# Chapter 3: Quantum Mechanics for Many-Body Systems

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https://www.phy.pku.edu.cn/xzli/TEACHING.htm

- The first chapter has already presented the tensor product structure of composite systems and the exchange requirements for identical particles.

- However, “merely writing down the tensor product and explicating the requirement of exchange symmetry" has not yet answered three further questions, which can imply many things in QM:

  1. Which states are the legitimate states of identical particles?

  2. Can the joint measurement predictions for these states be replaced by those for the states of the individual local subsystems? (The answer is obvious no nowadays, but in the history, this has induced quite some confusions).

  3. When the number of particles increases and interactions occur, how can we calculate the properties of a many-body system?

  These three questions lie at the heart of Q.M. for many-body systems. In the history, there are already many successes which we have achieved. Nowadays, it is also bringing new opportunities for physics. Therefore, we designed a Chapter for this topic.

# ◆ Outline

1. Which states of identical particles are legal? (Hilbert Space)

2. Why are local states insufficient to describe joint measurements? (Quantum Entanglement, EPR Paradox)

3. Bell Inequality

4. Occupation Number Representation?

5. Wave-Function Based Quantum Many-Body Methods?

6. The Path-Integral Method and its Advantage in Describing Many-Body systems

# 3.1 Which states of identical particles are legal?

- Before we start, let me ask you a fundamental question: are there proper quantum states for a subsystem (can be a single particle, can be number of particles) in the quantum system?

  → No!!! → But in practice, we still use single-particle states as the basis, upon which the many-body states are build …… (MBPT)

- We accept this convention for the time being. In our chapter for path-integral later, I think we will have a better expression for the quantum many-body problems. (现在，先按人们已形成的习惯讲)

## 3.1.1 Restriction from the permutation symmetry in a 2-particle system.

- In Chapter I, we mentioned, but we haven't detailed the restriction of the permutation of the symmetry on the many-body quantum states.
- Here, we detail this, starting from a 2-particle system.

# 3.1 Which states of identical particles are legal?

## 3.1.1 Restriction from the permutation symmetry in a 2-particle system.

- If we have two single-particle states, and we label them as $|\phi_1\rangle$ and $|\phi_2\rangle$
- The product states are: $|\phi_1\rangle_1|\phi_1\rangle_2$ $|\phi_1\rangle_1|\phi_2\rangle_2$ $|\phi_2\rangle_1|\phi_1\rangle_2$ $|\phi_2\rangle_1|\phi_2\rangle_2$
- The tensor product space is 4-dimensional.
- If we have *n* single-particle states, labelled as $|\phi_1\rangle, |\phi_2\rangle, |\phi_3\rangle, \cdots, |\phi_n\rangle$. The tensor product space will be $n^2$-dimensional.
- But, the tensor product space is not the Hilbert space of a quantum many-body system. We need to take care of permutation symmetry.
- For the problem of two single-particle states ($M$) for two particles ($N$), we have:

$\hat{P}_{12}(|\phi_1\rangle_1|\phi_2\rangle_2) = |\phi_2\rangle_1|\phi_1\rangle_2$ ⇒ The product state $|\phi_1\rangle_1|\phi_2\rangle_2$ is neither symmetric nor antisymmetric.

# 3.1 Which states of identical particles are legal?

## 3.1.1 Restriction from the permutation symmetry in a 2-particle system.

- Then, we need to make it symmetric (Boson) or anti-symmetric (Fermion)…(we neglect Anyon for the moment, it will be discussed later in the path-integral part)

$$\hat{P}_{12}|\Psi\rangle_B = |\Psi\rangle_B \qquad \hat{P}_{12}|\Psi\rangle_F = -|\Psi\rangle_F$$

- When we have two orbitals, the symmetric ones include:

$$|\phi_1\rangle_1|\phi_1\rangle_2 \qquad |\phi_2{}_1|\phi_2\rangle_2 \qquad \frac{|\phi_1\rangle_1|\phi_2\rangle_2 + |\phi_2\rangle_1|\phi_1\rangle_2}{\sqrt{2}}$$

- The Hilbert space for the bosonic system is 3-dimensional.

- The anti-symmetric ones include: $\frac{|\phi_1\rangle_1|\phi_2\rangle_2 - |\phi_2\rangle_1|\phi_1\rangle_2}{\sqrt{2}}$

- The Hilbert space for the fermionic system is 1-dimensional.

# 3.1 Which states of identical particles are legal?

## 3.1.1 Restriction from the permutation symmetry in a 2-particle system.

- The dimensionality of the Hilbert space of the Bosonic and Fermionic systems are different from the space of the product states.
- Some product states are many-body states, e.g. $|\phi_1\rangle_1|\phi_1\rangle_2$ $|\phi_2\rangle_1|\phi_2\rangle_2$
- But based on that, we have further restriction due to permutation symmetry.



In Chapter I, we have given this message. Here, we detail it more.

## 3.1.2 Spin must be included in the W.F.s.

- For electrons, it is the complete state—spatial and spin parts together—that must be antisymmetric under exchange. Therefore, the argument for the basis $|\phi_1\rangle, |\phi_2\rangle, |\phi_3\rangle, \cdots, |\phi_n\rangle$ include both DoFs.

$$\phi_{a\uparrow}(\mathbf{r},\sigma) = \varphi_a(\mathbf{r})\chi_\uparrow(\sigma), \qquad \phi_{a\downarrow}(\mathbf{r},\sigma) = \varphi_a(\mathbf{r})\chi_\downarrow(\sigma).$$

# 3.1 Which states of identical particles are legal?

## 3.1.2 Spin must be included in the W.F.s.

Spin-singlet state

$$\Psi(1,2) = \frac{1}{\sqrt{2}}[\phi_{a\uparrow}(1)\phi_{a\downarrow}(2) - \phi_{a\downarrow}(1)\phi_{a\uparrow}(2)] = \varphi_a(\mathbf{r}_1)\varphi_a(\mathbf{r}_2)\frac{\chi_\uparrow(1)\chi_\downarrow(2) - \chi_\downarrow(1)\chi_\uparrow(2)}{\sqrt{2}}.$$

- Besides the spin-singlet state, there are also spin-triplet states:

$$|\uparrow\uparrow\rangle, \qquad \frac{|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle}{\sqrt{2}}, \qquad |\downarrow\downarrow\rangle.$$

- For a two-electron system, there are two possible pairings:

| Spatial part | Spin part | Complete state |
|---|---|---|
| Symmetric $\Phi_+$ | Antisymmetric **singlet** | Antisymmetric |
| Antisymmetric $\Phi_-$ | Symmetric **triplet** | Antisymmetric |

- For more than two electrons:

The spatial and spin parts can also have mixed permutation symmetry, rather than being fully symmetric or antisymmetric.

For example, for a system of three electrons, exchange antisymmetry cannot be carried entirely by the spin degrees of freedom. A direct consequence is that three electrons cannot all occupy the same spatial orbital. Therefore, the above table cannot simply be reused for three electrons.

- However, the spin DoFs must addressed specifically in many-body quantum states!

→ Key message Sec. 3.1.2

# 3.1 Which states of identical particles are legal?

## 3.1.3 Extension to an $N$-particle system.

- At this moment, if you rethink what we have done, you may conclude that: we have detailed the many-body states in a two-particle system, and emphasized the importance of the spin DoFs.

Why two-particle, not three-particle, not four-particle?

Some people say that "the physics is the same". This is true. But, if I ask this person to give me the proper equations. Chances are, he/she can not. The true reason is that for these system, the permutation symmetry is just to hard to handle!

- When quantum mechanics was first applied to many-electron systems, exchanging identical particles became a serious mathematical challenge. Physicists had to track how wavefunctions behaved under permutations, and the growing use of group theory felt to some like a Gruppenpest—a "group-theory plague." For a system of N electrons, directly antisymmetrizing a product of single-particle states involves N! terms, which quickly becomes unwieldy.

# 3.1 Which states of identical particles are legal?

## 3.1.3 Extension to an $N$-particle system.

- At this time (late of 1920s), Slater's determinant offered an elegant escape. By placing single-electron orbitals in a determinant, physicists could write an antisymmetric wavefunction compactly: exchanging two electrons swaps two rows and automatically changes the sign, while putting two electrons in the same spin orbital makes the determinant vanish.

- The determinant did not make permutation symmetry or many-body interactions disappear, but it made the Pauli principle much easier to enforce in practical calculations.

$$\Psi_F(x_1,\ldots,x_N) = \frac{1}{\sqrt{N!}}\begin{vmatrix} \phi_1(x_1) & \phi_2(x_1) & \cdots & \phi_N(x_1) \\ \phi_1(x_2) & \phi_2(x_2) & \cdots & \phi_N(x_2) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_1(x_N) & \phi_2(x_N) & \cdots & \phi_N(x_N) \end{vmatrix}.$$

# 3.1 Which states of identical particles are legal?

## 3.1.3 Extension to an $N$-particle system.

- We have determinant (行列式) for the fermionic system. For the bosonic system, we have permanent (积和式).

$$A = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix}$$

$$\begin{matrix} \phi_1(x_1) & \phi_2(x_1) & \cdots & \phi_N(x_1) \\ \phi_1(x_2) & \phi_2(x_2) & \cdots & \phi_N(x_2) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_1(x_N) & \phi_2(x_N) & \cdots & \phi_N(x_N) \end{matrix}$$

- A permanent is just as compact as a determinant for writing down a many-particle wavefunction: it symmetrizes the state for bosons, while a determinant antisymmetrizes it for fermions.

$$\mathrm{perm}(A) = a_{11}a_{22}a_{33} + a_{11}a_{23}a_{32} + a_{12}a_{21}a_{33} + a_{12}a_{23}a_{31} + a_{13}a_{21}a_{32} + a_{13}a_{22}a_{31},$$

$$\det(A) = a_{11}a_{22}a_{33} - a_{11}a_{23}a_{32} - a_{12}a_{21}a_{33} + a_{12}a_{23}a_{31} + a_{13}a_{21}a_{32} - a_{13}a_{22}a_{31}.$$

$$\mathrm{perm}(A) = \sum_{\pi \in S_N} \prod_{i=1}^{N} a_{i,\pi(i)} \qquad \det(A) = \sum_{\pi \in S_N} \mathrm{sgn}(\pi) \prod_{i=1}^{N} a_{i,\pi(i)}.$$

Sec. 3.4!

$a_{ij} = \phi_j(x_i)$: **Rows correspond to particle coordinates, and columns correspond to single-particle orbitals.**

# 3.1 Which states of identical particles are legal?

## 3.1.3 Extension to an $N$-particle system.

- The difference is in using it. Determinants have powerful algebraic tools (given by Slater) and are generally efficient to compute; permanents lack many of those simplifications and are generally much harder to calculate.
- For bosons, repeated occupation of an orbital also requires care with normalization. So the permanent is not harder to write—it is usually harder to work with.



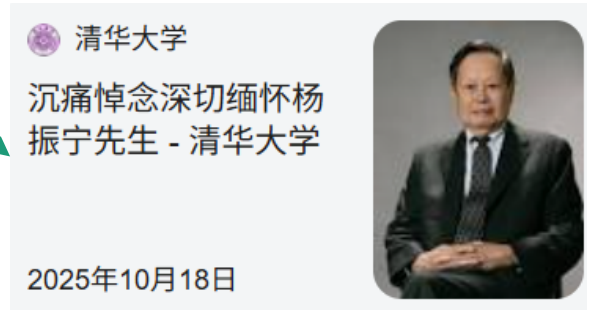
For the Wave Mechanics. With Path-Integral, it is the opposite: bosonic systems easier but fermionic systems harder. We will detail this in the Chapter of path-integral.

- For Sec. 3.1, our message is clear: 1) We have restrictions on the many-body W.F., leading to the result that the Hilbert space is smaller than the tensor product space. 2) For the bosonic system, we can address it using Permanents. For the fermionic system, using Slater Determinant.

# 3.1 Which states of identical particles are legal?

## 3.1.3 Extension to an $N$-particle system.

[1]何染尘,曾嘉熙,杨数,等.从杨李相变理论看量子多体问题中的置换对称性[J]物理与工程().DOI:10.27024/j.wlygc.2026.08.11.is.




# 从杨–李相变理论看量子多体问题中的置换对称性

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**摘　要**　量子多体系统的置换对称性不仅是其基本属性，也是量子力学的基本公设之一。基于这一对称性，系统可衍生出电子壳层结构及超流超固等新奇物态，也相应带来费米子符号问题等理论挑战。我们课题组近期基于杨–李相变理论对费米子符号问题开展了一系列研究，认识到置换对称性在当前量子多体理论方法中尚未被充分运用。事实上，这与上世纪20年代末“群灾”(Gruppenpest)的历史有关：置换群引入的繁琐计算使物理学家却步，直到1929年，斯莱特用行列式“帮物理学家消灭了群灾”，但代价是显式处理置换对称性的研究从此相对缺失。伴随着近年来来Borrmann等(1993)、Hirshberg等(2019)、熊羽诺和熊宏伟(2022)等工作的初期探索，人们重新开始基于置换群，并结合路径积分方法研究量子多体问题，尝试解决费米子符号问题。我们受此启发，将杨–李相变理论引入费米子符号问题及更广泛的量子多体问题研究中(何染尘等，2026)。借此纪念杨振宁先生的专栏，我们总结课题组这方面的相关工作，期望为未来量子多体问题研究提供新思路，并从中国科研工作者的视角，深切缅怀杨先生的学术贡献。

**关键词**　费米子符号问题；杨–李相变理论；李–杨零点；Slater行列式；置换对称性；路径积分方法

It is not necessary for you to understand this article now!!! But I do want to share with you some of our recent understanding of how to describe a many-body state, using W.F.s, and using path-integral, later.

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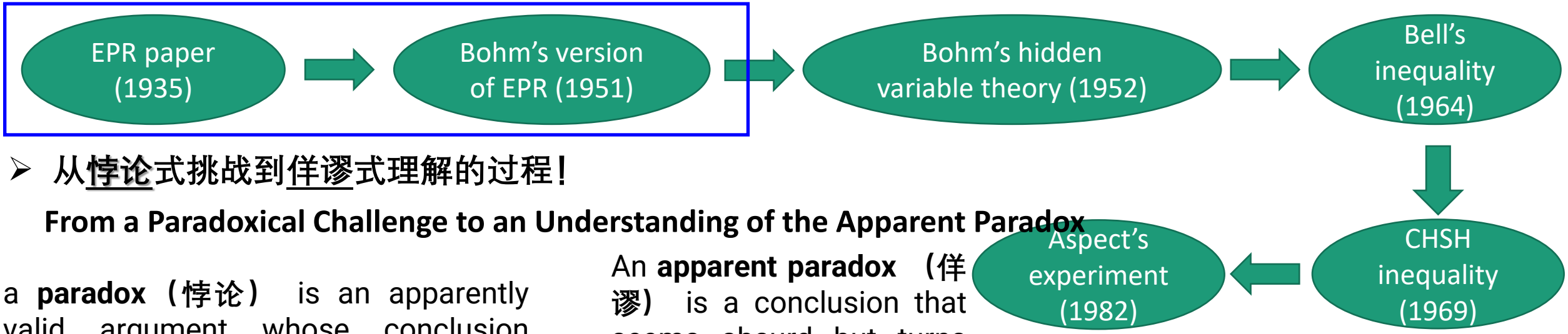
# 3.2 Why are local states insufficient to describe joint measurements?

## 3.2.1 The concept of quantum entanglement in its modern form

- This concept lies at the heart of all discussion in these two sections, i.e. Sec. 3.2 and Sec. 3.3.

## 3.2.2 The historical development of this concept of quantum entanglement




- 从悖论式挑战到佯谬式理解的过程！

**From a Paradoxical Challenge to an Understanding of the Apparent Paradox**

a **paradox**（悖论） is an apparently valid argument whose conclusion conflicts with reality, prompting us to question its premises. (开始)

An **apparent paradox** （佯谬) is a conclusion that seems absurd but turns out to be true once we understand it properly. (现在)

## 3.2.3 The question of EPR (as well as Bohm's version) in the modern language.

# 3.2 Why are local states insufficient to describe joint measurements?

## 3.2.1 The concept of quantum entanglement in its modern form

- In the simplest language, quantum entanglement simply refer to a many-body quantum state which can not be describe by a direct product of two or some single particle quantum states:

A clear point from the earlier discussions → $|\psi\rangle \neq |\phi\rangle \otimes |\varphi\rangle$



Against ⟷ Factorization

These states are entangled states. The phenomenon resulted from it, is called quantum entanglement (量子纠缠，剪不断理还乱).

- From this definition, it is also clear that the term which is contradictory to it (the entangled state) is the product state, where the individuals are not entangled.
- Now, we know that quantum entanglement is real. But in the history, it has taken people almost half a century to understand it and especially accept it.

# 3.2 Why are local states insufficient to describe joint measurements?

## 3.2.2 The historical development of this concept of quantum entanglement

- Starting point（江湖恩怨）: Solvey conference 1927.



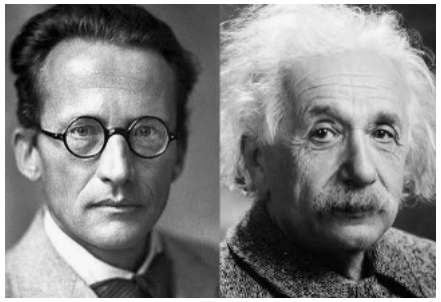
Bohr–Einstein debates

Article Talk

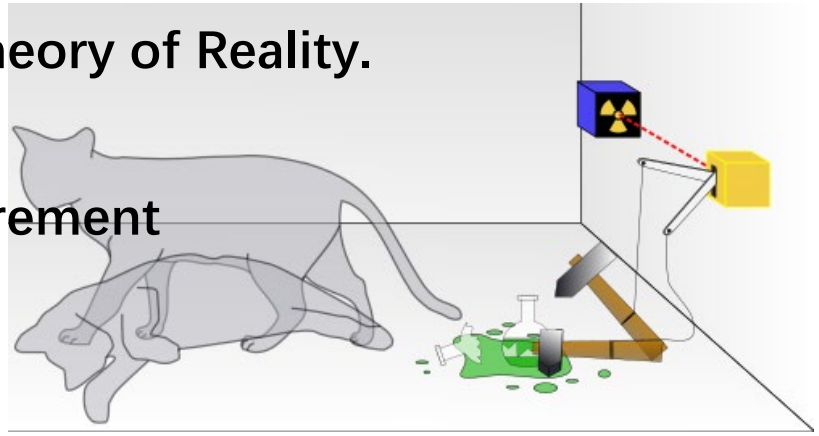
From Wikipedia, the free encyclopedia

The **Bohr–Einstein debates** were a series of public disputes about quantum mechanics between Albert Einstein and Niels Bohr. Their debates are remembered because of their



- Schrodinger's cat: Theory of Reality.



Postulate of the measurement

- EPR: Theory of Completeness.

Related to many-body problems

# 3.2 Why are local states insufficient to describe joint measurements?

## 3.2.2 The historical development of this concept of quantum entanglement

- **Suppose a theory accurately predicts the probability distribution of every experiment. Can this guarantee that it has completely described the physical reality of the system?** （假设一种理论准确预言了每次实验的概率分布。这能否保证它已经完整描述了系统的物理实在？）
- **EPR argued that this guarantee cannot be made directly.**（EPR 认为：不能直接作出这个保证。）
- **In the 1935 paper, they did not start from the premise that quantum mechanics miscalculates probabilities; instead, they used the perfect correlations predicted by quantum mechanics to question whether the quantum state already contains all the real information.**（他们并不以量子力学算错了概率为出发点；相反，他们利用量子力学给出的完美关联，质疑量子态是否已经包含一切真实信息。）
- **Same year, Schrödinger coined the term "entanglement (Verschränkung)" to describe the correlated states of quantum systems.**

# 3.2 Why are local states insufficient to describe joint measurements?

## 3.2.2 The historical development of this concept of quantum entanglement

- Thus, we can say that EPR brought the puzzling implications of entangled states into focus, while Schrödinger explicitly introduced and developed the concept of entanglement. Together, their work brought entanglement to the forefront of research in quantum mechanics.（提出了“纠缠”的概念，并且把关于“纠缠”的研究带入到了量子力学研究的视野！）

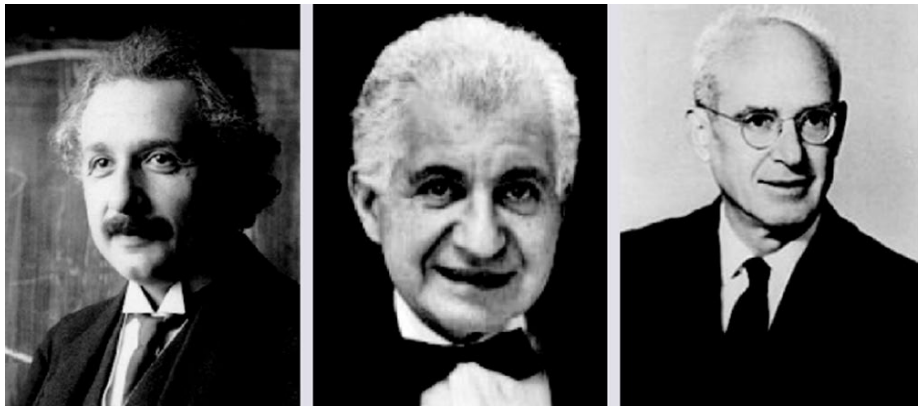


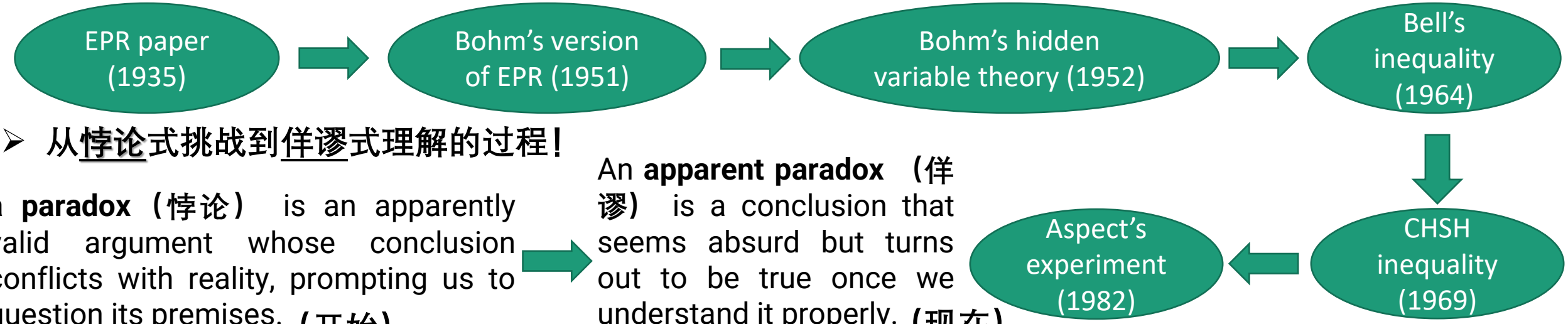
图 1　EPR 文章作者(从左至右)：爱因斯坦(A. Einstein)、波多尔斯基(B. Podolsky)和罗森(N. Rosen)

- Before EPR, entanglement was already implicit in the mathematical formalism of quantum mechanics. EPR turned it into a sharp physical and conceptual problem, and Schrödinger subsequently identified and emphasized entanglement as a distinct concept.

# 3.2 Why are local states insufficient to describe joint measurements?

## 3.2.2 The historical development of this concept of quantum entanglement

- People's attitude toward "quantum entanglement" evolved in a very funny way.

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- In short, the concept of quantum entanglement was inspired by the Einstein, Podolsky, and Rosen paper in 1935, to question Q.M. on where it is a complete theory. Making its alternative (hidden variable theory) popular for some years.
- Yet the Bell theorem and experimental tests that grew out of this challenge have provided strong support for the correlation predictions of standard quantum mechanics, while ruling out attempts to complete the theory with local hidden variables under the assumptions of Bell's theorem.

# 3.2 Why are local states insufficient to describe joint measurements?

## 3.2.3 The question of EPR (as well as Bohm's version) in the modern language

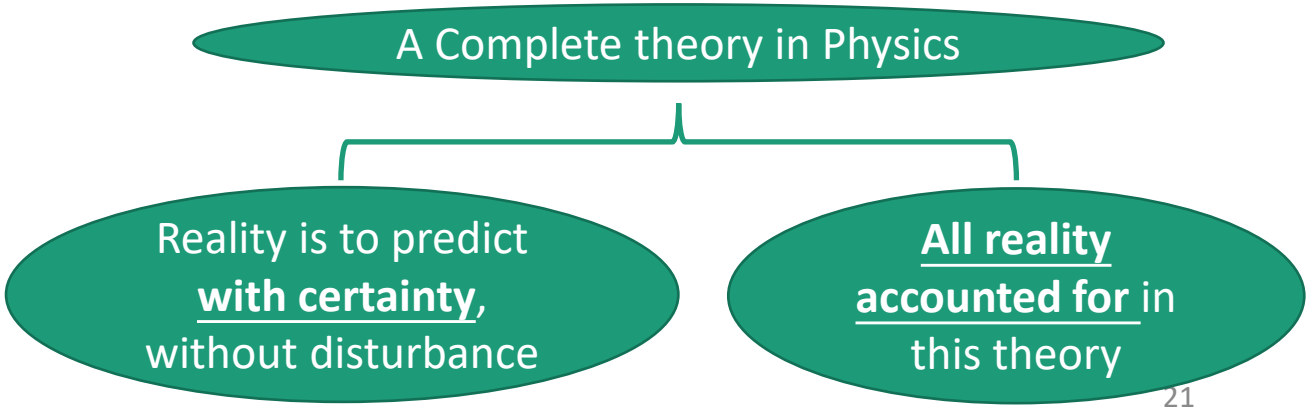
**Can Quantum-Mechanical Description of Physical Reality Be Considered Complete?**

A. EINSTEIN, B. PODOLSKY AND N. ROSEN, *Institute for Advanced Study, Princeton, New Jersey*

(Received March 25, 1935)

- EPR began with a criterion for physical reality: 1) if we can predict the value of a physical quantity with certainty, without disturbing a system in any way, then that quantity corresponds to an element of physical reality. 2) They also held that a complete theory must account for every element of physical reality.（实在性准则：如果不扰动一个系统，就能确定地预言某个物理量的值，那么这个物理量对应一个物理实在要素。他们还要求，完备理论必须表述物理实在的每一个要素。）

In a complete theory there is an element corresponding to each element of reality. A sufficient condition for the reality of a physical quantity is the possibility of predicting it with certainty, without disturbing the system. In quantum mechanics in the case of two physical quantities described by non-commuting operators, the knowledge of one precludes the knowledge of the other. Then either (1) the description of reality given by the wave function in



# 3.2 Why are local states insufficient to describe joint measurements?

## 3.2.3 The question of EPR (as well as Bohm's version) in the modern language




- Q. M. at that time, is already self-contained. But Einstein said, you are not perfect!
- In my eyes, a perfect theory should preserve some qualities. You do not have them!

$$|\psi^-\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow_z\rangle_A|\downarrow_z\rangle_B - |\downarrow_z\rangle_A|\uparrow_z\rangle_B\right)$$

- We can illustrate the argument using Bohm's later spin version. Suppose two widely separated particles, A and B, are in a spin-singlet state. Whenever Alice and Bob measure along the same direction, their results are opposite.



# 3.2 Why are local states insufficient to describe joint measurements?

## 3.2.3 The question of EPR (as well as Bohm's version) in the modern language

- If Alice measures along the z-axis, she can use her result to predict with certainty the outcome of Bob's measurement along z.

$$|\psi^-\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow_z\rangle_A|\downarrow_z\rangle_B - |\downarrow_z\rangle_A|\uparrow_z\rangle_B\right)$$




Question: In EPR $\hat{x}$、$\hat{p}$, in Bohm's version $\hat{S}_x$、$\hat{S}_z$, what is the point in common?

- If she instead measures along the x-axis, she can likewise predict with certainty the outcome of Bob's measurement along x.

I am Bob, if I do not believe that a remote Alice can control me, I will feel like being controlled by a hidden variable. Under some circumstance, e.g. that variable is fixed, my measurement can be with certain. I can have both $\hat{S}_x$ and $\hat{S}_z$ being real, according to the criterion of EPR.

# 3.2 Why are local states insufficient to describe joint measurements?

## 3.2.3 The question of EPR (as well as Bohm's version) in the modern language

- In other words, if Alice's distant choice between measuring z and measuring x does not change B's physical reality (here is a logic leap of EPR, assumption of locality), then her choice cannot determine which elements of reality B already possesses. By EPR's criterion, B's spin components along both z and x must correspond to elements of physical reality.

- Yet the usual quantum state cannot assign definite values to these two non-commuting spin components simultaneously. 然而，通常的量子态不能同时为这两个不对易的自旋分量指定确定值。

- Thus, given EPR's 1) reality criterion and the 2) assumption that a distant measurement does not disturb B, EPR would regard the quantum-state description of B as incomplete.因此，在实在性准则和远程不扰动等前提下，EPR 会认为量子态对 B 的描述不完备。

# 3.2 Why are local states insufficient to describe joint measurements?

## 3.2.3 The question of EPR (as well as Bohm's version) in the modern language

- **The problem of this argument: Can we use the assumption that a distant measurement does not disturb B to treat the outcomes predicted with certainty under two mutually exclusive measurement choices as elements of reality that B possesses simultaneously?**（将两种互斥测量选择下的确定预言，凭借远程不扰动要求，合并为 B 同时具有的实在要素。）
- **Bell's later work took the debate a step further: if this local picture of physical reality is formulated as a model satisfying local causality, measurement-setting independence, and related assumptions, it must obey a Bell inequality. Experiments, however, have observed violations of such inequalities.**（Bell 后来的工作使争论更进一步：若把这种局域物理图像落实为满足局域因果性、测量设置独立性等条件的模型，它会受到 Bell 不等式约束；实验却观察到违反。）
- **Thus, we can say that EPR brings a topic, Bell set up a physical theory to test it, and Quantum Entanglement becomes an important phenomenon.**

# 3.2 Why are local states insufficient to describe joint measurements?

## 3.2.3 The question of EPR (as well as Bohm's version) in the modern language

- **Still limitations (even now，即使今天，也有不完美): But this does not, by itself, prove that the quantum state is complete in every sense. Rather, the experiments rule out hidden-variable models that supplement the quantum state while satisfying Bell's locality condition and the other assumptions required for the inequality.**（但这也没有单独证明量子态在一切意义下都是完备的。只是说，实验证伪了借助隐变量将量子态进行局域处理这个理论。）

- **With these, we have clarified: 1) what quantum entanglement is by a definition? 2) the historical development of this concept; 3) the criticism of EPR and its logic.**



- **Next, we will use the Bell's inequality and the experiment of Aspect to conclude that many-body states in a quantum system should just be like what we have explained in Sec. 3.1.**

# ◆ Outline

1. Which states of identical particles are legal? (Hilbert Space)

2. Why are local states insufficient to describe joint measurements? (Quantum Entanglement, EPR Paradox)

3. Bell Inequality

4. Occupation Number Representation?

5. Wave-Function Based Quantum Many-Body Methods?

6. The Path-Integral Method and its Advantage in Describing Many-Body systems

# 3.3 Bell Inequality

## 3.3.1 The Hidden-Variable Theory of Bohm: A Final and Desperate Effort to Preserve the Classical Picture

- A central message given by EPR is that "If the wave function is not a complete description (since according to EPR, a complete theory should describe all reality), can we add physical variables that account for quantum statistics?"
- This bring the topic of hidden variable theory into attention. Actually, before EPR, de Broglie already has a pilot wave theory, which can be viewed as an early version of that. Later, von Neumann proved that constructing hidden variables in Q.M. is impossible. However, in the 1960s, Bell found a logic error in his proof. But anyway, with EPR, the hidden variable theory becomes a proper choice.
- In the 1950s, Bohm became the leading person in this field. In 1951, he proposed the spin version of EPR, as we used. In 1952, he also proposed a specific hidden-variable theory.

# 3.3 Bell Inequality

## 3.3.1 The Hidden-Variable Theory of Bohm: A Final and Desperate Effort to Preserve the Classical Picture

- In other words, EPR did not prove that such variables exist, nor did they construct a specific hidden-variable dynamics. In 1952, Bohm developed a concrete theory of this kind.
- Hidden-variable theories attempt to understand quantum mechanics within a deterministic framework, holding that the statistical character of the wave function arises from our ignorance of certain hidden variables. Such theories do not replace the wave function; rather, they supplement it with hidden variables, so that measurement outcomes are determined prior to measurement. However, Bell's theorem and its experimental verification confirm that any hidden-variable theory consistent with quantum mechanics must be nonlocal.
- Here, the trick is to suppose that the system possesses additional variables, denoted by λ, which are not specified by the wave function and may help determine individual measurement outcomes. This is the basic motivation for a hidden-variable description. A more complete description: $(\psi, \lambda)$.

# 3.3 Bell Inequality

## 3.3.1 The Hidden-Variable Theory of Bohm: A Final and Desperate Effort to Preserve the Classical Picture

- One example of the hidden variable theory is the Bohmian mechanics, where the hidden variable added to the usual quantum-state description is the actual particle position $X(t)$.

The two play different roles:

$$\underbrace{\psi(\mathbf{x},t)}_{\text{wave function: determines the guidance field}} \quad + \quad \underbrace{\mathbf{X}(t)}_{\text{actual position: the additional variable}}$$

- The **wave function** $\psi(\mathbf{x},t)$ obeys the Schrödinger equation and determines the velocity field through the guidance equation.
- The **actual position** $\mathbf{X}(t)$ specifies where the particle really is. Because the wave function alone does not specify this position, it is the additional hidden variable.

$$\psi^{(1)}(\mathbf{x},0) = \psi^{(2)}(\mathbf{x},0), \qquad \mathbf{X}^{(1)}(0) \neq \mathbf{X}^{(2)}(0).$$

- Here, two experiments can prepare exactly the same wave function but have different actual initial positions. They may therefore produce different trajectories and measurement outcomes. In quantum equilibrium, the actual positions are distributed according to $|\psi|^2$.

# 3.3 Bell Inequality

## 3.3.1 The Hidden-Variable Theory of Bohm: A Final and Desperate Effort to Preserve the Classical Picture

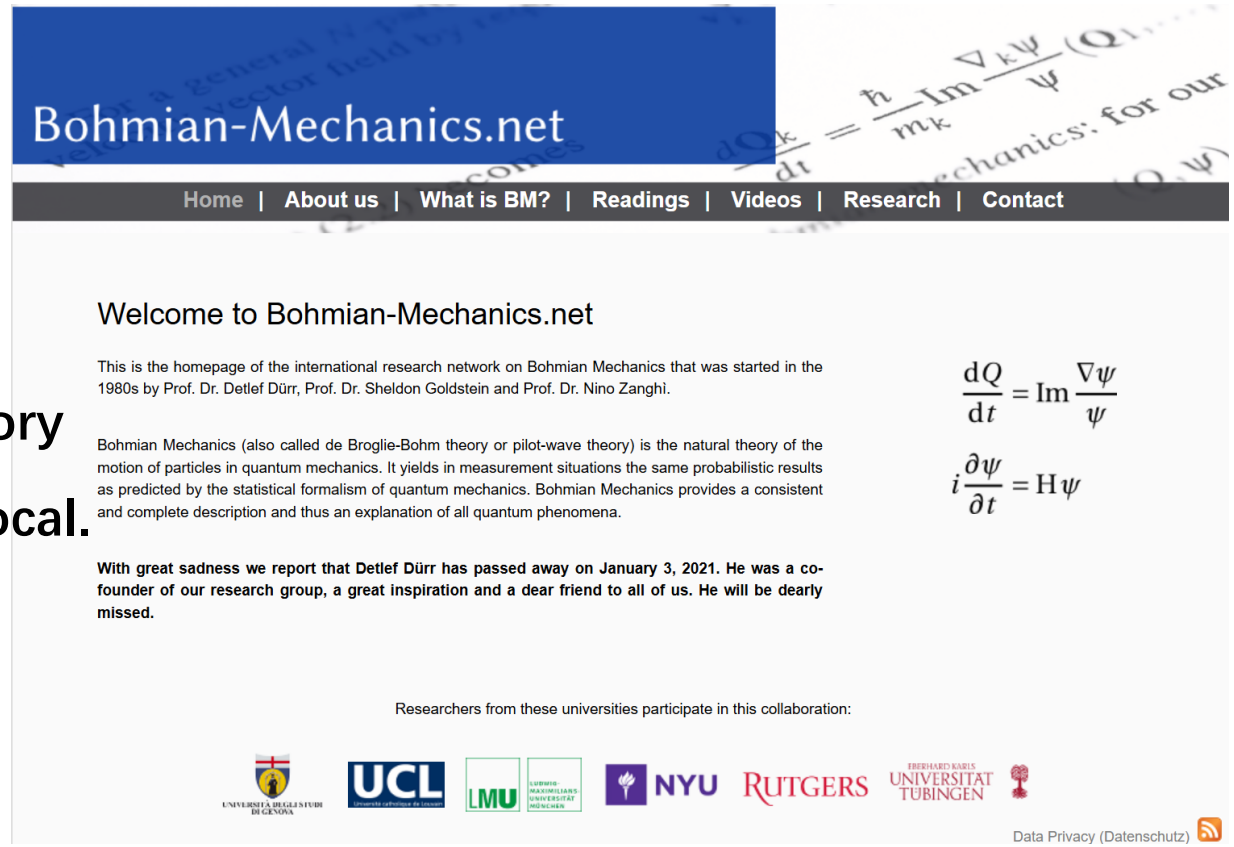
- Therefore, we can say that the Bohmian mechanics retains the wave function and adds actual particle positions as hidden variables. The wave function guides the motion, while the actual positions specify the configuration. Together, they determine the system's evolution.

- Now, the Bohmian mechanics is still alive !!!



However, Bell's theorem and its experimental verification confirm that any hidden-variable theory consistent with quantum mechanics must be nonlocal.

Bohm is also a feature in physics, who should not be forgotten.



# 3.3 Bell Inequality

## 3.3.1 The Hidden-Variable Theory of Bohm: A Final and Desperate Effort to Preserve the Classical Picture

Snapshot of the website. This Q is the X we use.

guidance equation

$$\frac{dQ}{dt} = \mathrm{Im}\frac{\nabla\psi}{\psi}$$

$$i\frac{\partial\psi}{\partial t} = \mathrm{H}\psi$$

1) de Broglie–Bohm theory（德布罗意-玻姆理论）或 pilot-wave theory（导波理论）

2) Deterministic trajectory with potential corrected by the quantum effects.

3) For $N$ particles, the hidden variables are their actual configuration:

$$\lambda = (\mathbf{X}_1, \mathbf{X}_2, \ldots, \mathbf{X}_N).$$

- I don't expect you to understand all these, but I want you to know these!

# 3.3 Bell Inequality

## 3.3.2 Bell's inequality

- For a long time, the hidden variable theory can coexist with QM.
- The turning point is in 1964, when Bell proposed an equation to test the validity of the hidden variable theory (with local assumption). A few years later, Aspect designed experiment to test it, and confirmed that entanglement is fundamental in QM and real.

ON THE EINSTEIN PODOLSKY ROSEN PARADOX*

J. S. BELL†
*Department of Physics, University of Wisconsin, Madison, Wisconsin*

(*Received 4 November* 1964)

- Now, we use a little bit of the modern language to explain how entangled state looks like. Then, follow the paper of Aspect to explain the Bell inequality, using an entangled photon pair.

$$\hat{H} = \hat{H}_1(x_1) + \hat{H}_2(x_2) = \hat{H}_1 \otimes \hat{I}_2 + \hat{I}_1 \otimes \hat{H}_2$$

→ There is no interaction between the subsystems, but we put them together.

# 3.3 Bell Inequality

## 3.3.2 Bell's inequality

$$\hat{H} = \hat{H}_1(x_1) + \hat{H}_2(x_2) = \hat{H}_1 \otimes \hat{I}_2 + \hat{I}_1 \otimes \hat{H}_2$$

$$E_{nm} = E_n(1) + E_m(2)$$

$$|\psi_n^{[1]}\rangle \otimes |\psi_m^{[2]}\rangle \equiv |n, m\rangle$$

$\Rightarrow$ Proper eigen state of the two-particle system when the two subsystems are not entangled.

$$\hat{H}_1(x_1) \Rightarrow |\psi_n^{[1]}\rangle$$

$$\hat{H}_2(x_2) \Rightarrow |\psi_m^{[2]}\rangle$$

- There are two ways to introduce entanglement: 1) exchange symmetry for identity particles (e.g. Slater determinant, be explained later, as long as the two subsystems are put together), 2) interactions.

$$\hat{H} = \hat{H}_1(x_1) + \hat{H}_2(x_2) + \hat{V}(x_1, x_2)$$

# 3.3 Bell Inequality

## 3.3.2 Bell's inequality

- Entangled Quantum State.

$$\widehat{H} = \begin{bmatrix} E_{11} & V_{12} & \cdots & V_{1N} \\ V_{21} & E_{22} & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots \\ V_{N1} & \cdots & \cdots & E_{NN} \end{bmatrix}$$

$$|B\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle \otimes |\downarrow\rangle - |\downarrow\rangle \otimes |\uparrow\rangle)$$

Extra notation: Spin DoF is not necessary, identity-particle neither

$$\Psi(\nu_1, \nu_2) = \frac{1}{\sqrt{2}}\{|x\rangle_1|x\rangle_2 + |y\rangle_1|y\rangle_2\}$$

Coupled photon

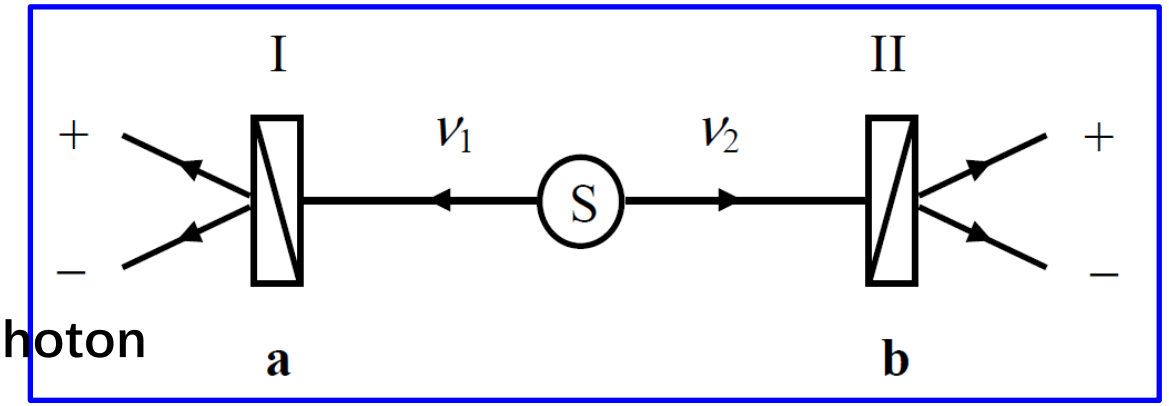
$$\widehat{H} = \widehat{H}_1(x_1) + \widehat{H}_2(x_2) + \widehat{V}(x_1, x_2)$$

$$|\psi_n^{[1]}\rangle \otimes |\psi_m^{[2]}\rangle \equiv |n, m\rangle$$

$$|m, n\rangle = |\beta\rangle, (\beta = 1, 2, \cdots, N = d_1 \times d_2)$$

$$|\psi\rangle = |\psi(1,2)\rangle = \sum_{j,l} C_{jl}|j(1)\rangle \otimes |l(2)\rangle$$

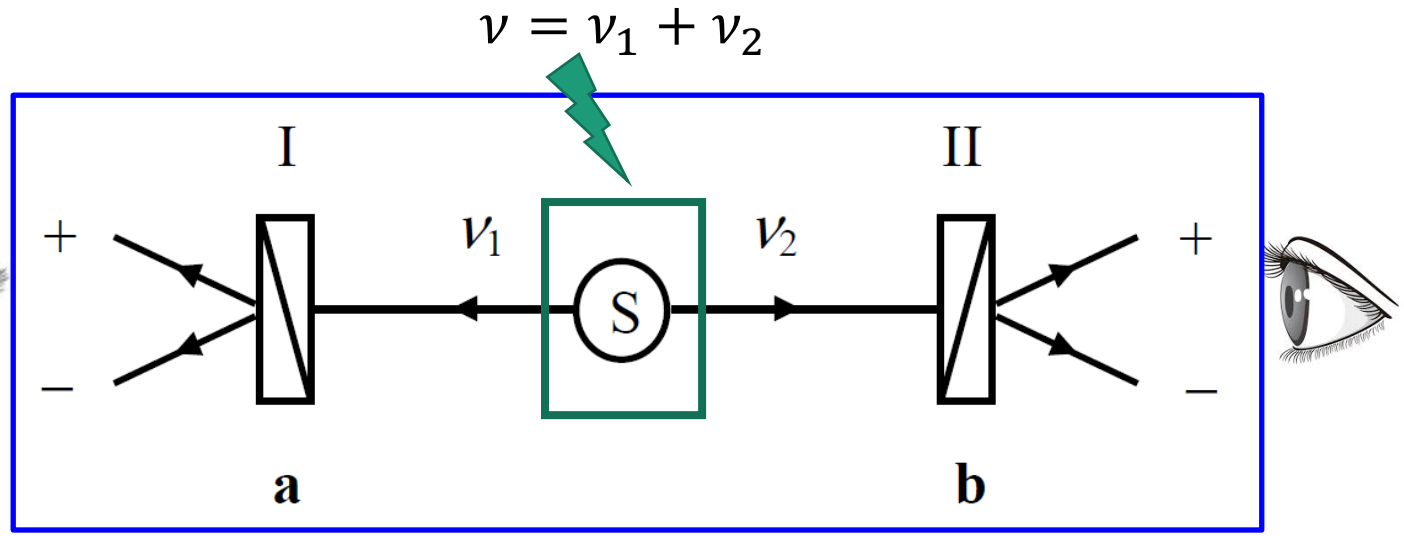
Experimental setup:



# 3.3 Bell Inequality

## 3.3.2 Bell's inequality

$$\Psi(\nu_1, \nu_2) = \frac{1}{\sqrt{2}}\{|x\rangle_1|x\rangle_2 + |y\rangle_1|y\rangle_2\}$$



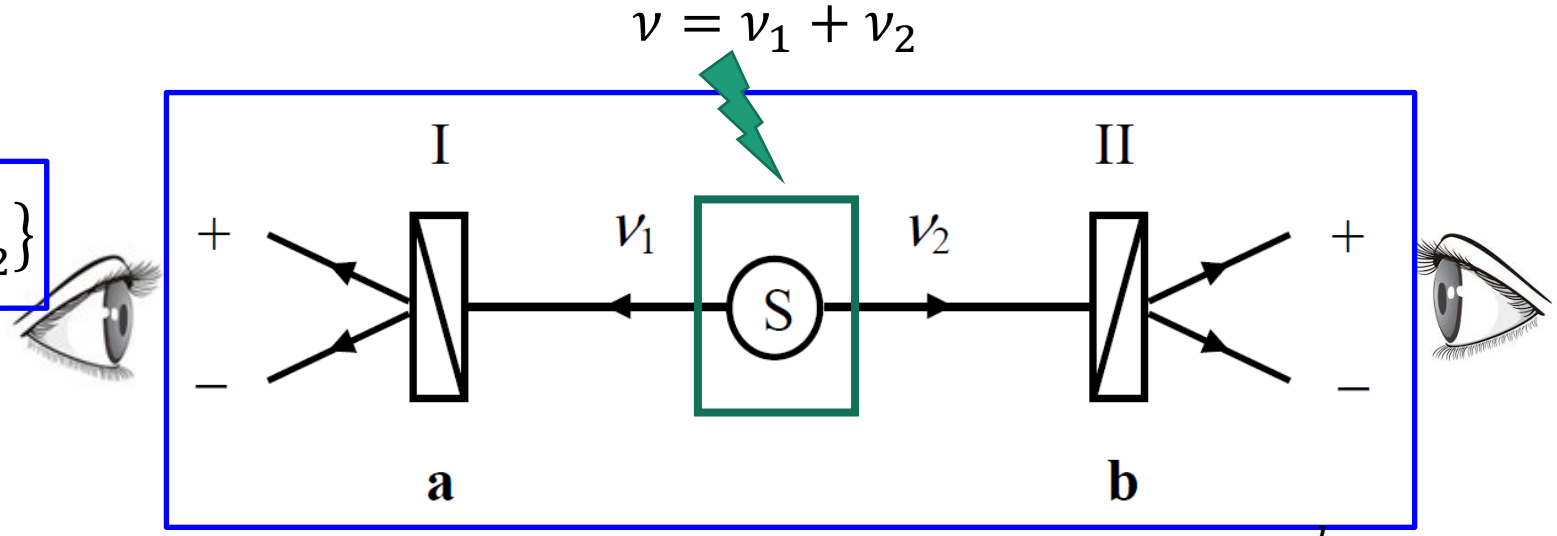

We perform linear polarization measurements on the two photons, with analysers / and //. The analyser /, in orientation a, is followed by two detectors, giving results + or -, corresponding to a linear polarization found parallel or perpendicular to a. The analyser //, in orientation b, acts similarly.

A two-output polarization analyzer, which separates the two orthogonal polarization components into different channels, allowing the ++, +-, -+, and −− outcomes to be recorded directly. In so doing, the correlation between the two events can be recorded and analyzed. It is this analysis of the correlation, which unravels the nature of quantum entanglement later.

# 3.3 Bell Inequality

## 3.3.2 Bell's inequality

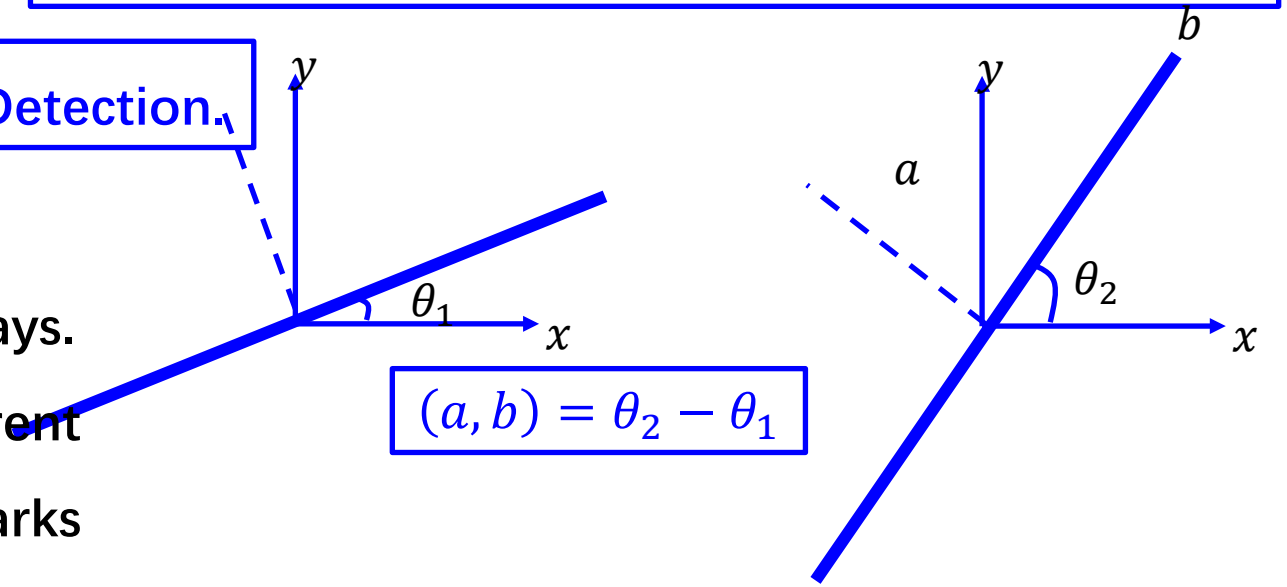
$$\Psi(\nu_1,\nu_2)=\frac{1}{\sqrt{2}}\{|x\rangle_1|x\rangle_2+|y\rangle_1|y\rangle_2\}$$




$$P_{++}(\mathbf{a},\mathbf{b})=P_{--}(\mathbf{a},\mathbf{b})=\frac{1}{2}\cos^2(\mathbf{a},\mathbf{b})$$

$$P_{+-}(\mathbf{a},\mathbf{b})=P_{-+}(\mathbf{a},\mathbf{b})=\frac{1}{2}\sin^2(\mathbf{a},\mathbf{b})$$

Joint Detection.



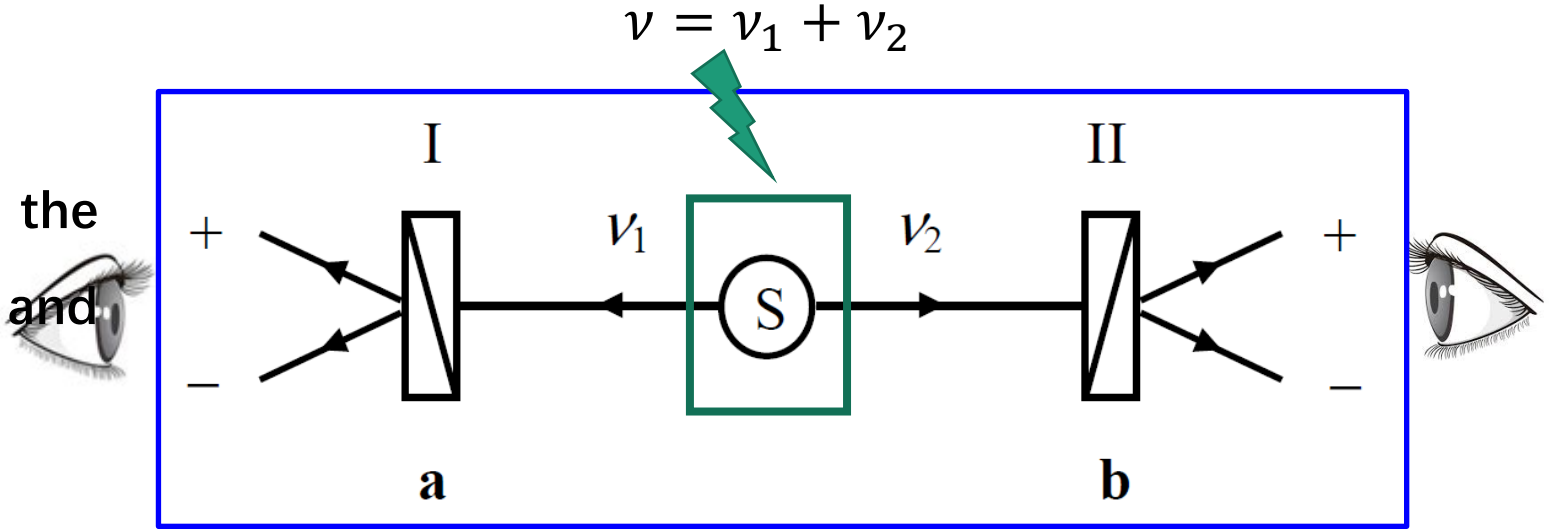

$$(a,b)=\theta_2-\theta_1$$

- This is the result of Q.M. we use nowadays.
- Hidden variable theory gives different results, which can be tested. This marks the fundamental difference between Bell and the others.

# 3.3 Bell Inequality

## 3.3.2 Bell's inequality

- For example, if we summarize the differences between EPR-Bohm and Bell.




- EPR–Bohm measurements along the same direction, and exhibit perfect anticorrelation

$$P(\uparrow_A,\downarrow_B) = \frac{1}{2}, \qquad P(\downarrow_A,\uparrow_B) = \frac{1}{2},$$

$$P(\uparrow_A,\uparrow_B) = P(\downarrow_A,\downarrow_B) = 0.$$

- Bell made the measurement directions on the two sides independently selectable and compared the joint correlations at different relative angles, thereby turning "whether the correlations can be explained by local hidden variables" into a testable question.

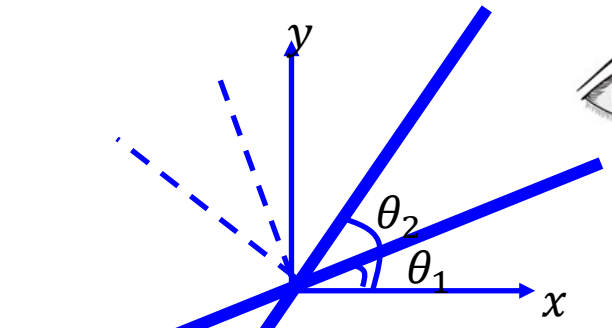
# 3.3 Bell Inequality

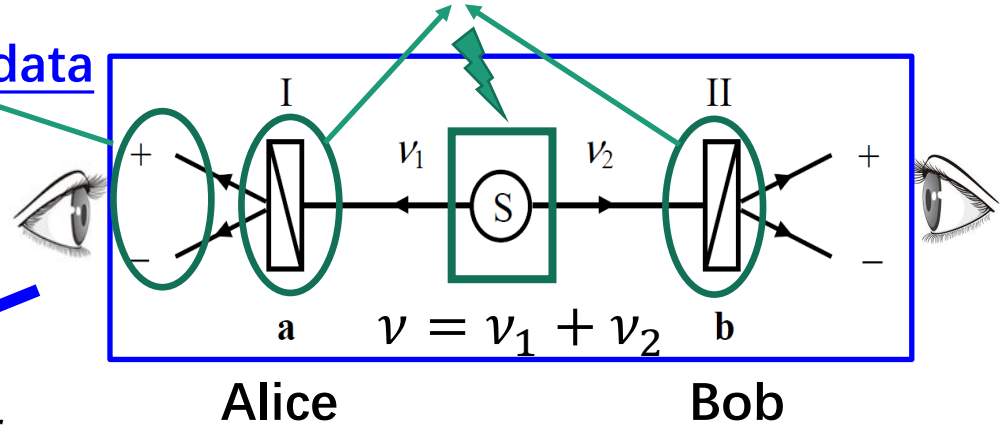
## 3.3.2 Bell's inequality

Joint Measurements!

Post-processing of the data

$|a\rangle_{1,\|}\langle a|_{1,\|}$ $|b\rangle_{2,\|}\langle b|_{2,\|}$




$$|a\rangle_{1,\|} = \cos\theta_1\,|x\rangle_1 + \sin\theta_1\,|y\rangle_1$$

$$|b\rangle_{2,\|} = \cos\theta_2\,|x\rangle_2 + \sin\theta_2\,|y\rangle_2$$

$$|a\rangle_{1,\|}|b\rangle_{2,\|}\langle a|_{1,\|}\langle b|_{2,\|}\left\{\frac{1}{\sqrt{2}}|x\rangle_1|x\rangle_2 + \frac{1}{\sqrt{2}}|y\rangle_1|y\rangle_2\right\}$$

$$P_{++}(\mathbf{a},\mathbf{b}) = P_{--}(\mathbf{a},\mathbf{b}) = \frac{1}{2}\cos^2(\mathbf{a},\mathbf{b})$$

$$P_{+-}(\mathbf{a},\mathbf{b}) = P_{-+}(\mathbf{a},\mathbf{b}) = \frac{1}{2}\sin^2(\mathbf{a},\mathbf{b})$$

$$\{\cos\theta_1\langle x|_1 + \sin\theta_1\langle y|_1\}\{\cos\theta_2\langle x|_2 + \sin\theta_2\langle y|_2\}\left\{\frac{1}{\sqrt{2}}|x\rangle_1|x\rangle_2 + \frac{1}{\sqrt{2}}|y\rangle_1|y\rangle_2\right\}$$

$$= \frac{1}{\sqrt{2}}\{\cos\theta_1\cos\theta_2 + \sin\theta_1\sin\theta_2\} = \frac{1}{\sqrt{2}}\cos(\theta_1 - \theta_2) = \frac{1}{\sqrt{2}}\cos(a,b)$$



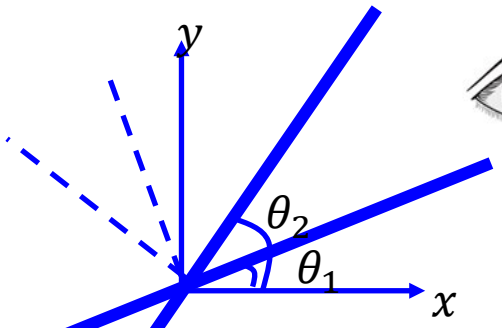
# 3.3 Bell Inequality

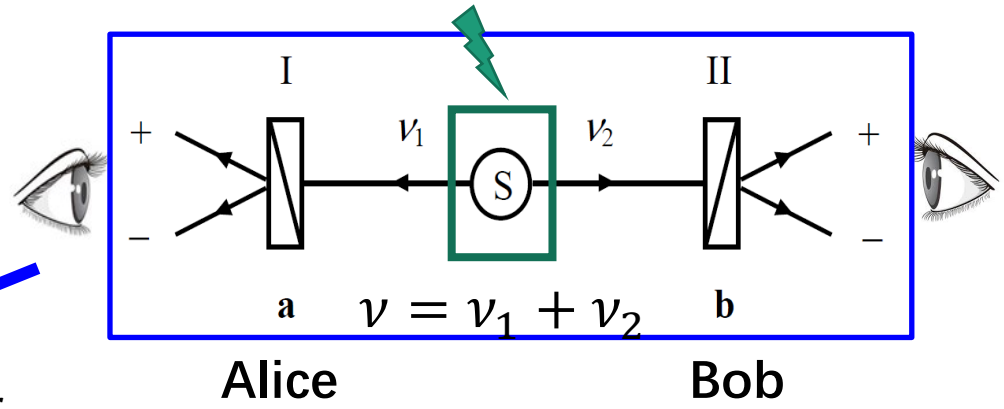
## 3.3.2 Bell's inequality

$|a\rangle_{1,\perp}\langle a|_{1,\perp}$ $|b\rangle_{2,\perp}\langle b|_{2,\perp}$

$$|a\rangle_{1,\perp} = -\sin\theta_1\,|x\rangle_1 + \cos\theta_1\,|y\rangle_1$$

$$|b\rangle_{2,\perp} = -\sin\theta_2\,|x\rangle_2 + \cos\theta_2\,|y\rangle_2$$




$$|a\rangle_{1,\perp}|b\rangle_{2,\perp}\langle a|_{1,\perp}\langle b|_{2,\perp}\left\{\frac{1}{\sqrt{2}}|x\rangle_1|x\rangle_2 + \frac{1}{\sqrt{2}}|y\rangle_1|y\rangle_2\right\}$$

$$P_{++}(\mathbf{a},\mathbf{b}) = P_{--}(\mathbf{a},\mathbf{b}) = \frac{1}{2}\cos^2(\mathbf{a},\mathbf{b})$$

$$P_{+-}(\mathbf{a},\mathbf{b}) = P_{-+}(\mathbf{a},\mathbf{b}) = \frac{1}{2}\sin^2(\mathbf{a},\mathbf{b})$$

$$\{-\sin\theta_1\langle x|_1 + \cos\theta_1\langle y|_1\}\{-\sin\theta_2\langle x|_2 + \cos\theta_2\langle y|_2\}\left\{\frac{1}{\sqrt{2}}|x\rangle_1|x\rangle_2 + \frac{1}{\sqrt{2}}|y\rangle_1|y\rangle_2\right\}$$

$$= \frac{1}{\sqrt{2}}\{(-\sin\theta_1)(-\sin\theta_2) + \cos\theta_1\cos\theta_2\} = \frac{1}{\sqrt{2}}\cos(\theta_1 - \theta_2) = \frac{1}{\sqrt{2}}\cos(a,b)$$

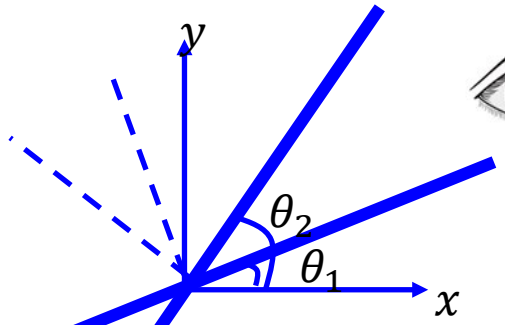
# 3.3 Bell Inequality

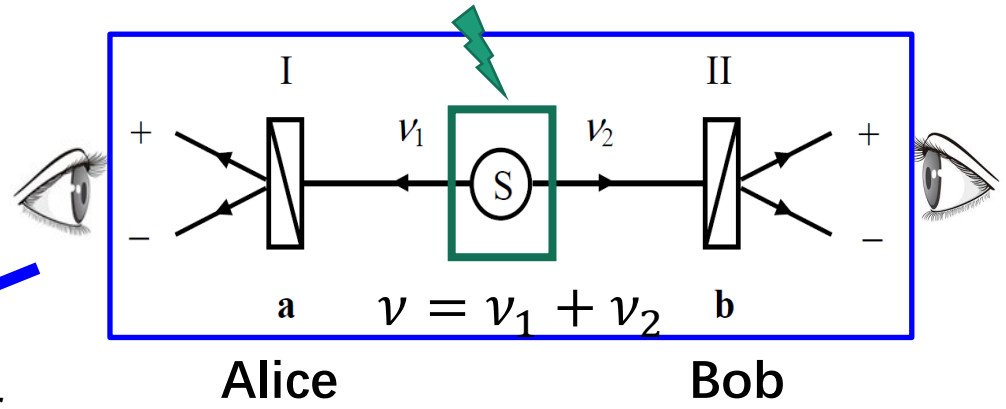
## 3.3.2 Bell's inequality

$|a\rangle_{1,\parallel}\langle a|_{1,\parallel}$ $|b\rangle_{2,\perp}\langle b|_{2,\perp}$

$$|a\rangle_{1,\parallel} = \cos\theta_1\,|x\rangle_1 + \sin\theta_1\,|y\rangle_1$$

$$|b\rangle_{2,\perp} = -\sin\theta_2\,|x\rangle_2 + \cos\theta_2\,|y\rangle_2$$




$$|a\rangle_{1,\parallel}|b\rangle_{2,\perp}\langle a|_{1,\parallel}\langle b|_{2,\perp}\left\{\frac{1}{\sqrt{2}}|x\rangle_1|x\rangle_2 + \frac{1}{\sqrt{2}}|y\rangle_1|y\rangle_2\right\}$$

$$P_{++}(\mathbf{a},\mathbf{b}) = P_{--}(\mathbf{a},\mathbf{b}) = \frac{1}{2}\cos^2(\mathbf{a},\mathbf{b})$$

$$P_{+-}(\mathbf{a},\mathbf{b}) = P_{-+}(\mathbf{a},\mathbf{b}) = \frac{1}{2}\sin^2(\mathbf{a},\mathbf{b})$$

$$\{\cos\theta_1\,\langle x|_1 + \sin\theta_1\,\langle y|_1\}\{-\sin\theta_2\,\langle x|_2 + \cos\theta_2\,\langle y|_2\}\left\{\frac{1}{\sqrt{2}}|x\rangle_1|x\rangle_2 + \frac{1}{\sqrt{2}}|y\rangle_1|y\rangle_2\right\}$$

$$= \frac{1}{\sqrt{2}}\{\cos\theta_1\,(-\sin\theta_2) + \sin\theta_1\cos\theta_2\} = \frac{1}{\sqrt{2}}\sin(\theta_1 - \theta_2) = \frac{1}{\sqrt{2}}\sin(a,b)$$

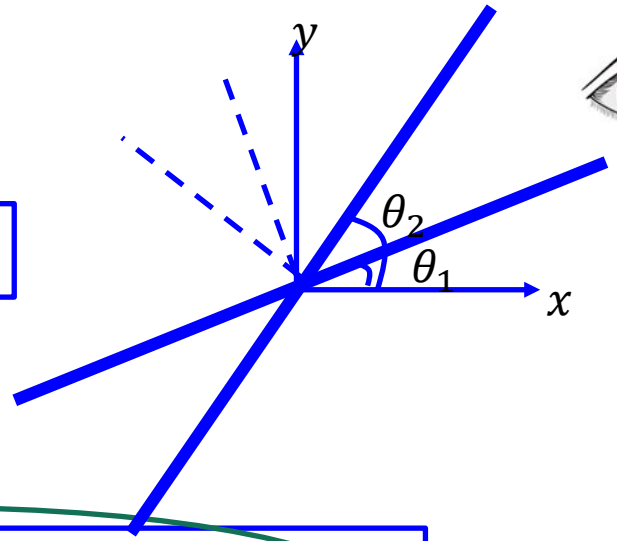
# 3.3 Bell Inequality

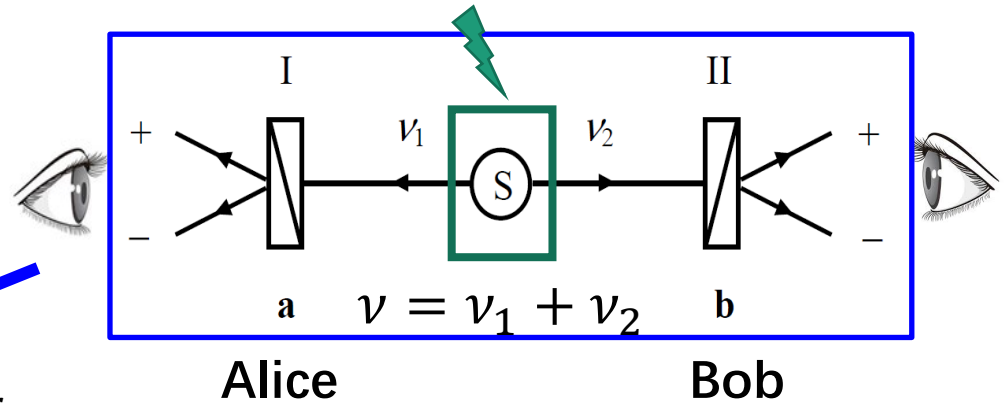
## 3.3.2 Bell's inequality

$|a\rangle_{1,\perp}\langle a|_{1,\perp}$ $|b\rangle_{2,\parallel}\langle b|_{2,\parallel}$

$$|a\rangle_{1,\perp} = -\sin\theta_1\,|x\rangle_1 + \cos\theta_1\,|y\rangle_1$$

$$|b\rangle_{2,\parallel} = \cos\theta_2\,|x\rangle_2 + \sin\theta_2\,|y\rangle_2$$




$$|a\rangle_{1,\perp}|b\rangle_{2,\parallel}\langle a|_{1,\perp}\langle b|_{1,\parallel}\left\{\frac{1}{\sqrt{2}}|x\rangle_1|x\rangle_2 + \frac{1}{\sqrt{2}}|y\rangle_1|y\rangle_2\right\}$$

$$P_{++}(\mathbf{a},\mathbf{b}) = P_{--}(\mathbf{a},\mathbf{b}) = \frac{1}{2}\cos^2(\mathbf{a},\mathbf{b})$$

$$P_{+-}(\mathbf{a},\mathbf{b}) = P_{-+}(\mathbf{a},\mathbf{b}) = \frac{1}{2}\sin^2(\mathbf{a},\mathbf{b})$$

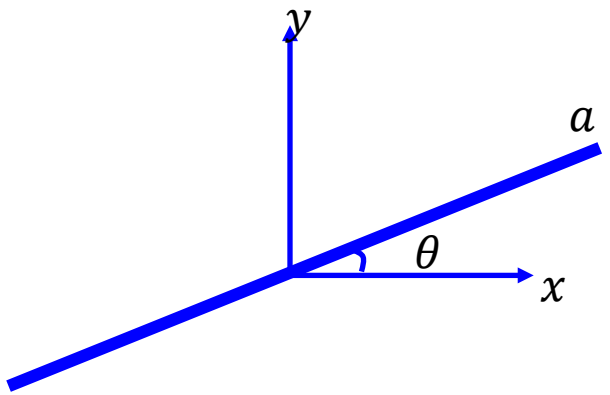
$$\left\{-\sin\theta_1\,\langle x|_1 + \cos\theta_1\,\langle y|_1\right\}\left\{\cos\theta_2\,\langle x|_2 + \sin\theta_2\,\langle y|_2\right\}\left\{\frac{1}{\sqrt{2}}|x\rangle_1|x\rangle_2 + \frac{1}{\sqrt{2}}|y\rangle_1|y\rangle_2\right\}$$

$$= \frac{1}{\sqrt{2}}\{(-\sin\theta_1)\cos\theta_2 + \cos\theta_1\sin\theta_2\} = -\frac{1}{\sqrt{2}}\sin(\theta_1 - \theta_2) = -\frac{1}{\sqrt{2}}\sin(a,b)$$

# 3.3 Bell Inequality

## 3.3.2 Bell's inequality

- Single Detection, and Reduced Density Matrix




$$|a\rangle_{1,\parallel}\langle a|_{1,\parallel}$$

$$|a\rangle_{1,\parallel} = \cos\theta\,|x\rangle_1 + \sin\theta\,|y\rangle_1$$

$$\hat{P}_+^a = |a\rangle_{1,\parallel}\langle a|_{1,\parallel} \Rightarrow |a\rangle_{1,\parallel}\langle a|_{1,\parallel}\left\{\frac{1}{\sqrt{2}}|x\rangle_1|x\rangle_2 + \frac{1}{\sqrt{2}}|y\rangle_1|y\rangle_2\right\} \Rightarrow P_+(a) = \langle\Phi^+|\left(\hat{P}_{+a}^A \otimes \hat{I}^B\right)|\Phi^+\rangle$$

$$P_+ = \left\{\frac{1}{\sqrt{2}}\langle x|_1\langle x|_2 + \frac{1}{\sqrt{2}}\langle y|_1\langle y|_2\right\}|a\rangle_{1,\parallel}\langle a|_{1,\parallel}\left\{\frac{1}{\sqrt{2}}|x\rangle_1|x\rangle_2 + \frac{1}{\sqrt{2}}|y\rangle_1|y\rangle_2\right\}$$

$$\left\{\cos\theta\,\langle x|_1 + \sin\theta\,\langle y|_1\right\}\left\{\tfrac{1}{\sqrt{2}}|x\rangle_1|x\rangle_2 + \tfrac{1}{\sqrt{2}}|y\rangle_1|y\rangle_2\right\} = \tfrac{1}{\sqrt{2}}\left\{\cos\theta\,|x\rangle_2 + \sin\theta\,|y\rangle_2\right\}$$

$$P_+ = \tfrac{1}{\sqrt{2}}\left\{\cos\theta_1\,\langle x|_2 + \sin\theta_1\,\langle x|_2\right\}\tfrac{1}{\sqrt{2}}\left\{\cos\theta_1\,|x\rangle_2 + \sin\theta_1\,|y\rangle_2\right\} = \frac{1}{2}(\cos^2\theta + \sin^2\theta) = \frac{1}{2}$$

**Same result for $P_-$. For single detection, the result does not depend on $\theta$!!!**

# 3.3 Bell Inequality

## 3.3.2 Bell's inequality

- Now, we have:

$$P_{++}(a,b) = P_{--}(a,b) = \frac{1}{2}\cos^2(a-b),$$

$$P_{+-}(a,b) = P_{-+}(a,b) = \frac{1}{2}\sin^2(a-b).$$

$P_{++}$ is the joint probability that, in the same round of the experiment, Alice obtains + and Bob obtains +. The sum of the probabilities of the four outcomes is 1.

- And if we take a single measurement, we have: $P(A=+\mid a,b) = P_{++} + P_{+-} = \frac{1}{2}$ $P(B=+\mid a,b) = 1/2$

The angular dependence does not appear in the probability of the single detection probability. It only appears in the joint detection.

- Now, we define a correlation function:

Let $A, B \in \{+1, -1\}$, and define the correlation function $E(a,b) = \langle AB \rangle_{a,b}$.

Equal outcomes contribute $+1$ to $E$, while opposite outcomes contribute $-1$.

# 3.3 Bell Inequality

## 3.3.2 Bell's inequality

- Now, we define a correlation function:

Let $A, B \in \{+1, -1\}$, and define the correlation function $E(a,b) = \langle AB \rangle_{a,b}$.

Equal outcomes contribute $+1$ to $E$, while opposite outcomes contribute $-1$.

Therefore,

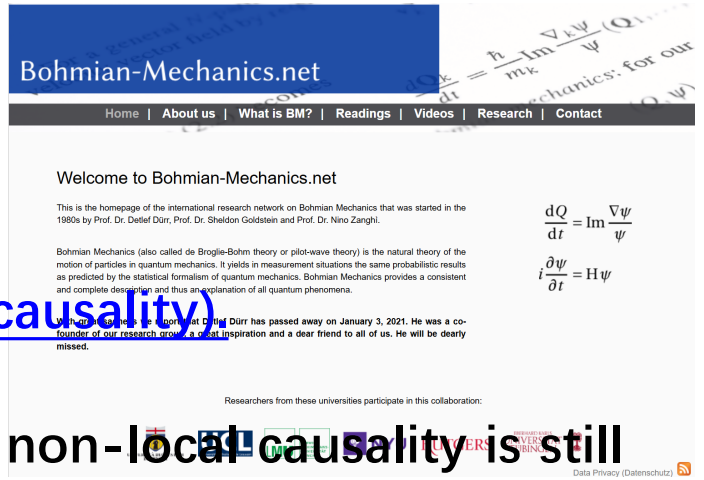
$$\begin{aligned} E_{\mathrm{QM}}(a,b) &= P_{++} + P_{--} - P_{+-} - P_{-+} \\ &= \cos^2(a-b) - \sin^2(a-b) \\ &= \boxed{\cos[2(a-b)]}. \end{aligned}$$

We now have a complete quantum prediction: as we vary the relative angle between the two analyzers, the correlation between their outcomes varies as $\cos[2(a-b)]$.

- Again, this is the result of the Q.M. we use nowadays.

# 3.3 Bell Inequality

## 3.3.2 Bell's inequality

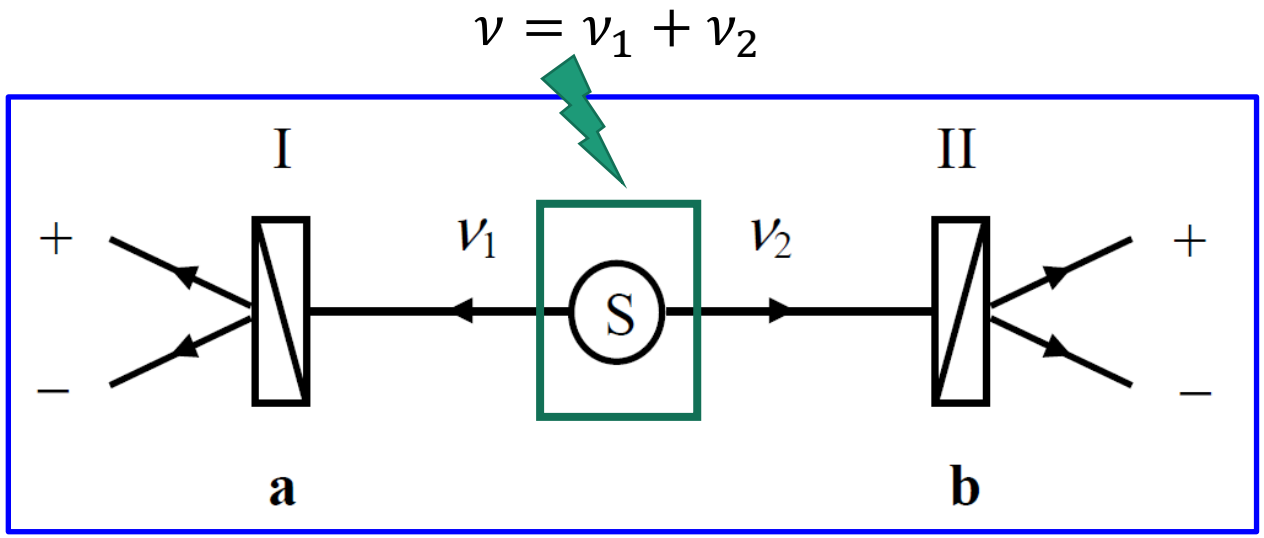



- Then, we look at the hidden variable theory (with assumption of local causality).
- Here, we emphasize local causality, since hidden variable theory with non-local causality is still alive, e.g. the Bohmian mechanics.
- We assume the hidden variable is $\lambda$, the value of this quantity gives us information of the quantum system beyond the description of the W.F.
- We do not specify the precise physical nature of the hidden variable $\lambda$. We treat it as additional information carried by a particle pair that is not fully described by the usual quantum state.
- Different experimental runs may have different values of $\lambda$, distributed according to a normalized probability density $\rho(\lambda)$. Nonnegativity and normalization are simply the basic requirements for a probability distribution.

$$\rho(\lambda) \geq 0 \qquad \int d\lambda \rho(\lambda) = 1$$

# 3.3 Bell Inequality

## 3.3.2 Bell's inequality



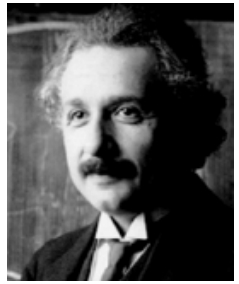

- Then, for this joint detection, we use a decisive model of the hidden variable theory to pass the main thought of Bell.

- Here, the outcomes are fixed once $\lambda$ and the measurement settings are specified.

- We still observe probabilities because we generally do not know the particular value of $\lambda$ in each run; instead, we average over many runs using $\rho(\lambda)$. In this way, quantum probabilities may be understood as arising from a statistical distribution over deeper deterministic states, rather than necessarily representing randomness that cannot be explained further.

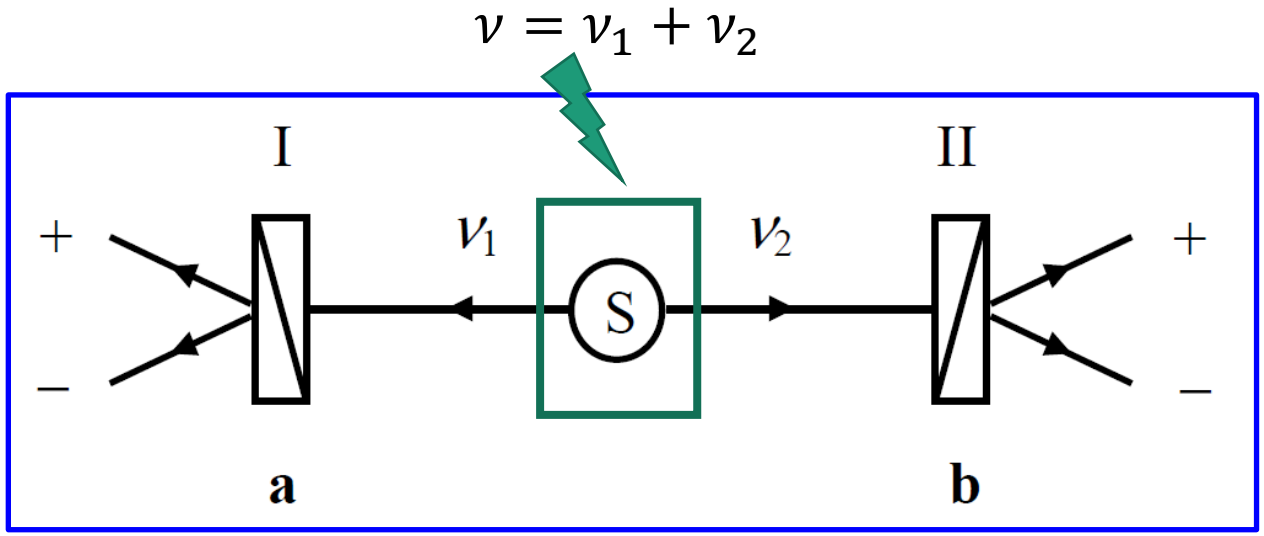
➡ Deny the fundamentality of the probability interpretation!





# 3.3 Bell Inequality

## 3.3.2 Bell's inequality




- Then, for each $\lambda$, Alice and Bob's detection gives results of:

$$A(a,\lambda) = \pm 1 \qquad B(b,\lambda) = \pm 1$$

- Alice's outcome depends only on her local setting $a$ and the shared information $\lambda$, not on Bob's distant setting $b$; the same applies to Bob's outcome. This is the locality assumption used here.

- Locality does not require $A$ and $B$ to be uncorrelated: their outcomes can be strongly correlated because the two sides share $\lambda$.

- But since this correlation is described mathematically in a different way from the Q.M. description, one can quantify this difference.

# 3.3 Bell Inequality

## 3.3.2 Bell's inequality

- Also, we need to emphasize that to compare experiments performed with different combinations of measurement angles, we must assume that the distribution of the shared information carried by the particle pairs is not changed by the experimenters' choices of measurement settings:

$$\rho(\lambda|a,b) = \rho(\lambda)$$

- This is called measurement-setting independence. It ensures that all the correlation functions $E(a,b)$ introduced below are averages over the same distribution $\rho(\lambda)$.

---

- With these, we can define the correlation function of the measurement. The integration is over $\lambda$. Therefore, so that we can do measurements for many trajectories, and obtain:

$$E_{\mathrm{L}}(a,b) = \int \mathrm{d}\lambda\, \rho(\lambda) A(a,\lambda) B(b,\lambda)$$

Here, we use the subscript L to stand for local causality.

- The contribution of Bell is that he realized if one believes the definition of the correlation function above, one can introduce an inequality to test the above thoughts based on local causality.

# 3.3 Bell Inequality

## 3.3.2 Bell's inequality

- His conclusion is that the inequality is in conflict with Q.M.

- Then, if we perform an experiment to test the validity of this inequality, one can test if the hidden-variable theory based on local causality is reasonable?

- One must say that this is a hhhhuuge achievement in the fundamental theory of Q.M.!!!

# 3.3 Bell Inequality

## 3.3.2 Bell's inequality

- One important point he took, which was given by Q.M., which was accepted by EPR, and which can be tested by experiment, is that if A and B are parallel to each other, one has:

$$P_{++}(\mathbf{a},\mathbf{b}) = P_{--}(\mathbf{a},\mathbf{b}) = \frac{1}{2}\cos^2(\mathbf{a},\mathbf{b})$$

$$P_{+-}(\mathbf{a},\mathbf{b}) = P_{-+}(\mathbf{a},\mathbf{b}) = \frac{1}{2}\sin^2(\mathbf{a},\mathbf{b})$$

$$\Rightarrow \quad \boldsymbol{A(n,\lambda) = B(n,\lambda)}$$

Meaning that the function is the same function, the angular dependence is the same!

- Then, he has: $\boldsymbol{E_{\mathrm{L}}(a,b) = \int \mathrm{d}\lambda\, \rho(\lambda) A(a,\lambda) A(b,\lambda)}$
- With this equation, one can choose three angles, i.e. $\boldsymbol{a}$, $\boldsymbol{b}$, and $\boldsymbol{c}$. Then, one has:

$$\boldsymbol{E_{\mathrm{L}}(a,b) - E_{\mathrm{L}}(a,c) = \int \mathrm{d}\lambda\, \rho(\lambda) A(a,\lambda)[A(b,\lambda) - A(c,\lambda)]}$$

- Since $\boldsymbol{\left(A(b,\lambda)\right)^2 = 1}$, one has:

$$\boldsymbol{A(b,\lambda) - A(c,\lambda) = A(b,\lambda)[1 - A(b,\lambda)A(c,\lambda)]}$$

# 3.3 Bell Inequality

## 3.3.2 Bell's inequality

- Therefore:

$$\boldsymbol{E_L(a,b) - E_L(a,c) = \int d\lambda\, \rho(\lambda) A(a,\lambda)[A(b,\lambda) - A(c,\lambda)]}$$

$$\boldsymbol{= \int d\lambda\, \rho(\lambda) A(a,\lambda) A(b,\lambda)[1 - A(b,\lambda)A(c,\lambda)]}$$

Either 0 or 2, always positive

$$\boldsymbol{\leq \int d\lambda\, \rho(\lambda) |A(a,\lambda) A(b,\lambda)| [1 - A(b,\lambda)A(c,\lambda)]}$$

- Since: $\boldsymbol{|A(a,\lambda)A(b,\lambda)| = 1}$

- One further has: $\boldsymbol{E_L(a,b) - E_L(a,c) \leq \int d\lambda\, \rho(\lambda)[1 - A(b,\lambda)A(c,\lambda)] = 1 - E_L(b,c)}$

- This is one inequality results from the hidden-variable theory with local causality assumed.

- If we put $\boldsymbol{E_{QM}(a,b)}$ in, we will find it is violated.

$$\begin{aligned} E_{\mathrm{QM}}(a,b) &= P_{++} + P_{--} - P_{+-} - P_{-+} \\ &= \cos^2(a-b) - \sin^2(a-b) \\ &= \boxed{\cos[2(a-b)]}. \end{aligned}$$

# 3.3 Bell Inequality

## 3.3.2 Bell's inequality

$$E_{\mathrm{QM}}(a,b) = P_{++} + P_{--} - P_{+-} - P_{-+}$$
$$= \cos^2(a-b) - \sin^2(a-b)$$
$$= \boxed{\cos[2(a-b)]}.$$

- For example, we set $\boldsymbol{a = 0^\circ}$, $\boldsymbol{b = 30^\circ}$, $\boldsymbol{c = 60^\circ}$. Then, we will have:

$$\boldsymbol{E_{\mathrm{QM}}(a,b) = \cos(60^\circ) = 1/2} \qquad \boldsymbol{E_{\mathrm{QM}}(a,c) = \cos(120^\circ) = -1/2} \qquad \boldsymbol{E_{\mathrm{QM}}(b,c) = \cos(60^\circ) = 1/2}$$

- Then, $\boldsymbol{E_{\mathrm{QM}}(a,b) - E_{\mathrm{QM}}(a,c) = 1}$ It is larger than: $\boldsymbol{1 - E_{\mathrm{QM}}(b,c) = 1/2}$

- In other words, the inequality which was proposed by assuming local causality in the hidden-variable theory is not respect by $\boldsymbol{E_{\mathrm{QM}}}$!!!

- For the first time, a quantitative criterion to test the hidden-variable theory and the Q.M. appeared!!!

- In the history, Bohm did not got a Nobel prize, neither did Bell. Aspect got one. But in my opinion, Bohm and Bell are both heroes. When judging physics, respect physics, and stay away from vanity and worldly honor!

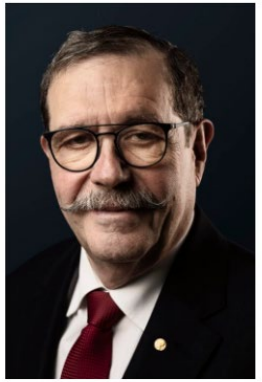
| 人物 | 主要贡献 | 与诺奖有关的事实 |
| --- | --- | --- |
| David Bohm | 1952 年提出具体的非局域隐变量理论 | 1992 年去世 |
| John Bell | 1964 年提出不等式，将局域性问题转化为可检验的约束 | 1990 年去世 |
| Aspect、Clauser、Zeilinger | 推进纠缠光子实验、Bell 不等式检验及量子信息研究 | 共同获得 2022 年诺贝尔物理学奖 |

In physics, the **Clauser–Horne–Shimony–Holt** (**CHSH**) **inequality** can be used in the proof of Bell's theorem, which states that certain consequences of entanglement in quantum mechanics cannot be reproduced by local hidden-variable theories. Experimental verification of the inequality being violated is seen as confirmation that nature cannot be described by such theories. CHSH stands for John Clauser, Michael Horne, Abner Shimony, and Richard Holt, who described it in a much-cited paper published in 1969.[1] They derived the CHSH inequality, which, as with John

**Abner Eliezer Shimony** (/ʃɪˈmoʊni/; March 10, 1928 – August 8, 2015) was an American physicist and philosopher. He specialized in quantum theory and

**Michael Allan Horne** (January 18, 1943 – January 19, 2019)[2] was an American quantum physicist, known for his work on the foundations of quantum mechanics.

# Nobel Prize in Physics 2022



© Nobel Prize Outreach. Photo: Stefan Bladh
Alain Aspect
Prize share: 1/3



© Nobel Prize Outreach. Photo: Stefan Bladh
John F. Clauser
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Anton Zeilinger
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**BELL'S THEOREM : THE NAIVE VIEW OF AN EXPERIMENTALIST**†

Alain Aspect

The Nobel Prize in Physics 2022 was awarded jointly to Alain Aspect, John F. Clauser and Anton Zeilinger "for experiments with entangled photons, establishing the violation of Bell inequalities and pioneering quantum information science"

- **Two keywords for the next: CHSH, and Aspect.**

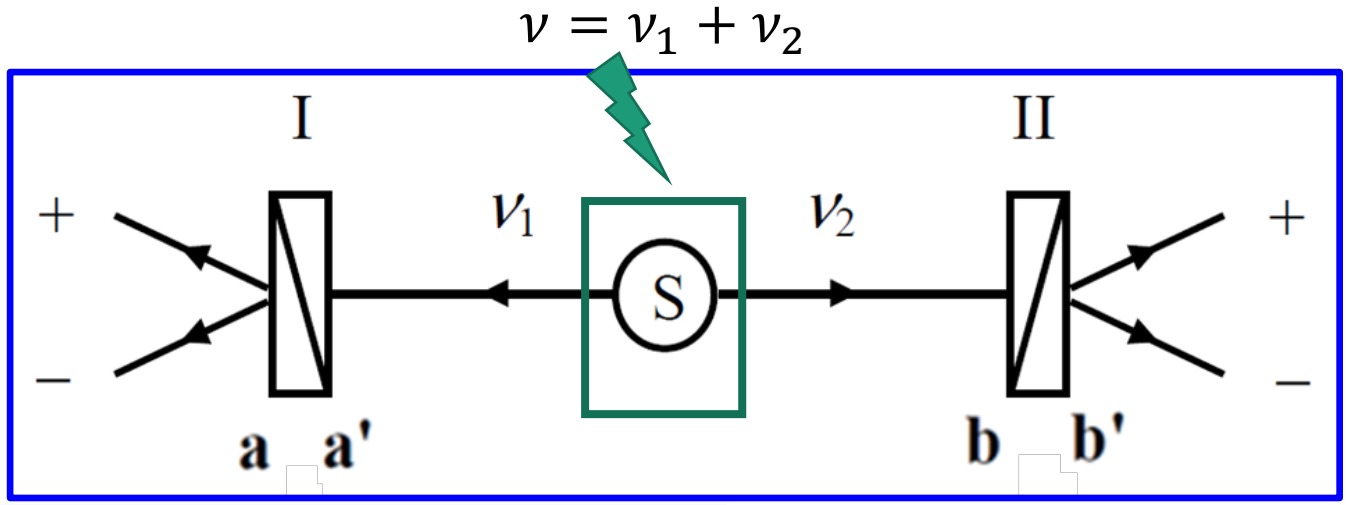
# 3.3 Bell Inequality

## 3.3.3 CHSH Inequality and Experiments

- The derivation in the previous section used $A(\boldsymbol{n}, \boldsymbol{\lambda}) = B(\boldsymbol{n}, \boldsymbol{\lambda})$, which requires the model to reproduce perfect correlations when both sides measure along the same direction.
- In a real experiment, however, imperfect state preparation, optical components, limited detection efficiency, and background counts can all make the measured correlations less than perfect.
- Therefore, a criterion which is robust to the experimental settings is desired.
- In 1969, Clauser, Horne, Shimony, and Holt proposed the CHSH inequality. It retains Bell's central question: How strong can the correlations across different measurement settings be in a local model? But it constructs a new combination of four setting pairs. Its derivation does not require perfect agreement, or perfect disagreement, between outcomes measured along the same direction.

# 3.3 Bell Inequality

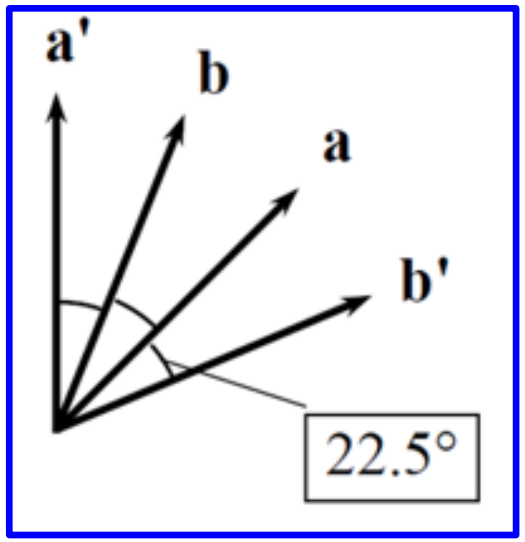
## 3.3.3 CHSH Inequality and Experiments




### 1. Experimental Setup

A source emits a pair of particles on each trial, sending one particle to Alice and the other to Bob. Alice chooses one of two measurement settings, $a$ or $a'$, while Bob chooses $b$ or $b'$. Each person obtains just one outcome on that trial, either $+1$ or $-1$.

| Participant | Available settings | Outcome on each trial |
|---|---|---|
| Alice | $a$ or $a'$ | $+1$ or $-1$ |
| Bob | $b$ or $b'$ | $+1$ or $-1$ |




The four possible pairs of settings are $(a, b)$, $(a, b')$, $(a', b)$, and $(a', b')$. By repeating the experiment for each pair, we can estimate the four correlations $E(a, b)$, $E(a, b')$, $E(a', b)$, and $E(a', b')$.

# 3.3 Bell Inequality

## 3.3.3 CHSH Inequality and Experiments

### 2. A Local Hidden-Variable Description

Let $\lambda$ denote a hidden variable carried by the particle pair. Its probability density is $\rho(\lambda)$, where

$$\rho(\lambda) \geq 0, \qquad \int \rho(\lambda)\, d\lambda = 1.$$

In a deterministic local hidden-variable model, for a given $\lambda$, Alice's two possible outcomes are $A(a, \lambda)$ and $A(a', \lambda)$, while Bob's are $B(b, \lambda)$ and $B(b', \lambda)$. For brevity, write them as $A$, $A'$, $B$, $B'$. Each takes a value of $+1$ or $-1$.

- **Locality:** Alice's outcome does not depend on whether Bob chooses $b$ or $b'$; likewise, Bob's outcome does not depend on Alice's choice.
- **Measurement-setting independence:** The distribution of $\lambda$ does not change according to which pair of settings is chosen. This allows all four correlations to be described using the same $\rho(\lambda)$.

# 3.3 Bell Inequality

## 3.3.3 CHSH Inequality and Experiments

### 3. The Algebraic Step

Especially defined quantity

First, consider the quantity

$$C(\lambda) = AB + AB' + A'B - A'B' = A(B + B') + A'(B - B').$$

Because $B$ and $B'$ are each either $+1$ or $-1$, one of $B + B'$ and $B - B'$ must be zero, while the other must be $+2$ or $-2$. Since $A, A' = \pm 1$, it follows that, for every $\lambda$,

$$C(\lambda) = +2 \text{ or } -2, \qquad \text{and therefore} \qquad |C(\lambda)| = 2.$$

Then, we will have: $|\langle C \rangle| = \left| \int \rho(\lambda) C(\lambda)\, d\lambda \right| \leq \int \rho(\lambda) |C(\lambda)|\, d\lambda = 2.$

Then, Define $E(a, b) = \langle AB \rangle$, with the other correlations defined in the same way. We obtain

$$\boxed{S \equiv |E(a, b) + E(a, b') + E(a', b) - E(a', b')| \leq 2}$$

**This is a commonly used form of the CHSH inequality.**

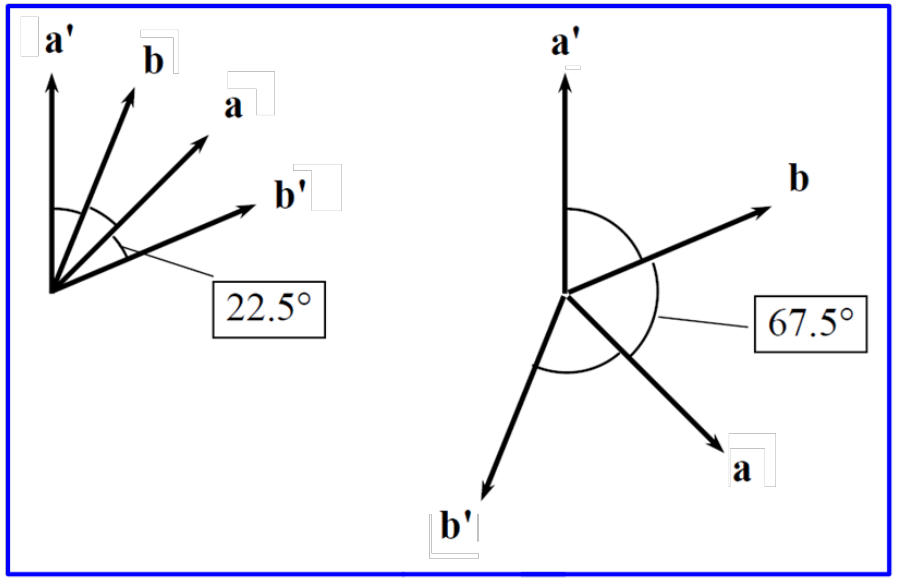
# 3.3 Bell Inequality

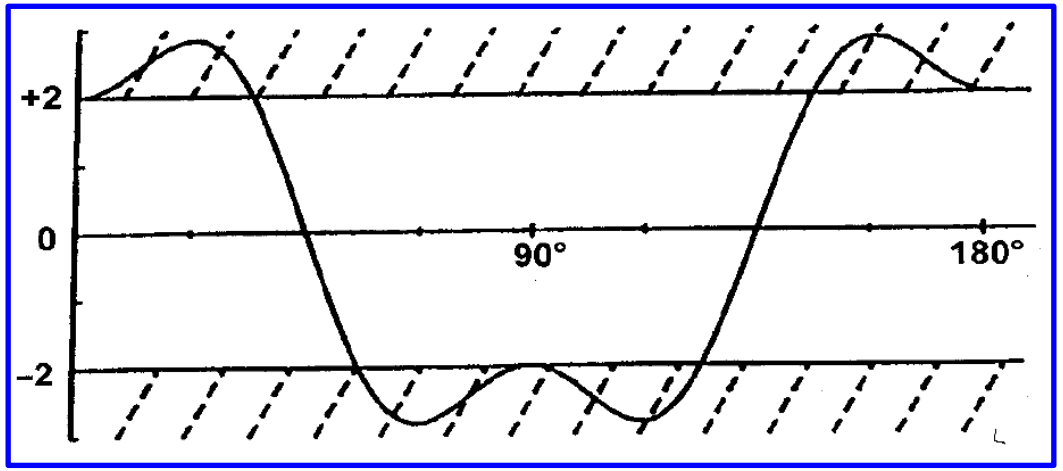
## 3.3.3 CHSH Inequality and Experiments

**A point to emphasize in class:** $C(\lambda)$ is a quantity used in the hidden-variable model's derivation. It is *not* a "sum of four outcomes" that can be read off in a single trial. On each trial, Alice and Bob choose only one setting each, so they obtain only one of the four products. The experiment estimates the four correlations through repeated trials with different setting pairs and then calculates $S$.

$$\boxed{S \equiv \left|E(a,b) + E(a,b') + E(a',b) - E(a',b')\right|}$$

$$\begin{aligned} E_{\mathrm{QM}}(a,b) &= P_{++} + P_{--} - P_{+-} - P_{-+} \\ &= \cos^2(a-b) - \sin^2(a-b) \\ &= \boxed{\cos[2(a-b)]}. \end{aligned}$$



# ◆ Outline

1. Which states of identical particles are legal?

(Hilbert Space)

2. Why are l… …neasurements?




现代物理学丛书

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卷Ⅱ

（第四版）

曾谨言 著

4. Occupation Number Representation?

5. Wave-Function Based Quantum Many-Body Methods?

6. The Path-Integral Method and its Advantage in Describing Many-Body systems

# 3.4 Occupation Number Representation

## 3.4.1 Group and the Rearrangement Theorem

### ➢ Definition of Group

**Definition 1.1 Group:**

Let $G$ be a collection of elements (operations), denoted as $G = \{\cdots, g, \cdots\}$, with a multiplication operation defined on $G$. If the elements of $G$ satisfy the following four conditions under this operation:

1. **Closure**: The product of any two elements (operations) remains within the set of such elements (operations).
2. **Associativity**: For any three elements (operations) $f$, $g$, and $h$, the relation $(fg)h = f(gh)$ holds.
3. **Existence of a Unique Identity Element**: There exists a unique identity element $e$ such that for every $f \in G$, $ef = fe = f$.
4. **Existence of a Unique Inverse**: For every $f \in G$, there exists a unique inverse $f^{-1} \in G$ such that $f^{-1}f = ff^{-1} = e$.

In this case, we call $G$ a **group**, where its elements are referred to as **group elements**, $e$ is the **identity element**, and $f^{-1}$ is the **inverse** of $f$.

**The set of permutations,**

$$P_{ij} = \begin{pmatrix} 1 & \cdots & i & \cdots & j & \cdots & N \\ 1 & \cdots & j & \cdots & i & \cdots & N \end{pmatrix}$$

**clearly, form a group.**

**The Group Theory will be detailed in Chapter 4.**

# 3.4 Occupation Number Representation

## 3.4.1 Group and the Rearrangement Theorem

### ➢ Rearrangement Theorem（重排定理）

**Theorem 1.1 Rearrangement Theorem:**

Let $G = \{\ldots, g_\alpha, \ldots\}$ be a group. For every $u \in G$, as $g_\alpha$ runs over all elements of $G$, the product $ug_\alpha$ yields each element of $G$ exactly once.

**Proof:**

The proof consists of two parts:

1. Every element of $G$ can be expressed as $ug_\alpha$ for some $g_\alpha \in G$.
2. Each element is produced exactly once.

**Part 1: Existence**

For any $g_\beta \in G$, we can choose $u^{-1}g_\beta \in G$, such that:

$$u(u^{-1}g_\beta) = (uu^{-1})g_\beta = eg_\beta = g_\beta.$$

Thus, every element $g_\beta$ is obtained as $ug_\alpha$ with $g_\alpha = u^{-1}g_\beta$.

**Part 2: Uniqueness**

Assume, for contradiction, that there exist distinct elements $g_\alpha \neq g'_\alpha$ in $G$ such that $ug_\alpha = ug'_\alpha$. Multiplying both sides on the left by $u^{-1}$ yields:

$$u^{-1}(ug_\alpha) = u^{-1}(ug'_\alpha) \implies (u^{-1}u)g_\alpha = (u^{-1}u)g'_\alpha \implies eg_\alpha = eg'_\alpha \implies g_\alpha = g'_\alpha,$$

which contradicts the assumption that $g_\alpha \neq g'_\alpha$. Hence, each element of $G$ is produced exactly once.

# 3.4 Occupation Number Representation

## 3.4.2 Permutation group and permutation symmetry

- The set of permutations form a group

$$\hat{H} = \hat{H}(\boldsymbol{r}_1, \boldsymbol{r}_2, \cdots, \boldsymbol{r}_i, \cdots, \boldsymbol{r}_j, \cdots, \boldsymbol{r}_N)$$

$$P_{ij} = \begin{pmatrix} 1 & \cdots & i & \cdots & j & \cdots & N \\ 1 & \cdots & j & \cdots & i & \cdots & N \end{pmatrix}$$

$$\hat{H}(\cdots, \boldsymbol{r}_i, \cdots, \boldsymbol{r}_j, \cdots) = \hat{H}(\cdots, \boldsymbol{r}_j, \cdots, \boldsymbol{r}_i, \cdots)$$

- And the physical consequences of this symmetry are:

$$|\psi(\boldsymbol{r}_1, \boldsymbol{r}_2, \cdots, \boldsymbol{r}_i, \cdots, \boldsymbol{r}_j, \cdots, \boldsymbol{r}_N)|^2 = |\psi(\boldsymbol{r}_1, \boldsymbol{r}_2, \cdots, \boldsymbol{r}_j, \cdots, \boldsymbol{r}_i, \cdots, \boldsymbol{r}_N)|^2$$

$$P_{ij}|\psi\rangle = \lambda|\psi\rangle$$

$\lambda = +1$ $\quad |\psi\rangle = |\psi_{\mathrm{S}}\rangle$ → Bosonic

$\lambda = -1$ $\quad |\psi\rangle = |\psi_{\mathrm{A}}\rangle$ → Fermionic

$$\psi(\boldsymbol{r}_1, \boldsymbol{r}_2) = \exp(\mathrm{i}\theta)\psi(\boldsymbol{r}_2, \boldsymbol{r}_1)$$

→ Anyonic

# 3.4 Occupation Number Representation

## 3.4.2 Permutation group and permutation symmetry

| Property | Bosons | Fermions |
|---|---|---|
| **Spin** | Integer | Half-integer |
| **Exchange symmetry** | $\Psi(1,2) = +\Psi(2,1)$ | $\Psi(1,2) = -\Psi(2,1)$ |
| **Occupation of one state** | $n_i = 0, 1, 2, \ldots$ | $n_i = 0, 1$ — Pauli exclusion |
| **Operator algebra** | $[a_i, a_j^\dagger] = \delta_{ij}$ | $\{c_i, c_j^\dagger\} = \delta_{ij}$ |
| **Quantum statistics** | Bose–Einstein | Fermi–Dirac |

We will detail them very soon.


A Brief History of Condensed Matter Physics

Guang-Shan Tian

April 17, 2024

翻译：凝聚态物理学简史——田光善

乐乐波色子

类比是一切创造力的源泉

32 人赞同了该文章 ›

# 3.4 Occupation Number Representation

## 3.4.2 Permutation group and permutation symmetry

- To truly understand these differences, one need to know how the many-body wave function looks like. The starting point (QM) is the Hamiltonian:

$$\hat{H}(\boldsymbol{r}_1, \boldsymbol{r}_2, \cdots, \boldsymbol{r}_N) = \sum_{j=1}^{N} \hat{H}_j(\boldsymbol{r}_j) + \frac{1}{2} \sum_{i \neq j} \widehat{W}_{ij}(\boldsymbol{r}_i, \boldsymbol{r}_j)$$

One can use either this part, or this part plus the mean field of the other part, to general a Hilbert space for single-particle quantum states. This gives me the following basis for particle $j$:

$$|u_1(j)\rangle, |u_2(j)\rangle, \cdots, |u_d(j)\rangle$$

- Basis set of the many-body wave function, tensor product Hilbert space:

$$|u_{j_1}, \cdots, u_{j_N}\rangle = |u_{j_1}(1)\rangle \otimes |u_{j_2}(2)\rangle \otimes \cdots \otimes |u_{j_N}(N)\rangle$$

$$P_{ij}|\cdots, u_i(i), \cdots, u_j(j)\rangle = |\cdots, u_i(j), \cdots, u_j(i), \cdots\rangle \neq \lambda |\cdots, u_i(i), \cdots, u_j(j)\rangle$$

- Therefore, as mentioned earlier, we need some linear combination of these product states（乘积态） to express the proper many-body states.

# 3.4 Occupation Number Representation

## 3.4.2 Permutation group and permutation symmetry

- We define this linear combination as:

$$\sum_{\hat{P}\in S_N} \lambda^{\hat{P}} \hat{P} \left| u_{j_1}, u_{j_2}, \cdots u_{j_N} \right\rangle$$

A simple produce state

$$|u_{j_1}, \cdots, u_{j_N}\rangle = |u_{j_1}(1)\rangle \otimes |u_{j_2}(2)\rangle \otimes \cdots \otimes |u_{j_N}(N)\rangle$$

$$\mathrm{s} = \begin{pmatrix} a_1, & a_2, & \cdots, & a_\mathrm{n} \\ b_1, & b_2, & \cdots, & b_\mathrm{n} \end{pmatrix} \Rightarrow \mathrm{s}^{-1} = \begin{pmatrix} b_1, & b_2, & \cdots, & b_\mathrm{n} \\ a_1, & a_2, & \cdots, & a_\mathrm{n} \end{pmatrix}$$

The order of $S_n$ is n!

$$\begin{pmatrix} e_1, & e_2, & \cdots, & e_\mathrm{m} \\ e_2, & e_3, & \cdots, & e_1 \end{pmatrix} \Rightarrow (e_1, \ e_2, \ \cdots, \ e_\mathrm{m})$$

$$\begin{pmatrix} 1, & 2, & 3, & 4, & 5, & 6 \\ 4, & 2, & 6, & 5, & 1, & 3 \end{pmatrix} = (1, \ 4, \ 5)(2)(3, \ 6)$$

$$(e_1, \ e_2, \ \cdots, \ e_\mathrm{m}) = \begin{pmatrix} e_1, & e_2, & e_3, & \cdots, & e_\mathrm{m} \\ e_2, & e_3, & e_4, & \cdots, & e_1 \end{pmatrix} = \begin{pmatrix} e_1, & e_2, & e_3, & \cdots, & e_\mathrm{m} \\ e_2, & e_1, & e_3, & \cdots, & e_\mathrm{m} \\ e_2, & e_1, & e_3, & \cdots, & e_\mathrm{m} \\ e_2, & e_3, & e_4, & \cdots, & e_1 \end{pmatrix} \Rightarrow \lambda^{\hat{P}}$$

$$= (e_1, \ e_3, \ \cdots, \ e_\mathrm{m})(e_1, \ e_2) = (e_1, \ e_4, \ \cdots, \ e_\mathrm{m})(e_1, \ e_3)(e_1, \ e_2)$$
$$= \cdots = (e_1, \ e_\mathrm{m})(e_1, \ e_{\mathrm{m}-1}) \cdots (e_1, \ e_3)(e_1, \ e_2)$$

# 3.4 Occupation Number Representation

## 3.4.2 Permutation group and permutation symmetry

- Then, making use of the rearrangement theorem, we can show that this wave function is symmetric.

$$\hat{P}_1 \sum_{\hat{P}\in S_N} \lambda^{\hat{P}} \hat{P} \left| u_{j_1}, u_{j_2}, \cdots u_{j_N} \right\rangle = \lambda^{\hat{P}_1^{-1}} \sum_{\hat{P}\in S_N} \lambda^{\hat{P}_1 \hat{P}} \hat{P}_1 \hat{P} \left| u_{j_1}, u_{j_2}, \cdots u_{j_N} \right\rangle = \lambda^{\hat{P}_1^{-1}} \sum_{\hat{P}\in S_N} \lambda^{\hat{P}} \hat{P} \left| u_{j_1}, u_{j_2}, \cdots u_{j_N} \right\rangle$$

Conclusion:

Rearrangement Theorem (重排定理)(to be explained in the next slide)

$$\sum_{\hat{P}\in S_N} \lambda^{\hat{P}} \hat{P} \left| u_{j_1}, u_{j_2}, \cdots u_{j_N} \right\rangle$$

Define the wave function of the Bosonic and Fermionic systems in a clean manner

Note: For identical anyons, the symmetry group is not permutation group (two consecutive pair exchange does not result in the original state).

# 3.4 Occupation Number Representation

## 3.4.3 Permanent, Determinant, and the Occupation Number Representation

- With these, we can introduce the concepts of determinant, permanent, and the occupation number representation for the bosonic and fermionic systems.

- The crucial restrictions are summarized in this table.

| Property | Bosons | Fermions |
|---|---|---|
| Spin | Integer | Half-integer |
| Exchange symmetry | $\Psi(1,2) = +\Psi(2,1)$ | $\Psi(1,2) = -\Psi(2,1)$ |
| Occupation of one state | $n_i = 0, 1, 2, \ldots$ | $n_i = 0, 1$ — Pauli exclusion |
| Operator algebra | $[a_i, a_j^\dagger] = \delta_{ij}$ | $\{c_i, c_j^\dagger\} = \delta_{ij}$ |
| Quantum statistics | Bose–Einstein | Fermi–Dirac |

- The starting point, is the symmetrized wave function of the bosonic and fermionic systems:

$$\hat{P}_1 \sum_{\hat{P}\in S_N} \lambda^{\hat{P}} \hat{P} \left| u_{j_1}, u_{j_2}, \cdots u_{j_N} \right\rangle = \lambda^{\hat{P}_1^{-1}} \sum_{\hat{P}\in S_N} \lambda^{\hat{P}_1\hat{P}} \hat{P}_1\hat{P} \left| u_{j_1}, u_{j_2}, \cdots u_{j_N} \right\rangle = \lambda^{\hat{P}_1^{-1}} \sum_{\hat{P}\in S_N} \lambda^{\hat{P}} \hat{P} \left| u_{j_1}, u_{j_2}, \cdots u_{j_N} \right\rangle$$

# 3.4 Occupation Number Representation

## 3.4.3 Permanent, Determinant, and the Occupation Number Representation

- We first look at the bosonic system:

We need to understand!

$$|\psi\rangle = \sqrt{\frac{1}{N!(n_1!n_2!\cdots n_d!)}} \times \sum_{P\in S_N} P|\underbrace{u_1(1), u_1(2), \cdots, u_1(n_1)}_{n_1};\times \underbrace{u_2(n_1+1), \cdots, u_2(n_1+n_2)}_{n_2};\cdots\rangle$$

$N$ positions, which gives me $N!$ terms of product states




Among them only $\frac{N!}{n_1!n_2!\cdots n_d!}$ terms are different from each other, they are the real occupation number configuration of the many-body state

The number of $n_1!\,n_2!\cdots n_d!$ stands for double counting of these

$n_1$ positions $n_2$ positions

$u_1 \cdots u_1$ $u_2 \cdots u_2 \cdots$ $u_d \cdots u_d$

$|n_1, n_2, \cdots, n_k\rangle$

The reason is that these orbitals give the same product state of $u_1 \cdots u_1 \; u_2 \cdots u_2 \cdots u_d \cdots u_d$

$n_1!$ vectors $n_2!$ vectors

On the other hand, when they do the inner product, they also give a result of $(n_1! n_2! \cdots n_d!)^2$.

Pictorially:




Therefore, we have:

$$\frac{1}{N!\,(n_1! n_2! \cdots n_d!)} \quad \frac{N!}{n_1! n_2! \cdots n_d!} (n_1! n_2! \cdots n_d!)^2$$

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As a result, to normalize the many-body wave function, we need this term.

$$|\psi\rangle = \sqrt{\frac{1}{N!(n_1! n_2! \cdots n_d!)}} \times \sum_{P \in \mathcal{S}_N} P | \underbrace{u_1(1), u_1(2), \cdots, u_1(n_1);}_{n_1} \times \underbrace{u_2(n_1+1), \cdots, u_2(n_1+n_2);}_{n_2} \cdots \rangle$$

Run over all the permutations!

$$|\psi\rangle = \sqrt{\frac{1}{N!(n_1!n_2!\cdots n_d!)}} \times \sum_{P\in S_N} P|\underbrace{u_1(1),u_1(2),\cdots,u_1(n_1);}_{n_1\uparrow} \times \underbrace{u_2(n_1+1),\cdots,u_2(n_1+n_2);}_{n_2\uparrow}\cdots\rangle$$

One example:

$$|\psi\rangle = \sqrt{\frac{1}{3!(2!\times 1!)}} \sum_{p\in S_3} p[u_1(1)u_1(2)u_2(3)]$$

$$I = \begin{pmatrix}1&2&3\\1&2&3\end{pmatrix}, \quad p_{12} = \begin{pmatrix}1&2&3\\2&1&3\end{pmatrix}, \quad p_{23} = \begin{pmatrix}1&2&3\\1&3&2\end{pmatrix}$$

$$p_{31} = \begin{pmatrix}1&2&3\\3&2&1\end{pmatrix}, \quad p_{123} = \begin{pmatrix}1&2&3\\2&3&1\end{pmatrix}, \quad p_{132} = \begin{pmatrix}1&2&3\\3&1&2\end{pmatrix}$$

$$\begin{aligned}
&= \frac{1}{2}\sqrt{\frac{1}{3}}[u_1(1)u_1(2)u_2(3) + u_1(1)u_1(3)u_2(2) + u_1(2)u_1(1)u_2(3) \\
&\quad + u_1(2)u_1(3)u_2(1) + u_1(3)u_1(1)u_2(2) + u_1(3)u_1(2)u_2(1)] \\
&= \frac{1}{\sqrt{3}}[u_1(1)u_1(2)u_2(3) + u_1(1)u_1(3)u_2(2) + u_1(2)u_1(3)u_2(1)],
\end{aligned}$$

**Test in details**

# 3.4 Occupation Number Representation

## 3.4.3 Permanent, Determinant, and the Occupation Number Representation

$$|\psi\rangle = \sqrt{\frac{1}{3!(2!\times 1!)}}\sum_{p\in S_3} p[u_1(1)u_1(2)u_2(3)]$$

$$= \frac{1}{2}\sqrt{\frac{1}{3}}[u_1(1)u_1(2)u_2(3)+u_1(1)u_1(3)u_2(2)+u_1(2)u_1(1)u_2(3)$$
$$+u_1(2)u_1(3)u_2(1)+u_1(3)u_1(1)u_2(2)+u_1(3)u_1(2)u_2(1)]$$
$$= \frac{1}{\sqrt{3}}[u_1(1)u_1(2)u_2(3)+u_1(1)u_1(3)u_2(2)+u_1(2)u_1(3)u_2(1)],$$

From this expression, we know that we can use the occupation number representation to denote the many-body wave function of the bosonic system in a simple and clean manner.

$$|\psi\rangle = |n_1, n_2, \cdots\rangle$$

$$|\psi\rangle = |n_1 = 2, n_2 = 1\rangle$$

$$|\psi\rangle = \sqrt{\frac{1}{N!(n_1!n_2!\cdots n_d!)}}\times\sum_{P\in S_N} P\underbrace{u_1(1),u_1(2),\cdots,u_1(n_1);}_{n_1\text{个}}\times\underbrace{u_2(n_1+1),\cdots,u_2(n_1+n_2);}_{n_2\text{个}}\cdots\rangle$$

由这组占据数产生的互不相同的粒子置换项

The mutually distinct particle permutation terms generated by this set of occupation numbers

$$\psi_{n_1\cdots n_N}(q_1,\cdots,q_N) = \sqrt{\frac{\prod n_i!}{N!}}\sum_P P[\varphi_{k_1}(q_1)\cdots\varphi_{k_N}(q_N)]$$

And the wave function can also be written as:

# 3.4 Occupation Number Representation

## 3.4.3 Permanent, Determinant, and the Occupation Number Representation

- For the three-particle fermionic system, we have:

$$|\psi_{\mathrm{A}}\rangle = |n_1, n_2, \cdots, n_\alpha, \cdots\rangle = \frac{1}{\sqrt{N!}} \sum_{P \in S_n} (-1)^{\delta_P} P(u_1(1)u_2(2)\cdots u_N(N))$$

$$= \frac{1}{\sqrt{N!}} \begin{vmatrix} u_1(1) & u_1(2) & \cdots & u_1(N) \\ u_2(1) & u_2(2) & \cdots & u_2(N) \\ \cdots & \cdots & \cdots & \cdots \\ u_N(1) & u_N(2) & \cdots & u_N(N) \end{vmatrix}$$

$$I = \begin{pmatrix} 1 & 2 & 3 \\ 1 & 2 & 3 \end{pmatrix}, \quad p_{12} = \begin{pmatrix} 1 & 2 & 3 \\ 2 & 1 & 3 \end{pmatrix}, \quad p_{23} = \begin{pmatrix} 1 & 2 & 3 \\ 1 & 3 & 2 \end{pmatrix} \quad p_{31} = \begin{pmatrix} 1 & 2 & 3 \\ 3 & 2 & 1 \end{pmatrix}, \quad p_{123} = \begin{pmatrix} 1 & 2 & 3 \\ 2 & 3 & 1 \end{pmatrix}, \quad p_{132} = \begin{pmatrix} 1 & 2 & 3 \\ 3 & 1 & 2 \end{pmatrix}$$

- This gives:

$$\Psi(1,2,3) = \frac{1}{\sqrt{6}}\big[u_1(1)u_2(2)u_3(3) + u_1(2)u_2(3)u_3(1) + u_1(3)u_2(1)u_3(2) - u_1(1)u_2(3)u_3(2) - u_1(2)u_2(1)u_3(3) - u_1(3)u_2(2)u_3(1)\big]$$

- The corresponding occupation number representation becomes:

$$|\Psi\rangle = |n_1 = 1, n_2 = 1, n_3 = 1\rangle$$

- With these, we conclude that occupation numbers give a good representation of the many-body state, with permutation symmetry taken into account!

# 3.4 Occupation Number Representation

## 3.4.4 Fock space, Creation and Annihilation Operators

- With occupation number representation defined, and the form of its wave function clarified, now we come to the "field-theory aspect" of this topic.
- The symmetrized many-body states are: $|n_1, n_2, \cdots, n_k\rangle$ , where: $N = \sum_i n_i$
- Based on them, we can define a Fock-space, which forms a basis for any many-body state.

For $N$ indistinguishable bosons in $M$ single-particle orbitals, a many-body basis state is uniquely specified by its occupation numbers, which satisfy $\sum_{i=1}^{M} n_i = N$ with $n_i \geq 0$. Counting these nonnegative integer solutions using the stars-and-bars method gives the dimension of the fixed-$N$ bosonic Hilbert space:

$$\dim \mathcal{H}_N^{\mathrm{B}} = \binom{N+M-1}{N}, \qquad \dim \mathcal{H}_N^{\mathrm{F}} = \binom{M}{N} \quad (N \leq M).$$

**$M$ choose $N$**

**$N+M-1$ choose $N$**

$$\mathcal{F}_{\mathrm{B}/F} = \bigoplus_{N=0}^{\infty} \mathcal{H}_N^{\mathrm{B}/F}$$

For example, when $N = 3$ and $M = 4$, In total, we arrange $N$ stars and $M-1$ bars.

$$**||*| \quad \longleftrightarrow \quad (n_1, n_2, n_3, n_4) = (2, 0, 1, 0).$$

# 3.4 Occupation Number Representation

## 3.4.4 Fock space, Creation and Annihilation Operators

**Classroom example: Four spin orbitals and two particles**

The number of fermionic basis states is $\binom{4}{2} = 6$, while the number of bosonic basis states is $\binom{5}{2} = 10$. For 10 fermions in 20 spin orbitals, there are already $\binom{20}{10} = 184{,}756$ basis states, even without interactions. Interactions make the problem harder still by coupling these basis states, so a list of single-particle energies is no longer sufficient to describe the system.

**From this, you can see how hard it is to perform man-body calculations (dimensionality is too high).**

For example, consider $N$ electrons in $M = 2N$ spin orbitals. The number of Slater determinants is

$$D = \binom{2N}{N} \sim \frac{4^N}{\sqrt{\pi N}}$$

The full configuration interaction (FCI) wave function is generally expanded in these determinants:

$$|\Psi\rangle = \sum_{I=1}^{D} C_I |I\rangle.$$

Thus, storing the coefficients $C_I$ alone requires space that grows exponentially with $N$, and solving the matrix eigenvalue problem involves a space of the same exponentially growing dimension. Although a two-body Hamiltonian is sparse and a full $D \times D$ matrix need not be stored, sparsity does not eliminate the exponential growth in the number of basis states $D$.

# 3.4 Occupation Number Representation

## 3.4.4 Fock space, Creation and Annihilation Operators

- With Fock space explained, we can define the creation and annihilation operators.
- These concepts were already explained in earlier discussions of the harmonic potential.

$$a_i^\dagger|\ldots,n_i,\ldots\rangle=\sqrt{n_i+1}\,|\ldots,n_i+1,\ldots\rangle,\qquad a_i|\ldots,n_i,\ldots\rangle=\sqrt{n_i}\,|\ldots,n_i-1,\ldots\rangle.$$

- Here, we note that the square-root coefficients arise from the normalization of symmetric many-body states. There is no need to assume that the particles are in a harmonic potential.
- In so doing, we arrive at a method to theoretically describe the many-body quantum state of the bosonic systems, with symmetry taken into account.

$$[a_i, a_j^+] = \delta_{ij}$$
$$[a_i, a_j] = [a_i^+, a_j^+] = 0$$

$$a_i a_i^+|n_1,n_2,\cdots,n_k\rangle$$
$$= a_i\sqrt{n_i+1}|n_1,n_2,\cdots,n_i+1,\cdots,n_k\rangle$$
$$= (n_i+1)|n_1,n_2,\cdots,n_i,\cdots,n_k\rangle$$

$$a_i^+ a_i|n_1,n_2,\cdots,n_k\rangle$$
$$= a_i^+\sqrt{n_i}|n_1,n_2,\cdots,n_i+1,\cdots,n_k\rangle$$
$$= n_i|n_1,n_2,\cdots,n_i,\cdots,n_k\rangle$$

Already explained in the harmonic potential part, the same algebra applies here.

# 3.4 Occupation Number Representation

## 3.4.4 Fock space, Creation and Annihilation Operators

$$|n_1 n_2 \cdots\rangle = \frac{1}{\sqrt{\prod_i n_i!}} (a_1^+)^{n_1} (a_2^+)^{n_2} \cdots |0\rangle$$

$$a_\alpha^+ |n_1 n_2 \cdots n_\alpha \cdots\rangle = \sqrt{n_\alpha + 1}\, |n_1 n_2 \cdots (n_\alpha + 1) \cdots\rangle$$

$$a_\alpha |n_1 n_2 \cdots n_\alpha \cdots\rangle = \sqrt{n_\alpha}\, |n_1 n_2 \cdots (n_\alpha - 1) \cdots\rangle$$

- Therefore, one can derive all properties of the bosonic system using:
- For the fermionic system, our starting point is also the permutation symmetry of the wave function of the occupation number basis. Here, the properties of the slater determinant can be used.

$$|\psi_A\rangle = \frac{1}{\sqrt{N!}} \begin{vmatrix} u_1(1) & u_1(2) & \cdots & u_1(N) \\ u_2(1) & u_2(2) & \cdots & u_2(N) \\ \cdots & \cdots & \cdots & \cdots \\ u_N(1) & u_N(2) & \cdots & u_N(N) \end{vmatrix}$$

$$|\alpha, \beta, \gamma, \cdots\rangle = -|\beta, \alpha, \gamma, \cdots\rangle$$

- Since the occupation number is either 0 or 1, the occupation representation can also be used.

And we have: $|\alpha, \beta, \gamma, \cdots\rangle = \hat{a}_\alpha^+ \hat{a}_\beta^+ \hat{a}_\gamma^+ \cdots |0\rangle$ $|\beta, \alpha, \gamma, \cdots\rangle = \hat{a}_\beta^+ \hat{a}_\alpha^+ \hat{a}_\gamma^+ \cdots |0\rangle$

- Since $|\alpha, \beta, \gamma, \cdots\rangle = -|\beta, \alpha, \gamma, \cdots\rangle$, we have: $\hat{a}_\alpha^+ \hat{a}_\beta^+ \hat{a}_\gamma^+ \cdots |0\rangle = -\hat{a}_\beta^+ \hat{a}_\alpha^+ \hat{a}_\gamma^+ \cdots |0\rangle$

When the two indices are equal, same logic holds.

$$\left[\hat{a}_\alpha^+ \hat{a}_\beta^+ + \hat{a}_\beta^+ \hat{a}_\alpha^+\right] |\gamma\rangle = 0$$

$$\hat{a}_\alpha^+ \hat{a}_\alpha^+ = -\hat{a}_\alpha^+ \hat{a}_\alpha^+$$

# 3.4 Occupation Number Representation

## 3.4.4 Fock space, Creation and Annihilation Operators

- Also, we can look at the adjunct state of them:

$$|\alpha,\beta,\gamma,\cdots\rangle = \hat{a}_\alpha^+\hat{a}_\beta^+\hat{a}_\gamma^+\cdots|0\rangle \qquad |\beta,\alpha,\gamma,\cdots\rangle = \hat{a}_\beta^+\hat{a}_\alpha^+\hat{a}_\gamma^+\cdots|0\rangle$$

$$\langle\cdots,\gamma,\beta,\alpha| = \langle 0|\hat{a}_\gamma\hat{a}_\beta\hat{a}_\alpha \qquad \hat{a}_\beta\hat{a}_\alpha + \hat{a}_\alpha\hat{a}_\beta = 0$$

- Then, if we define: $[\hat{a}_\beta,\hat{a}_\alpha]_+ = \hat{a}_\beta\hat{a}_\alpha + \hat{a}_\alpha\hat{a}_\beta$, the above analysis gives $[\hat{a}_\beta,\hat{a}_\alpha]_+ = [\hat{a}_\beta^+,\hat{a}_\alpha^+]_+ = \mathbf{0}$

- Also, since $a_\alpha|0\rangle = 0$ and more generally

$$a_\alpha|\beta\gamma\cdots\rangle = 0 \quad (\alpha\neq\beta\neq\gamma\neq\cdots)$$
$$a_\alpha|\alpha\beta\gamma\cdots\rangle = |\beta\gamma\cdots\rangle$$

We further have:

$$a_\beta a_\alpha^+ a_\beta^+ a_\gamma^+\cdots|0\rangle = -a_\beta a_\beta^+ a_\alpha^+ a_\gamma^+\cdots|0\rangle = -a_\alpha^+ a_\gamma^+\cdots|0\rangle$$
$$= -a_\alpha^+ a_\beta a_\beta^+ a_\gamma^+\cdots|0\rangle$$

$$(a_\beta a_\alpha^+ + a_\alpha^+ a_\beta)|\beta\gamma\cdots\rangle = 0$$

# 3.4 Occupation Number Representation

## 3.4.4 Fock space, Creation and Annihilation Operators

- Meanwhile, for those states when $\beta$ is empty, we have: $(a_\beta a_\alpha^+ + a_\alpha^+ a_\beta)\,|\,\gamma\delta\cdots\rangle = 0$

- Thus, for all kinds of states ($\beta$ is empty or not), when it was operated by $(a_\beta a_\alpha^+ + a_\alpha^+ a_\beta)$, one always zero. Therefore, we have $\left[\hat{a}_\beta, \hat{a}_\alpha^+\right]_+ = \mathbf{0}$, if $\beta \neq \alpha$.

- If $\beta = \alpha$, we have: $a_\alpha a_\alpha^+ \,|\,\alpha\beta\gamma\cdots\rangle = a_\alpha a_\alpha^+ a_\alpha^+ a_\beta^+ a_\gamma^+ \cdots |\,0\rangle = 0$

Also, we have:

$$a_\alpha^+ a_\alpha \,|\,\alpha\beta\gamma\cdots\rangle = a_\alpha^+ a_\alpha a_\alpha^+ a_\beta^+ a_\gamma^+ \cdots |\,0\rangle = a_\alpha^+ a_\beta^+ a_\gamma^+ \cdots |\,0\rangle = |\,\alpha\beta\gamma\cdots\rangle$$

- Therefore, $(a_\alpha a_\alpha^+ + a_\alpha^+ a_\alpha)\,|\,\alpha\beta\gamma\cdots\rangle = |\,\alpha\beta\gamma\cdots\rangle$

If $\alpha$ is empty, (next slide)

# 3.4 Occupation Number Representation

## 3.4.4 Fock space, Creation and Annihilation Operators

- If $\alpha$ is empty,

$$a_\alpha a_\alpha^+ \left|\beta\gamma\cdots\right\rangle = \left|\beta\gamma\cdots\right\rangle$$

$$a_\alpha^+ a_\alpha \left|\beta\gamma\cdots\right\rangle = 0$$

$$\Rightarrow \quad (a_\alpha a_\alpha^+ + a_\alpha^+ a_\alpha)\left|\beta\gamma\cdots\right\rangle = \left|\beta\gamma\cdots\right\rangle$$

- Therefore,

$$(a_\alpha a_\alpha^+ + a_\alpha^+ a_\alpha)\left|\alpha\beta\gamma\cdots\right\rangle = \left|\alpha\beta\gamma\cdots\right\rangle$$

$$(a_\alpha a_\alpha^+ + a_\alpha^+ a_\alpha)\left|\beta\gamma\cdots\right\rangle = \left|\beta\gamma\cdots\right\rangle$$

$$\Rightarrow \quad \left[a_\alpha, a_\alpha^+\right]_+ = 1$$

- This means that if we sum all these together, we get the rules for second quantization of the fermionic system:

$$\left[a_\alpha, a_\beta^+\right]_+ = \delta_{\alpha\beta}$$

$$\left[a_\alpha, a_\beta\right]_+ = \left[a_\alpha^+, a_\beta^+\right]_+ = 0$$

fermionic

$$\left[a_i, a_j^+\right] = \delta_{ij}$$

$$\left[a_i, a_j\right] = \left[a_i^+, a_j^+\right] = 0$$

bosonic

# 3.4 Occupation Number Representation

## 3.4.4 Fock space, Creation and Annihilation Operators

- One consequence of this permutation rule is that when the occupation number is changed, the changes of the bosonic and fermionic systems are different:

$$[a_\alpha, a_\beta^+]_+ = \delta_{\alpha\beta}$$
$$[a_\alpha, a_\beta]_+ = [a_\alpha^+, a_\beta^+]_+ = 0$$

fermionic

$$a_\alpha^+ \left| n_1 \cdots n_\alpha \cdots \right\rangle = (-1)^{\sum_{\nu=1}^{\alpha-1} n_\nu} \sqrt{1-n_\alpha} \left| n_1 \cdots (n_\alpha + 1) \cdots \right\rangle$$
$$= \begin{cases} 0, & n_\alpha = 1 \\ (-1)^{\sum_{\nu=1}^{\alpha-1} n_\nu} \left| n_1 \cdots 1_\alpha \cdots \right\rangle, & n_\alpha = 0 \end{cases}$$

$$[a_i, a_j^+] = \delta_{ij}$$
$$[a_i, a_j] = [a_i^+, a_j^+] = 0$$

bosonic

$$a_\alpha^+ \left| n_1 n_2 \cdots n_\alpha \cdots \right\rangle = \sqrt{n_\alpha + 1} \left| n_1 n_2 \cdots (n_\alpha + 1) \cdots \right\rangle$$
$$a_\alpha \left| n_1 n_2 \cdots n_\alpha \cdots \right\rangle = \sqrt{n_\alpha} \left| n_1 n_2 \cdots (n_\alpha - 1) \cdots \right\rangle$$

$$a_\alpha^+ \left| \cdots n_\alpha \cdots \right\rangle = (-1)^{\sum_{\nu=1}^{\alpha-1} n_\nu} \left| \cdots 1_\alpha \cdots \right\rangle \delta_{n_\alpha 0}$$

$$a_\alpha \left| \cdots n_\alpha \cdots \right\rangle = (-1)^{\sum_{\nu=1}^{\alpha-1} n_\nu} \left| \cdots 0_\alpha \cdots \right\rangle \delta_{n_\alpha 1}$$

The basis of many-body perturbation theory (MBPT)!!!

# 3.4 Occupation Number Representation

## 3.4.5 Dynamical Operators

- With these rules clarified, we now look at the dynamical operators. The starting point, is the many-body wave function:

$$\psi_{n_1\cdots n_N}(q_1,\cdots,q_N)=\sqrt{\frac{\prod n_i!}{N!}}\sum_P P[\varphi_{k_1}(q_1)\cdots\varphi_{k_N}(q_N)]$$

bosonic

$$=\frac{1}{\sqrt{N!}}\sum_P(-1)^{\delta_P}P[\varphi_\alpha(q_1)\varphi_\beta(q_2)\varphi_\gamma(q_3)\cdots]$$

fermionic

由这组占据数产生的互不相同的粒子置换项

- The mutually distinct particle permutation terms generated by this set of occupation numbers.

- We accept this notation of the quantum, and start from a one-body operator:

$$\hat{F}=\sum_{a=1}^{N}\hat{f}(a)$$

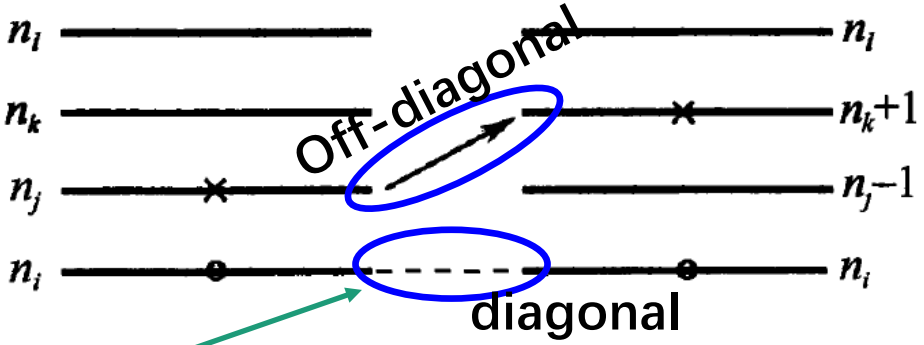
# 3.4 Occupation Number Representation

## 3.4.5 Dynamical Operators

There are N operators associated with each particle, whilst the particles are all the same!

- We first look at the bosonic system:

$$(\psi_{n_1' n_2' \cdots}, \hat{F}\psi_{n_1 n_2 \cdots}) = \sum_a (\psi_{n_1' n_2' \cdots}, \hat{f}(a)\psi_{n_1 n_2 \cdots}) = N(\psi_{n_1' n_2' \cdots}, \hat{f}(1)\psi_{n_1 n_2 \cdots})$$




- All the particles are identical, and it can involve the change of the occupation numbers changed by either 0 (diagonal) or 1 (off-diagonal).

They are the same!

- For the diagonal element, we have:

$$\bar{F} = (\psi_{n_1 n_2 \cdots}, \hat{F}\psi_{n_1 n_2 \cdots}) = N(\psi_{n_1 n_2 \cdots}, \hat{f}(1)\psi_{n_1 n_2 \cdots})$$

- We decipher this quantity by looking at the individual particles, and assume a state *k*.

$$f_{kk} = (\varphi_k(q_1), \hat{f}(1)\varphi_k(q_1)) = (\varphi_k, \hat{f}\varphi_k)$$

# 3.4 Occupation Number Representation

## 3.4.5 Dynamical Operators

- The trick, is to count how many terms will contribute to this dynamic variable by the diagonal part?

$$\bar{F} = (\psi_{n_1 n_2 \cdots}, \hat{F}\psi_{n_1 n_2 \cdots}) = N(\psi_{n_1 n_2 \cdots}, \hat{f}(1)\psi_{n_1 n_2 \cdots})$$

$$\psi_{n_1 \cdots n_N}(q_1, \cdots, q_N) = \sqrt{\frac{\prod_i n_i!}{N!}} \sum_P P[\varphi_{k_1}(q_1) \cdots \varphi_{k_N}(q_N)]$$

由这组占据数产生的互不相同的粒子置换项

$$|\psi\rangle = |n_1 = 2, n_2 = 1\rangle$$

$$\frac{1}{\sqrt{3}}\left[\varphi_1(1)\varphi_1(2)\varphi_2(3) + \varphi_1(1)\varphi_1(3)\varphi_2(2) + \varphi_1(2)\varphi_1(3)\varphi_2(1)\right]$$

$$\bar{F} = N \cdot \frac{\prod_i n_i!}{N!} \sum_k \frac{(N-1)!}{n_1! \cdots (n_k - 1)! \cdots} f_{kk} = \sum_k n_k f_{kk}$$

In this case, $k$ just goes over 1 and 2

$$f_{kk} = (\varphi_k(q_1), \hat{f}(1)\varphi_k(q_1)) = (\varphi_k, \hat{f}\varphi_k)$$

How many ways for the other N-1 particles to reside?

# 3.4 Occupation Number Representation

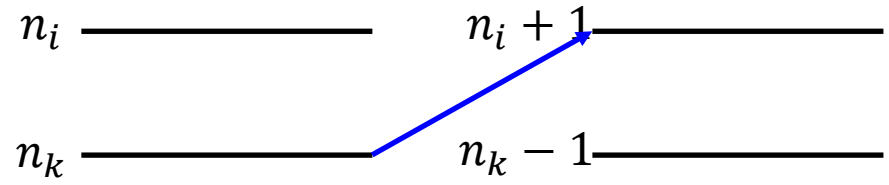
## 3.4.5 Dynamical Operators

- For the off-diagonal part of this one-body operator, we have:

$$(\psi_{\cdots(n_i+1)\cdots(n_k-1)\cdots}, \hat{F}\psi_{\cdots n_i\cdots n_k\cdots}) = N(\psi_{\cdots(n_i+1)\cdots(n_k-1)\cdots}, \hat{f}(1)\psi_{\cdots n_i\cdots n_k\cdots})$$

- We label this as $f_{ik}$, initial state is $k$, final state is $i$. The matrix element $f_{ik}$ is for particle $k$. There are in total $N$ particles.

$$\langle\cdots(n_k-1)\cdots(n_i+1)\cdots|\, a_\alpha^+ a_\beta \,|\cdots n_i\cdots n_k\cdots\rangle$$




- The initial state has occupation numbers: $(\ldots, n_i, \ldots, n_k, \ldots)$
- the final state has occupation numbers: $(\ldots, n_i + 1, \ldots, n_k - 1, \ldots)$
- In the initial-state term, coordinate 1 is associated with the state of $k$. Removing it from the initial occupation numbers leaves: $(\ldots, n_i, \ldots, n_k - 1, \ldots)$

# 3.4 Occupation Number Representation

## 3.4.5 Dynamical Operators

- In the final-state term, coordinate 1 is associated with the state of $i$. Removing it from the final occupation numbers leaves: $(\ldots,(n_i+1)-1,\ldots,n_k-1,\ldots)=(\ldots,n_i,\ldots,n_k-1,\ldots)$
- Therefore, the remaining $N-1$ coordinates have the same occupation numbers in the initial and final terms. This gives:

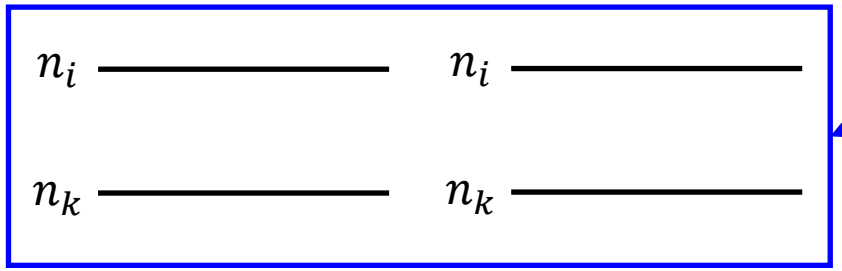
$$\bar{F}=N\sum_{i,k}\sqrt{\frac{n_1!\,n_2!\cdots(n_k-1)!\cdots(n_i+1)!\cdots n_d!}{N!}}\sqrt{\frac{n_1!\,n_2!\cdots n_k!\cdots n_i!\cdots n_d!}{N!}}$$
$$\frac{(N-1)!}{n_1!\,n_2!\cdots(n_k-1)!\cdots n_i!\cdots n_d!}f_{ik}$$
$$=\sqrt{n_k}\sqrt{n_i+1}f_{ik}$$

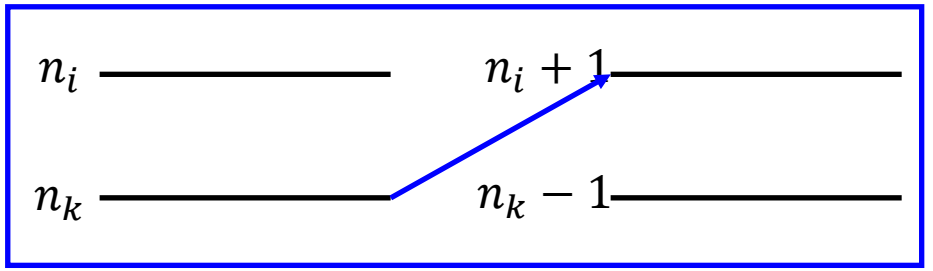
# 3.4 Occupation Number Representation

## 3.4.5 Dynamical Operators

- As a summary, for the one-body operator, we have this as the diagonal part:

$$\overline{F} = (\psi_{n_1 n_2 \cdots}, \hat{F}\psi_{n_1 n_2 \cdots}) = N(\psi_{n_1 n_2 \cdots}, \hat{f}(1)\psi_{n_1 n_2 \cdots})$$




, and this as the off-diagonal part:

$$(\psi_{\cdots(n_i+1)\cdots(n_k-1)\cdots}, \hat{F}\psi_{\cdots n_i \cdots n_k \cdots}) = N(\psi_{\cdots(n_i+1)\cdots(n_k-1)\cdots}, \hat{f}(1)\psi_{\cdots n_i \cdots n_k \cdots})$$

- They can be written as:

$$\hat{F}_{kk} = n_k f_{kk} \qquad \hat{F}_{ik} = \sqrt{n_i + 1}\sqrt{n_k} f_{ik}$$

$$\hat{F} = \sum_{\alpha\beta} f_{\alpha\beta} a_\alpha^+ a_\beta$$

# 3.4 Occupation Number Representation

## 3.4.5 Dynamical Operators

- These results can be double-checked by the rule of the creation and annihilation operators:

$$\begin{aligned}\bar{F} &= \langle \cdots n_k \cdots n_i \cdots | \hat{F} | \cdots n_i \cdots n_k \cdots \rangle \\ &= \sum_{\alpha\beta} f_{\alpha\beta} \langle \cdots n_k \cdots n_i \cdots | a_\alpha^+ a_\beta | \cdots n_i \cdots n_k \cdots \rangle \\ &= \sum_{\alpha} f_{\alpha\alpha} \langle \cdots n_k \cdots n_i \cdots | a_\alpha^+ a_\alpha | \cdots n_i \cdots n_k \cdots \rangle \\ &= \sum_{\alpha} f_{\alpha\alpha} \langle \cdots n_k \cdots n_i \cdots | n_\alpha | \cdots n_i \cdots n_k \cdots \rangle = \sum_{\alpha} f_{\alpha\alpha} n_\alpha\end{aligned}$$

$$\hat{F} = \sum_{\alpha\beta} f_{\alpha\beta} a_\alpha^+ a_\beta$$

Remind me: Need some explanation of this order

While in the earlier slide, we have:

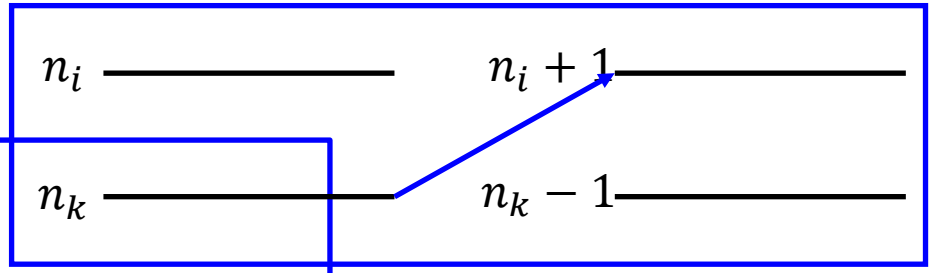
$$\bar{F} = N \cdot \frac{\prod_i n_i!}{N!} \sum_k \frac{(N-1)!}{n_1! \cdots (n_k - 1)! \cdots} f_{kk} = \sum_k n_k f_{kk}$$

→ The diagonal part of it agrees.

# 3.4 Occupation Number Representation

## 3.4.5 Dynamical Operators

- For the off-diagonal part, we also have:




$$\langle \cdots (n_k - 1) \cdots (n_i + 1) \cdots | \hat{F} | \cdots n_i \cdots n_k \cdots \rangle$$

$$= \sum_{\alpha\beta} f_{\alpha\beta} \langle \cdots (n_k - 1) \cdots (n_i + 1) \cdots | a_\alpha^+ a_\beta | \cdots n_i \cdots n_k \cdots \rangle$$

$$= \sum_{\alpha\beta} f_{\alpha\beta} \sqrt{n_i + 1}\, \delta_{\alpha i} \langle \cdots (n_k - 1) \cdots n_i \cdots | \cdots n_i \cdots (n_k - 1) \cdots \rangle \sqrt{n_k}\, \delta_{\beta k}$$

$$= \sqrt{(n_i + 1) n_k}\, f_{ik}$$

Earlier, we have:

$$\bar{F} = N \frac{\cdots n_i! \cdots (n_k - 1)! \cdots}{N!} \sqrt{(n_i + 1) n_k} \frac{(N-1)!}{\cdots n_i! \cdots (n_k - 1)! \cdots} f_{ik} = \sqrt{(n_i + 1) n_k}\, f_{ik}$$

Therefore, the off-diagonal part is also confirmed: ⇒ $\hat{F} = \sum_{\alpha\beta} f_{\alpha\beta} a_\alpha^+ a_\beta$

# 3.4 Occupation Number Representation

## 3.4.5 Dynamical Operators

- For two-body operator, $G=\sum_{a<b}^{N}\hat{g}(a,b)$ , we pick up a pair of particles:

$$\bar{G}=(\psi_{n_1 n_2\cdots},G\psi_{n_1 n_2\cdots})=\sum_{a<b}^{N}(\psi_{n_1 n_2\cdots},\hat{g}(a,b)\psi_{n_1 n_2\cdots})$$

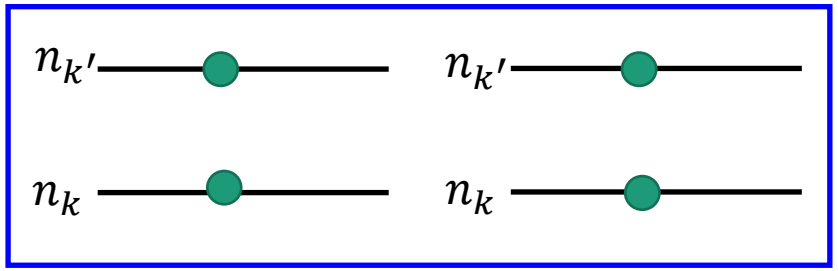
$$=\frac{N(N-1)}{2}(\psi_{n_1 n_2\cdots},\hat{g}(1,2)\psi_{n_1 n_2\cdots})$$

- We first look at the diagonal part of the two-body operator, meaning that the initial and final states are the same.

One on the state of $\varphi_k$

The other on $\varphi_{k'}$

约定 $k<k'$




For the rest N-2 particle, the number of arrangements is:

$$\frac{(N-2)!}{n_1!\cdots(n_k-1)!\cdots(n_{k'}-1)!\cdots}$$

# 3.4 Occupation Number Representation

## 3.4.5 Dynamical Operators

- This term contribute to G by:

$$\frac{N(N-1)}{2}\frac{\prod_i n_i!}{N!}\sum_{PP'}\left(P[\varphi_{k_1}(q_1)\cdots],\hat{g}(1,2)P'[\varphi_{k_1}(q_1)\cdots]\right)$$

$$=\frac{N(N-1)}{2}\frac{\prod_i n_i!}{N!}\sum_{k<k'}\frac{(N-2)!}{n_1!\cdots(n_k-1)!\cdots(n_{k'}-1)!\cdots}$$

$$\times\left(\begin{vmatrix}\varphi_k(q_1) & \varphi_{k'}(q_1)\\ \varphi_k(q_2) & \varphi_{k'}(q_2)\end{vmatrix}_+,\hat{g}(1,2)\begin{vmatrix}\varphi_k(q_1) & \varphi_{k'}(q_1)\\ \varphi_k(q_2) & \varphi_{k'}(q_2)\end{vmatrix}_+\right)$$

$$=\sum_{k<k'}n_k n_{k'}\{(\varphi_k(q_1)\varphi_{k'}(q_2),\hat{g}(1,2)\varphi_{k'}(q_2)\varphi_k(q_1))$$

$$+(\varphi_k(q_1)\varphi_{k'}(q_2);\hat{g}(1,2)\varphi_k(q_2)\varphi_{k'}(q_1))\}$$

$$=\sum_{k<k'}n_k n_{k'}\{\langle kk'|\hat{g}|k'k\rangle+\langle kk'|\hat{g}|kk'\rangle\}$$

$$\begin{vmatrix}\varphi_k(q_1) & \varphi_{k'}(q_1)\\ \varphi_k(q_2) & \varphi_{k'}(q_2)\end{vmatrix}_+\equiv\varphi_k(q_1)\varphi_{k'}(q_2)+\varphi_{k'}(q_1)\varphi_k(q_2)$$

$$\langle kk'|\hat{g}|k'k\rangle=\iint d\tau_1 d\tau_2\varphi_k^*(q_1)\varphi_{k'}^*(q_2)\hat{g}(1,2)\varphi_{k'}(q_2)\varphi_k(q_1)$$

$$\langle kk'|\hat{g}|kk'\rangle=\iint d\tau_1 d\tau_2\varphi_k^*(q_1)\varphi_{k'}^*(q_2)\hat{g}(1,2)\varphi_k(q_2)\varphi_{k'}(q_1)$$

Direct interaction term

Exchange term

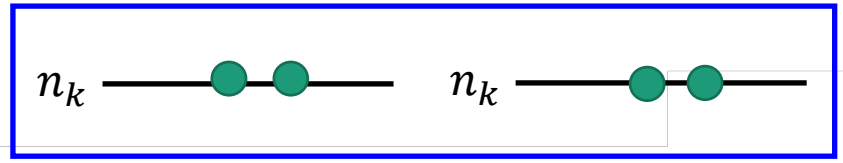
# 3.4 Occupation Number Representation

## 3.4.5 Dynamical Operators

- Also, we have the term when the two particles are on the same state:

$$\frac{N(N-1)}{2}\frac{\prod_i n_i!}{N!}\sum_k \frac{(N-2)!}{n_1!\cdots(n_k-2)!\cdots}\cdot(\varphi_k(q_1)\varphi_k(q_2),\hat{g}(1,2)\varphi_k(q_2)\varphi_k(q_1))$$

$$=\frac{1}{2}\sum n_k(n_k-1)\langle kk\,|\,\hat{g}\,|\,kk\rangle$$



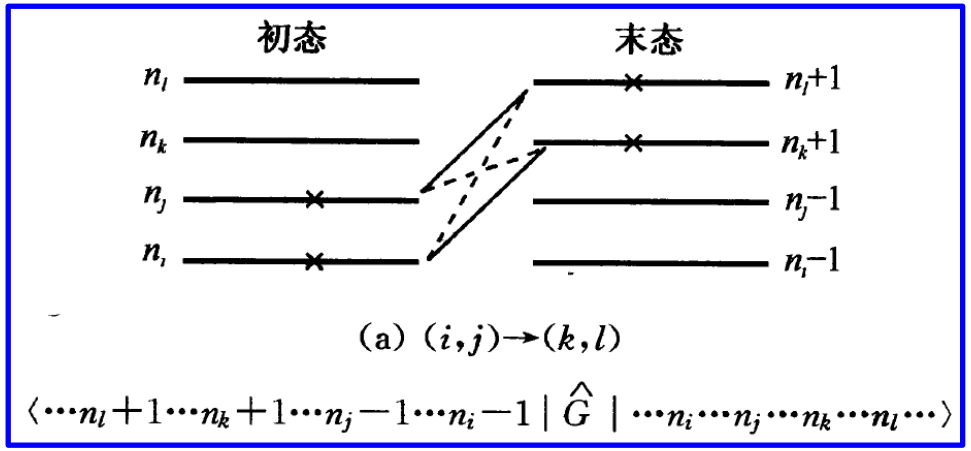

- Sum up these two, we have the following terms for the diagonal interaction of the two-body operator:

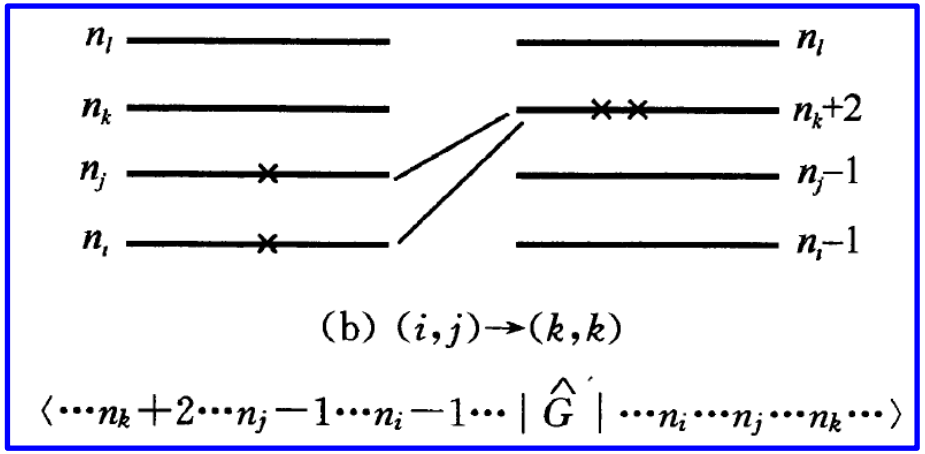
$$\bar{G}=\frac{1}{2}\sum_{k\neq k'} n_k n_{k'}\{\langle kk'\,|\,\hat{g}\,|\,k'k\rangle+\langle kk'\,|\,\hat{g}\,|\,kk'\rangle\}+\frac{1}{2}\sum_k n_k(n_k-1)\langle kk\,|\,\hat{g}\,|\,kk\rangle$$

The "Hartree-Fock" method for the bosonic system. For the fermionic system, we donot have this and the earlier pair wave function is antisymmetric. Will be detailed later for the electronic system.

# ◆ The Dynamical Operators, the Bosonic System

➢ Then, we look at the off-diagonal terms of the two-body interactions. By off-diagonal, all the excitations are taken into account. there are many possibilities:

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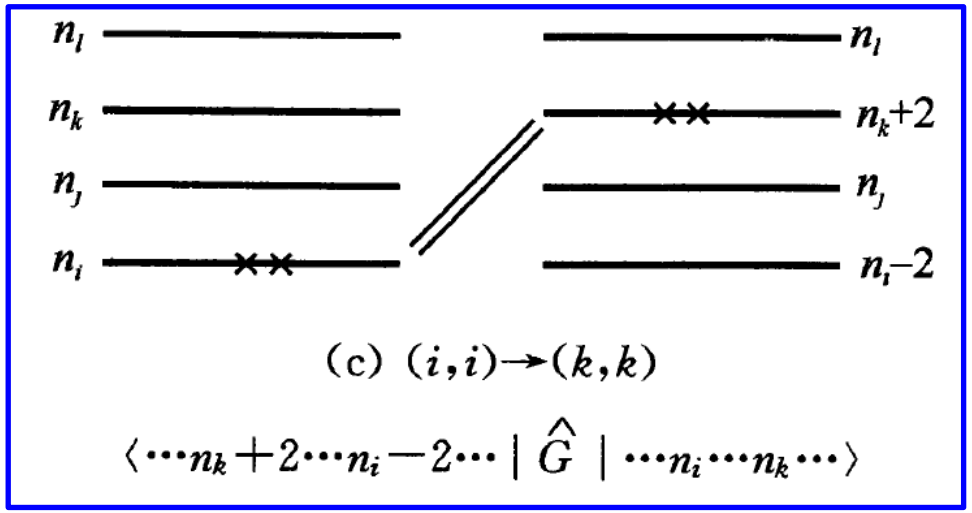
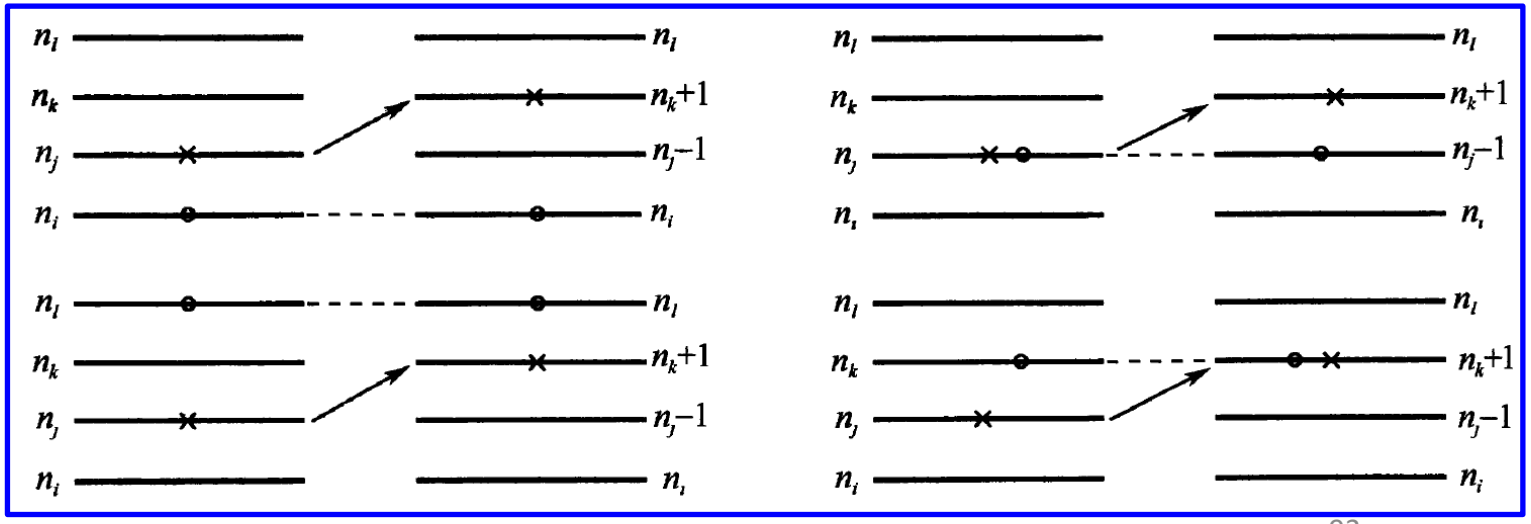


# The Dynamical Operators, the Bosonic System

- But in the end, what you get is that all the matrix elements can be described by:

$$\hat{G} = \frac{1}{2}\sum_{\alpha'\beta'\alpha\beta} g_{\alpha'\beta',\beta\alpha} a_{\alpha'}^{+} a_{\beta'}^{+} a_{\beta} a_{\alpha}$$

$$\begin{aligned} g_{\alpha'\beta',\beta\alpha} &\equiv \left(\varphi_{\alpha'}(q_1)\varphi_{\beta'}(q_2), \hat{g}(1,2)\varphi_{\beta}(q_2)\varphi_{\alpha}(q_1)\right) \\ &\equiv \langle \alpha'\beta' \mid \hat{g} \mid \beta\alpha \rangle \end{aligned}$$

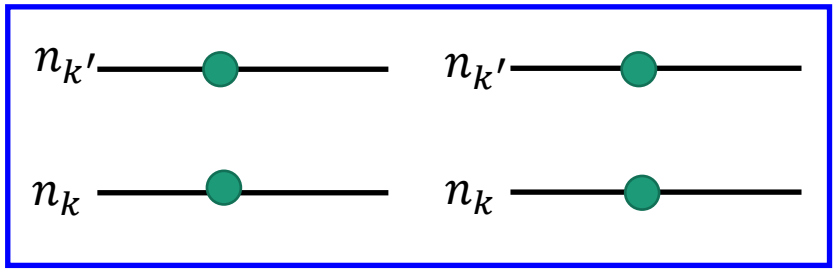
- For example, for the diagonal terms, we have:

$$\frac{1}{2}\sum_{\alpha\beta\alpha'\beta'} g_{\alpha'\beta',\beta\alpha} \langle \cdots n_\beta \cdots n_\alpha \cdots \mid a_{\alpha'}^{+} a_{\beta'}^{+} a_{\beta} a_{\alpha} \mid \cdots n_\alpha \cdots n_\beta \cdots \rangle$$

$$= \frac{1}{2}\sum_{\alpha\beta\alpha'\beta'} g_{\alpha'\beta',\alpha\beta} \cdot \langle \cdots n_\beta \cdots n_\alpha \cdots \mid a_{\alpha'}^{+} a_{\beta'}^{+} \mid \cdots n_\alpha - 1 \cdots n_\beta - 1 \cdots \rangle \sqrt{n_\alpha n_\beta}$$

$$= \frac{1}{2}\sum_{\alpha\beta\alpha'\beta'} g_{\alpha'\beta',\beta\alpha} \sqrt{n_\alpha n_\beta} (\delta_{\alpha'\alpha}\delta_{\beta'\beta} + \delta_{\alpha'\beta}\delta_{\beta'\alpha}) \sqrt{n_\alpha n_\beta}$$

$$= \frac{1}{2}\sum_{\alpha\beta} n_\alpha n_\beta (g_{\alpha\beta,\beta\alpha} + g_{\alpha\beta,\alpha\beta})$$



# ◆ The Dynamical Operators, the Bosonic System

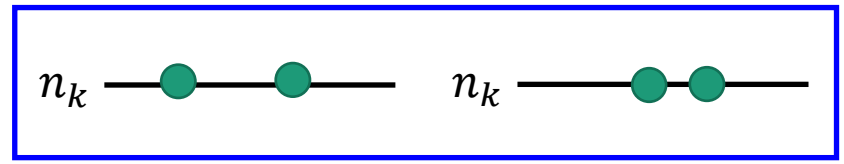
➢ And:

$$\frac{1}{2}\sum_{\alpha\beta\alpha'\beta'} g_{\alpha'\beta',\beta\alpha}\langle\cdots n_\alpha\cdots|\, a_{\alpha'}^{+}a_{\beta'}^{+}a_\beta a_\alpha \,|\cdots n_\alpha\cdots\rangle$$

$$=\frac{1}{2}\sum_{\alpha\beta\alpha'\beta'} g_{\alpha'\beta',\beta\alpha}\langle\cdots n_\alpha\cdots|\, a_{\alpha'}^{+},a_{\beta'}^{+}\,|\cdots n_\alpha-2\cdots\rangle\ \sqrt{n_\alpha(n_\alpha-1)}\,\delta_{\alpha\beta}$$

$$=\frac{1}{2}\sum_{\alpha\beta\alpha'\beta'} g_{\alpha'\beta',\beta\alpha}\ \sqrt{n_\alpha(n_\alpha-1)}\,\delta_{\alpha'\alpha}\delta_{\beta'\alpha}\ \sqrt{n_\alpha(n_\alpha-1)}\,\delta_{\alpha\beta}$$

$$=\frac{1}{2}\sum_{\alpha} n_\alpha(n_\alpha-1)\,g_{\alpha\alpha,\alpha\alpha}$$




➢ Sum up them, we have:

$$\bar{G}=\frac{1}{2}\sum_{\alpha\beta} n_\alpha n_\beta\left(g_{\alpha\beta,\beta\alpha}+g_{\alpha\beta,\alpha\beta}\right)+\frac{1}{2}\sum_{\alpha} n_\alpha(n_\alpha-1)\,g_{\alpha\alpha,\alpha\alpha}$$

$$\bar{G}=\frac{1}{2}\sum_{k\neq k'} n_k n_{k'}\left\{\langle kk'|\,\hat{g}\,|k'k\rangle+\langle kk'|\,\hat{g}\,|kk'\rangle\right\}+\frac{1}{2}\sum_{k} n_k(n_k-1)\langle kk|\,\hat{g}\,|kk\rangle$$

# ◆ The Dynamical Operators, the Fermionic System

- This is especially clear for the fermionic system. Since you read any literature for electronic structures, a sentence like “accurate many-body wave function is a linear combination of a series of Slater determinant”.

- In spite of this, for an easier introduction of the fermionic system, we still start from one single Slater determinant:

$$\psi_{\alpha\beta\gamma\cdots}(q_1, q_2, q_3, \cdots) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \varphi_\alpha(q_1) & \varphi_\alpha(q_2) & \varphi_\alpha(q_3) \cdots \\ \varphi_\beta(q_1) & \varphi_\beta(q_2) & \varphi_\beta(q_3) \cdots \\ \varphi_\gamma(q_1) & \varphi_\gamma(q_2) & \varphi_\gamma(q_3) \cdots \\ \vdots & \vdots & \vdots \end{vmatrix}$$

$$= \frac{1}{\sqrt{N!}} \sum_P (-1)^{\delta_P} P[\varphi_\alpha(q_1)\varphi_\beta(q_2)\varphi_\gamma(q_3)\cdots]$$

# ◆ The Dynamical Operators, the Fermionic System

- Based on this, we can analyze the diagonal/off-diagonal terms of the one-body/two-body operators.
- The occupation number representation is still a convenient method for us to understand the scattering processes.
- Below is the off-diagonal term of the one-body operator:

$$|\alpha\beta\gamma\cdots\rangle = a_\alpha^+ a_\beta^+ a_\gamma^+ \cdots |0\rangle$$

$$\langle\cdots\gamma\beta\alpha| = \langle 0|\cdots a_\gamma a_\beta a_\alpha$$

$$[a_\alpha, a_\beta^+]_+ = \delta_{\alpha\beta}$$

$$[a_\alpha, a_\beta]_+ = [a_\alpha^+, a_\beta^+]_+ = 0$$

$$\hat{F} = \sum_{\alpha\beta} f_{\alpha\beta} a_\alpha^+ a_\beta$$

$$\hat{G} = \frac{1}{2}\sum_{\alpha\beta\alpha'\beta'} g_{\alpha'\beta',\beta\alpha} a_{\alpha'}^+ a_{\beta'}^+ a_\beta a_\alpha$$

They act on the many-body wave functions. Therefore, different from the bosonic system, oddity of the exchange may play a role.

$$\langle\cdots 0_k\cdots 1_j\cdots|\hat{F}|\cdots 0_j\cdots 1_k\cdots\rangle \qquad (j<k)$$

$$= \sum_{\alpha\beta} f_{\alpha\beta}\langle\cdots 0_k\cdots 1_j\cdots|a_\alpha^+ a_\beta|\cdots 0_j\cdots 1_k\cdots\rangle$$

$$= \sum_{\alpha\beta} f_{\alpha\beta}\delta_{\alpha j}\delta_{\beta k}(-1)^{\sum_{i=1}^{j-1} n_i + \sum_{i=1}^{k-1} n_i} = (-1)^{\sum_{i=j+1}^{k-1} n_i} f_{jk}$$

$$f_{ik} = (\varphi_i, \hat{f}\varphi_k)$$

Off-diagonal, what for the diagonal?

# ◆ The Dynamical Operators, the Fermionic System

➢ Diagonal term of the two-body operator:

$$\bar{G} = (\psi_{n_1 n_2 \cdots}, \hat{G}\psi_{n_1 n_2 \cdots}) = \frac{N(N-1)}{2}(\psi_{n_1 n_2 \cdots}, \hat{g}(1,2)\psi_{n_1 n_2 \cdots})$$

$$= \frac{N(N-1)}{2}\frac{1}{N!}\sum_{k<k'}\left[\frac{(N-2)!}{n_1! \cdots (n_k-1)! \cdots (n_{k'}-1)! \cdots}\right]$$

$$\cdot \left( \begin{vmatrix} \varphi_k(q_1) & \varphi_{k'}(q_1) \\ \varphi_k(q_2) & \varphi_{k'}(q_2) \end{vmatrix}, \hat{g}(1,2) \begin{vmatrix} \varphi_k(q_1) & \varphi_{k'}(q_1) \\ \varphi_k(q_2) & \varphi_{k'}(q_2) \end{vmatrix} \right)$$

$$= \sum_{k<k'} n_k n_{k'} [(\varphi_k(q_1)\varphi_{k'}(q_2), \hat{g}(1,2)\varphi_{k'}(q_2)\varphi_k(q_1))$$

$$- (\varphi_k(q_1)\varphi_{k'}(q_2), \hat{g}(1,2)\varphi_k(q_2)\varphi_{k'}(q_1))]$$

$$= \sum_{k<k'} n_k n_{k'} [\langle kk' | \hat{g} | k'k \rangle - \langle kk' | \hat{g} | kk' \rangle]$$

$$= \frac{1}{2}\sum_{k \neq k'} n_k n_{k'} [\langle kk' | \hat{g} | k'k \rangle - \langle kk' | \hat{g} | kk' \rangle]$$

$n_{k'} = 1$ $n_{k'} = 1$

$n_k = 1$ $n_k = 1$

Hartree-Fock method, to be explained later.

# ◆ The Dynamical Operators, the Fermionic System

➢ This expression can be double-checked by derivations based on the occupation number representation.

$$\bar{G} = \langle \cdots n_2 n_1 \mid \hat{G} \mid n_1 n_2 \cdots \rangle$$

$$= \frac{1}{2} \sum_{\alpha\beta\alpha'\beta'} g_{\alpha'\beta',\beta\alpha} \langle \cdots n_2 n_1 \mid a_{\alpha'}^{+} a_{\beta'}^{+} a_{\beta} a_{\alpha} \mid n_1 n_2 \cdots \rangle$$

$$= \frac{1}{2} \Big[ \sum_{\substack{\alpha>\beta \\ \alpha'>\beta'}} + \sum_{\substack{\alpha<\beta \\ \alpha'<\beta'}} + \sum_{\substack{\alpha>\beta \\ \alpha'<\beta'}} + \sum_{\substack{\alpha<\beta \\ \alpha'>\beta'}} \Big] g_{\alpha'\beta',\beta\alpha} \cdot \langle \cdots n_2 n_1 \mid a_{\alpha'}^{+} a_{\beta'}^{+} a_{\beta} a_{\alpha} \mid n_1 n_2 \cdots \rangle$$

$$= \frac{1}{2} \Big[ \sum_{\substack{\alpha>\beta \\ \alpha'>\beta'}} + \sum_{\substack{\alpha<\beta \\ \alpha'<\beta'}} \Big] g_{\alpha'\beta',\beta\alpha} n_\alpha n_\beta \delta_{\alpha\alpha'} \delta_{\beta\beta'} - \frac{1}{2} \Big[ \sum_{\substack{\alpha>\beta \\ \alpha'<\beta'}} + \sum_{\substack{\alpha<\beta \\ \alpha'>\beta'}} \Big] g_{\alpha'\beta',\beta\alpha} n_\alpha n_\beta \delta_{\alpha\beta'} \delta_{\beta\alpha'}$$

$$= \frac{1}{2} \Big[ \sum_{\alpha>\beta} + \sum_{\alpha<\beta} \Big] g_{\alpha\beta,\beta\alpha} n_\alpha n_\beta - \frac{1}{2} \Big[ \sum_{\alpha>\beta} + \sum_{\alpha<\beta} \Big] g_{\alpha\beta,\alpha\beta} n_\alpha n_\beta$$

$$= \frac{1}{2} \sum_{\alpha\neq\beta} (g_{\alpha\beta,\beta\alpha} - g_{\alpha\beta,\alpha\beta}) n_\alpha n_\beta$$

$n_{k'} = 1$ $\quad$ $n_{k'} = 1$

$n_k = 1$ $\quad$ $n_k = 1$

# ◆ The Dynamical Operators, the Fermionic System

➢ For the off-diagonal matrix elements:

$$(\psi_{\cdots 0_i \cdots 0_j \cdots 1_k \cdots 1_l \cdots}, \hat{G}\psi_{\cdots 1_i \cdots 1_j \cdots 0_k \cdots 0_l \cdots}) \qquad (i<j, k<l)$$

$$=\frac{1}{2}N(N-1)(\psi_{\cdots 0_i \cdots 0_j \cdots 1_k \cdots 1_l \cdots}, \hat{g}(1,2)\psi_{\cdots 1_i \cdots 1_j \cdots 0_k \cdots 0_l \cdots})$$

$$\frac{1}{2}N(N-1)\frac{(N-2)!}{N!}(-1)^{\sum_{\nu=1}^{i-1}n_\nu+\sum_{\nu=1}^{j-1}n_\nu+\sum_{\nu=1}^{k-1}n_\nu+\sum_{\nu=1}^{l-1}n_\nu}$$

$$\cdot\left(\begin{vmatrix}\varphi_k(q_1) & \varphi_l(q_1)\\ \varphi_k(q_2) & \varphi_l(q_2)\end{vmatrix}, \hat{g}(1,2)\begin{vmatrix}\varphi_i(q_1) & \varphi_j(q_1)\\ \varphi_i(q_2) & \varphi_j(q_2)\end{vmatrix}\right)$$

$$=(-1)^{\sum_{\nu=i}^{j-1}n_\nu+\sum_{\nu=k}^{l-1}n_\nu}[\langle kl|\hat{g}|ji\rangle-\langle kl|\hat{g}|ij\rangle]$$

$$=(-1)^{\sum_{\nu=i+1}^{j-1}n_\nu+\sum_{\nu=k+1}^{l-1}n_\nu}[g_{kl,ji}-g_{kl,ij}]$$

$n_l = 0$ $\quad$ $n_l = 1$

$n_k = 0$ $\quad$ $n_k = 1$

$n_i = 1$ $\quad$ $n_i = 0$

$n_j = 1$ $\quad$ $n_j = 0$

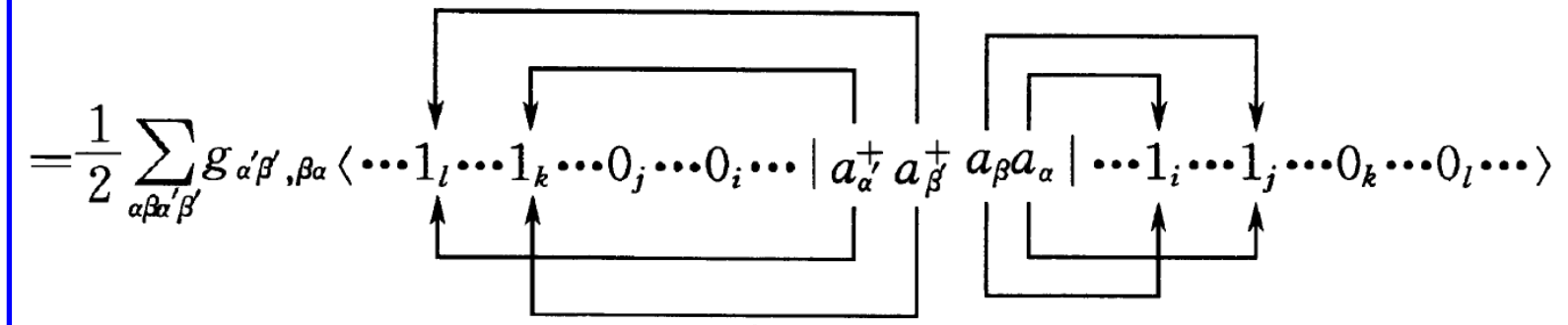
$$g_{kl,ji} = \int d\tau_1 d\tau_2 \varphi_k^*(q_1)\varphi_l^*(q_2)\hat{g}(1,2)\varphi_j(q_2)\varphi_i(q_1)$$

$$g_{kl,ij} = \int d\tau_1 d\tau_2 \varphi_k^*(q_1)\varphi_l^*(q_2)\hat{g}(1,2)\varphi_i(q_2)\varphi_j(q_1)$$

# ◆ The Dynamical Operators, the Fermionic System

➢ This can also be confirmed by:

$$\langle \cdots 1_l \cdots 1_k \cdots 0_j \cdots 0_i \cdots | \hat{G} | \cdots 1_i \cdots 1_j \cdots 0_k \cdots 0_l \cdots \rangle$$



$$= \frac{1}{2} \sum_{\alpha\beta\alpha'\beta'} g_{\alpha'\beta',\beta\alpha} \langle \cdots 1_l \cdots 1_k \cdots 0_j \cdots 0_i \cdots | a^+_{\alpha'} a^+_{\beta'} a_\beta a_\alpha | \cdots 1_i \cdots 1_j \cdots 0_k \cdots 0_l \cdots \rangle$$

$$= \frac{1}{2} \sum_{\alpha'\beta'\alpha\beta} g_{\alpha'\beta',\beta\alpha} (-1)^{\sum_{\nu=1}^{k-1} n_\nu + \sum_{\nu=1}^{l-1} n_\nu} (\delta_{\alpha' k}\delta_{\beta' l} - \delta_{\alpha' l}\delta_{\beta' k})(\delta_{\alpha i}\delta_{\beta j} - \delta_{\alpha j}\delta_{\beta i})(-1)^{\sum_{\nu=1}^{i-1} n_\nu + \sum_{\nu=1}^{j-1} n_\nu}$$

$$= \frac{1}{2} (g_{kl,ji} - g_{kl,ij} - g_{lk,ji} + g_{lk,ij}) (-1)^{\sum_{\nu=k}^{l-1} n_\nu + \sum_{\nu=i}^{j-1} n_\nu}$$

$$= (g_{kl,ji} - g_{kl,ij}) (-1)^{\sum_{\nu=k+1}^{l-1} n_\nu + \sum_{\nu=i+1}^{j-1} n_\nu}$$

# ◆ Coordinate Space Field Operator:

Originally: $\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\hat{x} + \frac{i}{\sqrt{2m\hbar\omega}}\hat{p}$

$\hat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\hat{x} - \frac{i}{\sqrt{2m\hbar\omega}}\hat{p}$

After all the discussions:

$$\hat{\psi}(\vec{r}) = \sum_{\alpha} \phi_\alpha(\vec{r})\,\hat{a}_\alpha \qquad \hat{\psi}^+(\vec{r}) = \sum_{\alpha} \phi_\alpha^*(\vec{r})\,\hat{a}_\alpha^+$$

$$\left[\hat{\psi}(\vec{r}), \hat{\psi}(\vec{r}')\right] = \left[\hat{\psi}^+(\vec{r}), \hat{\psi}^+(\vec{r}')\right] = 0$$

$$\left[\hat{\psi}(\vec{r}), \hat{\psi}^+(\vec{r}')\right] = \delta(\vec{r} - \vec{r}')$$

Or:

$$\left[\hat{\psi}(\vec{r}), \hat{\psi}(\vec{r}')\right]_+ = \left[\hat{\psi}^+(\vec{r}), \hat{\psi}^+(\vec{r}')\right]_+ = 0$$

$$\left[\hat{\psi}(\vec{r}), \hat{\psi}^+(\vec{r}')\right]_+ = \delta(\vec{r} - \vec{r}')$$

# ◆ Outline

1. Which states of identical particles are legal? (Hilbert Space)

2. Why are local states insufficient to describe joint measurements? (Quantum Entanglement, EPR Paradox)

3. Bell Inequality

4. Occupation Number Representation?

5. Wave-Function Based Quantum Many-Body Methods?

6. The Path-Integral Method and its Advantage in Describing Many-Body systems