

Quantum correlations at the mesoscopic and macroscopic levels

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Contents

1	Correlations of distinguishable particles	2
1.1	Entanglement	2
1.2	Quantum and classical correlations	4
1.3	Other types of quantum correlations	6
2	Systems of identical particles	6
2.1	Fock space	6
2.2	Second quantization	8
2.3	Hong-Ou-Mandel interference	9
2.4	N -particle interference	10
3	Correlations in many-body systems	11
3.1	Particle entanglement	11
3.2	Effectively distinguishable particles	12
3.3	Mode entanglement	13
3.4	Partial distinguishability	14

One of the features that distinguish quantum from classical theory is the strength of correlations that can exist between the results of measurement carried out on different subsystems. This was first pointed out by Einstein, Podolsky and Rosen [1] and further described by Schrödinger [2, 3] who introduced the notion of *entanglement*. In 1964, Bell proved that the degree of correlation allowed by entanglement is inconsistent with any local hidden variable theory [4]. An experimental demonstration of the violation of Bell's inequality was achieved by Aspect in 1981 [5].

While these (thought) experiments have focused on two entangled particles, the experimental, theoretical and computational tools developed over the last decades have allowed to tackle many-body quantum systems. As the number of constituents increases, so does the complexity of the states available to the system. Correlations are essential to characterize these states and to understand under which conditions large quantum systems can behave according to the predictions of classical thermodynamics.

In this lecture, we will introduce the basic tools for the characterization of correlations between parts of a quantum system, discuss the formalism which describes systems of identical particles and point out difficulties raised by the indistinguishability of the constituents.

1 Correlations of distinguishable particles

Classical random variables are said to be correlated if the expectation $E(XY)$ does not factorize into $E(X)E(Y)$ (note that absence of correlation does not guarantee independence, defined by $P(X=x, Y=y) = P(X=x)P(Y=y)$). Analogously, a quantum mechanical state is correlated if the expectation values of products of observables associated with different parts of the system do not factorize. We will see that such correlations can be of classical or quantum mechanical origin.

1.1 Entanglement

We consider two subsystems with Hilbert spaces \mathcal{H}_A and \mathcal{H}_B , whose common state $|\psi\rangle$ is therefore described by a vector in the tensor product space $\mathcal{H}_A \otimes \mathcal{H}_B$. Take an observable A acting on \mathcal{H}_A and an observable B acting on \mathcal{H}_B , if the state of the system can be written

$$|\psi\rangle = |\psi_A\rangle \otimes |\psi_B\rangle, \quad (1)$$

then it is clear that the expectation value of $A \otimes B$ factorizes:

$$\langle\psi|AB|\psi\rangle = \langle\psi_A|A|\psi_A\rangle \langle\psi_B|B|\psi_B\rangle. \quad (2)$$

States of the form (1) are called *separable pure states*. A pure state that is not separable is said to be *entangled*.

Remark: This definition depends on the separation of the system into two subsystems or *parties* and requires the overall system to be in a pure state.

Example: Two spin- $\frac{1}{2}$ particles with Hilbert spaces $\mathcal{H}_A = \mathcal{H}_B = \text{span}\{|\uparrow\rangle, |\downarrow\rangle\}$ such that $\mathcal{H}_A \otimes \mathcal{H}_B = \text{span}\{|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle\}$.

- $\frac{1}{\sqrt{2}}(|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle)$ is entangled.
- $\frac{1}{2}(|\uparrow\uparrow\rangle + |\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle + |\downarrow\downarrow\rangle) = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle) \otimes \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle)$ is separable.

A useful mathematical result when dealing with pure bipartite states is the Schmidt decomposition: any state $|\psi\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$ can be decomposed as

$$|\psi\rangle = \sum_k \sqrt{\lambda_k} |\psi_A^k\rangle \otimes |\psi_B^k\rangle, \quad (3)$$

where the λ_k are positive real numbers obeying $\sum_k \lambda_k = 1$ and the $|\psi_{A(B)}^k\rangle$ are orthonormal states in $\mathcal{H}_{A(B)}$. This follows from the singular value decomposition of a (not necessarily square) matrix. The number of non-zero λ_k coefficients is known as the *Schmidt rank* and is smaller than both $\dim \mathcal{H}_A$ and $\dim \mathcal{H}_B$.

Remark: The decomposition is not unique but the Schmidt coefficients are.

The reduced density matrices obtained by tracing out one of the subsystems are then easily expressed as:

$$\rho_A = \text{Tr}_B (|\psi\rangle \langle\psi|) = \sum_k \lambda_k |\psi_A^k\rangle \langle\psi_A^k|, \quad (4)$$

$$\rho_B = \text{Tr}_A (|\psi\rangle \langle\psi|) = \sum_k \lambda_k |\psi_B^k\rangle \langle\psi_B^k|, \quad (5)$$

where the coefficient λ_k appear as the weight of $|\psi_{A(B)}^k\rangle$ in the mixed states. One can show (as an exercise) that the following propositions are equivalent:

1. The pure state $|\psi\rangle$ is separable.
2. One λ_k is equal one, all others vanish, i.e. the Schmidt rank is one.
3. The reduced state ρ_A is pure, i.e. $\exists |\psi_A\rangle \in \mathcal{H}_A$, $\rho_A = |\psi_A\rangle\langle\psi_A|$, or equivalently $\rho_A^2 = \rho_A$, or equivalently $\text{Tr}(\rho_A^2) = \sum_k \lambda_k^2 = 1$.
4. Same thing with $A \leftrightarrow B$.

The quantity $\text{Tr}(\rho_A^2) = \text{Tr}(\rho_B^2) = \sum_k \lambda_k^2$ is the *purity* of the reduced states and can be used to quantify the entanglement between A and B : if it is equal to one, the state is separable and there is no entanglement whereas it reaches its minimum value $\min(\dim \mathcal{H}_A, \dim \mathcal{H}_B)^{-1}$ if all Schmidt coefficients are equal; the state is then said to be maximally entangled. Another important measure of entanglement is the *entropy of entanglement*, which is given by the von Neuman entropy of the reduced density matrices and therefore vanishes for separable states:

$$S = -\text{Tr}(\rho_A \log \rho_A) = -\text{Tr}(\rho_B \log \rho_B) = -\sum_k \lambda_k \log \lambda_k. \quad (6)$$

1.2 Quantum and classical correlations

The most general state of a quantum system is a mixed state represented by a density matrix ρ . This description allows for both classical and quantum correlations. We define *product states* on $\mathcal{H}_A \otimes \mathcal{H}_B$ as those states which can be written

$$\rho = \rho_A \otimes \rho_B. \quad (7)$$

They carry no correlations, quantum or classical. Indeed, for any choice of observables A and B acting on the respective subsystems, the expectation value of $A \otimes B$ factorizes: $\text{Tr}(\rho A \otimes B) = \text{Tr}(\rho_A A) \text{Tr}(\rho_B B)$. *Separable states* are those which can be written as mixtures of product states:

$$\rho = \sum_i p_i \rho_A^{(i)} \otimes \rho_B^{(i)}. \quad (8)$$

States which are not separable are called entangled.

Example: Consider the (pure) entangled state of two spin- $\frac{1}{2}$ particles

$$|\psi\rangle = \frac{1}{\sqrt{2}} (|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle) \quad (9)$$

and the separable mixed state

$$\rho = \frac{1}{2} |\uparrow\uparrow\rangle \langle\uparrow\uparrow| + \frac{1}{2} |\downarrow\downarrow\rangle \langle\downarrow\downarrow|. \quad (10)$$

In both cases, measurements of the z -component of the two spins are perfectly correlated (either both up or both down). The fact that the quantum correlations of state (9) are stronger than the classical ones of state (10) can be seen by considering measurements in an other basis. For measurements of the x -components of the spins, one finds (as an exercise) that state (9) still gives perfectly correlated results while state (10) gives completely uncorrelated results.

Contrary to the case of pure states, determining whether a mixed state ρ is separable is a difficult problem in general. Although any mixed state can be put into the form

$$\rho = \sum_i q_i |\psi^{(i)}\rangle \langle\psi^{(i)}| \quad (11)$$

by diagonalization, this decomposition is not unique. Entanglement measures must therefore be defined as optima over all decompositions. For example, *entanglement of formation* is the average entanglement entropy, minimized over all decompositions of ρ :

$$S_F(\rho) = \min_{\{q_i, |\psi^{(i)}\rangle\}} \sum_i q_i S(|\psi^{(i)}\rangle). \quad (12)$$

This minimization procedure is difficult in practice, which led to the introduction of the following criterion by Peres and Horodecki [6, 7]. If ρ is expanded in an orthonormal basis of $\mathcal{H}_A \otimes \mathcal{H}_B$ as

$$\rho = \sum_{i,j,k,l} p_{ij}^{kl} |\mathbf{i}\rangle \langle\mathbf{j}| \otimes |k\rangle \langle l|, \quad (13)$$

then its partial transpose with respect to subsystem A is defined by

$$\rho^{TA} = \sum_{i,j,k,l} p_{ij}^{kl} |\mathbf{j}\rangle \langle\mathbf{i}| \otimes |k\rangle \langle l|. \quad (14)$$

For separable states, ρ and ρ^{TA} have the same spectrum and, in particular, they only have positive eigenvalues. Therefore if ρ^{TA} has a negative eigenvalue, then ρ is entangled. The *negativity* is defined as the sum over negative eigenvalues of ρ^{TA} ,

$$\mathcal{N} = \sum_{\mu \in \text{sp}(\rho^{TA})} \frac{|\mu| - \mu}{2}, \quad (15)$$

and non-zero negativity is therefore a sufficient condition for entanglement.

1.3 Other types of quantum correlations

One can easily generalize the definition of entanglement to partitions into more than two subsystems. However the characterization of such *multipartite entanglement* can be extremely complex (see [8] for a comprehensive review on quantum entanglement). Moreover, apart from entanglement, there exists a whole hierarchy of quantum correlations. Quantum *discord* describes correlations found in separable mixed states that nevertheless go beyond what is classically possible [9, 10]. On the other hand, one can define quantum correlations that are stronger than simple entanglement: *EPR steering* refers to the ability to affect the results of measurements in a system A by acting locally on a system B , while *Bell nonlocality* describes correlations that cannot be explained by any local hidden variable theory, as witnessed by the violation of a Bell inequality [11, 12].

2 Systems of identical particles

Identical quantum particles are fundamentally indistinguishable from one another. However, the definition of entanglement relies on the existence of well identified parties that can be addressed individually. We briefly introduce the quantum mechanical formalism appropriate to describe systems of identical particles before we discuss the difficulties that it poses for the definition of entanglement.

2.1 Fock space

We consider a quantum system composed of N identical particles, each described by a single-particle Hilbert space \mathcal{H} . The N -particle Hilbert space is constructed by taking the tensor product of N copies of \mathcal{H} : $\mathcal{H}^{\otimes N} = \mathcal{H} \otimes \mathcal{H} \otimes \dots \mathcal{H}$. However, most states in $\mathcal{H}^{\otimes N}$ do not respect the indistinguishability of the constituents because each particle is implicitly given a

label corresponding to its position in the tensor product. For example, in state

$$|\psi\rangle = |\psi_1\rangle_1 \otimes |\psi_2\rangle_2 \otimes \dots \otimes |\psi_N\rangle_N, \quad (16)$$

the state $|\psi_i\rangle$ is associated with the particle carrying the label i . Acceptable physical states must be invariant under all permutations of these unphysical labels. For σ a permutation in S_N , we define the operator P_σ which reorders the tensor product according to σ :

$$P_\sigma |\psi_1\rangle_1 \otimes |\psi_2\rangle_2 \otimes \dots \otimes |\psi_N\rangle_N = |\psi_{\sigma^{-1}(1)}\rangle_1 \otimes |\psi_{\sigma^{-1}(2)}\rangle_2 \otimes \dots \otimes |\psi_{\sigma^{-1}(N)}\rangle_N. \quad (17)$$

We then require that all physical states $|\psi\rangle$ be invariant such operations, i.e.

$$\forall \sigma \in S_N, \quad |\langle \psi | P_\sigma | \psi \rangle|^2 = 1. \quad (18)$$

In other words, $|\psi\rangle$ must belong to a one-dimensional irreducible representation of S_N on $\mathcal{H}^{\otimes N}$. There are two possibilities:

$$P_\sigma |\psi\rangle = |\psi\rangle \quad \text{or} \quad P_\sigma |\psi\rangle = \text{sign}(\sigma) |\psi\rangle \quad (19)$$

and the projectors on the corresponding subspaces of $\mathcal{H}^{\otimes N}$ respectively read

$$S = \sum_{\sigma \in S_N} P_\sigma \quad \text{and} \quad A = \sum_{\sigma \in S_N} \text{sign}(\sigma) P_\sigma. \quad (20)$$

Particles whose state transforms according to the completely symmetric representation are called bosons and we denote the N -boson Hilbert space by $\mathcal{H}^{\vee N} = S\mathcal{H}^{\otimes N}$. Particles whose state transforms according to the sign representation are called fermions and we denote the N -fermion Hilbert space by $\mathcal{H}^{\wedge N} = A\mathcal{H}^{\otimes N}$.

Example: Two indistinguishable two-level systems with single-particle Hilbert space $\mathcal{H} = \text{span}\{|\uparrow\rangle, |\downarrow\rangle\}$.

Bosonic Hilbert space $\mathcal{H}^{\vee 2} = \text{span}\left\{|\uparrow\uparrow\rangle, \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle), |\downarrow\downarrow\rangle\right\}$

Fermionic Hilbert space $\mathcal{H}^{\wedge 2} = \text{span}\left\{\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)\right\}$

If the number of particles is not conserved, it is convenient to take the direct sum over the particle number N of the (bosonic or fermionic) N -particle Hilbert spaces, leading to the Fock space

$$\Gamma_{B,F}(\mathcal{H}) = \mathbb{C} \oplus \mathcal{H} \oplus \mathcal{H}^{\vee 2} \oplus \dots \oplus \mathcal{H}^{\vee N} \oplus \dots, \quad (21)$$

where the first term corresponds to $N = 0$ and is spanned by the vacuum state $|\emptyset\rangle$.

2.2 Second quantization

Since the unphysical labeling of particles has been erased by symmetrization, one can build a basis of the Fock space $\Gamma_{B,F}(\mathcal{H})$ by considering states with a given number of particles N_m in each state $|m\rangle$ (or *mode*) of an orthonormal basis of the single-particle Hilbert space \mathcal{H} . Therefore, rather than working with cumbersome symmetrized states, we use the Fock notation: for bosons,

$$|N_1, N_2, \dots, N_m, \dots\rangle_B \propto S \underbrace{|1\rangle \dots |1\rangle}_{N_1} \underbrace{|2\rangle \dots |2\rangle}_{N_2} \dots \underbrace{|m\rangle \dots |m\rangle}_{N_m} \dots, \quad (22)$$

while for fermions antisymmetrization imposes $N_m = 0$ or 1 , such that

$$|N_1, N_2, \dots, N_m, \dots\rangle_F \propto A \bigotimes_{\{m|N_m \neq 0\}} |m\rangle. \quad (23)$$

We can now define creation and annihilation operators which act on the Fock states by adding or removing a particle from mode m . For bosons these are analogous to the ladder operators of the harmonic oscillator:

$$\begin{aligned} a_m^\dagger |N_1, N_2, \dots, N_m, \dots\rangle_B &= \sqrt{N_m + 1} |N_1, N_2, \dots, N_m + 1, \dots\rangle \\ a_m |N_1, N_2, \dots, N_m, \dots\rangle_B &= \sqrt{N_m} |N_1, N_2, \dots, N_m - 1, \dots\rangle \\ a_m^\dagger a_m |N_1, N_2, \dots, N_m, \dots\rangle_B &= N_m |N_1, N_2, \dots, N_m, \dots\rangle \end{aligned} \quad (24)$$

and they obey the same commutation relations

$$[a_m, a_n] = [a_m^\dagger, a_n^\dagger] = 0, \quad [a_m, a_n^\dagger] = \delta_{mn}. \quad (25)$$

For fermions we have

$$\begin{aligned} a_m^\dagger |N_1, N_2, \dots, N_m, \dots\rangle_F &= \begin{cases} (-1)^{\sum_{i=1}^{m-1} N_i} |N_1, N_2, \dots, N_m + 1, \dots\rangle & \text{if } N_m = 0 \\ 0 & \text{if } N_m = 1 \end{cases} \\ a_m |N_1, N_2, \dots, N_m, \dots\rangle_F &= \begin{cases} 0 & \text{if } N_m = 0 \\ (-1)^{\sum_{i=1}^{m-1} N_i} |N_1, N_2, \dots, N_m - 1, \dots\rangle & \text{if } N_m = 1 \end{cases} \\ a_m^\dagger a_m |N_1, N_2, \dots, N_m, \dots\rangle_B &= N_m |N_1, N_2, \dots, N_m, \dots\rangle \end{aligned} \quad (26)$$

with the *anticommutation* relations

$$\{a_m, a_n\} = \{a_m^\dagger, a_n^\dagger\} = 0, \quad \{a_m, a_n^\dagger\} = \delta_{mn}. \quad (27)$$

Fock states can then be obtained by acting on the vacuum state $|\emptyset\rangle$ with the appropriate number of creation operators (and normalizing):

$$|N_1, N_2, \dots, N_m, \dots\rangle_{B,F} = \prod_m \frac{(a_m^\dagger)^{N_m}}{\sqrt{N_m!}} |\emptyset\rangle. \quad (28)$$

Example: The previously encountered states of two two-level bosons read $|2_{\uparrow}, 0_{\downarrow}\rangle_B = \frac{1}{\sqrt{2}}(a_{\uparrow}^{\dagger})^2 |\emptyset\rangle$, $|1_{\uparrow}, 1_{\downarrow}\rangle_B = a_{\uparrow}^{\dagger} a_{\downarrow}^{\dagger} |\emptyset\rangle$ and $|0_{\uparrow}, 2_{\downarrow}\rangle_B = \frac{1}{\sqrt{2}}(a_{\downarrow}^{\dagger})^2 |\emptyset\rangle$.

2.3 Hong-Ou-Mandel interference

In order to illustrate the physical consequences of the indistinguishability of particles, we discuss the 1987 experiment of Hong, Ou and Mandel [13] which demonstrated the ability of identical particles to interfere. We consider a beam splitter with input modes $|a\rangle$ and $|b\rangle$ and output modes $|c\rangle$ and $|d\rangle$, as represented in figure 1. The beam splitter realizes the following unitary transformation of the single-particle states:

$$|a\rangle \rightarrow \frac{1}{\sqrt{2}}(|c\rangle + |d\rangle), \quad |b\rangle \rightarrow \frac{1}{\sqrt{2}}(|c\rangle - |d\rangle). \quad (29)$$

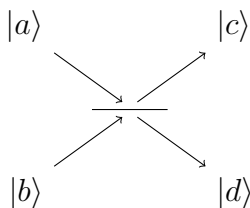


Figure 1: A beam splitter.

For two distinguishable particles arriving in a and b ,

$$|a\rangle \otimes |b\rangle \rightarrow \frac{1}{2}(|c\rangle \otimes |c\rangle - |c\rangle \otimes |d\rangle + |d\rangle \otimes |c\rangle - |d\rangle \otimes |d\rangle), \quad (30)$$

the distribution of results is as one would expect classically: the probability of observing both particles in the output c is $\frac{1}{4}$, the probability of observing both particles in d is also $\frac{1}{4}$ and the probability of observing one particle in c and one in d is $\frac{1}{2}$. However, if one considers the symmetrized state of two indistinguishable bosons, we find that both particles always exit through the same port:

$$\frac{1}{\sqrt{2}}(|a\rangle \otimes |b\rangle + |b\rangle \otimes |a\rangle) \rightarrow \frac{1}{\sqrt{2}}(|c\rangle \otimes |c\rangle - |d\rangle \otimes |d\rangle), \quad (31)$$

while for two indistinguishable fermions, they always leave in opposite ports:

$$\frac{1}{\sqrt{2}}(|a\rangle \otimes |b\rangle - |b\rangle \otimes |a\rangle) \rightarrow \frac{1}{\sqrt{2}}(|d\rangle \otimes |c\rangle - |c\rangle \otimes |d\rangle). \quad (32)$$

Equivalently, in the second quantized formulation, we start from the state $a_a^\dagger a_b^\dagger |\emptyset\rangle$, apply the transformation

$$a_a^\dagger \rightarrow \frac{1}{\sqrt{2}} (a_c^\dagger + a_d^\dagger), \quad a_b^\dagger \rightarrow \frac{1}{\sqrt{2}} (a_c^\dagger - a_d^\dagger). \quad (33)$$

Using the (anti)commutation relations, we obtain the output states $\frac{1}{2} \left((a_c^\dagger)^2 - (a_d^\dagger)^2 \right) |\emptyset\rangle$ for bosons and $a_d^\dagger a_c^\dagger |\emptyset\rangle$ for fermions. This ‘‘bunching’’ of bosons and ‘‘anti-bunching’’ of fermions is the result of destructive or constructive interference between the many-body transition amplitudes corresponding to both photons being reflected at the beam splitter and both being transmitted.

2.4 N -particle interference

The Hong-Ou-Mandel scenario can be extended to N particles in an N -port interferometer which performs the unitary transformation $U \in U(N)$. The corresponding relation between the creation operators of the input and output modes reads

$$a_m^\dagger \rightarrow \sum_n U_{mn} b_n^\dagger, \quad (34)$$

such that an initial Fock state

$$|1, 1, \dots, 1\rangle_{B,F} = \left(\prod_m a_m^\dagger \right) |\emptyset\rangle \quad \text{goes to} \quad \prod_m \left(\sum_n U_{mn} b_n^\dagger \right) |\emptyset\rangle. \quad (35)$$

The probability of observing exactly one particle in each output mode is given by the overlap with the corresponding Fock state and reads

$$P_B = \left| \sum_{\sigma \in S_N} \prod_{m=1}^N U_{m,\sigma(m)} \right|^2 = |\text{perm}(U)|^2 \quad \text{for bosons,} \quad (36)$$

$$P_F = \left| \sum_{\sigma \in S_N} \text{sign}(\sigma) \prod_{m=1}^N U_{m,\sigma(m)} \right|^2 = |\det(U)|^2 = 1 \quad \text{for fermions.} \quad (37)$$

These results can be interpreted as a sum over the amplitudes of many-particle paths where the particle in input i is sent to output $\sigma(i)$. For fermions, the interference is constructive since the Pauli principle forbids any other output. For bosons, the permanent of the unitary appears, a mathematical object which becomes increasingly difficult to compute as N

increases. The complexity of bosonic interference is behind the idea of “boson sampling” as a means to demonstrate the superiority of quantum devices over classical ones [14]. The result for distinguishable particles is obtained by summing the probabilities – rather than the probability amplitudes – of the many-particle paths: $P_D = \sum_{\sigma \in S_N} \left| \prod_{m=1}^N U_{m, \sigma(m)} \right|^2$. Contrary to the bosonic transition probability, this quantity can be computed efficiently.

3 Correlations in many-body systems

The study of correlations has played a major role our understanding of many-body quantum system [15–17]. For example, the scaling of the entanglement between a subsystem and the rest of the system with the size of the subsystem can be used to characterize quantum phases and determines the possibility to represent the state efficiently with a classical computer. Entanglement between subsystems has also been put forward to explain the ability of closed systems to thermalize, with entanglement and thermodynamic entropies being put in relation. While many results have been obtained with spin chains, where the individual spins are distinguishable through their fixed position, difficulties arise when considering correlations in systems of indistinguishable bosons or fermions. Although one can formally divide the particles into parties thanks to the tensor product structure between copies of the single-particle Hilbert spaces, this might not be physically meaningful given that the particles cannot always be addressed individually. We show under which conditions identical particles can meaningfully be divided into parties, introduce the notion of entanglement between modes and point out the relation between distinguishability and entanglement.

3.1 Particle entanglement

A first (naive?) approach to entanglement in a system of N identical particles is to embed the N -boson or N -fermion Hilbert space in $\mathcal{H}^{\otimes N}$ (i.e. use the first quantization formalism) and use the tensor product between copies of the single-particle Hilbert space to define parties. With this approach, symmetrization automatically creates entanglement between identical particles in different states and in particular, two fermions are always in an entangled state.

Example: Within this approach, the bosonic states $|\uparrow\uparrow\rangle$ and $|\downarrow\downarrow\rangle$ are separable but $\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$ is maximally entangled, and so is the fermionic state $\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$.

Although this correlation can hardly be considered to be physical, one can nevertheless ask what one learns from the reduced density matrices obtained by tracing out one or several particles in a many-particle state. For a N -particle state $\rho^{(N)}$, the reduced density matrix obtained by tracing out one factor of $\mathcal{H}^{\otimes N}$ is known as the $(N-1)$ -particle reduced density matrix $\rho^{(N-1)}$. Because of the symmetrization, it is a mixture of all states that can be obtained from $\rho^{(N)}$ by removing one particle:

$$\rho^{(N-1)} = \sum_m {}_N\langle m | \rho^{(N)} | m \rangle_N = \frac{1}{N} \sum_m a_m \rho^{(N)} a_m^\dagger. \quad (38)$$

Repeating this procedure, one arrives at the single-particle reduced density matrix

$$\rho^{(1)} = \frac{1}{N!} \sum_{m_1, \dots, m_{N-1}} a_{m_{N-1}} \dots a_{m_1} \rho^{(N)} a_{m_1}^\dagger \dots a_{m_{N-1}}^\dagger. \quad (39)$$

One can show that the matrix elements of $\rho^{(1)}$ can be expressed as

$$\langle n | \rho^{(1)} | m \rangle = \frac{1}{N} \text{Tr} (a_m^\dagger a_n \rho^{(N)}), \quad (40)$$

such that knowledge of the single-particle reduced density matrix suffices to calculate expectation values of single-particle observables $O = \sum_{m,n} o_{mn} a_m^\dagger a_n$. In general, knowledge of the n -particle reduced density matrix allows to compute expectation values of n -particle observables, i.e. observables which can be expressed in terms of products of n creation and n annihilation operators.

3.2 Effectively distinguishable particles

We now explain how we recover the usual definition of entanglement when two identical particles can be unambiguously distinguished. Suppose that the single-particle Hilbert space is written a direct sum of two orthogonal subspaces $\mathcal{H} = \mathcal{H}_A \oplus \mathcal{H}_B$, such that any single-particle state can be uniquely decomposed into the sum of a vector of \mathcal{H}_A and a vector of \mathcal{H}_B . The following isomorphism then holds for the Hilbert spaces of N bosons or fermions:

$$(\mathcal{H}_A \oplus \mathcal{H}_B)^{\vee \wedge N} \simeq \bigoplus_{N_A + N_B = N} \mathcal{H}_A^{\vee \wedge N_A} \otimes \mathcal{H}_B^{\vee \wedge N_B}. \quad (41)$$

This simply means that the state of N identical particles can be written as a superposition of states with N_A particles in \mathcal{H}_A and $N_B = N - N_A$ in \mathcal{H}_B , with N_A running from 0 to N . Note that the exchange symmetry between particles populating orthogonal subspaces is no longer explicit in this formulation. In particular, if two particles are and remain in orthogonal states (one in \mathcal{H}_A , the other in \mathcal{H}_B), then their exchange symmetry has no physical consequence: for all practical purposes their state can be written in $\mathcal{H}_A \otimes \mathcal{H}_B$ and the usual definition of entanglement applies. This is in particular true for spatially separated particles: a particle on Earth is not affected by the presence of an identical particle on the Moon.

Example: The state of two bosons, one on Earth and one on the Moon, reads $\frac{1}{\sqrt{2}} (|\psi_1, \text{Earth}\rangle \otimes |\psi_2, \text{Moon}\rangle + |\psi_2, \text{Moon}\rangle \otimes |\psi_1, \text{Earth}\rangle)$, but as long as the particles remain spatially separated one can equally well write $|\psi_1\rangle_{\text{Earth}} \otimes |\psi_2\rangle_{\text{Moon}}$.

Note that by considering only one term in the right-hand side of Eq. (41), we have made the assumption that the number of particles in \mathcal{H}_A and \mathcal{H}_B is fixed. Relaxing this assumption leads to the notion of mode entanglement.

3.3 Mode entanglement

Summing Eq. (41) over N , one can convince oneself that

$$\Gamma_{B,F}(\mathcal{H}) \simeq \Gamma_{B,F}(\mathcal{H}_A) \otimes \Gamma_{B,F}(\mathcal{H}_B), \quad (42)$$

i.e. the direct sum structure at the single-particle level leads to a tensor product structure at the many-particle level. Actually, we have already used this property without mentioning it when we introduced Fock states. Indeed the decomposition of the single-particle Hilbert space $\mathcal{H} = \bigoplus_m \text{span}\{|m\rangle\}$ allows us to decompose the Fock space as

$$\Gamma_{B,F}(\mathcal{H}) \simeq \bigotimes_m \Gamma_{B,F}(\text{span}\{|m\rangle\}). \quad (43)$$

Since each subspace $\text{span}\{|m\rangle\}$ has dimension one, the bosonic space $\text{span}\{|m\rangle\}^{\vee N_m}$ is spanned by only one state $|m\rangle^{\otimes N_m}$, which we denote $|N_m\rangle$. The fermionic space $\text{span}\{|m\rangle\}^{\wedge N_m}$ only exists if $N_m = 0$ or 1 and it is also spanned by a single state which we denote $|N_m\rangle$. This then justifies writing Fock states as $|N_1, N_2, \dots, N_m, \dots\rangle = |N_1\rangle \otimes |N_2\rangle \otimes \dots |N_m\rangle \otimes \dots$. By dividing the modes into two groups, one thus obtains an acceptable bipartition for the definition of entanglement.

Example: The output state of the Hong-Ou-Mandel experiment with indistinguishable bosons, $\frac{1}{\sqrt{2}}(|2_c, 0_d\rangle - |0_c, 2_d\rangle)$, is mode entangled with respect to the partition defined by modes c and d . The reduced density matrix for mode c reads $\rho_c = \frac{1}{2}(|2_c\rangle\langle 2_c| + |0_c\rangle\langle 0_c|)$ and mixes states with different numbers of particles.

Remark: Simple coupling between two modes is sufficient for mode entanglement to form, interactions between particles are not required. For example a single photon impinging in input a of a beam splitter yields the mode entangled state $\frac{1}{\sqrt{2}}(|1_c, 0_d\rangle + |0_c, 1_d\rangle)$.

3.4 Partial distinguishability

We now return to the Hong-Ou-Mandel experiment and consider two identical particles that can be made distinguishable through an additional degree of freedom. In a photonic Hong-Ou-Mandel experiment, this could be the polarization or the temporal overlap of the incoming wavepackets. We assume that the beam splitter does not affect this “label”. The initial state reads

$$\frac{1}{\sqrt{2}}(|a, \alpha\rangle \otimes |b, \beta\rangle \pm |b, \beta\rangle \otimes |a, \alpha\rangle), \quad (44)$$

where $|\alpha\rangle$ and $|\beta\rangle$ are the label states of the particles entering in input a and b , respectively.

One can easily show (as an exercise) that the probability of a coincidence event (both detectors c and d click) is given by $P = \frac{1}{2}(1 \mp |\langle\alpha|\beta\rangle|^2)$. If $|\langle\alpha|\beta\rangle|^2 = 0$, the two particles are in orthogonal label states and are therefore perfectly distinguishable from one another and we recover the classical probability of $\frac{1}{2}$. If $|\langle\alpha|\beta\rangle|^2 = 1$, the particles are perfectly indistinguishable and we recover the bosonic ($P = 0$) or fermionic ($P = 1$) result. For intermediate values of $|\langle\alpha|\beta\rangle|^2$, the particles are said to be partially distinguishable.

If we now formally calculate the reduced density matrix for the position degree of freedom of the initial state, tracing out the label, we find, in the (non-symmetrized) basis $\{|a\rangle \otimes |b\rangle, |b\rangle \otimes |a\rangle\}$,

$$\rho = \frac{1}{2} \begin{pmatrix} 1 & \pm |\langle\alpha|\beta\rangle|^2 \\ \pm |\langle\alpha|\beta\rangle|^2 & 1 \end{pmatrix}. \quad (45)$$

The purity of this reduced density matrix is $\frac{1}{2}(1 + |\langle\alpha|\beta\rangle|^4)$. For indistinguishable labels $|\langle\alpha|\beta\rangle|^2 = 1$, we have a pure state, while for orthogonal labels $|\langle\alpha|\beta\rangle|^2 = 0$, it is maximally mixed. The degree of entanglement of the position and label degrees of freedom thus reflects the distinguishability of the particles. For partially distinguishable particles, the coherences (off-diagonal elements) of the reduced density matrix correspond to the contrast of Hong-Ou-Mandel dip or peak.

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