Notations for today's lecture

(1) A complete set of
single-particle states;
$\psi_i(\mathbf{x})$ where i $\in$ { 1, 2, 3, ..., ∞ }
(E_i = the quantum numbers
for this state)

(2) The *field* for a spin-0 boson;
(this is not a wave function ---
it's an ***operator*** in the Hilbert
space of N particle states);

$$\Psi(\mathbf{x}) = \sum_i \psi_i(\mathbf{x})\, b_i$$

(3) The N particle *wave function* ;

$$\Phi(x_1 , x_2 , x_3 , \ldots , x_N ; t)$$

Summary from the previous lecture

The quantum many-particle problem in first quantized form, for bosons :

■ Understand that the symmetry of the wave function (*for bosons*) implies that the basis states depend only on the list of occupation numbers ...

$$\Phi_{\{n\}}(\{x\}) = \sqrt{\frac{\prod n_i!}{N!}} \sum_P \psi_1(x_1)\cdots\psi_k(x_k)\cdots\psi_N(x_N)$$

quantum nos. E_k

■ We can expand $\Phi(\{x\},t)$ in occupation-number basis states ...

$$\Phi(\{x\};t) = \sum_{\{n\}}{}' f_N(\{n\};t)\, \Phi_{\{n\}}(\{x\})$$

where $f_N(\{n\},t)$ is a probability amplitude.

1b. THE MANY-PARTICLE HILBERT SPACE ; CREATION AND ANNIHILATION OPERATORS ; SECOND QUANTIZATION

bosons!

- The index i labels a single-particle state.
- Basis states : $|n_1 n_2 n_3 \ldots\rangle$ or $|\{n\}\rangle$

  where $\sum_{i=1}^{\infty} n_i = N$
- Orthonormality

  $$\langle \{n'\} | \{n\} \rangle = \delta(n_1', n_1)\, \delta(n_2', n_2) \ldots \delta(n_k', n_k) \ldots$$

  $$= \prod_{i=1}^{\infty} \delta(n_i', n_i) \quad \text{Kronecker delta}$$
- Completeness $\sum'_{\{n\}} |\{n\}\rangle\langle\{n\}| = \mathbb{1}$

We have seen creation and annihilation operators twice before.

- a and $a^\dagger$ for a harmonic oscillator;

  $[a, a^\dagger] = 1$;

  $|n\rangle = (a^\dagger)^n |0\rangle / \sqrt{n!}$.
- $a_{\mathbf{k}\sigma}$ and $a^\dagger_{\mathbf{k}\sigma}$ for the photon field ;

  $[a_{\mathbf{k}\sigma}, a^\dagger_{\mathbf{k}'\sigma'}] = \delta_{\mathbf{k},\mathbf{k}'}\, \delta_{\sigma,\sigma'}$;

  |multi photon state>

  $= (a^\dagger_{\mathbf{k}'\sigma'})^n |\text{vacuum}\rangle / \sqrt{n!}$.

Now, for a third time ,

- b_i and $b^\dagger_i$ for the boson field.

Now define the quantized field for this boson, in the Schroedinger picture,

$$\Psi(x) = \sum_{i=1}^{\infty} \psi_i(x)\ b_i$$

where $[b_i , b^\dagger_j] = \delta_{ij}$

(all other CR's are 0)

Note that

$$[\Psi(x),\Psi^\dagger(x')] = \delta^3(x-x')$$

Annihilation and creation operators

$$[b_i, b_j^+] = \delta_{ij}.$$

$$[b_i, b_j] = 0 \quad \text{and} \quad [b_i^+, b_j^+] = 0.$$

$$[\Psi(x), \Psi^+(x')] = \sum_i \sum_j \underbrace{[b_i, b_j^+]}_{\delta_{ij}} \psi_i(x) \psi_j^+(x')$$

$$= \sum_i \psi_i(x) \psi_i^+(x')$$

$$= \delta^3(x - x')$$

The wave function of an N boson state

Denote the state by $| \alpha >$.

The definition of the wave function is

$$\Phi_\alpha(\{x\}\,;t) =$$

$$< 0 \,|\, e^{itH/\hbar}\,\Psi(x_1)\Psi(x_2)\ldots\Psi(x_N)e^{-itH/\hbar}\,|\, \alpha >$$

(Trick question: Is this the Schroedinger picture or the Heisenberg picture?)

Note that Φ_α is not an expectation value.

The N factors of Ψ annihilate the particles, leaving $| 0 >$.

Now, what is equation for time evolution?

$$\underline{H} = \sum_{[ij]} b_i^{+} < i\,|T|\,j > b_j + \tfrac{1}{2} \sum_{[ijkl]} b_i^{+}\, b_j^{+} < ij\,|V|\,kl > b_l b_k$$

Be sure to understand that $\underline{H}$ is the Hamiltonian of the field theory ("second quantization") , which is *not* the N-particle Hamiltonian,

$$H_N = \sum_k T_k + \tfrac{1}{2} {\sum_{k,l}}' V(x_k, x_l) \, .$$

("first quantization") .

Theorem.

The second quantized theory is equivalent to the first quantized theory.

Proof

First , let’s rewrite the Hamiltonian in terms of the field $\Psi(x)$.

$$\underline{H} = H^{(1)} + H^{(2)}$$

$$H^{(1)} = \sum_{ij} \langle i|T|j\rangle b_i^+ b_j$$

$$= \int \Psi^+(x)\, T_x\, \Psi(x)\, d^3x$$

$$\langle i|T|j\rangle = \int \psi_i^*(x)\, T_x\, \psi_j(x)\, d^3x$$

$$H^{(2)} = \frac{1}{2} \sum_{ijkl} \underbrace{\langle ij|V|kl\rangle}_{\int \psi_i^*(x)\, \psi_j^*(x')\, V(x,x')\, \psi_k(x)\, \psi_l(x')\, d^3x\, d^3x'} b_i^+ b_j^+ b_l b_k$$

$$= \frac{1}{2} \int \Psi^+(x)\, \Psi^+(x')\, V(x,x')\, \Psi(x')\, \Psi(x)\, d^3x\, d^3x'$$

Proof continues

Next, let's consider N = 1.

$$\Phi_\alpha(\vec{x},t) = \langle 0 | e^{iHt/\hbar}\, \Psi(\vec{x})\, e^{-iHt/\hbar} | \alpha \rangle$$

$$i\hbar \frac{\partial \Phi_\alpha}{\partial t} = i\hbar \langle 0 | e^{iHt/\hbar}\, \frac{i}{\hbar}[H, \Psi]\, e^{-iHt/\hbar} | \alpha \rangle$$

$$[H^{(1)}, \Psi(\vec{x})] = \int [\Psi^\dagger(x') T_{x'} \Psi(x'), \Psi(x)]\, d^3x'$$

$$[AB, C] = A[B,C] + [A,C]B$$

Proof continues.

$$[H^{(1)}, \Psi(\vec{x})] = \int \{ \Psi^\dagger(x') [T\Psi(x'), \Psi(x)] + [\Psi^\dagger(x'), \Psi(x)]\, T\Psi(x') \}\, d^3x'$$

$$= \int - \delta^3(x'-x)\, T\Psi(x)\, d^3x' = - T_x \Psi(x)$$

$$i\hbar \frac{\partial \Phi_\alpha}{\partial t} = i\hbar \langle 0 | e^{iHt/\hbar} \left(-\frac{i}{\hbar} T_x \Psi(x)\right) e^{-iHt/\hbar} | \alpha \rangle$$

$$= T_x\, \Phi_\alpha(x,t)$$ as it should be.

Result :

$i\hbar\, \partial\Phi_\alpha/\partial t = T_x\, \Phi_\alpha(x)$;

Q.E.D. for N = 1

Proof continues.
Now, let's consider N = 2.

$$\Phi_\beta(x_1 x_2 t) = \langle 0 | e^{iHt/\hbar} \Psi(x_1)\Psi(x_2) e^{-iHt/\hbar} | \beta \rangle$$

$$i\hbar \frac{\partial \Phi_\beta}{\partial t} = i\hbar \langle 0 | e^{iHt/\hbar} \frac{i}{\hbar}[H, \Psi(x_1)\Psi(x_2)] e^{-iHt/\hbar} | \beta \rangle$$

$$[H^{(1)}, \Psi(x_1)\Psi(x_2)] = [H^{(1)}, \Psi(x_1)]\Psi(x_2) + \Psi(x_1)[H^{(1)}, \Psi(x_2)]$$

$$= -T_{x_1}\Psi(x_1)\,\Psi(x_2) - \Psi(x_1)\,T_{x_2}\Psi(x_2)$$

So the contribution from $H^{(1)}$ is

$$i\hbar \frac{i}{\hbar}(-)\,(T_{x_1} + T_{x_2}) \langle 0 | e^{iHt/\hbar} \Psi(x_1)\Psi(x_2) e^{-iHt/\hbar} | \beta \rangle$$

$$= (T_{x_1} + T_{x_2})\,\Phi_\beta(x_1 x_2 t)$$

Q.E.D. for $N = 2$ if $V_2 = 0$

Now the contribution from $H^{(2)}$ $\longrightarrow$

$$i\hbar \langle 0| e^{iHt/\hbar} \frac{i}{\hbar}[H^{(2)}, \Psi(x_1)\Psi(x_2)] e^{-iHt/\hbar} |\beta\rangle$$

Now, $[H^{(2)}, \Psi_1\Psi_2] = \underbrace{[H^{(2)}, \Psi_1]}_{(A)}\Psi_2 + \underbrace{\Psi_1[H^{(2)}, \Psi_2]}_{(B)}$

(A) $$[H^{(2)}, \Psi_1] = \int d^3x\, d^3x'\, \frac{1}{2} V(x,x') \left[\Psi^+(x)\Psi^+(x')\Psi(x)\Psi(x'), \Psi(x_1)\right]$$

⋮ ~~Homework Problem~~

$$= \{-\Psi^+(x)\delta^3(x'-x_1) - \Psi^+(x')\delta^3(x-x_1)\}\Psi(x)\Psi(x')$$

Both terms have Ψ^+ as the left most factor.

But $\langle 0|\Psi^+ = 0$. So (A) = 0.

(B) $$\Psi(x_1)[H^{(2)}, \Psi(x_2)] = \int d^3x\, d^3x'\, \frac{1}{2} V(x,x')$$

$$\times \Psi(x_1)\{-\Psi^+(x)\delta^3(x'-x_2) - \Psi^+(x')\delta^3(x-x_2)\}\Psi(x)\Psi(x')$$

Because $\langle 0|\Psi^+ = 0$,

I can replace $\Psi(x_1)\Psi^+(x) \to \delta^3(x_1-x)$

and $\Psi(x_1)\Psi^+(x') \to \delta^3(x_1-x')$.

Therefore

$$(B) = i\hbar \frac{i}{\hbar}(-)\langle 0| e^{iHt/\hbar}\int d^3x\, d^3x'\, \frac{1}{2} V(x,x')\Psi(x)\Psi(x') e^{-iHt/\hbar} \{\delta^3(x_1-x)\delta^3(x_2-x') + \delta^3(x_1-x')\delta^3(x-x_2)\}|\beta\rangle$$

$$= \frac{1}{2}V(x_1,x_2)\Phi_\beta(x_1,x_2) + \frac{1}{2}V(x_2,x_1)\Phi_\beta(x_2,x_1)$$

$$= V(x_1,x_2)\,\Phi_\beta(x_1,x_2)$$

Result :

$$i\hbar\, \partial\Phi_\beta / \partial t =$$

$$(T_{x1} + T_{x2})\ \Phi_\beta(x_1, x_2)$$

$$+ V(x_1, x_2)\ \Phi_\beta(x_1, x_2)$$

Q.E.D. for N = 2.

By induction...
The second quantized theory is equivalent to the first quantized theory.

If they are equivalent, what is the advantage?

1c. FERMIONS

Start again with the first quantized N-body Hamiltonian ,

$$H = \sum_k T_k + \tfrac{1}{2} \sum'_{kl} V(x_k, x_l)$$

(T and V would be matrices w. r. t. spin space.)

Now add the ***antisymmetry*** of the of the wave function $\Phi(x_1\, x_2 \ldots x_k \ldots x_N\, ; t)$,

$$\Phi(\ldots x_k \ldots x_l \ldots ; t)$$
$$= - \Phi(\ldots x_l \ldots x_k \ldots ; t) \;\; **$$

*for any pair , k and l ; **for fermions**.*

** The exchange of coordinates must also include spin indices, which are suppressed in this notation.

Fermions are easier than bosons because the occupation numbers are more limited:

For any single-particle state i, n_i can only be 0 or 1 .

That's the *Pauli exclusion principle*.

It is a consequence of the antisymmetry of the wave function.

$$\ldots \psi_E(x_k) \ldots \psi_{E'}(x_l) \ldots$$

must be equal to

$$- \ldots \psi_E(x_l) \ldots \psi_{E'}(x_k) \ldots$$

If E' = E then the N-body wave function would be 0; i.e., it's *not an allowed state*.

Theorem.

The anticommutation relations of the **fermion field** imply that the N-fermion **wave function** is antisymmetric with respect to interchanges of particle coordinates.

Proof. $A_{ji} = \langle 0|\ldots\Psi(x_j)\ldots\Psi(x_i)\ldots|\alpha\rangle$

Pull $\Psi(x_i)$ to the left.

$$\Psi(x')\,\Psi(x_i) + \Psi(x_i)\,\Psi(x') = 0$$

$$\therefore\ \Psi(x')\,\Psi(x_i) = -\,\Psi(x_i)\,\Psi(x')\ ;$$

so pick up a minus sign each time $\Psi(x_i)$ moves one step to the left.

$\Rightarrow$ Factor $(-1)^{n+1}$ when $\Psi(x_i)$ is to the left of $\Psi(x_j)$.

Then move $\Psi(x_j)$ to the right.

$\Rightarrow$ Additional factor of $(-1)^n$.

Result:

$$A_{ji} = -\langle 0|\ldots\Psi(x_i)\ldots\Psi(x_j)\ldots|\alpha\rangle = -\,A_{ij} \qquad \|$$

Homework due Friday, February 5 ...

Problem 13.

(a) Consider the state $c_i^\dagger\ c_j^\dagger\ |0\rangle$,
where i and j are labels for single particle states and $c_i^\dagger$ is an *electron* creation operator. Determine the 2-particle wave function.

(b) Write down a reasonable approximation for the wave function of a helium atom in its ground state.

(c) Verify that the wave function in (b) is antisymmetric under exchange.

$\{c_i, c_j\}=0 \qquad \{c_i^\dagger\ c_j^\dagger\}=0 \qquad \{c_i, c_j^\dagger\}=\delta_{ij}$