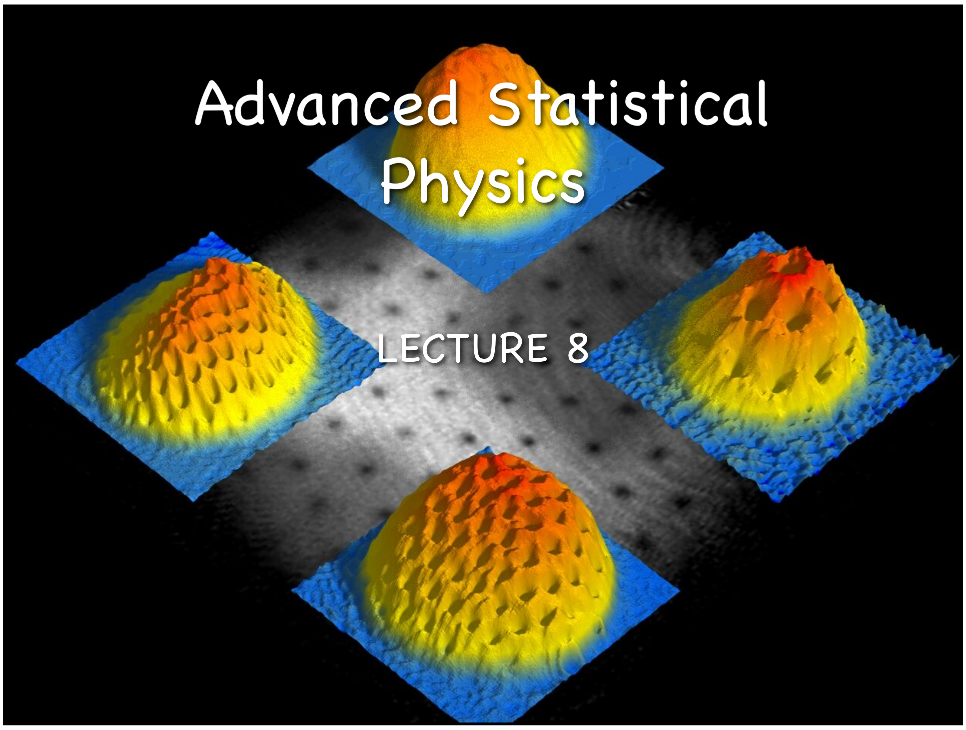

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Outline:

- "Second" quantization; creation, annihilation (or destruction) and the number operators
- Commutators ⇔ quantum statistics
- Indistinguishability of quantum particles
- Fock space, Occupation number representation
- Operators written in terms of creation and destruction operators

- Scope: to recognize the necessity of a quantum statistical formalism/approach and to introduct the second quantization formalism which allows for the treatment of quantum open systems where the number of particles in not conserved: Grand canonical ensemble

2

2

The second-quantization formalism

- In the contest of relativistic quantum field theory, where it was originally invented, the formalism of "second quantization" embodies new physics, such as the possibility of creation of particle-antiparticle pairs

- In a quantum statistical mechanics context it is the formalism which more naturally allows for the description of systems where the number of particle is not conserved

- Moreover it allows one to keep track in an automatic way of the effects of the relevant (Bose-Einstein or Fermi-Dirac) statistics. The formalism of "second quantization" thus permits a considerable simplification in the description of many-body systems, but in the end, it involves merely a reformulation of the original Schrödinger equation
- Basic elements:
  - Creation or destruction operators in a single particle state λ: $\hat{a}_\lambda^+ ; \hat{a}_\lambda$

  (Creation or destruction operators at a given space-point: $\hat{\Psi}^+(\vec{r}); \hat{\Psi}(\vec{r})$)

  - The overall statistical properties are included in fundamental commutation relations of these creation and annihilation operators.

3

3

Why a "second" quantization?

- The term "second quantization" is a bit confusing at first. How do you quantize something that is already quantized? The answer to this question is that in second quantization it is as if you were quantizing a different thing than in first quantization

- In ordinary non-relativistic point particle quantum mechanics, we "first" quantize by making the position of a classical particle x and its momentum p operators on a Hilbert space. The elements of the Hilbert space describe the possible states of the one particle system; the coordinate representation of a state is called the wave function for the system in that state; the wave function is just a function (probability amplitude)

- In the process of second quantization, the attention goes from states to creation and annihilation operators, where x and p are their indices… it is as if states were replaced by field operators

- The set of states, on which these new operators can operate, live in a direct sum of Hilbert spaces, the Fock space

4

4

The commutator

- We begin by formulating and solving the following simple problem: Suppose an operator a satisfies $[a,a^+]=aa^+-a^+a=1$ (a^+ denotes the conjugate of a, and [.,.] is, of course, the commutator... moreover $[a,a]=[a^+,a^+]=0$)

- The problem is to find the eigenvalues of the operator a^+a, and the related eigenvectors

- We first note that, if $|\alpha\rangle$ is a normalized eigenvector with $a^+a\,|\alpha\rangle = \alpha|\alpha\rangle$ then $\alpha= \langle\alpha|\, a^+a\, |\alpha\rangle = \|\, a|\alpha\rangle \,\|^2 \geq 0$
that is, the eigenvalues are all real and nonnegative

- Using the identity [AB,C]=A[B,C]+[A,C]B we observe that

$$\left[a^+a,a\right]=a^+\left[\cancel{a,a}\right]+\left[a^+,a\right]a=-\left[a,a^+\right]a=-a$$
$$\left[a^+a,a^+\right]=a^+\left[a,a^+\right]+\left[\cancel{a^+,a^+}\right]a=a^+$$

or

$$(a^+a)a=a(a^+a-1)$$
$$(a^+a)a^+=a^+(a^+a+1)$$

5

5

- From the first equation we have, for an eigenvector $|\alpha\rangle$,

$$(a^+a)a|\alpha\rangle=a(a^+a-1)|\alpha\rangle=a(\alpha-1)|\alpha\rangle=(\alpha-1)a|\alpha\rangle$$

therefore $a|\alpha\rangle$ is an eigenvector with eigenvalue $(\alpha-1)$, unless $a|\alpha\rangle = 0$

- Similarly $a^+|\alpha\rangle$ is an eigenvector with eigenvalue $(\alpha+1)$, unless $a^+|\alpha\rangle = 0$

$$(a^+a)a^+|\alpha\rangle=a^+(a^+a+1)|\alpha\rangle=a^+(\alpha+1)|\alpha\rangle=(\alpha+1)a^+|\alpha\rangle$$

- The norm of $a|\alpha\rangle$ is found from $\left\|a|\alpha\rangle\right\|^2=\langle\alpha|a^+a|\alpha\rangle=\alpha\langle\alpha|\alpha\rangle=\alpha$

$$\left\|a|\alpha\rangle\right\|=\sqrt{\alpha}$$

- Similarly, $\left\|a^+|\alpha\rangle\right\|=\sqrt{\alpha+1}$ (*)

- Now, suppose that $a^n|\alpha\rangle\neq 0$ for all n. Then by repeated application of a, $a^n|\alpha\rangle$ is an eigenvector of a^+a with eigenvalue $(\alpha-n)$. This contradicts the fact that the eigenvalues of a^+a are all real and nonnegative, because $(\alpha-n)<0$ for sufficiently large n

6

6

Bosonic occupation

- Therefore we must have $a^n|\alpha\rangle \neq 0$ but $a^{n+1}|\alpha\rangle = 0$ for some nonnegative integer n

- Let $|\alpha-n\rangle = a^n|\alpha\rangle / \|a^n|\alpha\rangle\|$, so that $|\alpha-n\rangle$ is a normalized eigenvector with eigenvalue $(\alpha-n)$; then

$$\sqrt{\alpha - n} = \left\| a|\alpha - n\rangle \right\| = 0 \quad \Rightarrow \alpha = n$$

  this shows that the eigenvalue of a^+a must be nonnegative integers, and that there is a "ground state" $|0\rangle$ such that $a|0\rangle = 0$

- By repeatedly applying a^+ to $|0\rangle$ we see that $(a^+)^n|0\rangle$ has the eigenvalue n and, because of Eq.(*), it is never zero. Thus the eigenvalues of a^+a are 0,1,2,3,…; in general

$$\boxed{|n\rangle = \frac{1}{\sqrt{n!}}\left(a^+\right)^n|0\rangle}$$

- Note that we could have included arbitrary phase factors in the definition of $|n\rangle$; our convention here is to make them unity

7

7

- With the previous definition, the $|n\rangle$ are orthonormal … (suppose $n \geq m$)

By using $[a,a^+]=1$ m times (check!)

$$\sqrt{n!\,m!}\left\langle n \middle| m \right\rangle = \left\langle 0 \middle| a^n (a^+)^m \middle| 0 \right\rangle \stackrel{\downarrow}{=} \left\langle 0 \middle| a^{n-1} (a^+)^m a \middle| 0 \right\rangle + m\left\langle 0 \middle| a^{n-1} (a^+)^{m-1} \middle| 0 \right\rangle =$$

$$= m\left\langle 0 \middle| a^{n-1} (a^+)^{m-1} \middle| 0 \right\rangle = \cdots = m(m-1)\ldots 2\cdot 1\left\langle 0 \middle| a^{n-m} \middle| 0 \right\rangle = \delta_{nm}\, m!$$

  … and satisfy:

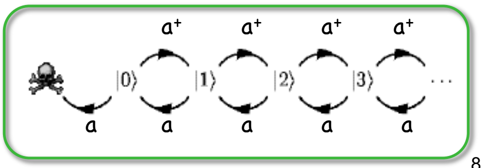
$$a^+|n\rangle = \sqrt{n+1}\,|n+1\rangle$$

$$a|n\rangle = \sqrt{n}\,|n-1\rangle$$

$$a^+a|n\rangle = n|n\rangle$$

- In later applications a^+a will be interpreted as the operator associated with the number of particles of a certain kind, in which case a^+ and a are called "creation" and "destruction" (annihilation) operators, respectively

Action of the commuting (bosonic) creation and destruction operators in the occupation number space



8

8

The anti-commutator

- Suppose instead that a satisfies $\{a,a^+\}=aa^++a^+a=1$ (a^+ denotes the conjugate of a, and $\{.,.\}$ is the anti-commutator; moreover let $\{a,a\}= \{a^+,a^+\}=0$)

- The problem is to find the eigenvalues of the operator a^+a, and the related eigenvectors

- We again note that, if $|\alpha\rangle$ is a normalized eigenvector with $a^+a\,|\alpha\rangle = \alpha|\alpha\rangle$ then $\alpha= \langle\alpha|\, a^+a\,|\alpha\rangle = \|\, a|\alpha\rangle\, \|^2 \geq 0$; that is, the eigenvalues are all real and nonnegative

- We note also that

$$\{a,a\}|\alpha\rangle = 2aa|\alpha\rangle = 0 \quad \Rightarrow \quad aa|\alpha\rangle = 0$$
$$\{a^+,a^+\}|\alpha\rangle = 2a^+a^+|\alpha\rangle = 0 \quad \Rightarrow \quad a^+a^+|\alpha\rangle = 0$$

9

9

Fermionic occupation

- Therefore

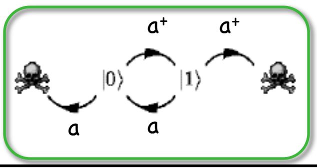
$$\alpha^2|\alpha\rangle = \left(a^+a\right)^2|\alpha\rangle = \left(a^+a\right)\left(a^+a\right)|\alpha\rangle = a^+\left(aa^+\right)a|\alpha\rangle =$$
$$= a^+\left(1-a^+a\right)a|\alpha\rangle = \left(a^+a\right)|\alpha\rangle = \alpha|\alpha\rangle \quad \Rightarrow \quad \alpha = 0,1$$

Thus the eigenvalues of a^+a are only: 0,1

- This is equivalent to what is obtained assuming Fermi statistics

- In summary we have:
$$a^+|0\rangle = |1\rangle$$
$$a|1\rangle = |0\rangle$$
$$a^+a|n\rangle = n|n\rangle \quad n = 0,1$$

Action of the anticommuting (fermionic) creation and destruction operators in the occupation number space



10

10

Identical particles

- Identical particles: particles which behave in exactly the same way under similar physical conditions and therefore cannot be distinguished by any objective measurement

- In classical mechanics, with well-known initial conditions, the *state* of a particle is determined for all times by Hamilton's equations of motion. The particle is always identifiable, since its orbit can be (in principle) calculated. In this sense, classical identical particles (with the same masses, charges, spatial extensions etc.) can always be distinguished

- Within quantum mechanics, in contrast, the fundamental **principle of indistinguishability** holds. This principle states that identical particles are not distinguishable

- In quantum mechanics, *Physically relevant* are exclusively the measurable quantities of a physical system: expectation values of observables or scalar products of states. They must not change if the numbering of two identical particles in the *N*-particle state is exchanged. Otherwise, there would be a measurement procedure which would distinguish between the two identical particles.

11

11

Systems of indistinguishable particles

- The Hilbert space of states for a system of N identical particles is the space $\mathcal{H}_N$ of complex, square integrable function, defined in the configuration space of the N particles.

- The wave function $\psi_N(\mathbf{r}_1,\mathbf{r}_2,..,\mathbf{r}_N)$, which represent the probability amplitude for finding particles at the N positions $\{\mathbf{r}_1,\mathbf{r}_2,..,\mathbf{r}_N\}$, must satisfy

$$\langle \psi_N | \psi_N \rangle = \int d^3\vec{r}_1 \cdots d^3\vec{r}_N \left|\psi_N(\vec{r}_1,\vec{r}_2,\cdots,\vec{r}_N)\right|^2 < +\infty$$

- The Hilbert space $\mathcal{H}_N$ is simply the N^{th} tensor product of the single-particle Hilbert space $\mathcal{H}$

$$\mathcal{H}_N = \mathcal{H} \otimes \mathcal{H} \otimes \mathcal{H} \otimes \ldots \otimes \mathcal{H}$$

- If $\{| i \rangle\}$ is an orthonormal basis of $\mathcal{H}$, the orthonormal basis of $\mathcal{H}_N$ is constructed from the tensor product

- These basis states have the wave functions:

$$\psi_{i_1\cdots i_N}(\vec{r}_1,\cdots,\vec{r}_N) = \langle \vec{r}_1 \cdots \vec{r}_N | i_1 \cdots i_N \rangle = \left(\langle \vec{r}_1 | \otimes \cdots \otimes \langle \vec{r}_N |\right)\left(|i_1\rangle \otimes \cdots \otimes |i_N\rangle\right) = \phi_{i_1}(\vec{r}_1)\cdots\phi_{i_N}(\vec{r}_N)$$

12

12

- The overlap of two vectors of the basis is given by

$$\langle i_1 \cdots i_N | i'_1 \cdots i'_N \rangle = \left(\langle i_1 | \otimes \cdots \otimes \langle i_N | \right) \left(| i'_1 \rangle \otimes \cdots \otimes | i'_N \rangle \right) = \langle i_1 | i'_1 \rangle \cdots \langle i_N | i'_N \rangle$$

- and the completeness of the basis is obtained from the tensor product of the completeness relation for the basis {| i ⟩}

$$\sum_{i_1 \cdots i_N} | i_1 \cdots i_N \rangle \langle i_1 \cdots i_N | = 1$$

- Physically it is clear that the space $\mathcal{H}_N$ is generated by a linear combination of products of single-particle wave functions

- Thus far, in defining the Hilbert space $\mathcal{H}_N$, we have not taken into account the symmetry property of the wave function: only totally symmetric or anti-symmetric states are observed in nature

- The wave function of N Bosons is totally symmetric and thus satisfies

$$\boxed{\psi(\vec{r}_{P1}, \cdots, \vec{r}_{PN}) = \psi(\vec{r}_1, \cdots, \vec{r}_N)}$$

where (P1,…,PN) represent any permutation P of the set (1,…,N)

13

13

- The wave function of N Fermions is anti-symmetric under exchange of any pair of particles:

$$\boxed{\psi(\vec{r}_{P1}, \cdots, \vec{r}_{PN}) = (-1)^P \psi(\vec{r}_1, \cdots, \vec{r}_N)}$$

here, $(-1)^P$ denotes the sign, or parity, of the permutation P, and is defined as (-1) elevated to the number of transpositions of two elements which brings the permutation (P1,…,PN) to its original form (1,…,N)

- It can be proven within the context of quantum field theory that given general assumption of locality, causality and Lorentz invariance, particles with integer spin (0,1,2,…) are Bosons and particles with half-integer spin (1/2,3/2,…) are Fermions (spin-statistics theorem)

- For convenience we shall adopt the following unified notation for Bosons or Fermions:

$$\psi(\vec{r}_{P1}, \cdots, \vec{r}_{PN}) = \zeta^P \psi(\vec{r}_1, \cdots, \vec{r}_N)$$

where P is the parity of the permutation, and ζ is +1 or -1 for Bosons or Fermions respectively

14

14

- These symmetry requirements imply corresponding restrictions of the Hilbert space $\mathcal{H}_N$ of N-particle system. A wave function $\psi(\mathbf{r}_1,\mathbf{r}_2,..,\mathbf{r}_N)$ of $\mathcal{H}_N$ belongs to the Hilbert space of N Bosons, $\mathcal{B}_N$, or the Hilbert space of N Fermions, $\mathcal{F}_N$, if it is symmetric or anti-symmetric respectively under a permutation of the particles.

- We will define the symmetrization operator $\mathcal{P}_B$ and the antisymmetrization operator $\mathcal{P}_F$ in $\mathcal{H}_N$ by their action on the wave function $\psi(\mathbf{r}_1,\mathbf{r}_2,..,\mathbf{r}_N)$

$$\boxed{\mathcal{P}_{\left\{ B \atop F \right\}}\psi(\vec{r}_1,\cdots,\vec{r}_N) := \frac{1}{N!}\sum_P \zeta^P \psi(\vec{r}_{P1},\cdots,\vec{r}_{PN})}$$

- For example, for two Bosons: $\mathcal{P}_B\psi(\vec{r}_1,\vec{r}_2) = \frac{1}{2}\left[\psi(\vec{r}_1,\vec{r}_2)+\psi(\vec{r}_2,\vec{r}_1)\right]$

- and for two Fermions: $\mathcal{P}_F\psi(\vec{r}_1,\vec{r}_2) = \frac{1}{2}\left[\psi(\vec{r}_1,\vec{r}_2)-\psi(\vec{r}_2,\vec{r}_1)\right]$

- $\mathcal{P}_B$ and $\mathcal{P}_F$ may be shown to be projector operators; these operators project $\mathcal{H}_N$ onto the Hilbert (sub)space of Bosons $\mathcal{B}_N$ and the Hilbert space Fermions, $\mathcal{F}_N$.

15

15

- Using these projectors, a system of Bosons or Fermions, with one particle in state $| i_1 \rangle$, one in state $| i_2 \rangle$, … and one in state $| i_N \rangle$, is represented as follows:

$$\boxed{\left| i_1 \cdots i_N \right\rangle_{\left\{ S \atop A \right\}}} := \sqrt{N!}\,\mathcal{P}_{\left\{ B \atop F \right\}}\left| i_1 \cdots i_N \right\rangle = \frac{1}{\sqrt{N!}}\sum_P \zeta^P \left| i_{P1} \right\rangle \otimes \cdots \otimes \left| i_{PN} \right\rangle$$

- The Pauli exclusion principle, that two Fermions cannot occupy the same state is automatically satisfied for anti-symmetric states. Suppose that two states are identical, for example $| i_1 \rangle = | i_2 \rangle = | i \rangle$, then

$$\left| i_1 i_2 \cdots i_N \right\rangle_A = \sqrt{N!}\,\mathcal{P}_F \left| i_1 i_2 \cdots i_N \right\rangle = -\sqrt{N!}\,\mathcal{P}_F \left| i_2 i_1 \cdots i_N \right\rangle = 0$$

and no acceptable many-Fermion state exists in this case

- From $\mathcal{B}_N = \mathcal{P}_B\mathcal{H}_N$ and $\mathcal{F}_N = \mathcal{P}_F\mathcal{H}_N$ it follows that if $| i_1 \dots i_N \rangle$ is a orthogonal basis of the Hilbert space $\mathcal{H}_N$, then $\mathcal{P}_{B(F)} | i_1 \dots i_N \rangle$ is a orthogonal basis of $\mathcal{B}_N$ ($\mathcal{F}_N$), in fact…

16

16

- …the scalar product of two basis vectors constructed from the same basis {| i ⟩} is

$$ {}_{\left\{ S \atop A \right\}}\langle i_1' \cdots i_N' | i_1 \cdots i_N \rangle_{\left\{ S \atop A \right\}} = N! \langle i_1' \cdots i_N' | \mathcal{P}^2_{\left\{ B \atop F \right\}} | i_1 \cdots i_N \rangle = N! \langle i_1' \cdots i_N' | \mathcal{P}_{\left\{ B \atop F \right\}} | i_1 \cdots i_N \rangle = \sum_P \zeta^P \langle i_1' | i_{P1} \rangle \cdots \langle i_N' | i_{PN} \rangle $$

  because of the orthogonality of the basis {| i ⟩} , the only non-vanishing terms are the permutations P such that

$$ i_1' = i_{P1}, \cdots, i_N' = i_{PN} $$

- For Fermions, since there is at most one particle per state | i ⟩ , no two identical states can be present in the set { i_1 … i_N } and therefore, there exists only one permutation P which transforms i_1 … i_N into i'_1 … i'_N . The sum thus reduces to one term, and if the states | i_j ⟩ are normalized, we obtain

$$ {}_A\langle i_1' \cdots i_N' | i_1 \cdots i_N \rangle_A = (-1)^P $$

- For Bosons, many particles may be in the same state, and therefore, any permutation which does interchange particles in the same state contributes to the sum. If the set { i_1 … i_N } represent a system with n_1 Bosons in the state | i_1 ⟩ , … , n_p Bosons in the state | i_p ⟩ , where i_1 … i_p are distinct, the overlap is given by

$$ {}_S\langle i_1' \cdots i_N' | i_1 \cdots i_N \rangle_S = n_1! n_2! \cdots n_p! $$

17

17

- Finally, an orthonormal basis for the Hilbert space $\mathcal{B}_N$ or $\mathcal{F}_N$ is obtained:

$$ \boxed{| i_1 \cdots i_N)} := \frac{1}{\sqrt{\prod_i n_i!}} | i_1 \cdots i_N \rangle_{\left\{ S \atop A \right\}} = \frac{1}{\sqrt{N! \prod_i n_i!}} \sum_P \zeta^P | i_{P1} \rangle \otimes \cdots \otimes | i_{PN} \rangle $$

- The overlap between a tensor product | j_1 … j_N ⟩ constructed from a basis | j ⟩ (in $\mathcal{H}_N$) and the symmetrized or anti-symmetrized | i_1 … i_N) is

$$ \langle j_1 \cdots j_N | i_1 \cdots i_N) = \frac{1}{\sqrt{N! \prod_i n_i!}} \sum_P \zeta^P \langle j_1 | i_{P1} \rangle \cdots \langle j_N | i_{PN} \rangle = \frac{1}{\sqrt{N! \prod_i n_i!}} S(\langle j_m | i_n \rangle) $$

  where $S(M_{mn})$ denotes a permanent for Bosons $\mathrm{Per}(M_{mn}) = \sum_P M_{1,P1} \cdots M_{N,PN}$

  and a determinant for Fermions $\det(M_{mn}) = \sum_P (-1)^P M_{1,P1} \cdots M_{N,PN}$

- In coordinate representation, we thus obtain a basis of permanent wave functions for Bosons

$$ \psi_{i_1 \cdots i_N}(\vec{r}_1 \cdots \vec{r}_N) = \langle \vec{r}_1 \cdots \vec{r}_N | i_1 \cdots i_N) = \frac{1}{\sqrt{N! \prod_i n_i!}} \mathrm{Per}\left(\phi_{i_m}(\vec{r}_n)\right) $$

  and a basis of Slater determinants for Fermions

$$ \psi_{i_1 \cdots i_N}(\vec{r}_1 \cdots \vec{r}_N) = \langle \vec{r}_1 \cdots \vec{r}_N | i_1 \cdots i_N) = \frac{1}{\sqrt{N!}} \det\left(\phi_{i_m}(\vec{r}_n)\right) $$

18

18

Creation and annihilation operators

- Creation and annihilation operators provide a convenient representation of the many-particle states and many-body operators

- For each single-particle state $|\lambda\rangle$ of the single-particle space $\mathcal{H}$, we define a Boson or Fermion creation operator by its action on any symmetrized or anti-symmetrized state of $\mathcal{B}_N$ or $\mathcal{F}_N$ as follows

$$\boxed{a_\lambda^+ |\lambda_1 \cdots \lambda_N)_{S(A)} := \sqrt{n_\lambda + 1}\,|\lambda \lambda_1 \cdots \lambda_N)_{S(A)}}$$

Note: a^+_λ by definition acts on the first position in $|...)_{S(A)}$ and therefore also a_λ

where n_λ is the occupation number of the state $|\lambda\rangle$ in $|\lambda_1 \dots \lambda_N\rangle$

- Physically this operator adds a particle in state $|\lambda\rangle$ to the state on which it operates, and symmetrizes or anti-symmetrizes the new state (this depends on the commutation or anti-commutation rules that it satisfies). For example, in the case of fermions the previous eq. takes the simpler form:

$$a_\lambda^+ |\lambda_1 \cdots \lambda_N\rangle_A = \begin{cases} |\lambda \lambda_1 \cdots \lambda_N\rangle_A & \text{if the state } |\lambda\rangle \text{ is not in } |\lambda_1 \dots \lambda_N\rangle_A \\ 0 & \text{if the state } |\lambda\rangle \text{ is already in } |\lambda_1 \dots \lambda_N\rangle_A \end{cases}$$

19

19

The Fock space

- It is useful to define the vacuum state, denoted with $|0\rangle$, which represent a state with zero particles; the creation operator acting on $|0\rangle$ creates a particle in the state $|\lambda\rangle$

$$a_\lambda^+|0\rangle = |\lambda\rangle$$

- The creation (annihilation) operators do not operate within one space $\mathcal{B}_N$ or $\mathcal{F}_N$, but rather operate from any space $\mathcal{B}_N$ or $\mathcal{F}_N$ to $\mathcal{B}_{N+1}$ or $\mathcal{F}_{N+1}$ ($\mathcal{B}_{N-1}$ or $\mathcal{F}_{N-1}$). Hence it is useful to define the Fock space as the direct sum of the Boson or Fermion spaces

$$\mathcal{B} = \mathcal{B}_0 \oplus \mathcal{B}_1 \oplus \mathcal{B}_2 \oplus \cdots = \oplus_{n=0}^{\infty} \mathcal{B}_n \qquad \mathcal{F} = \mathcal{F}_0 \oplus \mathcal{F}_1 \oplus \mathcal{F}_2 \oplus \cdots = \oplus_{n=0}^{\infty} \mathcal{F}_n$$

where by definition $\mathcal{B}_0 = \mathcal{F}_0 = |0\rangle$ and $\mathcal{B}_1 = \mathcal{F}_1 = \mathcal{H}$

- A general state $|\phi\rangle$ of the Fock space is a linear combination of states with any number of particles. For example, the state

$$|\phi\rangle = \tfrac{1}{2}|0\rangle + \tfrac{1}{\sqrt{2}}|\lambda\rangle + \tfrac{1}{2}|\lambda\mu\rangle$$

belongs to the Fock space and represents a system of particles in which there is a prob. 1/4 for having no particle, prob. 1/2 for having one particle in state $|\lambda\rangle$, and prob. 1/4 for having two particles in state $|\lambda\ \mu\rangle$

20

20

- Any basis vector $|\lambda_1 \ldots \lambda_N)$ in $\mathcal{B}_N$ or $\mathcal{F}_N$ may be generated by repeated action of the creator operators on the vacuum $|0\rangle$ ...

$$|\lambda_1 \cdots \lambda_N) = \frac{1}{\sqrt{\prod_\lambda n_\lambda!}} a^+_{\lambda_1} a^+_{\lambda_2} \cdots a^+_{\lambda_N} |0\rangle$$

thus the creation operators generate the entire Fock space by repeated action on the vacuum

- The symmetry or anti-symmetry properties of the many-particle states impose commutation or anti-commutation relations between the creation operators... consider the un-normalized state

$$|\lambda_1 \cdots \lambda_N\rangle_{\left\{ S \atop A \right\}} = a^+_{\lambda_1} a^+_{\lambda_2} \cdots a^+_{\lambda_N} |0\rangle \quad \left(= \sqrt{N!}\,\mathcal{P}_{\left\{ B \atop F \right\}} |\lambda_1 \cdots \lambda_N) \right)$$

for any state $|\lambda_1 \ldots \lambda_N\rangle_{S(A)}$ and any single particle states $|\lambda\rangle$ and $|\mu\rangle$, we obtain

$$a^+_\lambda a^+_\mu |\lambda_1 \cdots \lambda_N\rangle_{S(A)} = |\lambda \mu \lambda_1 \cdots \lambda_N\rangle_{S(A)} = \zeta |\mu \lambda \lambda_1 \cdots \lambda_N\rangle_{S(A)} = \zeta a^+_\mu a^+_\lambda |\lambda_1 \cdots \lambda_N\rangle_{S(A)}$$

thus for Bosons, the creation operators commute whereas for Fermions they anti-commute

$$\boxed{\left[a^+_\lambda, a^+_\mu\right]_{-\zeta} = a^+_\lambda a^+_\mu - \zeta\, a^+_\mu a^+_\lambda = 0}$$

21

21

- The commutations relations of annihilation operators follow immediately form the adjoint of the previous equation
- To close the algebra of the creation and annihilation operators, we need to evaluate the commutators of creation and annihilation operators ...

$$a^+_\mu a_\lambda |\lambda_1 \cdots \lambda_N\rangle_{S(A)} = \sum_{i=1}^N \zeta^{i-1} \delta_{\lambda\lambda_i} |\mu \lambda_1 \cdots \lambda_{i-1} \lambda_{i+1} \cdots \lambda_N\rangle_{S(A)}$$

$$a_\lambda a^+_\mu |\lambda_1 \cdots \lambda_N\rangle_{S(A)} = a_\lambda |\mu \lambda_1 \cdots \lambda_N\rangle_{S(A)} = \delta_{\lambda\mu} |\lambda_1 \cdots \lambda_N\rangle_{S(A)} + \sum_{i=1}^N \zeta^i \delta_{\lambda\lambda_i} |\mu \lambda_1 \cdots \lambda_{i-1} \lambda_{i+1} \cdots \lambda_N\rangle_{S(A)} =$$

$$= \delta_{\lambda\mu} |\lambda_1 \cdots \lambda_N\rangle_{S(A)} + \zeta \sum_{i=1}^N \zeta^{i-1} \delta_{\lambda\lambda_i} |\mu \lambda_1 \cdots \lambda_{i-1} \lambda_{i+1} \cdots \lambda_N\rangle_{S(A)} = \delta_{\lambda\mu} |\lambda_1 \cdots \lambda_N\rangle_{S(A)} + \zeta a^+_\mu a_\lambda |\lambda_1 \cdots \lambda_N\rangle_{S(A)}$$

hence

$$a_\lambda a^+_\mu |\lambda_1 \cdots \lambda_N\rangle_{S(A)} = (\delta_{\lambda\mu} + \zeta\, a^+_\mu a_\lambda) |\lambda_1 \cdots \lambda_N\rangle_{S(A)}$$

for any state $|\lambda_1 \ldots \lambda_N\rangle_{S(A)}$, so the creation and annihilation operators satisfy the operator equations

$$\boxed{\left[a_\lambda, a^+_\mu\right]_{-\zeta} = a_\lambda a^+_\mu - \zeta\, a^+_\mu a_\lambda = \delta_{\lambda\mu}}$$

... we have "walked" along the "inverse path" of the simple problems introduced at the beginning of this lecture

22

22

A new basis

- Consider a transformation which transform the orthonormal basis $\{|\lambda\rangle\}$ into another basis $\{|\mu\rangle\}$ as follows $|\mu\rangle = \sum_\lambda \langle\lambda|\mu\rangle|\lambda\rangle$
- By this eq. and the definition of the creation operators

$$a_\mu^+|\mu_1\cdots\mu_N\rangle_{S(A)} = |\mu\mu_1\cdots\mu_N\rangle_{S(A)} = \sum_\lambda \langle\lambda|\mu\rangle|\lambda\mu_1\cdots\mu_N\rangle_{S(A)} = \sum_\lambda \langle\lambda|\mu\rangle a_\lambda^+|\mu_1\cdots\mu_N\rangle_{S(A)}$$

- Thus the creation operators satisfy the operator equation: $a_\mu^+ = \sum_\lambda \langle\lambda|\mu\rangle a_\lambda^+$

  and the annihilation operators satisfy the adjoint equation $a_\mu = \sum_\lambda \langle\mu|\lambda\rangle a_\lambda$
- Commutation and anti-commutation relations for these new operators are

$$\left[a_\mu, a_{\mu'}^+\right]_{-\xi} = \sum_{\lambda\lambda'} \langle\mu|\lambda\rangle\langle\lambda'|\mu'\rangle \underbrace{\left[a_\lambda, a_{\lambda'}^+\right]_{-\xi}}_{\delta_{\lambda\lambda'}} = \sum_\lambda \langle\mu|\lambda\rangle\langle\lambda|\mu'\rangle = \langle\mu|\mu'\rangle = \delta_{\mu\mu'}$$

  and similarly $\left[a_\mu^+, a_{\mu'}^+\right]_{-\xi} = \left[a_\mu, a_{\mu'}\right]_{-\xi} = 0$
- If $\{|\mu\rangle\}$ is orthonormal we obtain the usual commutation relations and the transformation is called canonical

23

23

Field operators

- Of particular importance is the $\{|r\rangle\}$ basis; the creation and annihilation operators are traditionally denoted by $\hat{\Psi}^+(\vec{r})$ *and* $\hat{\Psi}(\vec{r})$ and are called field operators
- Their commutation relations are $\left[\hat{\Psi}^+(\vec{r}), \hat{\Psi}^+(\vec{r}')\right]_{-\xi} = \left[\hat{\Psi}(\vec{r}), \hat{\Psi}(\vec{r}')\right]_{-\xi} = 0$

  and $\left[\hat{\Psi}(\vec{r}), \hat{\Psi}^+(\vec{r}')\right]_{-\xi} = \langle\vec{r}|\vec{r}'\rangle = \delta(\vec{r}-\vec{r}')$
- The expansion of these operators on a basis $\{|\lambda\rangle\}$ is $\longrightarrow$ where $\phi_\lambda(\mathbf{r})$ is the wave function of the state $|\lambda\rangle$

$$\hat{\Psi}^+(\vec{r}) = \sum_\lambda \langle\lambda|\vec{r}\rangle a_\lambda^+ = \sum_\lambda \phi_\lambda^*(\vec{r}) a_\lambda^+$$

$$\hat{\Psi}(\vec{r}) = \sum_\lambda \langle\vec{r}|\lambda\rangle a_\lambda = \sum_\lambda \phi_\lambda(\vec{r}) a_\lambda$$

- Loosely speaking, $\hat{\Psi}^+(\vec{r})$ is the sum of all possible ways to add a particle to the system at position $\mathbf{r}$ through any of the basis states $\phi(\mathbf{r})$
- In some sense the quantum field operators express the essence of the wave/particle duality in quantum physics: on the one hand they act on the Fock space to build wave functions, but on the other hand they exhibit the commutator properties associated with particles

24

24

A basis for all operators

- A fundamental property of creation and annihilation operators is that they provide a basis for all operators in the Fock space; that is, any operator can be expressed as a linear combination of the set of all products of the creation and annihilation operators

- A convenient technique for representing an operator in terms of creation and annihilation operators is to first use a basis in which it is diagonal and then transform to a general basis

- At first consider the number operator, its action is to count the number of particles n_λ in state $|\lambda\rangle$:

$$\hat{n}_\lambda \left|\lambda_1 \cdots \lambda_N\right\rangle_{S(A)} = a_\lambda^+ a_\lambda \left|\lambda_1 \cdots \lambda_N\right\rangle_{S(A)} = \sum_{i=1}^{N} \zeta^{i-1} \delta_{\lambda \lambda_i} a_\lambda^+ \left|\lambda_1 \cdots \lambda_{i-1}\, \lambda_{i+1} \cdots \lambda_N\right\rangle_{S(A)} =$$

$$= \left(\sum_{i=1}^{N} \delta_{\lambda \lambda_i} \right) \left|\lambda_1 \cdots \lambda_{i-1}\, \lambda_i\, \lambda_{i+1} \cdots \lambda_N\right\rangle_{S(A)} = n_\lambda \left|\lambda_1 \cdots \lambda_N\right\rangle_{S(A)}$$

- The following operator thus counts the total number of particles in a state of the Fock space

$$\boxed{\hat{N} = \sum_\lambda a_\lambda^+ a_\lambda}$$

25

25

- We now consider a one-body operator which is diagonal in the orthonormal basis $\{|\lambda\rangle\}$:

$$\hat{U}|\lambda\rangle = U_\lambda |\lambda\rangle \qquad U_\lambda = \langle \lambda | \hat{U} | \lambda \rangle$$

for states in $\mathcal{H}_N$ (see supplementary material)

$$\langle \lambda_1' \cdots \lambda_N' | \hat{U} | \lambda_1 \cdots \lambda_N \rangle = \langle \lambda_1' \cdots \lambda_N' | \sum_l \hat{U}_l | \lambda_1 \cdots \lambda_N \rangle = \sum_{l=1}^{N} \langle \lambda_l' | \hat{U}_l | \lambda_l \rangle \left(\prod_{k \neq l} \langle \lambda_k' | \lambda_k \rangle \right) =$$

$$= \sum_{l=1}^{N} U_{\lambda_l} \langle \lambda_l' | \lambda_l \rangle \left(\prod_{k \neq l} \langle \lambda_k' | \lambda_k \rangle \right) = \sum_{l=1}^{N} U_{\lambda_l} \left(\prod_{k} \langle \lambda_k' | \lambda_k \rangle \right) = \left(\sum_{l=1}^{N} U_{\lambda_l} \right) \langle \lambda_1' \cdots \lambda_N' | \lambda_1 \cdots \lambda_N \rangle$$

for symmetric states we thus obtain

$${}_{\left\{ S \atop A \right\}}\langle \lambda_1' \cdots \lambda_N' | \hat{U} | \lambda_1 \cdots \lambda_N \rangle_{\left\{ S \atop A \right\}} = N! \langle \lambda_1' \cdots \lambda_N' | \mathcal{P}_{\left\{ B \atop F \right\}} \hat{U} \mathcal{P}_{\left\{ B \atop F \right\}} | \lambda_1 \cdots \lambda_N \rangle = N! \langle \lambda_1' \cdots \lambda_N' | \mathcal{P}^2_{\left\{ B \atop F \right\}} \hat{U} | \lambda_1 \cdots \lambda_N \rangle =$$

$$= N! \langle \lambda_1' \cdots \lambda_N' | \mathcal{P}_{\left\{ B \atop F \right\}} \hat{U} | \lambda_1 \cdots \lambda_N \rangle = \sum_P \zeta^P \sum_{l=1}^{N} \left(\prod_{k \neq l} \langle \lambda_{Pk}' | \lambda_k \rangle \right) \langle \lambda_{Pl}' | \hat{U}_l | \lambda_l \rangle = \left(\sum_{l=1}^{N} U_{\lambda_l} \right) \sum_P \zeta^P \prod_k \langle \lambda_{Pk}' | \lambda_k \rangle =$$

$$= \left(\sum_{l=1}^{N} U_{\lambda_l} \right) {}_{\left\{ S \atop A \right\}}\langle \lambda_1' \cdots \lambda_N' | \lambda_1 \cdots \lambda_N \rangle_{\left\{ S \atop A \right\}} = \left(\sum_\lambda U_\lambda n_\lambda \right) {}_{\left\{ S \atop A \right\}}\langle \lambda_1' \cdots \lambda_N' | \lambda_1 \cdots \lambda_N \rangle_{\left\{ S \atop A \right\}} = {}_{\left\{ S \atop A \right\}}\langle \lambda_1' \cdots \lambda_N' | \sum_\lambda U_\lambda \hat{n}_\lambda | \lambda_1 \cdots \lambda_N \rangle_{\left\{ S \atop A \right\}}$$

26

26

- Since this equality holds for any states, we obtain the operator identity:

$$\boxed{\hat{U} = \sum_{\lambda} U_{\lambda} \hat{n}_{\lambda} = \sum_{\lambda} \langle \lambda | \hat{U} | \lambda \rangle a_{\lambda}^{+} a_{\lambda}}$$

For example a local one-body potential in the coordinate basis or the kinetic energy operator in the momentum basis or the Hamiltonian in the basis of its eigenstates turns out to be respectively:

$$\hat{U} = \int d\vec{r}\, U(\vec{r}) \hat{\Psi}^{+}(\vec{r}) \hat{\Psi}(\vec{r}) \qquad \hat{T} = \sum_{\vec{p}} \frac{\vec{p}^{2}}{2m} a_{\vec{p}}^{+} a_{\vec{p}} \qquad \hat{H} = \sum_{n} \varepsilon_{n} a_{n}^{+} a_{n}$$

- We may now transform from the diagonal representation to a general basis:

$$\hat{U} = \sum_{\lambda} U_{\lambda} a_{\lambda}^{+} a_{\lambda} = \sum_{\lambda} U_{\lambda} \left(\sum_{\mu} \langle \mu | \lambda \rangle b_{\mu}^{+} \right) \left(\sum_{\mu'} \langle \lambda | \mu' \rangle b_{\mu'} \right) = \sum_{\mu\mu'} \left(\sum_{\lambda} \langle \mu | \lambda \rangle U_{\lambda} \langle \lambda | \mu' \rangle \right) b_{\mu}^{+} b_{\mu'} = \sum_{\mu\mu'} \langle \mu | \hat{U} | \mu' \rangle b_{\mu}^{+} b_{\mu'}$$

and, for example, the kinetic energy in the coordinate basis becomes:

$$\hat{T} = \int d\vec{r}\,' d\vec{r}\, \hat{\Psi}^{+}(\vec{r}\,') \langle \vec{r}\,' | \tfrac{\hat{\vec{p}}^{2}}{2m} | \vec{r} \rangle \hat{\Psi}(\vec{r}) = -\tfrac{\hbar^{2}}{2m} \int d\vec{r}\,' d\vec{r}\, \hat{\Psi}^{+}(\vec{r}\,') \nabla^{2} \delta(\vec{r} - \vec{r}\,') \hat{\Psi}(\vec{r}) =$$

$$= -\tfrac{\hbar^{2}}{2m} \int d\vec{r}\, \hat{\Psi}^{+}(\vec{r}) \nabla^{2} \hat{\Psi}(\vec{r})$$

27

27

- Similarly, a two-body operator may be expressed in terms of creation and annihilation operators; using the basis in which it is diagonal

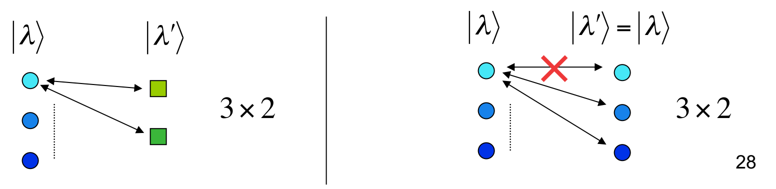
$$\hat{V}_{\lambda\lambda'} | \lambda \lambda' \rangle = V_{\lambda\lambda'} | \lambda \lambda' \rangle \quad V_{\lambda\lambda'} = \langle \lambda \lambda' | \hat{V}_{\lambda\lambda'} | \lambda \lambda' \rangle \qquad \left(\hat{V} = \frac{1}{2} \sum_{\lambda \neq \lambda'} \hat{V}_{\lambda\lambda'} \right)$$

we calculate a general matrix element as before

$$_{\left\{ S \atop A \right\}}\langle \lambda_1' \cdots \lambda_N' | \hat{V} | \lambda_1 \cdots \lambda_N \rangle_{\left\{ S \atop A \right\}} = \sum_{P} \zeta^{P} \frac{1}{2} \sum_{m \neq n}^{N} \left(\prod_{k \neq m,n} \langle \lambda_{Pk}' | \lambda_k \rangle \right) \langle \lambda_{Pm}' \lambda_{Pn}' | \hat{V}_{\lambda_m \lambda_n} | \lambda_m \lambda_n \rangle = \left(\frac{1}{2} \sum_{m \neq n}^{N} V_{\lambda_m \lambda_n} \right) {}_{\left\{ S \atop A \right\}}\langle \lambda_1' \cdots \lambda_N' | \lambda_1 \cdots \lambda_N \rangle_{\left\{ S \atop A \right\}}$$

the multiplicative factor is a sum over all <u>distinct</u> pairs of particles present in the state $|\lambda_1 \ldots \lambda_N\rangle_{S(A)}$ so we need to construct an operator which counts the number of pairs of particles in the states $|\lambda\rangle$ and $|\lambda'\rangle$ …

if $|\lambda\rangle$ and $|\lambda'\rangle$ are different, the number of pairs is $n_{\lambda} n_{\lambda'}$ whereas if $|\lambda\rangle = |\lambda'\rangle$, the number of pairs is $n_{\lambda}(n_{\lambda} - 1)$;



28

28

- hence the operator which counts pairs may be written

$$\hat{n}_\lambda \hat{n}_{\lambda'} - \delta_{\lambda\lambda'}\hat{n}_\lambda = a_\lambda^+ a_\lambda a_{\lambda'}^+ a_{\lambda'} - \delta_{\lambda\lambda'} a_\lambda^+ a_\lambda =$$
$$= a_\lambda^+ (\delta_{\lambda\lambda'} + \zeta a_{\lambda'}^+ a_\lambda) a_{\lambda'} - \delta_{\lambda\lambda'} a_\lambda^+ a_\lambda = \zeta\, a_\lambda^+ a_{\lambda'}^+ a_\lambda a_{\lambda'} = a_\lambda^+ a_{\lambda'}^+ a_{\lambda'} a_\lambda$$

and hence we have found the following operator identity

$$\hat{V} = \frac{1}{2}\sum_{\lambda\mu} \langle \lambda\mu | \hat{V} | \lambda\mu \rangle a_\lambda^+ a_\mu^+ a_\mu a_\lambda$$

- transforming from the diagonal representation to an arbitrary basis one obtains

$$\boxed{\hat{V} = \frac{1}{2}\sum_{\lambda\mu\nu\rho} \langle \lambda\mu | \hat{V} | \nu\rho \rangle a_\lambda^+ a_\mu^+ a_\rho a_\nu}$$

- An example is a two-body interaction potential which is diagonal in the coordinate representation:

$$\hat{V} = \frac{1}{2}\int d\vec{r}\, d\vec{r}\,' v(\vec{r} - \vec{r}\,')\hat{\Psi}^+(\vec{r})\hat{\Psi}^+(\vec{r}\,')\hat{\Psi}(\vec{r}\,')\hat{\Psi}(\vec{r})$$

29

29

- We remember now that being $\langle \vec{p} | \vec{r} \rangle = \frac{1}{(2\pi\hbar)^3} e^{-\frac{i}{\hbar}\vec{p}\cdot\vec{r}} = \frac{1}{(2\pi)^3} e^{-i\vec{p}\cdot\vec{r}}$

for simplicity ħ=1

- The field operators in the momentum basis are

$$\hat{\Psi}^+(\vec{r}) = \sum_\lambda \langle \lambda | \vec{r} \rangle a_\lambda^+ \quad \Rightarrow \quad \hat{\Psi}^+(\vec{r}) = \int \frac{d\vec{p}}{(2\pi)^3} e^{-i\vec{p}\cdot\vec{r}} a_{\vec{p}}^+$$
$$\hat{\Psi}(\vec{r}) = \sum_\lambda \langle \vec{r} | \lambda \rangle a_\lambda \quad \Rightarrow \quad \hat{\Psi}(\vec{r}) = \int \frac{d\vec{p}}{(2\pi)^3} e^{i\vec{p}\cdot\vec{r}} a_{\vec{p}}$$

it follows that

$$\hat{V} = \frac{1}{2}\int d\vec{r}\, d\vec{r}\,' v(\vec{r} - \vec{r}\,') \int \frac{d\vec{p}_1}{(2\pi)^3} \int \frac{d\vec{p}_2}{(2\pi)^3} \int \frac{d\vec{p}_3}{(2\pi)^3} \int \frac{d\vec{p}_4}{(2\pi)^3} e^{-i(\vec{p}_1 - \vec{p}_4)\cdot\vec{r}} e^{-i(\vec{p}_2 - \vec{p}_3)\cdot\vec{r}\,'} a_{\vec{p}_1}^+ a_{\vec{p}_2}^+ a_{\vec{p}_3} a_{\vec{p}_4}$$

And being that

$$\int d\vec{r}\, d\vec{r}\,' \, v(\vec{r} - \vec{r}\,')\, e^{-i(\vec{p}_1 - \vec{p}_4)\cdot\vec{r}} e^{-i(\vec{p}_2 - \vec{p}_3)\cdot\vec{r}\,'} =$$

$\vec{x} = \vec{r} - \vec{r}\,'$

$$= \int d\vec{r}\,' \int d\vec{x}\, v(\vec{x})\, e^{-i(\vec{p}_1 - \vec{p}_4)\cdot\vec{x}} e^{-i[(\vec{p}_2 - \vec{p}_3) + (\vec{p}_1 - \vec{p}_4)]\cdot\vec{r}\,'} =$$
$$= \hat{v}(\vec{p}_1 - \vec{p}_4) \int d\vec{r}\,' e^{-i[(\vec{p}_2 - \vec{p}_3) + (\vec{p}_1 - \vec{p}_4)]\cdot\vec{r}\,'} =$$
$$= \hat{v}(\vec{p}_1 - \vec{p}_4)\;\; \delta\left[(\vec{p}_2 - \vec{p}_3) + (\vec{p}_1 - \vec{p}_4)\right]$$

30

30

- It follows that:

$$\hat{V} = \frac{1}{2}\int \frac{d\vec{p}_1}{(2\pi)^3}\int \frac{d\vec{p}_2}{(2\pi)^3}\int \frac{d\vec{p}_3}{(2\pi)^3}\int \frac{d\vec{p}_4}{(2\pi)^3}\hat{v}(\vec{p}_1 - \vec{p}_4)\delta[(\vec{p}_2 - \vec{p}_3) + (\vec{p}_1 - \vec{p}_4)]a^+_{\vec{p}_1}a^+_{\vec{p}_2}a_{\vec{p}_3}a_{\vec{p}_4}$$

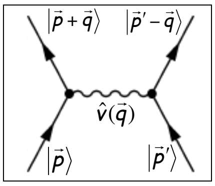
- Let: $\vec{p}_1 = \vec{p} + \vec{q} \quad \vec{p}_2 = \vec{p}' - \vec{k} \quad \vec{p}_3 = \vec{p}' \quad \vec{p}_4 = \vec{p}$

$$\Rightarrow \quad \vec{q} = \vec{k} \quad \vec{p}_2 = \vec{p}' - \vec{k} = \vec{p}' - \vec{q}$$

then

$$\hat{V} = \frac{1}{2}\int \frac{d\vec{q}}{(2\pi)^3}\int \frac{d\vec{p}'}{(2\pi)^3}\int \frac{d\vec{p}}{(2\pi)^3}\hat{v}(\vec{q})\, a^+_{\vec{p}+\vec{q}}a^+_{\vec{p}'-\vec{q}}a_{\vec{p}'}a_{\vec{p}}$$

A graphical representation of the two-body interaction in second quantization:
Under momentum conservation the incoming states p and p' are with probability amplitude $\hat{v}(\vec{q})$ scattered into the outgoing states p+q and p'-q



- From the "first" to the "second" quantization Hamiltonian:

$$\hat{H} = -\frac{\hbar^2}{2m}\sum_{i=1}^{N}\nabla_i^2 + \frac{1}{2}\sum_{i\neq j}^{N} v(\vec{r}_i - \vec{r}_j) \quad \Rightarrow \quad \boxed{\hat{H} = \sum_{\vec{p}}\frac{\vec{p}^2}{2m}a^+_{\vec{p}}a_{\vec{p}} + \frac{1}{2V}\sum_{\vec{q}\,\vec{p}'\vec{p}}\hat{v}_{\vec{q}}\, a^+_{\vec{p}+\vec{q}}a^+_{\vec{p}'-\vec{q}}a_{\vec{p}'}a_{\vec{p}}}$$

31

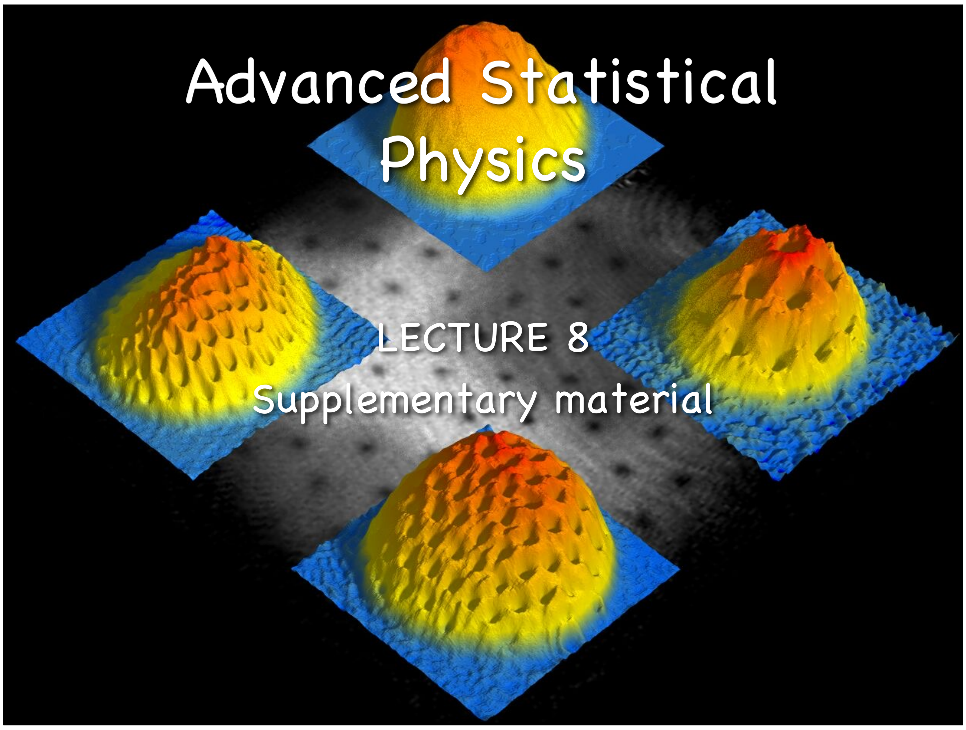
31

Lecture 8: Suggested books

- T. Guénault "Basic Superfluids", Taylor & Francis
- D.R. Tilley and J. Tilley "Superfluidity and Superconductivity", IOP publishing Ltd (1990)
- W. Nolting "Fundamentals of Many-Body Physics", Springer
- J.W. Negele, H. Orland "Quantum Many-Particle Systems", Perseus Books

32

32



33

Many-body operators

- Consider matrix elements of many-body operators in the basis of $\mathcal{H}_N$: $| i_1 \dots i_N \rangle = | i_1 \rangle \otimes | i_2 \rangle \otimes \dots \otimes | i_N \rangle$

- From these, the representation of operators in the spaces $\mathcal{B}_N$ and $\mathcal{F}_N$ follow straightforwardly using $\mathcal{P}_B$ and $\mathcal{P}_F$

- Let $\hat{O}$ be an arbitrary operator in $\mathcal{B}_N$ or $\mathcal{F}_N$. Independent of whether the particles are Bosons or Fermions, their indistinguishability implies that $\hat{O}$ is invariant under any permutation of the particles. Thus for any state and any permutation P

$$\left\langle i_{P1} \cdots i_{PN} \middle| \hat{O} \middle| i'_{P1} \cdots i'_{PN} \right\rangle = \left\langle i_1 \cdots i_N \middle| \hat{O} \middle| i'_1 \cdots i'_N \right\rangle$$

- We begin by considering the case of one-body operators: $\hat{U}$ is a one-body operator if its action on a state $| i_1 \dots i_N \rangle$ of N particles is the sum of the action of $\hat{U}$ on each particle

$$\hat{U} | i_1 \cdots i_N \rangle = \sum_i \hat{U}_i | i_1 \cdots i_N \rangle$$

where the operator $\hat{U}_i$ operates only on the i^{th} particle.

34

34

- For example, the kinetic energy operator in the momentum basis, act as

$$\hat{T}|\vec{p}_1 \cdots \vec{p}_N\rangle = \sum_i \frac{\vec{p}_i^{\,2}}{2m}|\vec{p}_1 \cdots \vec{p}_N\rangle$$

and a local one-body potential in the coordinate basis act as

$$\hat{V}^{(1)}|\vec{r}_1 \cdots \vec{r}_N\rangle = \sum_i V^{(1)}(\vec{r}_i)|\vec{r}_1 \cdots \vec{r}_N\rangle$$

- The matrix element of a one-body operator Û between two states is given by

$$\langle i_1 \cdots i_N|\hat{U}|i_1' \cdots i_N'\rangle = \sum_{l=1}^{N}\langle i_1 \cdots i_N|\hat{U}_l|i_1' \cdots i_N'\rangle = \sum_{l=1}^{N}\left(\prod_{k \neq l}\langle i_k|i_k'\rangle\right)\langle i_l|\hat{U}_l|i_l'\rangle$$

and thus for non-orthogonal states: $\longrightarrow$ $\dfrac{\langle i_1 \cdots i_N|\hat{U}|i_1' \cdots i_N'\rangle}{\langle i_1 \cdots i_N|i_1' \cdots i_N'\rangle} = \sum_{l=1}^{N}\dfrac{\langle i_l|\hat{U}_l|i_l'\rangle}{\langle i_l|i_l'\rangle}$

so the one-body operator Û is entirely determined by its matrix elements ⟨ i | Û | i' ⟩ in the single-particle Hilbert space $\mathcal{H}$.

- Similarly, an operator Â, is a two-body operator if the action of Â on a state | i_1 … i_N ⟩ of N particles is the sum of the action of Â on all distinct pairs of particles

$$\hat{A}|i_1 \cdots i_N\rangle = \sum_{1 \le m < n \le N}\hat{A}_{mn}|i_1 \cdots i_N\rangle$$

where $\hat{A}_{mn}$ operates only on particles m and n

35

35

- The restriction m < n yields a summation over distinct pairs. The symmetry requirement on Â implies that $\hat{A}_{mn} = \hat{A}_{nm}$ and the previous expression can be written as

$$\hat{A}|i_1 \cdots i_N\rangle = \frac{1}{2}\sum_{1 \le m \neq n \le N}\hat{A}_{mn}|i_1 \cdots i_N\rangle$$

- The matrix elements of Â are given by

$$\langle i_1 \cdots i_N|\hat{A}|i_1' \cdots i_N'\rangle = \frac{1}{2}\sum_{m \neq n}^{N}\langle i_1 \cdots i_N|\hat{A}_{mn}|i_1' \cdots i_N'\rangle = \frac{1}{2}\sum_{m \neq n}^{N}\left(\prod_{k \neq m,n}\langle i_k|i_k'\rangle\right)\langle i_m i_n|\hat{A}_{mn}|i_m' i_n'\rangle$$

and for non-orthogonal states

$$\frac{\langle i_1 \cdots i_N|\hat{A}|i_1' \cdots i_N'\rangle}{\langle i_1 \cdots i_N|i_1' \cdots i_N'\rangle} = \frac{1}{2}\sum_{m \neq n}^{N}\frac{\langle i_m i_n|\hat{A}_{mn}|i_m' i_n'\rangle}{\langle i_m|i_m'\rangle\langle i_n|i_n'\rangle}$$

thus a two-body operator is entirely determined by its matrix elements ⟨ i j | Â | i' j' ⟩ in the Hilbert space $\mathcal{H}_2$ of two-particle systems

- Further, a two-body interaction is said to be local when it is diagonal in configuration space:

$$\langle \vec{r}_1 \vec{r}_2|\hat{V}|\vec{r}_3 \vec{r}_4\rangle = \delta(\vec{r}_1 - \vec{r}_3)\delta(\vec{r}_2 - \vec{r}_4)v(\vec{r}_1 - \vec{r}_2)$$

in this case we have $\hat{V}|\vec{r}_1 \cdots \vec{r}_N\rangle = \dfrac{1}{2}\sum_{1 \le i \neq j \le N}v(\vec{r}_i - \vec{r}_j)|\vec{r}_1 \cdots \vec{r}_N\rangle$

36

36