Week 3

PHY 635 Many-body Quantum Mechanics of Degenerate Gases
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2.3 Quantum Fields

Let us expand our assembly of the second quantized Hamiltonian in (2.21) again

$$\hat{H} = \sum_{nm} \langle \varphi_n | \hat{A} | \varphi_m \rangle \hat{a}_n^\dagger \hat{a}_m + \sum_{nmlk} \langle \varphi_n \varphi_m | \hat{B} | \varphi_l \varphi_k \rangle \hat{a}_m^\dagger \hat{a}_n^\dagger \hat{a}_l \hat{a}_k \tag{2.23}$$

Using the position space representation of $|\varphi_n\rangle$, this becomes

$$\hat{H} = \sum_{nm} \int dx \; \varphi_n^*(x) \hat{A}(x) \varphi_m(x) \hat{a}_n^\dagger \hat{a}_m + \sum_{nmlk} \int dx \int dy \; \varphi_n^*(x) \varphi_m^*(y) \hat{B}(x,y) \varphi_l(x) \varphi_k(y) \hat{a}_n^\dagger \hat{a}_m^\dagger \hat{a}_l \hat{a}_k \tag{2.24}$$

We now lump together the position space single particle basis functions $\varphi_n(x)$ and operators $\hat{a}_n$ into the

Field Operator

$$\hat{\Psi}(x) = \sum_n \varphi_n(x) \hat{a}_n \tag{2.25}$$

Using this notation, the Hamiltonian is

$$\hat{H} = \int dx \; \hat{\Psi}^\dagger(x) \hat{A}(x) \hat{\Psi}(x) + \int dx \int dy \; \hat{\Psi}^\dagger(y) \hat{\Psi}^\dagger(x) \hat{B}(x,y) \hat{\Psi}(x) \hat{\Psi}(y) \tag{2.26}$$

For the same case as (2.16) we have:

Hamiltonian for particles in a 1D harmonic trap (with interactions)

$$\hat{H} = \int dx \; \hat{\Psi}^\dagger(x) \underbrace{\left[-\frac{\hbar^2}{2m} \nabla_x^2 + V(x) \right]}_{\equiv \hat{H}_o} \hat{\Psi}(x) + \frac{1}{2} \int dx \int dy \; \hat{\Psi}^\dagger(y) \hat{\Psi}^\dagger(x) U(x-y) \hat{\Psi}(x) \hat{\Psi}(y) \tag{2.27}$$

- Field operator is also simply the annihilation operator for the position-basis. Think of it as annihilating a particle at position "x". To see this consider the state $|\, x \,\rangle = \hat{\Psi}^\dagger(x)|\, 0 \,\rangle = \sum_n \varphi_n(x)\hat{a}_n^\dagger|\, 0 \,\rangle$. If we now consider the overlapp of two of these states we have

$$\langle\, y \,|\, x \,\rangle = \langle\, 0 \,|\sum_{nm} \varphi_m^*(y)\varphi_n(x)\hat{a}_m\hat{a}_n^\dagger|\, 0 \,\rangle. \tag{2.28}$$

Using the orthogonality of Fock states, this reduces to $\langle\, y \,|\, x \,\rangle = \sum_n \varphi_n^*(y)\varphi_n(x) \overset{\text{see QM book}}{=} \delta(x-y)$. Since the states only overlap for $x = y$, they must be position eigenstates.

- All three descriptions (2.12), (2.14), (2.27) are fully equivalent, which is "best" depends on the problem.

- Using (2.8) and $\sum_n \varphi_n(x)\varphi_n^*(y) = \delta(x-y)$ we can show

Commutation relations for field operators

$$\begin{aligned} \text{Bosons}: \left[\hat{\Psi}(x), \hat{\Psi}^\dagger(y)\right] &= \delta(x-y), \qquad \left[\hat{\Psi}(x), \hat{\Psi}(y)\right] = 0 \\ \text{Fermions}: \left\{\hat{\Psi}(x), \hat{\Psi}^\dagger(y)\right\} &= \delta(x-y), \qquad \left\{\hat{\Psi}(x), \hat{\Psi}(y)\right\} = 0 \end{aligned} \tag{2.29}$$

2.3.1 Examples of Quantum Fields

Advantages/strengths of quantum field concept:

- Naturally deals with particle creation/anhilation and conversion. Different Fock-states (2.2) can be viewed as different excited states of the underlying the field.

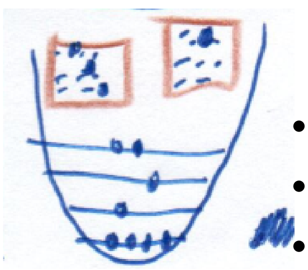
- Formulated in time and space (t, $\mathbf{x}$), quantum fields can naturally address spatial and temporal coherence properties (e.g. see chapter 3).

- Can conveniently formulate Lorentz-invariant (relativistic) theories and take care of causality.

Examples:

Example A: Harmonically trapped dilute Bose gas

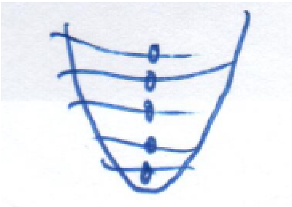
$$\hat{\Psi}(x) = \sum_n \underbrace{\varphi_n(x)}_{\text{SHO modes}} \hat{a}_n$$



- typically atom number conserved and non-relativistic
- Field operator useful to describe coherence and condensation.
- Atom number may fluctuate if part of the system external.

Examples cont:

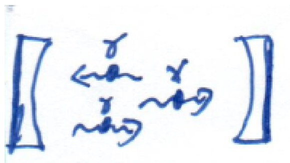
Example B: Harmonically trapped dilute Fermi gas.



We expect here that Fermi blocking or the Pauli exclusion principle play a crucial role. These first two examples are the sole focus of this lecture. The remaining ones are listed to provide links to other lectures.

Example C: Quantized light field / electric field in QED, Quantum Optics

$$\hat{\vec{E}}(\vec{r},t) = \sum_k \vec{\epsilon}_k \mathcal{E}_k \hat{a}_k e^{-i\omega_k t + i\mathbf{k}\cdot\mathbf{r}} + \text{H.c.}$$



where,

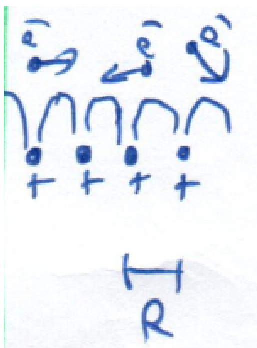
$\vec{\epsilon}_k$ - Polarization vector, $\mathcal{E}_k$ - Amplitude, $e^{-i\omega_k t + i\mathbf{k}\cdot\mathbf{r}}$ - Plane wave (Photon-mode)

Example D: Relativistic spin $\frac{1}{2}$ field (e.g. quarks/electrons)

$$\hat{\Psi}_\alpha(x) = \sum_{s=\pm\frac{1}{2}} \int \frac{d^3p}{(2\pi)^3 2p_0} \left(\underbrace{e^{-ipx} u_\alpha(p,s)\hat{a}(p,s)}_{\text{particle}} + \underbrace{e^{ipx} v_\alpha(p,s)\hat{a}^\dagger(p,s)}_{\text{anti-particle}} \right)$$

where α - spin index, x - 4-vector(t,$\mathbf{x}$), $u_\alpha(p,s)$ - Spinor

Example E: Non-relativistic electron gas in condensed-matter



$$\hat{\Psi}_\sigma(x) = \sum_n \int dk \;\; \hat{a}_{nk} \;\; \underbrace{u_{nk}(r)}_{\text{Bloch-function}} \;\; \underbrace{e^{ikx}}_{\text{plane-wave}} \;\; \underbrace{\chi_\sigma}_{\text{spin}}$$

where, n - Band index, $u_{nk}(r)$ - Bloch function with periodicity R

$$u_{nk}(r+R) = u_{nk}(r)$$

- Quantum fields are operators and thus on the same level as an Observable in single body quantum mechanics.
- A specific physical situation requires us in principle to specify also an underlying (many-body)

quantum state $|\,\psi\,\rangle$.

- With that we can then evaluate specific expectation values involving the quantum field.

Example: Interplay of quantum field and quantum state: Consider N Bosonic atoms in a 1D harmonic trap as in Example A above.
Using (2.10) and (2.25), we can show that the total number of atoms is:

$$N = \int dx \hat{\Psi}^{\dagger}(x)\hat{\Psi}(x). \tag{2.30}$$

This motivates viewing $\hat{\rho}(x) = \hat{\Psi}^{\dagger}(x)\hat{\Psi}(x)$ as operator for the density of atoms.
We shall see two sources of fluctuations for this density: One due to the underlying quantum state of the field, and one due to the discreteness of the individual atoms. To measure local density, we count atoms in a small region of size L as shown in the figure, to find the local number of atoms in this region

$$\hat{n}_{\text{loc}}(x_0) = \int_{x_0}^{x_0+L} dx \hat{\Psi}^{\dagger}(x)\hat{\Psi}(x), \tag{2.31}$$

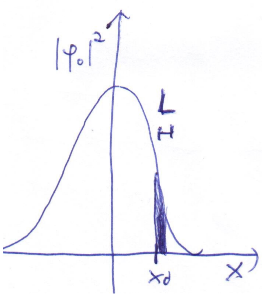
and then use $\hat{\rho} = n_{\text{loc}}(x_0)/L$ to get a density. Let us define the local number uncertainty

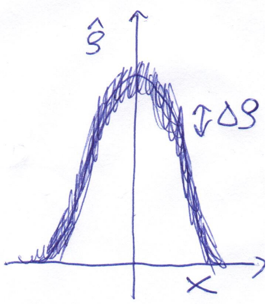
$$\Delta n_{\text{loc}}(x_0)^2 = \langle \hat{n}_{\text{loc}}(x_0)^2 \rangle - \langle \hat{n}_{\text{loc}}(x_0) \rangle^2. \tag{2.32}$$

You should have seen similar expressions for e.g. position uncertainty ΔX in basic QM.

Case (i): Quantum state $\psi = |\,N, 0, 0, 0 \cdots\rangle$, i.e. all N atoms are in the ground state. We can see a mean local number $\langle \hat{\rho} \rangle = N p_{\text{loc}}$ and an uncertainty $\Delta n_{\text{loc}}(x_0) = \sqrt{N(p_{\text{loc}} - p_{\text{loc}}^2)}$, where $p_{\text{loc}} = \int_0^L du |\varphi_0(x_0 + u)|^2$ is the single atom probability to be in the chosen region. The uncertainty arises because the density measurement is based on a finite sample number of atoms.
Case (ii): Quantum state $\psi = [|\,N-k, 0, 0, 0 \cdots\rangle + |\,N+k, 0, 0, 0 \cdots\rangle]/\sqrt{2}$ for $k < N$. Now the atom number itself is uncertain. We find again $\langle \hat{\rho} \rangle = N p_{\text{loc}}$ but this time $\Delta n_{\text{loc}}(x_0) = \sqrt{N(p_{\text{loc}} - p_{\text{loc}}^2) + k^2 p_{\text{loc}}^2}$. Thus while we can have the same mean density, increasing k increases the density fluctuations. This now happens because of the quantum state itself.

Note that all the properties above changed based on quantum state.





- As we see later, often the detailed specification of the underlying quantum state can be avoided however, by simply postulating certain properties of expectation values of field operators, and then working with those.

2.3.2 Dynamics of quantum fields

Here the field operators are mainly a way to re-write the Hamiltonian. Much of the usual methodology of quantum mechanics can be applied as before.

E.g. Consider the Heisenberg picture[1] for the field operator in (2.27): $i\hbar\dot{\hat{\Psi}} = [\hat{\Psi}, \hat{H}]$:

Heisenberg equation for Field operator

$$i\hbar\dot{\hat{\Psi}}(x,t) = \hat{H}_0\hat{\Psi}(x,t) + \int d^3y\ \hat{\Psi}^\dagger(y,t)U(x-y)\hat{\Psi}(y,t)\hat{\Psi}(x,t) \tag{2.33}$$

- We have made use of the commutation relation (2.29).
- We shall begin exploring BEC from here in chapter 3.

Example: Non-interacting evolution of atom-field (thus the Hamiltonian is as in (2.16) but with $U = 0$)
Insert $\hat{\Psi}(x) = \sum_n \varphi_n(x)\hat{a}_n$ into (3.38).

$$i\hbar\sum_n \varphi_n(x)\dot{\hat{a}}_n = \hat{H}_0\left(\sum_n \varphi_n(x)\hat{a}_n\right) \tag{2.34}$$

$$= \sum_n \underbrace{\hat{H}_0\varphi_n(x)}_{=E_n\varphi_n(x)}\ \hat{a}_n \tag{2.35}$$

$$\tag{2.36}$$

Multiplying by $\int dx\varphi_m^*(x)$

$$i\hbar\dot{\hat{a}}_m = E_m\hat{a}_m \tag{2.37}$$

$$\implies \hat{a}_m(t) = \hat{a}(0)e^{-i\frac{E_m t}{\hbar}} \tag{2.38}$$

$$\implies \hat{\Psi}(x,t) = \sum_n \varphi_n(x)e^{-i\frac{E_n t}{\hbar}}\hat{a}(0) \tag{2.30b}$$

The number of cases where (2.30) can be solved is limited. But we also still have:

[1] If unfamiliar, please revise all three QM dynamical pictures (Schrödinger-, Heisenberg-, Interaction picture)

Time-evolution operator:

$$\hat{U}(t, t_0) = \mathcal{T}\left[\exp\left[-i\int_{t_0}^{t} dt' \hat{H}(t')\right]\right] \tag{2.39}$$

- Evolves a (many-body) quantum state in time

$$|\,\psi(t)\,\rangle = \hat{U}(t, t_0)|\,\psi(t_0)\,\rangle$$

- $\hat{H}$ & initial/final states can be written using field operators.
- We can move to the interaction picture to replace $\hat{H}(t')$ with some (weaker) interaction $\hat{V}$(t') in (2.31).
- Then expand exponential in a power series → time-dependent perturbation theory, Feynman diagrams (not here).

2.3.3 Observables and Green's functions[1]

1. As usual in QM, all physical observations related to a quantum field can be written as expectation value of an operator.
2. In 2.2.1 we showed of all operators can be expressed by creation-(destruction-) operator $\hat{a}^\dagger(\hat{a})$.
3. These in turn can all be expressed through field operators.

All up, a huge list of phenomena can be understood from correlation functions:

Green's function: Roughly of the form

$$G^{(n)}(x_1 t, ..., x_n t | x_1' t', ..., x_n' t') = \langle \hat{\Psi}^\dagger(x_n,' t'), ..., \hat{\Psi}^\dagger(x_1,' t') | \hat{\Psi}(x_n, t), ..., \hat{\Psi}(x_1, t) \rangle \tag{2.40}$$

There are lots and lots of alternative definitions.

2.3.4 Spin-statistics theorem

This really belongs to the realm of relativistic quantum mechanics or particle physics, but we could not resist sketching it here. You know that:

[1]See Bruus and Flensberg

Spin-statistics theorem:

$$\begin{aligned} \underline{\text{Half-integer spin particles}} &= \underline{\text{Fermions}}\ (s = \tfrac{1}{2}, \tfrac{3}{2}, etc.) \\ \underline{\text{Integer spin particles}} &= \underline{\text{Bosons}}\ (s = 0, 1, 2, etc.) \end{aligned} \tag{2.41}$$

This follows necessarily from casuality and Lorentz invariance.

Rough sketch of the proof:

- Hamiltonian density $\hat{H} = \int d^4x \hat{\mathscr{H}}(x)$ (where $x = (t, \mathbf{x})$) must obey $\left[\hat{\mathscr{H}}(x), \hat{\mathscr{H}}(y)\right] = 0$ for $(x-y)^2 = c^2\Delta t^2 - \Delta x^2 < 0$. (A)
(This means space-like seperated events cannot affect each other.)

- Quantum fields obey specific transformation laws under Lorentz-transformations Λ (4x4 matrix), depending on spin of the field.

$$U(\Lambda)\hat{\Psi}^\dagger(x)U^{-1}(\Lambda) = \hat{\Psi}^\dagger(\Lambda x) \qquad \text{(spin zero)}$$
$$U(\Lambda)\hat{\Psi}^\dagger_s(x)U^{-1}(\Lambda) = \sum_{s'} \underbrace{D_{ss'}(\Lambda^{-1})}_{\equiv\ representation\ matrix} \hat{\Psi}^\dagger_{s'}(\Lambda x) \qquad \text{(spin 1/2)}$$

- It turns out that (A) works out if

$$\left[\hat{\Psi}(x), \hat{\Psi}^\dagger(y)\right] = 0 \qquad \text{for } (x-y)^2 < 0 \qquad \text{(integer spin)}$$
$$\left\{\hat{\Psi}(x), \hat{\Psi}^\dagger(y)\right\} = 0 \qquad \text{for } (x-y)^2 < 0 \qquad \text{(half-integer spin)}$$

2.3.5 Notation overview-I

We have introduced a lot of different but similar symbols for single vs many body states and operators. We will attempt to stick to the following notation:

Notation:

$\vert w_n\rangle, \vert\varphi_n\rangle, w_n(\mathbf{x}), \varphi_n(\mathbf{x})$	Single particle bases and their position representation.
$\vert\psi\rangle$, $\psi(\mathbf{x}_1, \mathbf{x}_2, ...)$	Many-body state and its (1st quantized) position representation.
$\hat{\Psi}(\mathbf{x})$	Field operator
$\hat{b}, \hat{b}^\dagger$	Harmonic oscillator ladder operator.
$\hat{a}_n, \hat{a}^\dagger_n, \hat{c}_n, \hat{c}^\dagger_n$	Creation and anhilation operators for various bases $\vert w_n\rangle, \vert\varphi_n\rangle$