[\psi_{\alpha}\left(x_{1}\right) \psi_{\beta}\left(x_{1}\right)-\psi_{\beta}\left(x_{1}\right) \psi_{\alpha}\left(x_{1}\right)\right] \\
& \sim 0 \\
\psi_{S} & =\frac{1}{\sqrt{2}}\left[\psi_{\alpha}\left(x_{1}\right) \psi_{\beta}\left(x_{2}\right)+\psi_{\beta}\left(x_{1}\right) \psi_{\alpha}\left(x_{2}\right)\right] \\
& \sim \frac{1}{\sqrt{2}}\left[\psi_{\alpha}\left(x_{1}\right) \psi_{\beta}\left(x_{1}\right)+\psi_{\beta}\left(x_{1}\right) \psi_{\alpha}\left(x_{1}\right)\right] \\
& \sim \sqrt{2} \psi_{\alpha}\left(x_{1}\right) \psi_{\beta}\left(x_{1}\right)
\end{aligned}
$$

## Comparison with the distinguishable case

- Distinguishable at same position

$$
\psi=\psi_{\alpha}\left(x_{1}\right) \psi_{\beta}\left(x_{1}\right) \quad \psi^{*} \psi=\psi_{\alpha}^{*}\left(x_{1}\right) \psi_{\alpha}\left(x_{1}\right) \psi_{\beta}^{*}\left(x_{1}\right) \psi_{\beta}\left(x_{1}\right)
$$

- Antisymmetric

$$
\psi_{A}^{*} \psi_{A}=0
$$

particles are more separated

- Symmetric

$$
\psi_{s}^{*} \psi_{s}=2 \psi^{*} \psi
$$

particles are more closed to each other

## spin wavefunction

- The spin states:
- singlet is anti-symmetric under interchange

$$
\frac{1}{\sqrt{2}}\left(\chi_{+}^{(1)} \chi_{-}^{(2)}-\chi_{-}^{(1)} \chi_{+}^{(2)}\right)
$$

- triplet is symmetric under interchange

$$
\begin{aligned}
& \chi_{+}^{(1)} \chi_{+}^{(2)} \\
& \frac{1}{\sqrt{2}}\left(\chi_{+}^{(1)} \chi_{-}^{(2)}+\chi_{-}^{(1)} \chi_{+}^{(2)}\right) \\
& \chi_{-}^{(1)} \chi_{-}^{(2)}
\end{aligned}
$$

## Exchange force

- spatial wavefunction

$$
\begin{aligned}
& \psi_{S}=\frac{1}{\sqrt{2}}\left[\psi_{\alpha}\left(x_{1}\right) \psi_{\beta}\left(x_{2}\right)+\psi_{\beta}\left(x_{1}\right) \psi_{\alpha}\left(x_{2}\right)\right] \\
& \psi_{A}=\frac{1}{\sqrt{2}}\left[\psi_{\alpha}\left(x_{1}\right) \psi_{\beta}\left(x_{2}\right)-\psi_{\beta}\left(x_{1}\right) \psi_{\alpha}\left(x_{2}\right)\right]
\end{aligned}
$$

- Combining spin part together

| spatial | spin | total |
| :---: | :---: | :---: |
| sym | asym(singlet) | asym |
| asym | sym(triplet) | asym |

## spatial-spin wavefunctions

- The probability density for $\mathrm{x}_{1} \sim \mathrm{x}_{2}$ is very small for spin triplet.

- The probability density for $\mathrm{x}_{1} \sim \mathrm{x}_{2}$ is slightly higher for spin singlet.




## Coulomb interaction

- $V$ for interparticle interaction is positive (same polarity)
- To reduce potential energy, separated particles are favored
- The spatial wavefunction is antisymmetric and the spin part is symmetric
- Called "exchange" interaction



## Hartree theory

- To deal with the electron-electron interaction in a muliti-electron atom
- The effect is included in a local potential generated by all electrons
- The potential should obeys the properties

$$
\begin{array}{rlrl}
V(r) & =-\frac{Z e^{2}}{4 \pi \varepsilon_{0} r} & V(r) & =-\frac{e^{2}}{4 \pi \varepsilon_{0} r} \\
r & \rightarrow 0 & r & \rightarrow \infty
\end{array}
$$

## Procedures I

- With the guessed/modified $\mathrm{V}(\mathrm{r})$, one numerically solve all eigenstates $\psi_{\alpha}, \psi_{\beta}, \psi_{\gamma}$ and associated eigenenergies $E_{\alpha}, E_{\beta}, E_{\gamma}$
- Use Pauli exclusive principle to assign total wavefunction without considering particle interactions(but not antisymmetrized)
- Electron charge distributions are obtained from

$$
\left|\psi_{\alpha}\right|^{2},\left|\psi_{\beta}\right|^{2},\left|\psi_{\gamma}\right|^{2}
$$

## Procedures 2

- With charge distribution, the potential satisfies

$$
\nabla^{2} V=\frac{\rho}{\varepsilon_{0}} \quad \rho=\rho_{0}-e n_{e}
$$

- Go back to step I with the modified $V$ and recursively to obtain a converged V and $\psi_{\alpha}, \psi_{\beta}, \psi_{\gamma}$


## Bose system

- Bosons obey symmetrized wave functions

$$
\psi_{S}=\frac{1}{\sqrt{2}}\left[\psi_{\alpha}\left(x_{1}\right) \psi_{\beta}\left(x_{2}\right)+\psi_{\beta}\left(x_{1}\right) \psi_{\alpha}\left(x_{2}\right)\right]
$$

- We may put them in the same state $\alpha=\beta$

$$
\begin{aligned}
\psi_{S} & =\frac{1}{\sqrt{2}}\left[\psi_{\beta}\left(x_{1}\right) \psi_{\beta}\left(x_{2}\right)+\psi_{\beta}\left(x_{1}\right) \psi_{\beta}\left(x_{2}\right)\right] \\
& =\sqrt{2} \psi_{\beta}\left(x_{1}\right) \psi_{\beta}\left(x_{2}\right)
\end{aligned}
$$

- The probability density

$$
\psi_{S}^{*} \psi_{S}=2 \psi_{\beta}^{*}\left(x_{1}\right) \psi_{\beta}^{*}\left(x_{2}\right) \psi_{\beta}\left(x_{1}\right) \psi_{\beta}\left(x_{2}\right)
$$

## Distinguishable case

- For distinguishable particles, the wavefunction is

$$
\psi=\psi_{\alpha}\left(x_{1}\right) \psi_{\beta}\left(x_{2}\right)=\psi_{\beta}\left(x_{1}\right) \psi_{\beta}\left(x_{2}\right)
$$

- The probability density is

$$
\psi^{*} \psi=\psi_{\beta}^{*}\left(x_{1}\right) \psi_{\beta}^{*}\left(x_{2}\right) \psi_{\beta}\left(x_{1}\right) \psi_{\beta}\left(x_{2}\right)
$$

- Indistinguashability increases the probability

$$
\psi_{s}^{*} \psi_{s}=2 \psi^{*} \psi
$$

## N -particle case

- Symmetrized N -particle wavefuncitons

$$
\psi_{s}=\frac{1}{\sqrt{N!}}(N!) \psi_{\beta}\left(x_{1}\right) \psi_{\beta}\left(x_{2}\right) \cdots \psi_{\beta}\left(x_{N}\right)
$$

- Probability density
$\psi_{s}^{*} \psi_{s}=(N!) \psi_{\beta}^{*}\left(x_{1}\right) \psi_{\beta}^{*}\left(x_{2}\right) \cdots \psi_{\beta}^{*}\left(x_{N}\right) \psi_{\beta}\left(x_{1}\right) \psi_{\beta}\left(x_{2}\right) \cdots \psi_{\beta}\left(x_{N}\right)$
- Enhancement in probability

$$
\psi_{S}^{*} \psi_{s}=(N!) \psi^{*} \psi
$$

## Probability Enhancement

- For I-particle $\quad P_{1}=\psi_{\beta}^{*} \psi_{\beta}$
- For N -particle $P_{N}=N!P_{1}^{N}=N!\left(\psi_{\beta}^{*} \psi_{\beta}\right)^{N}$
- For $\mathrm{N}+\mathrm{I}$ particle $P_{N+1}=(N+1)!P_{1}^{N+1}=(N+1) N!P_{1}^{N} P_{1}$

$$
=(N+1) P_{N} P_{1}
$$

- The probability for more bosons joining together is enhanced


## 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 $\mathrm{T}=0$, 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 (pl, p2,...) 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 $p_{i}=I$ and the others vanish, $\mathrm{S}=\mathrm{O}$.


## maximal entropy

- The entropy has a maximal value

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

- 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.

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

- 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 $\mathrm{d}^{2}-1$ 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 $A_{I}$ 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 $A_{1}$ in $\Psi$ is

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

- reduced density matrix

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

## entangled state

- entangled state is a pure state

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

- 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 $\rho_{I}$ 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

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

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$$
\begin{gathered}
P_{a b}=\left|\Psi\left(q_{a}, q_{b}, t\right)\right| \\
P_{a}\left(q_{a}, t\right)=\int d q_{b} P_{a b}\left(q_{a}, q_{b}, t\right)
\end{gathered}
$$

- 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 (I999).
- 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 $\mathrm{X}_{\mathrm{l}, 2}$ 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 $a$.

