Week 2

PHY 635 Many-body Quantum Mechanics of Degenerate Gases
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2 Quantum Many-Body Formalism

2.1 Second Quantisation

In principle we could work out most of many-body quantum mechanics using (anti-) symmetrized wave functions such as Eq. (1.32). We could generalise that expression to more particles using the

(Anti-) Symmetrization Operator

$$\hat{P}_{\{\frac{B}{F}\}}\psi\left(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, , , \mathbf{x}_N\right) = \mathcal{N}\sum_{\mathcal{P}} \xi^{\mathcal{P}}\psi\left(\mathbf{x}_{\mathcal{P}(1)}, \mathbf{x}_{\mathcal{P}(2)}, ..., \mathbf{x}_{\mathcal{P}(N)}\right) \tag{2.1}$$

$\xi = -1$ (for Fermions) or $\xi = +1$ (for Bosons),
$\mathcal{P} =$ Permutation of $\{1, 2, ..., N\}$, (e.g. $\{1, 3, 2, 4, ..., N\}$),
$\xi^P \leftarrow \xi$ to the power of parity of permutation.
The normalisation factor is $\mathcal{N} = 1/\sqrt{N!\prod_k n_k!}$, where the $\prod$ part is 1 for Fermions.

In practice, such a formalism gets cumbersome quickly. Discouraging example: Write the bosonic states for three particles in three states A, B, C. The only meaningful information in an (anti-) symmetrized many-body wave function is how many particles (not "which") are in which single-particle basis states ϕ_n. We thus introduce:

(Occupation) Number representation

$$|\,\mathbf{N}\,\rangle = |\,N_0, N_1, ...,\rangle, \tag{2.2}$$

which denotes a state where N_0 particles are in state $|\,\phi_0\,\rangle$, N_1 particles are in state $|\,\phi_1\,\rangle$ etc. The vector[a] $\mathbf{N} = [N_0, N_1, N_2, \ldots]^T$ just groups all these numbers. The space of all $\{|\,N_0, ...\rangle\}$ is called the Fock Space.

[a] The superscript ^{T} means "transposed", turning the row I write into a column vector.

- Correct (anti-) symmetrisation is automatically implied in these states

Example (Bosons): If we explicitly write the Fock state in terms of single particles states in the position representation, we get:

$$\langle \mathbf{x} \,|\, 2100... \rangle = \frac{1}{\sqrt{3}}[\phi_0(\mathbf{x_1})\phi_\mathbf{0}(\mathbf{x_2})\phi_\mathbf{1}(\mathbf{x_3}) + \phi_\mathbf{0}(\mathbf{x_1})\phi_\mathbf{0}(\mathbf{x_3})\phi_\mathbf{1}(\mathbf{x_2}) + \phi_\mathbf{0}(\mathbf{x_2})\phi_\mathbf{0}(\mathbf{x_3})\phi_\mathbf{1}(\mathbf{x_1})]$$

We also define one special number state, the vacuum, which has no particles in any state

$$|\, 0 \,\rangle = |\, 0...0 \,\rangle. \tag{2.3}$$

Now define

Creation and Destruction Operators

creation operator for Bosons:
$$a_n^\dagger |\, N_0 N_1 ... \,\rangle = \sqrt{N_n + 1} |\, N_0 N_1 ... (N_n + 1) ... \,\rangle \tag{2.4}$$

annihilation operator for Bosons:
$$a_n |\, N_0 N_1 ... \,\rangle = \sqrt{N_n} |\, N_0 N_1 ... (N_n - 1) ... \,\rangle \tag{2.5}$$

creation operator for Fermions:
$$a_n^\dagger |\, N_0 N_1 ... \,\rangle = (-1)^{\sum_{k<n} N_k} (1 - N_n) |\, N_0 N_1 ... (N_n + 1) ... \,\rangle \tag{2.6}$$

annihilation operator for Fermions:
$$a_n |\, N_0 N_1 ... \,\rangle = (-1)^{\sum_{k<n} N_k} N_n |\, N_0 N_1 ... (N_n - 1) ... \,\rangle \tag{2.7}$$

- The last two relations already incorporate the Pauli inclusion principle on the level of the operators.
- The sign factors appearing for Fermions take care of the fact that a state that is anti-symmetric under exchange of particles $\mathbf{x_1} \leftrightarrow \mathbf{x_2}$, such as $\langle \mathbf{x} \,|\, 11 \,\rangle = \frac{1}{2}\big(\phi_a(\mathbf{x_1})\phi_\mathbf{b}(\mathbf{x_2}) - \phi_\mathbf{b}(\mathbf{x_1})\phi_\mathbf{a}(\mathbf{x_2})\big)$, then is also automatically anti-symmetric under exchange of state labels $a \leftrightarrow b$.

From these definitions, we can show

Commutation Relations

$$[\hat{a}_i, \hat{a}_j] = 0, \quad [\hat{a}_i^\dagger, \hat{a}_j^\dagger] = 0, \quad [\hat{a}_i, \hat{a}_j^\dagger] = \delta_{ij} \qquad \text{(Bosons)}$$
$$\{\hat{a}_i, \hat{a}_j\} = 0, \quad \{\hat{a}_i^\dagger, \hat{a}_j^\dagger\} = 0, \quad \{\hat{a}_i, \hat{a}_j^\dagger\} = \delta_{ij} \qquad \text{(Fermions)} \tag{2.8}$$

- To proof these, apply both sides to a general "test" Fock state.
- We used the

  Anti-Commutator: $\{\hat{A}, \hat{B}\} = \hat{A}\hat{B} + \hat{B}\hat{A}$

- For Bosons this is inspired by the S.H.O ladder operators (1.12) for harmonic oscillator states. They share the commutator algebra with bosonic many-body creation operators.
- Using operatrs $\hat{a}^\dagger$, we can span the entire Fock space:

$$| N_0 N_1 N_2 ... \rangle = \frac{(\hat{a}_0^\dagger)^{N_0} (\hat{a}_1^\dagger)^{N_1} (\hat{a}_2^\dagger)^{N_2} ... | 0 \rangle}{\sqrt{N_0! N_1! N_2! ...}} \tag{2.9}$$

- Fock-states obey orthonormality

$$\langle N_0' N_1' N_2' ... | N_0 N_1 N_2 ... \rangle = \delta_{N_0 N_0'} \delta_{N_1 N_1'} \delta_{N_2 N_2'} ...$$

By combining operators from above, we can define the

Particle number operator

$$\hat{N}_k = \hat{a}_k^\dagger \hat{a}_k, \tag{2.10}$$

which fulfills $\hat{N}_k | \mathbf{N} \rangle = N_k | \mathbf{N} \rangle$.

- Thus Fock states are eigenstates of all the number operators $\hat{N}_k$, with the number of particles in single particle state $| \varphi_k \rangle$ as eigenvalues.
- We finally can define the total number operator

$$\hat{N} = \sum_k \hat{N}_k \tag{2.11}$$

2.1.1 N-Body Operators

Second quantisation now means to re-write everything in terms of creation and destruction operators

Consider a generic 2-body Hamiltonian (in the first quantised form), e.g.

$$\hat{H} = -\frac{\hbar^2}{2m} (\boldsymbol{\nabla}_{x_1}^2 + \boldsymbol{\nabla}_{x_2}^2) + V(\mathbf{x}_1) + V(\mathbf{x}_2) + U(\mathbf{x}_1, \mathbf{x}_2) \tag{2.12}$$

where $\boldsymbol{\nabla}_{x_1}^2$ and $\boldsymbol{\nabla}_{x_2}^2$ are kinetic energies of particle 1,2. V($\mathbf{x}_1$), V($\mathbf{x}_2$) are some external potentials (e.g. harmonic trap, gravity), and U($\mathbf{x}_1$, $\mathbf{x}_2$) is an interaction potential.
We can distinguish here:

Operator types
Single-body Operators (e.g. kinetic energy, potential energy), that are a sum of identical replica acting on each particle:

$$\hat{O}_1 = \sum_k \hat{o}^{(k)}, \text{ where } \hat{o}^{(k)} \text{ acts on a particle k.} \tag{2.13}$$

and a Two-body operator (Interaction potential), that contains both $\hat{\mathbf{x}}_1$ and $\hat{\mathbf{x}}_2$, $\hat{O}_2 = \sum_{kl} \hat{o}^{(kl)}$.

- More generally, there can be N-body operators for any N, but typically the two above are sufficient.
- It is possible to express any first quantised Hamiltonian such as Eq. (2.12) in second quantised form, i.e. using $\hat{a}$, $\hat{a}^\dagger$. To see how, we need to realize:

Equality of operators: Operators $\hat{O}$ are maps in Hilbert Space $\implies$ they are identical if all matrix-elements such as $\langle \phi_A | \hat{O} | \phi_B \rangle$, for all states A and B, are the same.

2.2 Second Quantised Hamiltonian

Let us assume $\hat{H} = \hat{A} + \hat{B}$, where $\hat{A} = \sum_k \hat{\mathcal{A}}^k$ is a single-body and $\hat{B} = \sum_{kl} \hat{\mathcal{B}}^{kl}$ a two-body operator. This results in

Second-Quantised Hamiltonian

$$\hat{H} = \sum_{nm} A_{nm} \hat{a}_n^\dagger \hat{a}_m + \sum_{nmlk} B_{nm,lk} \hat{a}_m^\dagger \hat{a}_n^\dagger \hat{a}_l \hat{a}_k \tag{2.14}$$

$$\begin{aligned} &\text{with single-body matrix-elements: } A_{nm} = \langle \phi_n | \hat{\mathcal{A}} | \phi_m \rangle, \\ &\text{and two-body matrix-elements: } B_{nm,lk} = \langle \phi_n \phi_m | \hat{\mathcal{B}} | \phi_l \phi_k \rangle. \end{aligned} \tag{2.15}$$

Example: Consider N identical particles in a 1-D harmonic trap, interacting with $U(\mathbf{x}_1,\mathbf{x}_2) = U_0 \exp(\frac{-|\mathbf{x}_1-\mathbf{x}_2|^2}{2\eta^2})$. First quantised Hamiltonian:

$$\hat{H} = \sum_{k=1}^{N}\left(-\frac{\hbar^2}{2m}\nabla^2_{\mathbf{x}_k} + V(\mathbf{x}_k)\right) + \frac{1}{2}\sum_{k,l=1}^{N} U(\mathbf{x}_k,\mathbf{x}_l) \tag{2.16}$$

$V(\mathbf{x}_k) = \frac{1}{2}m\omega^2\mathbf{x}_k^2$. We want to use the Harmonic oscillator basis (1.9) to define our $\hat{a}, \hat{a}^\dagger$. In the notation used for Eq. (2.15):

$$\hat{\mathcal{A}} = -\frac{\hbar^2}{2m}\nabla^{\mathbf{2}}_{\mathbf{x}} + V(\hat{\mathbf{x}}) = \hat{H}_{0,osc},$$
$$\hat{\mathcal{B}} = U(\hat{\mathbf{x}},\hat{\mathbf{y}}).$$

Thus,

$$\mathcal{A}_{nm} = \langle\, \phi_n\,|H_{0,osc}|\, \phi_m\,\rangle = E_m\langle\, \phi_n\,|\, \phi_m\,\rangle = \delta_{nm}E_m, \cdots \tag{2.17}$$

Example continued:
...and

$$\mathcal{B}_{nm,lk} = \langle\, \phi_n\phi_m\,|\hat{B}|\, \phi_l\phi_k\,\rangle$$
$$= \int d^3\mathbf{x}\int d^3\mathbf{y}\;\; \phi_n^*(\mathbf{x})\phi_m^*(\mathbf{y})\frac{U(\mathbf{x},\mathbf{y})}{2}\phi_n(\mathbf{x})\phi_m(\mathbf{y})$$

The latter expression is quite complicated, involving many oscillator states and the Gaussian interaction potential, but can in principle be evaluated, at the very least numerically.
Hence, for the 1D case for simplicity:

$$\hat{H} = \sum_n \hbar\omega(n+\frac{1}{2})\hat{a}_n^\dagger\hat{a}_n + \sum_{nmlk} B_{nm,lk}\hat{a}_m^\dagger\hat{a}_n^\dagger\hat{a}_l\hat{a}_k \tag{2.18}$$

<u>Exercise:</u> For $2 \le N \le 3$, explicitly confirm that the matrix elements of operators Eq. (2.16) and Eq. (2.18) are the same between a few pairs of Fock-states Eq. (2.2).

In the same manner, any first quantized many-body Hamiltonian can be converted to second quantized form for any choice of single-particle basis.

2.2.1 Basis Changes

We can always change the single particle basis underlying our second quantisation with a unitary transformation

$$|\,\phi_l\,\rangle = \sum_m u_{lm}|\,w_m\,\rangle \quad u_{lm} = \langle\, w_m\,|\,\phi_l\,\rangle \tag{2.19}$$

Define one set of operators for each, e.g.

$$\langle\, x\,|\hat{a}_n^\dagger|\,0\,\rangle = \phi_n(x) \quad \langle\, x\,|\hat{c}_n^\dagger|\,0\,\rangle = w_n(x)$$

We can show the following

Basis Transformation for Second-Quantised Operators

$$\begin{aligned} \hat{a}_l^\dagger &= \sum_m u_{lm}\hat{c}_m^\dagger \\ \Longrightarrow\ \hat{a} &= \sum_m u_{lm}^*\hat{c}_m \end{aligned} \tag{2.20}$$

Example: Let us rewrite the Hamiltonian Eq. (2.18) in the previous example 1.13 in the momentum basis. Hence we have a continuous form of the transformation Eq. (2.19):

$$\begin{aligned} \phi_l(x) &= \int u_l(k)e^{ikx}dk \qquad \text{since } \langle\, x\,|\,W(k)\,\rangle = \exp\left[ikx\right] \\ u_l(k) &= \frac{1}{2\pi}\int e^{-ikx}\phi_l(x)dx = \tilde{\phi}_l(k) \quad \leftarrow \quad \text{(Momentum space oscillator eigenfunction)} \end{aligned}$$

i.e: $u_{lm} \to u_l(k)$ [m-index became continuous momentum "k" and $\sum_m \to \int dk$]
Hence we have $\hat{a}_l^\dagger = \int u_l(k)\hat{c}^\dagger(k)dk$. The single-body term of Eq. (2.18) becomes

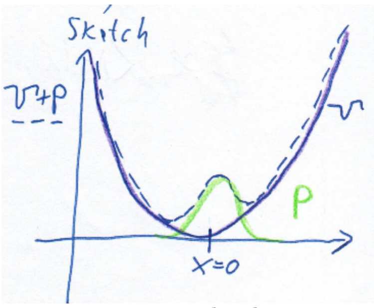
$$\begin{aligned} \sum_n \underbrace{\hbar\omega(n+\frac{1}{2})}_{=E_n}\hat{a}_n^\dagger\hat{a}_n &= \sum_n E_n\int dk\int dk' u_n(k)u_n^*(k')\hat{c}^\dagger(k)\hat{c}(k') \\ &= \int dk\int dk' h(k,k')\hat{c}^\dagger(k)\hat{c}(k') \\ h(k,k') &= \sum_n E_n u_n(k)u_n^*(k') \end{aligned}$$

This term describes the transitions between different momenta, as expected since momentum states are not eigenstates of the single-particle Hamiltonian $\hat{H}_{0,osc}$.

2.2.2 Application: Fermi Blocking vs Bose-Enhancement

Let us consider again N atoms in a harmonic trap, ignore interactions but add a small perturbing potential $P(x) = P_0 \exp\left(-\frac{x^2}{2\eta^2}\right)$. So Eq. (2.16) becomes

$$\hat{H} = \sum_{k=1}^{N} \left(-\frac{\hbar^2}{2m} \nabla^2_{x_k} + V(x_k) + P(x_k) \right) \tag{2.21}$$



left: Sketch of trap and perturbing potential.

We can separately determine the contribution of P(x) to the single body operator and find

$$\hat{H} = [\sum_n E_n \hat{a}^\dagger_n \hat{a}_m + \sum_{nm} \kappa_{nm} \hat{a}^\dagger_n \hat{a}_m]$$
$$\kappa_{nm} = \int dx \ \phi^*_n(x) P(x) \phi_m(x) \tag{2.22}$$

In general, κ_{nm} may be non-zero for $n \neq m$, hence the perturbation induces transitions between oscillator states n, m.

Fermions:

top: What is the transition amplitude from $|\,A\,\rangle = |\,1,1,0,0,...\,\rangle \rightarrow |\,B\,\rangle = |\,2,0,0,0,...\,\rangle$ for Fermions? We consider the following matrix element of the Hamiltonian:

$$\langle\, B\,|\hat{H}|\,A\,\rangle = \langle\, 0\,|\hat{a}_0\hat{a}_0(\sum_{nm} \kappa_{nm}\hat{a}^\dagger_n\hat{a}_m)\hat{a}^\dagger_0\hat{a}_1|\,0\,\rangle = 0.$$

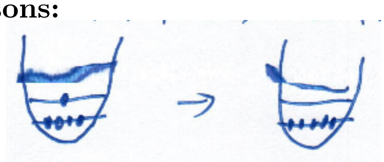
We can see that it must be zero in multiple ways:

1. $= 0$ from $\{\hat{a}_i, \hat{a}_j\} = 0$ in Eq. (2.8)
2. or $= \langle\, 1\,|\hat{a}_0 = [\hat{a}^\dagger_0|\,1\,\rangle]^* = 0$ from Eq. (2.7)
3. or we say $\langle\, 2, 0, 0, ...\,|$ for Fermions didn't make sense to begin with.

Either way, this demonstrates:

Fermi blocking: Fermionic particles cannot make a transition into a state already occupied by another particle.

Bosons:



top: What is the transition amplitude from $|\,A'\,\rangle = |\,N,1,0,0,...\,\rangle \rightarrow |\,B'\,\rangle = |\,N+1,0,0,0,...\,\rangle$ for Bosons?
The corresponding matrix element to the one above is:

$$\langle\,B'\,|\hat{H}|\,A'\,\rangle = \langle\,N+1,0,0,..\,|\sum_{nm}\kappa_{nm}\hat{a}_n^\dagger\hat{a}_m|\,N,1,0,...\,\rangle$$
$$\stackrel{Eq.\ (2.4)-(2.5)}{=} \langle\,N+1,0,0,...\,|\kappa_{01}\sqrt{N+1}\times 1|\,N+1,0,0,...\,\rangle = \sqrt{N+1}\kappa_{01}$$

We see that there is

Bose-Enhancement: The quantum transition amplitude of a Boson into a single-body state already occupied by N other identical Bosons is enhanced by a factor $\sqrt{N+1}$