

Chapter 1

Second Quantization

1.1 Creation and Annihilation Operators in Quantum Mechanics

We will begin with a quick review of creation and annihilation operators in the non-relativistic linear harmonic oscillator. Let a and a^\dagger be two operators acting on an abstract Hilbert space of states, and satisfying the commutation relation

$$[a, a^\dagger] = 1 \quad (1.1)$$

where by “1” we mean the identity operator of this Hilbert space. The operators a and a^\dagger are not self-adjoint but are the adjoint of each other.

Let $|\alpha\rangle$ be a state which we will take to be an eigenvector of the Hermitian operators $a^\dagger a$ with eigenvalue α which is a real number,

$$a^\dagger a |\alpha\rangle = \alpha |\alpha\rangle \quad (1.2)$$

Hence,

$$\alpha = \langle \alpha | a^\dagger a | \alpha \rangle = \|a |\alpha\rangle\|^2 \geq 0 \quad (1.3)$$

where we used the fundamental axiom of Quantum Mechanics that the norm of all states in the physical Hilbert space is positive. As a result, the eigenvalues α of the eigenstates of $a^\dagger a$ must be non-negative real numbers.

Furthermore, since for all operators A , B and C

$$[AB, C] = A[B, C] + [A, C]B \quad (1.4)$$

we get

$$[a^\dagger a, a] = -a \quad (1.5)$$

$$[a^\dagger a, a^\dagger] = a^\dagger \quad (1.6)$$

i.e., a and a^\dagger are “eigen-operators” of $a^\dagger a$. Hence,

$$(a^\dagger a) a = a (a^\dagger a - 1) \quad (1.7)$$

$$(a^\dagger a) a^\dagger = a^\dagger (a^\dagger a + 1) \quad (1.8)$$

Consequently we find

$$(a^\dagger a) a|\alpha\rangle = a (a^\dagger a - 1) |\alpha\rangle = (\alpha - 1) a|\alpha\rangle \quad (1.9)$$

Hence the state $a|\alpha\rangle$ is an eigenstate of $a^\dagger a$ with eigenvalue $\alpha - 1$, provided $a|\alpha\rangle \neq 0$. Similarly, $a^\dagger|\alpha\rangle$ is an eigenstate of $a^\dagger a$ with eigenvalue $\alpha + 1$, provided $a^\dagger|\alpha\rangle \neq 0$. This also implies that

$$|\alpha - 1\rangle = \frac{1}{\sqrt{\alpha}} a|\alpha\rangle \quad (1.10)$$

$$|\alpha + 1\rangle = \frac{1}{\sqrt{\alpha + 1}} a^\dagger|\alpha\rangle \quad (1.11)$$

Let us assume that

$$a^n |\alpha\rangle \neq 0, \quad \forall n \in \mathbb{Z}^+ \quad (1.12)$$

Hence, $a^n|\alpha\rangle$ is an eigenstate of $a^\dagger a$ with eigenvalue $\alpha - n$. However, $\alpha - n < 0$ if $\alpha < n$, which contradicts our earlier result that all these eigenvalues must be non-negative real numbers. Hence, for a given α there must exist an integer n such that $a^n|\alpha\rangle \neq 0$ but $a^{n+1}|\alpha\rangle = 0$, where $n \in \mathbb{Z}^+$. Let

$$|\alpha - n\rangle = \frac{1}{\|a^n|\alpha\rangle\|} a^n|\alpha\rangle \Rightarrow a^\dagger a |\alpha - n\rangle = (\alpha - n) |\alpha - n\rangle \quad (1.13)$$

where

$$\|a^n|\alpha - n\rangle\| = \sqrt{\alpha - n} \quad (1.14)$$

But

$$a|\alpha - n\rangle = -\frac{1}{\|a^n|\alpha\rangle\|} a^{n+1}|\alpha\rangle = 0 \Rightarrow \boxed{\alpha = n} \quad (1.15)$$

In other words the allowed eigenvalues of $a^\dagger a$ are the non-negative integers.

Let us now define the ground state $|0\rangle$, as the state annihilated by a ,

$$a|0\rangle = 0 \quad (1.16)$$

Then, an arbitrary state $|n\rangle$ is

$$|n\rangle = \frac{1}{\sqrt{n!}} (a^\dagger)^n |0\rangle \quad (1.17)$$

which has the inner product

$$\langle n|m\rangle = \delta_{n,m} n! \quad (1.18)$$

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In summary, we found that creation and annihilation operators obey

$$a^\dagger |n\rangle = \sqrt{n+1} |n+1\rangle \quad (1.19)$$

$$a |n\rangle = \sqrt{n} |n-1\rangle \quad (1.20)$$

$$a^\dagger a |n\rangle = n |n\rangle \quad (1.21)$$

$$(1.22)$$

and thus their matrix elements are

$$\langle m | a^\dagger | n \rangle = \sqrt{n+1} \delta_{m,n+1} \quad \langle m | a | n \rangle = \sqrt{n} \delta_{m,n-1} \quad (1.23)$$

1.1.1 The Linear harmonic Oscillator

The Hamiltonian of the Linear Harmonic Oscillator is

$$H = \frac{P^2}{2m} + \frac{1}{2} m \omega^2 X^2 \quad (1.24)$$

where X and P , the coordinate and momentum Hermitian operators satisfy canonical commutation relations,

$$[X, P] = i\hbar \quad (1.25)$$

We now define the creation and annihilation operators a^\dagger and a as

$$a = \frac{1}{\sqrt{2}} \left[\sqrt{\frac{m\omega}{\hbar}} X + i \frac{P}{\sqrt{m\omega\hbar}} \right] \quad (1.26)$$

$$a^\dagger = \frac{1}{\sqrt{2}} \left[\sqrt{\frac{m\omega}{\hbar}} X - i \frac{P}{\sqrt{m\omega\hbar}} \right] \quad (1.27)$$

which satisfy

$$[a, a^\dagger] = 1 \quad (1.28)$$

Since

$$X = \sqrt{\frac{\hbar}{2m\omega}} (a + a^\dagger) \quad (1.29)$$

$$P = \sqrt{\frac{m\omega\hbar}{2}} \frac{(a - a^\dagger)}{i} \quad (1.30)$$

the Hamiltonian takes the simple form

$$H = \hbar\omega \left(a^\dagger a + \frac{1}{2} \right) \quad (1.31)$$

The eigenstates of the Hamiltonian are constructed easily using our results since all eigenstates of $a^\dagger a$ are eigenstates of H . Thus, the eigenstates of H are the eigenstates of $a^\dagger a$,

$$H |n\rangle = \hbar\omega \left(n + \frac{1}{2} \right) |n\rangle \quad (1.32)$$

with eigenvalues

$$E_n = \hbar\omega \left(n + \frac{1}{2} \right) \quad (1.33)$$

where $n = 0, 1, \dots$

The ground state $|0\rangle$ is the state annihilated by a ,

$$a|0\rangle \equiv \frac{1}{2} \left[\sqrt{\frac{m\omega}{\hbar}} X + i \frac{P}{\sqrt{m\omega\hbar}} \right] |0\rangle = 0 \quad (1.34)$$

Since

$$\langle x|P|\phi\rangle = -i\hbar \frac{d}{dx} \langle x|\phi\rangle \quad (1.35)$$

we find that $\psi_0(x) = \langle x|0\rangle$ satisfies

$$\left(x + \frac{\hbar}{m\omega} \frac{d}{dx} \right) \psi_0(x) = 0 \quad (1.36)$$

whose (normalized) solution is

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar} \right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2} \quad (1.37)$$

The wave functions $\psi_n(x)$ of the excited states $|n\rangle$ are

$$\begin{aligned} \psi_n(x) &= \langle x|n\rangle = \frac{1}{\sqrt{n!}} \langle x|(a^\dagger)^n|0\rangle \\ &= \frac{1}{\sqrt{n!}} \left(\frac{m\omega}{2\hbar} \right)^{n/2} \left(x - \frac{\hbar}{m\omega} \frac{d}{dx} \right)^n \psi_0(x) \end{aligned} \quad (1.38)$$

Creation and annihilation operators are very useful. Let us consider for instance the anharmonic oscillator whose Hamiltonian is

$$H = \frac{P^2}{2m} + \frac{1}{2}m\omega^2 X^2 + \lambda X^4 \quad (1.39)$$

Let us compute the eigenvalues E_n to lowest order in perturbation theory in powers of λ . The first order shift ΔE_n is

$$\begin{aligned} \Delta E_n &= \lambda \langle n|X^4|n\rangle + O(\lambda^2) \\ &= \lambda \left(\frac{\hbar}{2m\omega} \right)^2 \langle n|(a + a^\dagger)^4|n\rangle + \dots \\ &= \lambda \left(\frac{\hbar}{2m\omega} \right)^2 \{ \langle n|a^\dagger a^\dagger a a|n\rangle + \text{other terms with two } a's \text{ and two } a^\dagger's \} + \dots \\ &= \lambda \left(\frac{\hbar}{2m\omega} \right)^2 (6n^2 + 6n + 3) + \dots \end{aligned} \quad (1.40)$$

1.1.2 Many Harmonic Oscillators

It is trivial to extend these ideas to the case of many harmonic oscillators, which is a crude model of an elastic solid. Consider a system of N identical linear harmonic oscillators of mass M and frequency ω , with coordinates $\{Q_i\}$ and momenta $\{P_i\}$, where $i = 1, \dots, N$. These operators satisfy the commutation relations

$$[Q_j, Q_k] = [P_j, P_k] = 0, \quad [Q_j, P_k] = i\hbar\delta_{jk} \quad (1.41)$$

where $j, k = 1, \dots, N$. The Hamiltonian is

$$H = \sum_{i=1}^N \frac{P_i^2}{2M_i} + \frac{1}{2} \sum_{i,j=1}^N V_{ij} Q_i Q_j \quad (1.42)$$

where V_{ij} is a symmetric positive definite matrix, $V_{ij} = V_{ji}$.

We will find the spectrum (and eigenstates) of this system by changing variables to normal modes and using creation and annihilation operators for the normal modes. To this end we will first rescale coordinates and momenta so as to absorb the particle mass M :

$$x_i = \sqrt{M_i} Q_i \quad (1.43)$$

$$p_i = \frac{P_i}{\sqrt{M_i}} \quad (1.44)$$

$$U_{ij} = \frac{1}{\sqrt{M_i M_j}} V_{ij} \quad (1.45)$$

which also satisfy

$$[x_j, p_j] = i\hbar\delta_{jk} \quad (1.46)$$

and

$$H = \sum_{i=1}^N \frac{p_i^2}{2} + \frac{1}{2} \sum_{i,j=1}^N U_{ij} x_i x_j \quad (1.47)$$

We now get to normal mode variables by means of an orthogonal transformation C_{jk} , *i.e.* $[C^{-1}]_{jk} = C_{kj}$,

$$\begin{aligned} \tilde{x}_k &= \sum_{j=1}^N C_{kj} x_j, & \tilde{p}_k &= \sum_{j=1}^N C_{kj} p_j \\ \sum_{i=1}^N C_{ki} C_{ji} &= \delta_{kj}, & \sum_{i=1}^N C_{ik} C_{ij} &= \delta_{kj} \end{aligned} \quad (1.48)$$

Since the matrix U_{ij} is real symmetric and positive definite, its eigenvalues, which we will denote by ω_k^2 (with $k = 1, \dots, N$), are all non-negative, $\omega_k^2 \geq 0$. The eigenvalue equation is

$$\sum_{i,j=1}^N C_{ki} C_{lj} U_{ij} = \omega_k^2 \delta_{kl}, \quad (\text{no sum over } k) \quad (1.49)$$

Since the transformation is orthogonal, it preserves the commutation relations

$$[\tilde{x}_j, \tilde{x}_k] = [\tilde{p}_j, \tilde{p}_k] = 0, \quad [\tilde{x}_j, \tilde{p}_k] = i\hbar\delta_{jk} \quad (1.50)$$

and the Hamiltonian is now diagonal

$$H = \frac{1}{2} \sum_{i=1}^N (\tilde{p}_i^2 + \omega_i^2 \tilde{x}_i^2) \quad (1.51)$$

We now define creation and annihilation operators for the normal modes

$$\begin{aligned} a_j &= \frac{1}{\sqrt{2\hbar}} \left(\sqrt{\omega_j} \tilde{x}_j + \frac{i}{\sqrt{\omega_j}} \tilde{p}_j \right) \\ a_j^\dagger &= \frac{1}{\sqrt{2\hbar}} \left(\sqrt{\omega_j} \tilde{x}_j - \frac{i}{\sqrt{\omega_j}} \tilde{p}_j \right) \\ \tilde{x}_j &= \sqrt{\frac{\hbar}{2\omega_j}} (a_j + a_j^\dagger) \\ \tilde{p}_j &= -i\sqrt{\frac{\hbar\omega_j}{2}} (a_j - a_j^\dagger) \end{aligned} \quad (1.52)$$

where, once again,

$$[a_j, a_k] [a_j^\dagger, a_k^\dagger] = 0, \quad [a_j, a_k^\dagger] = \delta_{jk} \quad (1.53)$$

and the normal mode Hamiltonian takes the standard form

$$H = \sum_{j=1}^N \hbar\omega_j \left(a_j^\dagger a_j + \frac{1}{2} \right) \quad (1.54)$$

The eigenstates of the Hamiltonian are labelled by the eigenvalues of $a_j^\dagger a_j$ for each normal mode j , $|n_1, \dots, n_N\rangle \equiv |\{n_j\}\rangle$. Hence,

$$H|n_1, \dots, n_N\rangle = \sum_{j=1}^N \hbar\omega_j \left(n_j + \frac{1}{2} \right) |n_1, \dots, n_N\rangle \quad (1.55)$$

where

$$|n_1, \dots, n_N\rangle = \left[\prod_{j=1}^N \frac{(a_j^\dagger)^{n_j}}{\sqrt{n_j!}} \right] |0, \dots, 0\rangle \quad (1.56)$$

The ground state of the system, which we will denote by $|0\rangle$, is the state in which all normal modes are in their ground state,

$$|0\rangle \equiv |0, \dots, 0\rangle \quad (1.57)$$

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Thus, the ground state $|0\rangle$ is annihilated by the annihilation operators of all normal modes,

$$a_j|0\rangle = 0, \quad \forall j \quad (1.58)$$

and the ground state energy of the system E_{gnd} is

$$E_{\text{gnd}} = \sum_{j=1}^N \frac{1}{2} \hbar \omega_j \quad (1.59)$$

The energy of the excited states is

$$E(n_1, \dots, n_N) = \sum_{j=1}^N \hbar \omega_j n_j + E_{\text{gnd}} \quad (1.60)$$

We can now regard the state $|0\rangle$ as the *vacuum state* and the excited states $|n_1, \dots, n_N\rangle$ as a state with n_j *excitations* (or particles) of type j . In this context, the excitations are called *phonons*. A *single-phonon* state of type j will be denoted by $|j\rangle$, is

$$|j\rangle = a_j^\dagger |0\rangle = |0, \dots, 0, 1_j, 0, \dots, 0\rangle \quad (1.61)$$

This state is an eigenstate of H ,

$$H|j\rangle = H a_j^\dagger |0\rangle = (\hbar \omega_j + E_{\text{gnd}}) a_j^\dagger |0\rangle = (\hbar \omega_j + E_{\text{gnd}}) |j\rangle \quad (1.62)$$

with *excitation* energy $\hbar \omega_j$. Hence, an arbitrary state $|n_1, \dots, n_N\rangle$ can also be regarded as a collection of non-interacting particles (or excitations), each carrying an energy equal to the excitation energy (relative to the ground state energy). The total number of phonons in a given state is measured by the number operator

$$\hat{N} = \sum_{j=1}^N a_j^\dagger a_j \quad (1.63)$$

Notice that although the number of oscillators is fixed (and equal to N) the number of excitations may differ greatly from one state to another.

We now note that the state $|n_1, \dots, n_N\rangle$ can also be represented as

$$|n_1, \dots, n_k, \dots\rangle \equiv \frac{1}{\sqrt{n_1! n_2! \dots}} | \overbrace{1 \dots 1}^{n_1}, \overbrace{2 \dots 2}^{n_2} \dots \rangle \quad (1.64)$$

We will see below that this form appears naturally in the quantization of systems of identical particles. Eq.(1.64) is *symmetric* under the exchange of labels of the phonons. Thus, phonons are *bosons*.

1.2 The Quantized Elastic Solid

We will now consider the problem of an elastic solid in the approximation of continuum elasticity, *i.e.* we will be interested in vibrations on wavelengths long compared to the inter-atomic spacing. At the classical level, the physical state of this system is determined by specifying the local three-component vector *displacement field* $\vec{u}(\vec{r}, t)$, which describes the local displacement of the atoms away from their equilibrium positions, and by the velocities of the atoms, $\frac{\partial \vec{u}}{\partial t}(\vec{r}, t)$. The classical Lagrangian L for an isotropic solid is

$$L = \int d^3r \frac{\rho}{2} \left(\frac{\partial u}{\partial t} \right)^2 - \frac{1}{2} \int d^3r [K \nabla_i u_j \nabla_i u_j + \Gamma \nabla_i u_i \nabla_j u_j] \quad (1.65)$$

where ρ is the mass density, K and Γ are two elastic moduli.

The classical equations of motion are

$$\frac{\delta L}{\delta u_i} = \frac{\partial}{\partial t} \left(\frac{\delta L}{\delta \dot{u}_i} \right) \quad (1.66)$$

which have the explicit form of a wave equation

$$\rho \frac{\partial^2 u_i}{\partial t^2} - K \nabla^2 u_i - \Gamma \nabla_i \vec{\nabla} \cdot \vec{u} = 0 \quad (1.67)$$

We now define the *canonical momentum* $\Pi_i(\vec{r}, t)$

$$\Pi_i(\vec{r}, t) = \frac{\delta L}{\delta \dot{u}_i} = \rho \dot{u}_i \quad (1.68)$$

which *in this case* coincides with the linear momentum density of the particles. The classical Hamiltonian H is

$$H = \int d^3r \Pi_i(\vec{r}, t) \frac{\partial \vec{u}}{\partial t}(\vec{r}, t) - L = \int d^3r \left[\frac{\vec{\Pi}^2}{2\rho} + \frac{K}{2} (\nabla_i \vec{u})^2 + \frac{\Gamma}{2} (\vec{\nabla} \cdot \vec{u})^2 \right] \quad (1.69)$$

In the quantum theory, the displacement field $\vec{u}(\vec{r})$ and the canonical momentum $\vec{\Pi}(\vec{r})$ become operators acting on a Hilbert space, obeying the equal-time commutation relations

$$\left[u_i(\vec{r}), u_j(\vec{R}) \right] = \left[\Pi_i(\vec{r}), \Pi_j(\vec{R}) \right] = 0, \quad \left[u_i(\vec{r}), \Pi_j(\vec{R}) \right] = i\hbar \delta(\vec{r} - \vec{R}) \delta_{ij} \quad (1.70)$$

Due to the translational invariance of the continuum solid, the canonical transformation to normal modes is found essentially by Fourier transforms. Thus we write

$$\tilde{u}_i(\vec{p}) = \int d^3r e^{-i\vec{p}\cdot\vec{r}} u_i(\vec{r}) \quad (1.71)$$

$$\tilde{\Pi}_i(\vec{p}) = \int d^3r e^{-i\vec{p}\cdot\vec{r}} \Pi_i(\vec{r}) \quad (1.72)$$

Using the representations of the Dirac δ -function

$$\delta^3(\vec{r} - \vec{R}) = \int \frac{d^3p}{(2\pi)^3} e^{i\vec{p}\cdot(\vec{r}-\vec{R})} \quad (1.73)$$

$$(2\pi)^3 \delta^3(\vec{p} - \vec{q}) = \int d^3r e^{-i(\vec{p}-\vec{q})\cdot\vec{r}} \quad (1.74)$$

we can write

$$u_i(\vec{r}) = \frac{1}{\sqrt{\rho}} \int \frac{d^3p}{(2\pi)^3} e^{i\vec{p}\cdot\vec{r}} \tilde{u}_i(\vec{p}) \quad (1.75)$$

$$\Pi_i(\vec{r}) = \sqrt{\rho} \int \frac{d^3p}{(2\pi)^3} e^{i\vec{p}\cdot\vec{r}} \tilde{\Pi}_i(\vec{p}) \quad (1.76)$$

where we have scaled out the density for future convenience. On the other hand, since $u_i(\vec{r})$ and $\Pi_i(\vec{r})$ are real (and Hermitian)

$$u_i(\vec{r}) = u_i^\dagger(\vec{r}), \quad \Pi_i(\vec{r}) = \Pi_i^\dagger(\vec{r}) \quad (1.77)$$

their Fourier transformed fields $\tilde{u}_i(\vec{p})$ and $\tilde{\Pi}_i(\vec{p})$ obey

$$\tilde{u}_i^\dagger(\vec{p}) = \tilde{u}_i(-\vec{p}), \quad \tilde{\Pi}_i^\dagger(\vec{p}) = \tilde{\Pi}_i(-\vec{p}) \quad (1.78)$$

with equal-time commutation relations

$$[\tilde{u}_j(\vec{p}), \tilde{u}_k(\vec{q})] = [\tilde{\Pi}_j(\vec{p}), \tilde{\Pi}_k(\vec{q})] = 0, \quad [\tilde{u}_j(\vec{p}), \tilde{\Pi}_k(\vec{q})] = i\hbar(2\pi)^3 \delta^3(\vec{p} + \vec{q}) \delta_{jk} \quad (1.79)$$

In terms of the Fourier transformed fields the Hamiltonian has the form

$$H = \int \frac{d^3p}{(2\pi)^3} \left(\frac{1}{2} \tilde{\Pi}_i(-\vec{p}) \tilde{\Pi}_i(\vec{p}) + \frac{1}{2} \omega_{ij}^2(\vec{p}) \tilde{u}_i(-\vec{p}) \tilde{u}_j(\vec{p}) \right) \quad (1.80)$$

where

$$\omega_{ij}^2(\vec{p}) = \frac{K}{\rho} \vec{p}^2 \delta_{ij} + \frac{\Gamma}{\rho} p_i p_j \quad (1.81)$$

The 3×3 matrix ω_{ij}^2 has two eigenvalues:

1.

$$\omega_L^2(\vec{p}) = \left(\frac{K + \Gamma}{\rho} \right) \vec{p}^2 \quad (1.82)$$

with eigenvector parallel to the unit vector $\vec{p}/|\vec{p}|$

2.

$$\omega_T^2(\vec{p}) = \left(\frac{K}{\rho} \right) \vec{p}^2 \quad (1.83)$$

with a two-dimensional degenerate space spanned by the mutually orthogonal unit vectors $\vec{e}_1(\vec{p})$ and $\vec{e}_2(\vec{p})$, both orthogonal to \vec{p} :

$$\vec{e}_\alpha(\vec{p}) \cdot \vec{p} = 0, \quad (\alpha = 1, 2), \quad \vec{e}_1(\vec{p}) \cdot \vec{e}_2(\vec{p}) = 0 \quad (1.84)$$

We can now expand the displacement field $\tilde{u}(\vec{p})$ into a *longitudinal* component

$$\tilde{u}_i^L(\vec{p}) = \tilde{u}_L(\vec{p}) \frac{p_i}{|\vec{p}|} \quad (1.85)$$

and two *transverse* components

$$\tilde{u}_i^T(\vec{p}) = \sum_{\alpha=1,2} \tilde{u}_\alpha^T(\vec{p}) e_i^\alpha(\vec{p}) \quad (1.86)$$

The canonical momenta $\tilde{\Pi}_i(\vec{p})$ can also be expanded into one longitudinal component $\tilde{\Pi}_L(\vec{p})$ and two transverse components $\tilde{\Pi}_\alpha^T(\vec{p})$. As a result the Hamiltonian can be decomposed into a sum of two terms,

$$H = H_L + H_T \quad (1.87)$$

- H_L involves only the longitudinal component of the field and momenta

$$H_L = \frac{1}{2} \int \frac{d^3p}{(2\pi)^3} \left\{ \tilde{\Pi}_L(-\vec{p}) \tilde{\Pi}_L(\vec{p}) + \omega_L^2(\vec{p}) \tilde{u}_L(-\vec{p}) \tilde{u}_L(\vec{p}) \right\} \quad (1.88)$$

- H_T involves only the transverse components of the field and momenta

$$H_T = \frac{1}{2} \int \frac{d^3p}{(2\pi)^3} \sum_{\alpha=1,2} \left\{ \tilde{\Pi}_\alpha^T(-\vec{p}) \tilde{\Pi}_\alpha^T(\vec{p}) + \omega_T^2(\vec{p}) \tilde{u}_\alpha^T(-\vec{p}) \tilde{u}_\alpha^T(\vec{p}) \right\} \quad (1.89)$$

We can now define creation and annihilation operators for both longitudinal and transverse components

$$\begin{aligned} a_L(\vec{p}) &= \frac{1}{\sqrt{2\hbar}} \left(\sqrt{\omega_L(\vec{p})} \tilde{u}_L(\vec{p}) + \frac{i}{\sqrt{\omega_L(\vec{p})}} \tilde{\Pi}_L(\vec{p}) \right) \\ a_L(\vec{p})^\dagger &= \frac{1}{\sqrt{2\hbar}} \left(\sqrt{\omega_L(\vec{p})} \tilde{u}_L(-\vec{p}) - \frac{i}{\sqrt{\omega_L(\vec{p})}} \tilde{\Pi}_L(-\vec{p}) \right) \\ a_T^\alpha(\vec{p}) &= \frac{1}{\sqrt{2\hbar}} \left(\sqrt{\omega_T(\vec{p})} \tilde{u}_T^\alpha(\vec{p}) + \frac{i}{\sqrt{\omega_T(\vec{p})}} \tilde{\Pi}_T^\alpha(\vec{p}) \right) \\ a_T^\alpha(\vec{p})^\dagger &= \frac{1}{\sqrt{2\hbar}} \left(\sqrt{\omega_T(\vec{p})} \tilde{u}_T^\alpha(-\vec{p}) - \frac{i}{\sqrt{\omega_T(\vec{p})}} \tilde{\Pi}_T^\alpha(-\vec{p}) \right) \end{aligned} \quad (1.90)$$

which obey standard commutation relations:

$$\begin{aligned} [a_L(\vec{p}), a_L(\vec{q})] &= [a_L(\vec{p})^\dagger, a_L(\vec{q})^\dagger] = 0 \\ [a_L(\vec{p}), a_L(\vec{q})^\dagger] &= (2\pi)^3 \delta^3(\vec{p} - \vec{q}) \\ [a_T^\alpha(\vec{p}), a_T^\beta(\vec{q})] &= [a_T^\alpha(\vec{p})^\dagger, a_T^\beta(\vec{q})^\dagger] = 0 \\ [a_T^\alpha(\vec{p}), a_T^\beta(\vec{q})^\dagger] &= (2\pi)^3 \delta^3(\vec{p} - \vec{q}) \delta_{\alpha\beta} \\ [a_L(\vec{p}), a_T^\alpha(\vec{q})] &= [a_L(\vec{p}), a_T^\alpha(\vec{q})^\dagger] = 0 \end{aligned} \quad (1.91)$$

where $\alpha, \beta = 1, 2$.

Conversely we also have

$$\begin{aligned}
\tilde{u}_L(\vec{p}) &= \sqrt{\frac{\hbar}{2\omega_L(\vec{p})}} (a_L(\vec{p}) + a_L(-\vec{p})^\dagger) \\
\tilde{\Pi}_L(\vec{p}) &= -i \sqrt{\frac{\hbar\omega_L(\vec{p})}{2}} (a_L(\vec{p}) - a_L(-\vec{p})^\dagger) \\
\tilde{u}_T^\alpha(\vec{p}) &= \sqrt{\frac{\hbar}{2\omega_T(\vec{p})}} (a_T^\alpha(\vec{p}) + a_T^\alpha(-\vec{p})^\dagger) \\
\tilde{\Pi}_T^\alpha(\vec{p}) &= -i \sqrt{\frac{\hbar\omega_T(\vec{p})}{2}} (a_T^\alpha(\vec{p}) - a_T^\alpha(-\vec{p})^\dagger)
\end{aligned} \tag{1.92}$$

The Hamiltonian now reads

$$\begin{aligned}
H &= \frac{1}{2} \int \frac{d^3p}{(2\pi)^3} \hbar\omega_L(\vec{p}) (a_L(\vec{p})^\dagger a_L(\vec{p}) + a_L(\vec{p}) a_L(\vec{p})^\dagger) \\
&\quad + \frac{1}{2} \int \frac{d^3p}{(2\pi)^3} \hbar\omega_T(\vec{p}) \sum_{\alpha=1,2} (a_T^\alpha(\vec{p})^\dagger a_T^\alpha(\vec{p}) + a_T^\alpha(\vec{p}) a_T^\alpha(\vec{p})^\dagger) \\
&= E_{\text{gnd}} + \int \frac{d^3p}{(2\pi)^3} \left(\hbar\omega_L(\vec{p}) a_L(\vec{p})^\dagger a_L(\vec{p}) + \sum_{\alpha=1,2} \hbar\omega_T(\vec{p}) a_T^\alpha(\vec{p})^\dagger a_T^\alpha(\vec{p}) \right)
\end{aligned} \tag{1.93}$$

The ground state $|0\rangle$ has energy E_{gnd} ,

$$E_{\text{gnd}} = V \int \frac{d^3p}{(2\pi)^3} \frac{1}{2} (\hbar\omega_L(\vec{p}) + 2\hbar\omega_T(\vec{p})) \tag{1.94}$$

where we have used that

$$\lim_{\vec{p} \rightarrow 0} \delta^3(\vec{p}) = \frac{V}{(2\pi)^3} \tag{1.95}$$

As before the ground state is annihilated by all annihilation operators

$$a_L(\vec{p})|0\rangle = 0, \quad a_T^\alpha(\vec{p})|0\rangle = 0 \tag{1.96}$$

and it will be regarded as the state without phonons.

There are three one-phonon states with wave vector \vec{p} :

- One *longitudinal* phonon state

$$|L, \vec{p}\rangle = a_L(\vec{p})^\dagger |0\rangle \tag{1.97}$$

with energy $E_L(\vec{p})$

$$E_L(\vec{p}) = \hbar\omega_L(\vec{p}) = v_L \hbar|\vec{p}| \tag{1.98}$$

where

$$v_L = \sqrt{\frac{K + \Gamma}{\rho}} \quad (1.99)$$

is the speed of the longitudinal phonon,

- Two *transverse* phonon states

$$|T, \alpha, \vec{p}\rangle = a_T^\alpha(\vec{p})^\dagger |0\rangle \quad (1.100)$$

one for each polarization, with energy $E_T(\vec{p})$

$$E_T(\vec{p}) = \hbar\omega_T(\vec{p}) = v_T \hbar|\vec{p}| \quad (1.101)$$

where

$$v_T = \sqrt{\frac{K}{\rho}} \quad (1.102)$$

is the speed of the transverse phonons.

The energies of the longitudinal and transverse phonon we found vanish as $\vec{p} \rightarrow 0$. These are *acoustic* phonons and the speeds v_L and v_T are speeds of sound. Notice that if the elastic modulus $\Gamma = 0$ all three states become degenerate. If in addition we were to have considered the effects of lattice anisotropies, the two transverse branches may no longer be degenerate as in this case.

Similarly we can define multi-phonon states, with either polarization. For instance a state with two longitudinal phonons with momenta \vec{p} and \vec{q} is

$$|L, \vec{p}, \vec{q}\rangle = a_L(\vec{p})^\dagger a_L(\vec{q})^\dagger |0\rangle \quad (1.103)$$

This state has energy $\hbar\omega_L(\vec{p}) + \hbar\omega_L(\vec{q})$ above the ground state.

Finally, let us define the linear momentum operator \vec{P} , for phonons of either longitudinal or transverse polarization,

$$\vec{P} = \int \frac{d^3p}{(2\pi)^3} \hbar\vec{p} \left(a_L(\vec{p})^\dagger a_L(\vec{p}) + \sum_{\alpha=1,2} a_T^\alpha(\vec{p})^\dagger a_T^\alpha(\vec{p}) \right) \quad (1.104)$$

This operator obeys the commutation relations

$$\begin{aligned} [\vec{P}, a_L(\vec{k})^\dagger] &= \hbar\vec{k}a_L(\vec{k})^\dagger \\ [\vec{P}, a_T^\alpha(\vec{k})^\dagger] &= \hbar\vec{k}a_T^\alpha(\vec{k})^\dagger \\ [\vec{P}, a_L(\vec{k})] &= -\hbar\vec{k}a_L(\vec{k}) \\ [\vec{P}, a_T^\alpha(\vec{k})] &= -\hbar\vec{k}a_T^\alpha(\vec{k}) \end{aligned} \quad (1.105)$$

and commutes with the Hamiltonian

$$[\vec{P}, H] = 0 \quad (1.106)$$

Hence \vec{P} is a conserved quantity. Moreover, using the commutation relations and the expressions for the displacement fields it is easy to show that

$$[\vec{P}, u_i(\vec{x})] = i\hbar \vec{\nabla} u_i(\vec{x}) \quad (1.107)$$

which implies that \vec{P} is the generator of infinitesimal displacements. Hence, it is the linear momentum operator.

It is easy to see that \vec{P} annihilates the ground state

$$\vec{P}|0\rangle = 0 \quad (1.108)$$

which means that the ground state has zero momentum. In other terms, the ground state is translationally invariant (as it should).

Using the commutation relations it is easy to show that

$$\vec{P}|L, \vec{k}\rangle = \hbar\vec{k}|L, \vec{k}\rangle, \quad \vec{P}|T, \alpha, \vec{k}\rangle = \hbar\vec{k}|T, \alpha, \vec{k}\rangle \quad (1.109)$$

which allows us to identify the momentum carried by a phonon with $\hbar\vec{k}$ where \vec{k} is the label of the Fourier transform.

Finally, we notice that we can easily write down an expression for the displacement field $u_i(\vec{r})$ and the canonical momentum $\Pi_i(\vec{r})$ in terms of creation and annihilation operators for longitudinal and transverse phonons:

$$\begin{aligned} u_i(\vec{r}) &= \frac{1}{\sqrt{\rho}} \int \frac{d^3p}{(2\pi)^3} \sqrt{\frac{\hbar}{2\omega_L(p)}} \frac{p_i}{|\vec{p}|} (a_L(\vec{p})e^{i\vec{p}\cdot\vec{r}} - a_L(\vec{p})^\dagger e^{-i\vec{p}\cdot\vec{r}}) \\ &\quad + \frac{1}{\sqrt{\rho}} \int \frac{d^3p}{(2\pi)^3} \sqrt{\frac{\hbar}{2\omega_T(p)}} \sum_{\alpha=1,2} e_i^\alpha(\vec{p}) (a_T^\alpha(\vec{p})e^{i\vec{p}\cdot\vec{r}} - a_T^\alpha(\vec{p})^\dagger e^{-i\vec{p}\cdot\vec{r}}) \end{aligned} \quad (1.110)$$

which is known as a mode expansion. There is a similar expression for the canonical momentum $\Pi_i(\vec{r})$.

In summary, after quantizing the elastic solid we found that the quantum states of this system can be classified in terms of a set of excitations, the longitudinal and transverse phonons. These states carry energy and momentum (as well as polarization) and hence behave as particles. For these reason we will regard these excitations as the *quasi-particles* of this system. We will see that quasi-particles arise generically in interacting many-body system. One problem we will be interested in is in understanding the relation between the properties of the ground state and the quantum numbers of the quasiparticles.

1.3 Indistinguishable Particles

Let us consider now the problem of a system of N *identical* non-relativistic particles. For the sake of simplicity I will assume that the physical state of *each* particle j is described by its position \vec{x}_j relative to some reference frame. This case is easy to generalize.

The wave function for this system is $\Psi(x_1, \dots, x_N)$. If the particles are *identical* then the *probability density*, $|\Psi(x_1, \dots, x_N)|^2$, must be invariant (*i.e.*, unchanged) under arbitrary exchanges of the labels that we use to identify (or designate) the particles. In quantum mechanics, the particles do not have well defined trajectories. Only the states of a physical system are well defined. Thus, even though at some initial time t_0 the N particles may be localized at a set of well defined positions x_1, \dots, x_N , they will become delocalized as the system evolves. Furthermore the Hamiltonian itself is *invariant* under a permutation of the particle labels. Hence, *permutations* constitute a *symmetry* of a many-particle quantum mechanical system. In other terms, identical particles are indistinguishable in quantum mechanics. In particular, the *probability density* of *any* eigenstate must remain invariant if the labels of any pair of particles are exchanged. If we denote by P_{jk} the operator that exchanges the labels of particles j and k , the wave functions must change under the action of this operator *at most* by a phase factor. Hence, we must require that

$$P_{jk}\Psi(x_1, \dots, x_j, \dots, x_k, \dots, x_N) = e^{i\phi}\Psi(x_1, \dots, x_j, \dots, x_k, \dots, x_N) \quad (1.111)$$

Under a further exchange operation, the particles return to their initial labels and we recover the original state. This sample argument then requires that $\phi = 0, \pi$ since 2ϕ must not be an observable phase. We then conclude that there are two possibilities: either Ψ is *even* under permutation and $P\Psi = \Psi$, or Ψ is *odd* under permutation and $P\Psi = -\Psi$. Systems of identical particles which have wave functions which are *even* under a pairwise permutation of the particle labels are called *bosons*. In the other case, Ψ *odd* under pairwise permutation, they are *Fermions*. It must be stressed that these arguments only show that the requirement that the state Ψ be either even or odd is only a *sufficient* condition. It turns out that under special circumstances (*e.g.* in one and two-dimensional systems) other options become available and the phase factor ϕ may take values different from 0 or π . These particles are called *anyons*. For the moment the only cases in which they may exist appears to be in situations in which the particles are restricted to move on a line or on a plane. In the case of *relativistic* quantum field theories, the requirement that the states have well defined *statistics* (or *symmetry*) is demanded by a very deep and fundamental theorem which links the *statistics* of the states of the *spin* of the field. This is known as the *spin-statistics* theorem and it is actually an *axiom* of relativistic quantum mechanics (and field theory).

1.4 Fock Space

We will now discuss a procedure, known as *Second Quantization*, which will enable us to keep track of the symmetry of the states of systems of many identical particles in a simple way. Let us consider a system of N identical non-relativistic particles. The wave functions in the coordinate representation are $\Psi(x_1, \dots, x_N)$ where the labels x_1, \dots, x_N denote both the coordinates and the spin states of the particles in the state $|\Psi\rangle$. For the sake of definiteness we will discuss physical systems describable by Hamiltonians \hat{H} of the form

$$\hat{H} = -\frac{\hbar^2}{2m} \sum_{j=1}^N \nabla_j^2 + \sum_{j=1}^N V(x_j) + \sum_{j,k} U(x_j - x_k) + \dots \quad (1.112)$$

Let $\{\phi_n(x)\}$ be the wave functions for a complete set of one-particle states. Then an arbitrary N -particle state can be expanded in a basis which is the tensor product of the one-particle states, namely

$$\Psi(x_1, \dots, x_N) = \sum_{\{n_j\}} C(n_1, \dots, n_N) \phi_{n_1}(x_1) \dots \phi_{n_N}(x_N) \quad (1.113)$$

Thus, if Ψ is symmetric (antisymmetric) under an arbitrary exchange $x_j \leftrightarrow x_k$, the coefficients $C(n_1, \dots, n_N)$ must be symmetric (antisymmetric) under the exchange $n_j \leftrightarrow n_k$.

A set of N -particle basis states with well defined permutation symmetry is the properly symmetrized or antisymmetrized tensor product

$$|\Psi_1, \dots, \Psi_N\rangle \equiv |\Psi_1\rangle \times |\Psi_2\rangle \times \dots \times |\Psi_N\rangle = \frac{1}{\sqrt{N!}} \sum_P \xi^P |\Psi_{P(1)}\rangle \times \dots \times |\Psi_{P(N)}\rangle \quad (1.114)$$

where the sum runs over the set of all possible permutation P . The weight factor ξ is $+1$ for *bosons* and -1 for *fermions*. Notice that, for fermions, the N -particle state vanishes if two particles are in the same one-particle state. This is the *Pauli Exclusion Principle*.

The inner product of two N -particle states is

$$\begin{aligned} \langle \chi_1, \dots, \chi_N | \psi_1, \dots, \psi_N \rangle &= \frac{1}{N!} \sum_{P, Q} \xi^{P+Q} \langle \chi_{Q(1)} | \psi_{P(1)} \rangle \dots \langle \chi_{Q(N)} | \psi_{P(N)} \rangle = \\ &= \sum_{P'} \xi^{P'} \langle \chi_1 | \psi_{P(1)} \rangle \dots \langle \chi_N | \psi_{P(N)} \rangle \end{aligned} \quad (1.115)$$

where $P' = P + Q$ denotes the permutation resulting from the composition of the permutations P and Q . Since P and Q are arbitrary permutations, P' spans the space of all possible permutations as well.

It is easy to see that Eq.(1.115) is nothing but the *permanent* (*determinant*) of the matrix $\langle \chi_j | \psi_k \rangle$ for *symmetric* (*antisymmetric*) states, *i.e.*,

$$\langle \chi_1, \dots, \chi_N | \psi_1, \dots, \psi_N \rangle = \left| \begin{array}{ccc} \langle \chi_1 | \psi_1 \rangle & \dots & \langle \chi_1 | \psi_N \rangle \\ \vdots & & \vdots \\ \langle \chi_N | \psi_1 \rangle & \dots & \langle \chi_N | \psi_N \rangle \end{array} \right|_{\xi} \quad (1.116)$$

In the case of antisymmetric states, the inner product is the familiar *Slater determinant*.

Let us denote by $\{|\alpha\rangle\}$ a complete set of orthonormal one-particle states. They satisfy

$$\langle \alpha | \beta \rangle = \delta_{\alpha\beta} \quad \sum_{\alpha} |\alpha\rangle \langle \alpha| = 1 \quad (1.117)$$

The N -particle states are $\{|\alpha_1, \dots, \alpha_N\rangle\}$. Because of the symmetry requirements, the labels α_j can be arranged in the form of a monotonic sequence $\alpha_1 \leq \alpha_2 \leq \dots \leq \alpha_N$ for *bosons*, or in the form of a *strict* monotonic sequence $\alpha_1 < \alpha_2 < \dots < \alpha_N$ for *fermions*. Let n_j be an integer which counts how many particles are in the j -th one-particle state. The *boson* states $|\alpha_1, \dots, \alpha_N\rangle$ must be normalized by a factor of the form

$$\frac{1}{\sqrt{n_1! \dots n_N!}} |\alpha_1, \dots, \alpha_N\rangle \quad (\alpha_1 \leq \alpha_2 \leq \dots \leq \alpha_N) \quad (1.118)$$

and n_j are non-negative integers. For *fermions* the states are

$$|\alpha_1, \dots, \alpha_N\rangle \quad (\alpha_1 < \alpha_2 < \dots < \alpha_N) \quad (1.119)$$

and $n_j = 0 > 1$. These N -particle states are complete and orthonormal

$$\frac{1}{N!} \sum_{\alpha_1, \dots, \alpha_N} |\alpha_1, \dots, \alpha_N\rangle \langle \alpha_1, \dots, \alpha_N| = \hat{I} \quad (1.120)$$

where the sum over the α 's is unrestricted and the operator \hat{I} is the identity operator in the space of N -particle states.

We will now consider the more general problem in which the number of particles N is not fixed a-priori. Rather, we will consider an *enlarged* space of states in which the number of particles is allowed to fluctuate. In the language of Statistical Physics what we are doing is to go from the *Canonical Ensemble* to the *Grand Canonical Ensemble*. Thus, let us denote by \mathcal{H}_0 the Hilbert space with no particles, \mathcal{H}_1 the Hilbert space with only one particle and, in general, \mathcal{H}_N the Hilbert space for N -particles. The direct sum of these spaces \mathcal{H}

$$\mathcal{H} = \mathcal{H}_0 \oplus \mathcal{H}_1 \oplus \dots \oplus \mathcal{H}_N \oplus \dots \quad (1.121)$$

is usually called *Fock space*.

An arbitrary state $|\psi\rangle$ in Fock space is the sum over the subspaces \mathcal{H}_N ,

$$|\psi\rangle = |\psi^{(0)}\rangle + |\psi^{(1)}\rangle + \dots + |\psi^{(N)}\rangle + \dots \quad (1.122)$$

The subspace with no particles is a one-dimensional space spanned by the vector $|0\rangle$ which we will call the *vacuum*. The subspaces with well defined number of particles are defined to be orthogonal to each other in the sense that the *inner product* in *Fock space*

$$\langle \chi | \psi \rangle \equiv \sum_{j=0}^{\infty} \langle \chi^{(j)} | \psi^{(j)} \rangle \quad (1.123)$$

vanishes if $|\chi\rangle$ and $|\psi\rangle$ belong to different subspaces.

1.5 Creation and Annihilation Operators

Let $|\phi\rangle$ be an arbitrary *one-particle state*, i.e. $|\phi\rangle \in \mathcal{H}_1$. Let us define the *creation operator* $\hat{a}^\dagger(\phi)$ by its action on an arbitrary state in Fock space

$$\hat{a}^\dagger(\phi)|\psi_1, \dots, \psi_N\rangle = |\phi, \psi_1, \dots, \psi_N\rangle \quad (1.124)$$

Clearly, $\hat{a}^\dagger(\phi)$ maps the N -particle state with proper symmetry $|\psi_1, \dots, \psi_N\rangle$ to the $N+1$ -particle state $|\phi, \psi_1, \dots, \psi_N\rangle$, also with proper symmetry. The *destruction* or *annihilation operator* $\hat{a}(\phi)$ is then defined as the *adjoint* of $\hat{a}^\dagger(\phi)$,

$$\langle \chi_1, \dots, \chi_{N-1} | \hat{a}(\phi) | \psi_1, \dots, \psi_N \rangle = \langle \psi_1, \dots, \psi_N | \hat{a}^\dagger(\phi) | \chi_1, \dots, \chi_{N-1} \rangle^* \quad (1.125)$$

Hence

$$\begin{aligned} \langle \chi_1, \dots, \chi_{N-1} | \hat{a}(\phi) | \psi_1, \dots, \psi_N \rangle &= \langle \psi_1, \dots, \psi_N | \phi, \chi_1, \dots, \chi_{N-1} \rangle^* = \\ &= \left| \begin{array}{cccc} \langle \psi_1 | \phi \rangle & \langle \psi_1 | \chi_1 \rangle & \cdots & \langle \psi_1 | \chi_{N-1} \rangle \\ \vdots & \vdots & & \vdots \\ \langle \psi_N | \phi \rangle & \langle \psi_N | \chi_1 \rangle & \cdots & \langle \psi_N | \chi_{N-1} \rangle \end{array} \right|_{\xi}^* \end{aligned} \quad (1.126)$$

We can now expand the permanent (or determinant) to get

$$\begin{aligned} \langle \chi_1, \dots, \chi_{N-1} | \hat{a}(\phi) | \psi_1, \dots, \psi_N \rangle &= \\ &= \sum_{k=1}^N \xi^{k-1} \langle \psi_k | \phi \rangle \left| \begin{array}{ccc} \langle \psi_1 | \chi_1 \rangle & \cdots & \langle \psi_1 | \chi_{N-1} \rangle \\ \vdots & & \vdots \\ \cdots & (\text{no } \psi_k) & \cdots \\ \langle \psi_N | \chi_1 \rangle & \cdots & \langle \psi_N | \chi_{N-1} \rangle \end{array} \right|_{\xi}^* \\ &= \sum_{k=1}^N \xi^{k-1} \langle \psi_k | \phi \rangle \langle \chi_1, \dots, \chi_{N-1} | \psi_1, \dots, \hat{\psi}_k, \dots, \psi_N \rangle \end{aligned} \quad (1.127)$$

where $\hat{\psi}_k$ indicates that ψ_k is *absent*.

Thus, the destruction operator is given by

$$\hat{a}(\phi)|\psi_1, \dots, \psi_N\rangle = \sum_{k=1}^N \xi^{k-1} \langle \phi | \psi_k \rangle |\psi_1, \dots, \hat{\psi}_k, \dots, \psi_N\rangle \quad (1.128)$$

With these definitions, we can easily see that the operators $\hat{a}^\dagger(\phi)$ and $\hat{a}(\phi)$ obey the commutation relations

$$\hat{a}^\dagger(\phi_1)\hat{a}^\dagger(\phi_2) = \xi \hat{a}^\dagger(\phi_2)\hat{a}^\dagger(\phi_1) \quad (1.129)$$

Let us introduce the notation

$$[\hat{A}, \hat{B}]_{-\xi} \equiv \hat{A}\hat{B} - \xi \hat{B}\hat{A} \quad (1.130)$$

where \hat{A} and \hat{B} are two arbitrary operators. For $\xi = +1$ (*bosons*) we have the *commutator*

$$[\hat{a}^\dagger(\phi_1), \hat{a}^\dagger(\phi_2)]_{+1} \equiv [\hat{a}^\dagger(\phi_1), \hat{a}^\dagger(\phi_2)] = 0 \quad (1.131)$$

while for $\xi = -1$ it is the *anticommutator*

$$[\hat{a}^\dagger(\phi_1), \hat{a}^\dagger(\phi_2)]_{-1} \equiv \{\hat{a}^\dagger(\phi_1), \hat{a}^\dagger(\phi_2)\} = 0 \quad (1.132)$$

Similarly for any pair of arbitrary one-particle states $|\phi_1\rangle$ and $|\phi_2\rangle$ we get

$$[\hat{a}(\phi_1), \hat{a}(\phi_2)]_{-\xi} = 0 \quad (1.133)$$

It is also easy to check that the following identity holds

$$[\hat{a}(\phi_1), \hat{a}^\dagger(\phi_2)]_{-\xi} = \langle \phi_1 | \phi_2 \rangle \quad (1.134)$$

So far we have not picked any particular representation. Let us consider the *occupation number representation* in which the states are labelled by the number of particles n_k in the single-particle state k . In this case, we have

$$|n_1, \dots, n_k, \dots\rangle \equiv \frac{1}{\sqrt{n_1! n_2! \dots}} |\overbrace{1 \dots 1}^{n_1}, \overbrace{2 \dots 2}^{n_2} \dots\rangle \quad (1.135)$$

In the case of *bosons*, the n_j 's can be any non-negative integer, while for *fermions* they can only be equal to zero or one. In general we have that if $|\alpha\rangle$ is the α th single-particle state, then

$$\begin{aligned} \hat{a}_\alpha^\dagger |n_1, \dots, n_\alpha, \dots\rangle &= \sqrt{n_\alpha + 1} |n_1, \dots, n_\alpha + 1, \dots\rangle \\ \hat{a}_\alpha |n_1, \dots, n_\alpha, \dots\rangle &= \sqrt{n_\alpha} |n_1, \dots, n_\alpha - 1, \dots\rangle \end{aligned} \quad (1.136)$$

Thus for both *fermions* and *bosons*, \hat{a}_α annihilates all states with $n_\alpha = 0$, while for *fermions* \hat{a}_α^\dagger annihilates all states with $n_\alpha = 1$.

The commutation relations

$$[\hat{a}_\alpha, \hat{a}_\beta] = [\hat{a}_\alpha^\dagger, \hat{a}_\beta^\dagger] = 0 \quad [\hat{a}_\alpha, \hat{a}_\beta^\dagger] = \delta_{\alpha\beta} \quad (1.137)$$

apply for bosons, while the anticommutation relations

$$\{\hat{a}_\alpha \hat{a}_\beta\} = \{\hat{a}_\beta^\dagger, \hat{a}_\alpha^\dagger\} = 0 \quad \{\hat{a}_\alpha, \hat{a}_\beta^\dagger\} = \delta_{\alpha\beta} \quad (1.138)$$

apply for fermions. Here, $\{\hat{A}, \hat{B}\}$ is the anticommutator of the operators \hat{A} and \hat{B}

$$\{\hat{A}, \hat{B}\} \equiv \hat{A}\hat{B} + \hat{B}\hat{A} \quad (1.139)$$

If a unitary transformation is performed in the space of one-particle state vectors, then a unitary transformation is *induced* in the space of the operators themselves, *i.e.*, if $|\chi\rangle = \alpha|\psi\rangle + \beta|\phi\rangle$, then

$$\begin{aligned} \hat{a}(\chi) &= \alpha^* \hat{a}(\psi) + \beta^* \hat{a}(\phi) \\ \hat{a}^\dagger(\chi) &= \alpha \hat{a}^\dagger(\psi) + \beta \hat{a}^\dagger(\phi) \end{aligned} \quad (1.140)$$

and we say that $\hat{a}^\dagger(\chi)$ transforms like the *ket* $|\chi\rangle$ while $\hat{a}(\chi)$ transforms like the *bra* $\langle\chi|$.

For example, we can pick as the complete set of one-particle states the momentum states $\{|\vec{p}\rangle\}$. This is “momentum space”. With this choice the commutation relations are

$$\begin{aligned} [\hat{a}^\dagger(\vec{p}), \hat{a}^\dagger(\vec{q})]_{-\xi} &= [\hat{a}(\vec{p}), \hat{a}(\vec{q})]_{-\xi} = 0 \\ [\hat{a}(\vec{p}), \hat{a}^\dagger(\vec{q})]_{-\xi} &= (2\pi)^d \delta^d(\vec{p} - \vec{q}) \end{aligned} \quad (1.141)$$

where d is the dimensionality of space. In this representation, an N -particle state is

$$|\vec{p}_1, \dots, \vec{p}_N\rangle = \hat{a}^\dagger(\vec{p}_1) \dots \hat{a}^\dagger(\vec{p}_N)|0\rangle \quad (1.142)$$

On the other hand, we can also pick the one-particle states to be eigenstates of the position operators, *i.e.*,

$$|\vec{x}_1, \dots, \vec{x}_N\rangle = \hat{a}^\dagger(\vec{x}_1) \dots \hat{a}^\dagger(\vec{x}_N)|0\rangle \quad (1.143)$$

In position space, the operators satisfy

$$\begin{aligned} [\hat{a}^\dagger(\vec{x}_1), \hat{a}^\dagger(\vec{x}_2)]_{-\xi} &= [\hat{a}(\vec{x}_1), \hat{a}(\vec{x}_2)]_{-\xi} = 0 \\ [\hat{a}(\vec{x}_1), \hat{a}^\dagger(\vec{x}_2)]_{-\xi} &= \delta^d(\vec{x}_1 - \vec{x}_2) \end{aligned} \quad (1.144)$$

This is the position space or coordinate representation. A transformation from position space to momentum space is the Fourier transform

$$|\vec{p}\rangle = \int d^d x |\vec{x}\rangle \langle \vec{x} | \vec{p}\rangle = \int d^d x |\vec{x}\rangle e^{i\vec{p}\cdot\vec{x}} \quad (1.145)$$

and, conversely

$$|\vec{x}\rangle = \int \frac{d^d p}{(2\pi)^d} |\vec{p}\rangle e^{-i\vec{p}\cdot\vec{x}} \quad (1.146)$$

Then, the operators themselves obey

$$\begin{aligned} \hat{a}^\dagger(\vec{p}) &= \int d^d x \hat{a}^\dagger(\vec{x}) e^{i\vec{p}\cdot\vec{x}} \\ \hat{a}^\dagger(\vec{x}) &= \int \frac{d^d p}{(2\pi)^d} \hat{a}^\dagger(\vec{p}) e^{-i\vec{p}\cdot\vec{x}} \end{aligned} \quad (1.147)$$

1.6 General Operators in Fock Space

Let $A^{(1)}$ be an operator acting on one-particle states. We can always define an *extension* \hat{A} of $A^{(1)}$ acting on any arbitrary state $|\psi\rangle$ of the N -particle Hilbert space \mathcal{H}_N as follows:

$$\hat{A}|\psi\rangle \equiv \sum_{j=1}^N |\psi_1\rangle \times \dots \times A^{(1)}|\psi_j\rangle \times \dots \times |\psi_N\rangle \quad (1.148)$$

For instance, if the one-particle basis states $\{|\psi_j\rangle\}$ are eigenstates of \hat{A} with eigenvalues $\{a_j\}$ we get

$$\hat{A}|\psi\rangle = \left(\sum_{j=1}^N a_j \right) |\psi\rangle \quad (1.149)$$

We wish to find an expression for an arbitrary operator \hat{A} in terms of creation and annihilation operators. Let us first consider the operator $A_{\alpha\beta}^{(1)} = |\alpha\rangle\langle\beta|$ which acts on one-particle states. The operators $A_{\alpha\beta}^{(1)}$ form a basis of the space of operators acting on one-particle states. Then, the N -particle extension of $A_{\alpha\beta}^{(1)}$ is

$$\hat{A}_{\alpha\beta}|\psi\rangle = \sum_{j=1}^N |\psi_1\rangle \times \dots \times |\alpha\rangle \times \dots \times |\psi_N\rangle \langle\beta|\psi_j\rangle \quad (1.150)$$

Thus

$$\hat{A}_{\alpha\beta}|\psi\rangle = \sum_{j=1}^N |\psi_1, \dots, \overbrace{\alpha}^j, \dots, \psi_N\rangle \langle\beta|\psi_j\rangle \quad (1.151)$$

In other words, we can replace the one-particle state $|\psi_j\rangle$ from the basis with the state $|\alpha\rangle$ at the price of a weight factor, the overlap $\langle\beta|\psi_j\rangle$. This operator has a very simple expression in terms of creation and annihilation operators. Indeed,

$$\hat{a}^\dagger(\alpha)\hat{a}(\beta)|\psi\rangle = \sum_{k=1}^N \xi^{k-1} \langle\beta|\psi_k\rangle |\alpha, \psi_1, \dots, \psi_{k-1}, \psi_{k+1}, \dots, \psi_N\rangle \quad (1.152)$$

We can now use the symmetry of the state to write

$$\xi^{k-1} |\alpha, \psi_1, \dots, \psi_{k-1}, \psi_{k+1}, \dots, \psi_N\rangle = |\psi_1, \dots, \overbrace{\alpha}^k, \dots, \psi_N\rangle \quad (1.153)$$

Thus the operator $\hat{A}_{\alpha\beta}$, the extension of $|\alpha\rangle\langle\beta|$ to the N -particle space, coincides with $\hat{a}^\dagger(\alpha)\hat{a}(\beta)$

$$\hat{A}_{\alpha\beta} \equiv \hat{a}^\dagger(\alpha)\hat{a}(\beta) \quad (1.154)$$

We can use this result to find the extension for an arbitrary operator $A^{(1)}$ of the form

$$A^{(1)} = \sum_{\alpha,\beta} |\alpha\rangle\langle\alpha|A^{(1)}|\beta\rangle \langle\beta| \quad (1.155)$$

we find

$$\hat{A} = \sum_{\alpha,\beta} \hat{a}^\dagger(\alpha)\hat{a}(\beta)\langle\alpha|A^{(1)}|\beta\rangle \quad (1.156)$$

Hence the coefficients of the expansion are the matrix elements of $A^{(1)}$ between arbitrary one-particle states. We now discuss a few operators of interest.

1. *The Identity Operator:*

The Identity Operator $\hat{1}$ of the one-particle Hilbert space

$$\hat{1} = \sum_{\alpha} |\alpha\rangle\langle\alpha| \quad (1.157)$$

becomes the *number operator* \hat{N}

$$\hat{N} = \sum_{\alpha} \hat{a}^\dagger(\alpha)\hat{a}(\alpha) \quad (1.158)$$

In position and in momentum space we find

$$\hat{N} = \int \frac{d^d p}{(2\pi)^d} \hat{a}^\dagger(\vec{p})\hat{a}(\vec{p}) = \int d^d x \hat{a}^\dagger(\vec{x})\hat{a}(\vec{x}) = \int d^d x \hat{\rho}(\vec{x}) \quad (1.159)$$

where $\hat{\rho}(x) = \hat{a}^\dagger(\vec{x})\hat{a}(\vec{x})$ is the *particle density operator*.

2. *The Linear Momentum Operator:*

In the space \mathcal{H}_1 , the linear momentum operator is

$$\hat{p}_j^{(1)} = \int \frac{d^d p}{(2\pi)^d} p_j |\vec{p}\rangle\langle\vec{p}| = \int d^d x |\vec{x}\rangle \frac{\hbar}{i} \partial_j \langle\vec{x}| \quad (1.160)$$

Thus, we get that the total linear momentum operator \hat{P}_j is

$$\hat{P}_j = \int \frac{d^d p}{(2\pi)^d} p_j \hat{a}^\dagger(\vec{p}) \hat{a}(\vec{p}) = \int d^d x \hat{a}^\dagger(\vec{x}) \frac{\hbar}{i} \partial_j \hat{a}(\vec{x}) \quad (1.161)$$

3. Hamiltonian:

The one-particle Hamiltonian $H^{(1)}$

$$H^{(1)} = \frac{\vec{p}^2}{2m} + V(\vec{x}) \quad (1.162)$$

has the matrix elements

$$\langle \vec{x} | H^{(1)} | \vec{y} \rangle = -\frac{\hbar^2}{2m} \nabla^2 \delta^d(\vec{x} - \vec{y}) + V(\vec{x}) \delta^d(\vec{x} - \vec{y}) \quad (1.163)$$

Thus, in Fock space we get

$$\hat{H} = \int d^d x \hat{a}^\dagger(\vec{x}) \left[-\frac{\hbar^2}{2m} \nabla^2 + V(\vec{x}) \right] \hat{a}(\vec{x}) \quad (1.164)$$

in position space. In momentum space we can define

$$\tilde{V}(\vec{q}) = \int d^d x V(\vec{x}) e^{-i\vec{q}\cdot\vec{x}} \quad (1.165)$$

the Fourier transform of the potential $V(x)$, and get

$$\hat{H} = \int \frac{d^d p}{(2\pi)^d} \frac{\vec{p}^2}{2m} \hat{a}^\dagger(\vec{p}) \hat{a}(\vec{p}) + \int \frac{d^d p}{(2\pi)^d} \int \frac{d^d q}{(2\pi)^d} \tilde{V}(\vec{q}) \hat{a}^\dagger(\vec{p} + \vec{q}) \hat{a}(\vec{p}) \quad (1.166)$$

The last term has a very simple physical interpretation. When acting on a one-particle state with well-defined momentum, say $|\vec{p}\rangle$, the potential term yields another one-particle state with momentum $\vec{p} + \vec{q}$, where \vec{q} is the *momentum transfer*, with amplitude $\tilde{V}(\vec{q})$. This *process* is usually depicted by the diagram of Fig.1.1.

4. Two-Body Interactions:

A two-particle interaction is an operator $\hat{V}^{(2)}$ which acts on the space of two-particle states \mathcal{H}_2 , which has the form

$$V^{(2)} = \frac{1}{2} \sum_{\alpha, \beta} |\alpha, \beta\rangle V^{(2)}(\alpha, \beta) \langle \alpha, \beta| \quad (1.167)$$

The methods developed above yield an extension of $V^{(2)}$ to Fock space of the form

$$\hat{V} = \frac{1}{2} \sum_{\alpha, \beta} \hat{a}^\dagger(\alpha) \hat{a}^\dagger(\beta) \hat{a}(\beta) \hat{a}(\alpha) V^{(2)}(\alpha, \beta) \quad (1.168)$$

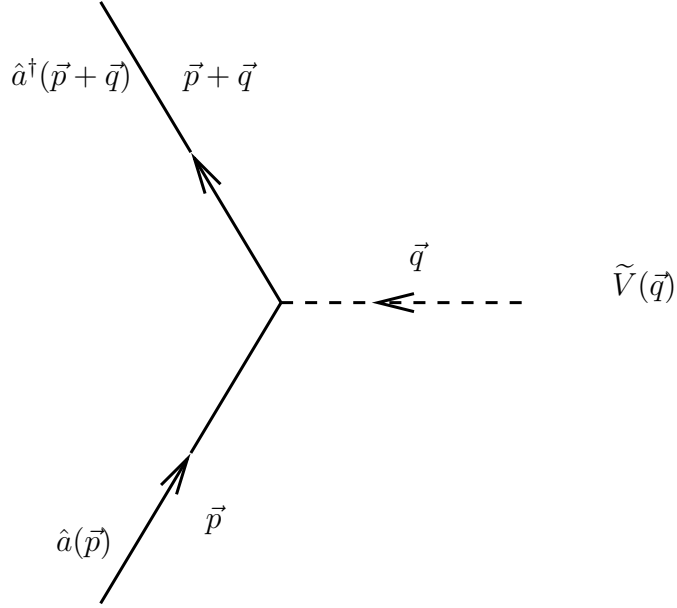


Figure 1.1: One-body scattering.

In position space, ignoring spin, we get

$$\begin{aligned} \hat{V} &= \frac{1}{2} \int d^d x \int d^d y \hat{a}^\dagger(\vec{x}) \hat{a}^\dagger(\vec{y}) \hat{a}(\vec{y}) \hat{a}(\vec{x}) V^{(2)}(\vec{x}, \vec{y}) \\ &\equiv \frac{1}{2} \int d^d x \int d^d y \hat{\rho}(\vec{x}) V^{(2)}(\vec{x}, \vec{y}) \hat{\rho}(\vec{y}) + \frac{1}{2} \int d^d x V^{(2)}(\vec{x}, \vec{x}) \hat{\rho}(\vec{x}) \end{aligned} \quad (1.169)$$

where we have used the commutation relations. In momentum space we find instead

$$\hat{V} = \frac{1}{2} \int \frac{d^d p}{(2\pi)^d} \int \frac{d^d q}{(2\pi)^d} \int \frac{d^d k}{(2\pi)^d} \tilde{V}(\vec{k}) \hat{a}^\dagger(\vec{p} + \vec{k}) \hat{a}^\dagger(\vec{q} - \vec{k}) \hat{a}(\vec{q}) \hat{a}(\vec{p}) \quad (1.170)$$

where $\tilde{V}(\vec{k})$ is only a function of the momentum transfer \vec{k} . This is a consequence of translation invariance. In particular for a Coulomb interaction,

$$V^{(2)}(\vec{x}, \vec{y}) = \frac{e^2}{|\vec{x} - \vec{y}|} \quad (1.171)$$

for which

$$\tilde{V}(\vec{k}) = \frac{4\pi e^2}{k^2} \quad (1.172)$$

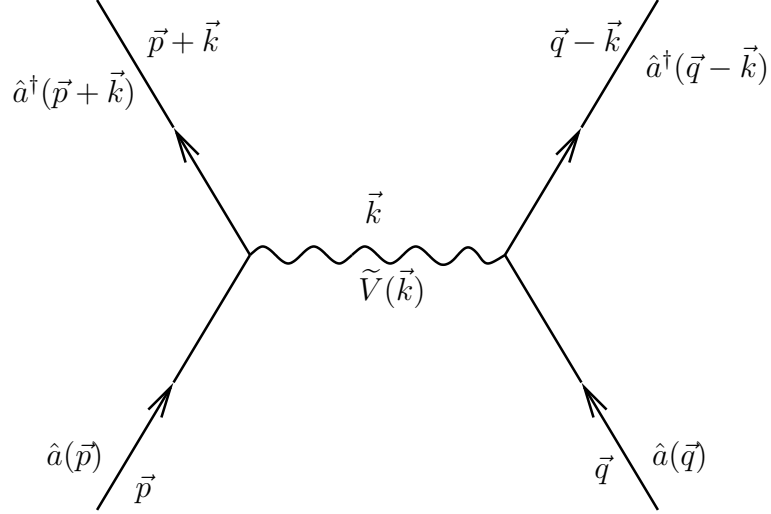


Figure 1.2: Two-body interaction.

1.7 Non-Relativistic Field Theory and Second Quantization

We can now reformulate the problem of an N -particle system as a non-relativistic field theory. The procedure described in the previous section is commonly known as Second Quantization. If the (identical) particles are *bosons*, the operators $\hat{a}(\phi)$ obey *canonical commutation relations*. If the (identical) particles are *Fermions*, the operators $\hat{a}(\phi)$ obey *canonical anticommutation relations*. In position space, it is customary to represent $\hat{a}^\dagger(\phi)$ by the operator $\hat{\psi}(\vec{x})$ which obeys the equal-time algebra

$$\begin{aligned} \left[\hat{\psi}(\vec{x}), \hat{\psi}^\dagger(\vec{y}) \right]_{-\xi} &= \delta^d(\vec{x} - \vec{y}) \\ \left[\hat{\psi}(\vec{x}), \hat{\psi}(\vec{y}) \right]_{-\xi} &= \left[\hat{\psi}^\dagger(\vec{x}), \hat{\psi}^\dagger(\vec{y}) \right]_{-\xi} = 0 \end{aligned} \quad (1.173)$$

In this framework, the one-particle Schrödinger equation becomes the classical field equation

$$\left[i\hbar \frac{\partial}{\partial t} + \frac{\hbar^2}{2m} \nabla^2 - V(\vec{x}) \right] \psi = 0 \quad (1.174)$$

Can we find a Lagrangian density \mathcal{L} from which the one-particle Schrödinger equation follows as its classical equation of motion? The answer is yes and \mathcal{L} is

given by

$$\mathcal{L} = i\hbar\psi^\dagger \overleftrightarrow{\partial}_t \psi - \frac{\hbar^2}{2m} \vec{\nabla}\psi^\dagger \cdot \vec{\nabla}\psi - V(\vec{x})\psi^\dagger\psi \quad (1.175)$$

Its Euler-Lagrange equations are

$$\partial_t \frac{\delta\mathcal{L}}{\delta\partial_t\psi^\dagger} = -\vec{\nabla} \cdot \frac{\delta\mathcal{L}}{\delta\vec{\nabla}\psi^\dagger} + \frac{\delta\mathcal{L}}{\delta\psi^\dagger} \quad (1.176)$$

which are equivalent to the field Equation Eq. 1.174. The canonical momenta $\pi(x)$ and $\pi^\dagger(y)$ are

$$\pi_\psi = \frac{\delta\mathcal{L}}{\delta\partial_t\psi^\dagger} = -i\hbar\psi \quad (1.177)$$

and

$$\pi_\psi^\dagger = \frac{\delta\mathcal{L}}{\delta\partial_t\psi} = i\hbar\psi^\dagger \quad (1.178)$$

Thus, the (equal-time) canonical commutation relations are

$$\left[\hat{\psi}(\vec{x}), \hat{\pi}(\vec{y}) \right]_{-\xi} = i\hbar\delta(\vec{x} - \vec{y}) \quad (1.179)$$

which require that

$$\left[\hat{\psi}(\vec{x}), \hat{\psi}^\dagger(\vec{y}) \right]_{-\xi} = \delta^d(\vec{x} - \vec{y}) \quad (1.180)$$

1.8 Non-Relativistic Fermions at Zero Temperature

The results of the previous sections tell us that the action for non-relativistic fermions (with two-body interactions) is (in $D = d + 1$ space-time dimensions)

$$\begin{aligned} S &= \int d^D x \left[\hat{\psi}^\dagger i\hbar\partial_t \hat{\psi} - \frac{\hbar^2}{2m} \vec{\nabla}\hat{\psi}^\dagger \cdot \vec{\nabla}\hat{\psi} - V(\vec{x})\hat{\psi}^\dagger(x)\hat{\psi}(x) \right] \\ &\quad - \frac{1}{2} \int d^D x \int d^D x' \hat{\psi}^\dagger(x)\hat{\psi}^\dagger(x')U(x-x')\hat{\psi}(x')\hat{\psi}(x) \end{aligned} \quad (1.181)$$

where $U(x-x')$ represents instantaneous pair-interactions,

$$U(x-x') \equiv U(\vec{x}-\vec{x}')\delta(x_0-x'_0) \quad (1.182)$$

The Hamiltonian \hat{H} for this system is

$$\begin{aligned} \hat{H} &= \int d^d x \left[\frac{\hbar^2}{2m} \vec{\nabla}\hat{\psi}^\dagger \cdot \vec{\nabla}\hat{\psi} + V(\vec{x})\hat{\psi}^\dagger(\vec{x})\hat{\psi}(\vec{x}) \right] \\ &\quad + \frac{1}{2} \int d^d x \int d^d x' \hat{\psi}^\dagger(x)\hat{\psi}^\dagger(x')U(x-x')\hat{\psi}(x')\hat{\psi}(x) \end{aligned} \quad (1.183)$$

For *Fermions* the fields $\hat{\psi}$ and $\hat{\psi}^\dagger$ satisfy equal-time canonical anticommutation relations

$$\{\hat{\psi}(\vec{x}), \hat{\psi}^\dagger(\vec{x}')\} = \delta(\vec{x} - \vec{x}') \quad (1.184)$$

while for *Bosons* they satisfy

$$[\hat{\psi}(\vec{x}), \hat{\psi}^\dagger(\vec{x}')] = \delta(\vec{x} - \vec{x}') \quad (1.185)$$

In both cases, the Hamiltonian \hat{H} commutes with the total number operator $\hat{N} = \int d^d x \hat{\psi}^\dagger(x) \hat{\psi}(x)$ since \hat{H} conserves the total number of particles. The Fock space picture of the many-body problem is equivalent to the Grand Canonical Ensemble of Statistical Mechanics. Thus, instead of fixing the number of particles we can introduce a Lagrange multiplier μ , the chemical potential, to weigh contributions from different parts of the Fock space. Thus, we define the operator \tilde{H} .

$$\tilde{H} \equiv \hat{H} - \mu \hat{N} \quad (1.186)$$

In a Hilbert space with fixed \hat{N} this amounts to a shift of the energy by μN . We will now allow the system to choose the sector of the Fock space but with the requirement that the *average* number of particles $\langle \hat{N} \rangle$ is fixed to be some number \bar{N} . In the thermodynamic limit ($N \rightarrow \infty$), μ represents the difference of the ground state energies between two sectors with $N + 1$ and N particles respectively. The modified Hamiltonian \tilde{H} is (for *spinless fermions*)

$$\begin{aligned} \tilde{H} &= \int d^d x \hat{\psi}^\dagger(\vec{x}) \left[-\frac{\hbar^2}{2m} \nabla^2 + V(\vec{x}) - \mu \right] \hat{\psi}(\vec{x}) \\ &+ \frac{1}{2} \int d^d x \int d^d y \hat{\psi}^\dagger(\vec{x}) \hat{\psi}^\dagger(\vec{y}) U(\vec{x} - \vec{y}) \hat{\psi}(\vec{y}) \hat{\psi}(\vec{x}) \end{aligned} \quad (1.187)$$

1.9 The Ground State of a System of Free Fermions

Let us discuss now the very simple problem of finding the ground state for a system of N spinless *free* fermions. In this case, the pair-potential vanishes and, if the system is isolated, so does the potential $V(\vec{x})$. In general there will be a complete set of one-particle states $\{|\alpha\rangle\}$ and, in this basis, \hat{H} is

$$\hat{H} = \sum_{\alpha} E_{\alpha} \hat{a}_{\alpha}^{\dagger} a_{\alpha} \quad (1.188)$$

where the index α labels the one-particle states by increasing order of their single-particle energies

$$E_1 \leq E_2 \leq \dots \leq E_n \leq \dots \quad (1.189)$$

Since we are dealing with fermions, we cannot put more than one particle in each state. Thus the state the *lowest* energy is obtained by filling up all the first

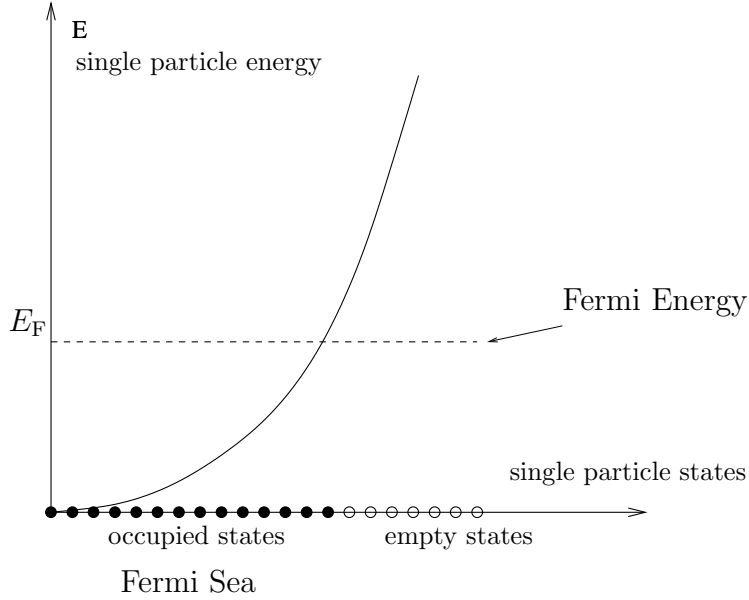


Figure 1.3: The Fermi Sea.

N single particle states. Let $|\text{gnd}\rangle$ denote this ground state

$$|\text{gnd}\rangle = \prod_{\alpha=1}^N \hat{a}_{\alpha}^{\dagger} |0\rangle \equiv \hat{a}_1^{\dagger} \cdots \hat{a}_N^{\dagger} |0\rangle = |\overbrace{1 \dots 1}^N, 00 \dots\rangle \quad (1.190)$$

The energy of this state is E_{gnd} with

$$E_{\text{gnd}} = E_1 + \cdots + E_N \quad (1.191)$$

The energy of the top-most occupied single particle state, E_N , is called the *Fermi energy* of the system and the set of occupied states is called the *filled Fermi sea*.

1.10 Excited States

A state like $|\psi\rangle$

$$|\psi\rangle = |\overbrace{1 \dots 1}^{N-1} 0 10 \dots\rangle \quad (1.192)$$

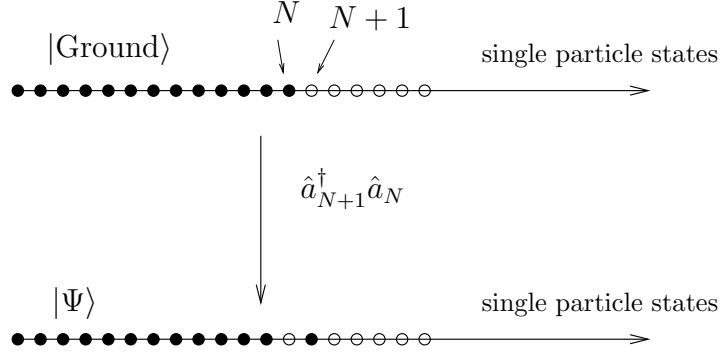


Figure 1.4: An excited (particle-hole) state.

is an excited state. It is obtained by removing one particle from the single particle state N (thus leaving a *hole* behind) and putting the particle in the unoccupied single particle state $N + 1$. This is a state with one *particle-hole pair*, and it has the form

$$|1 \dots 1010 \dots\rangle = \hat{a}_{N+1}^\dagger \hat{a}_N |\text{gnd}\rangle \quad (1.193)$$

The energy of this state is

$$E_\psi = E_1 + \dots + E_{N-1} + E_{N+1} \quad (1.194)$$

Hence

$$E_\psi = E_{\text{gnd}} + E_{N+1} - E_N \quad (1.195)$$

and, since $E_{N+1} \geq E_N$, $E_\psi \geq E_{\text{gnd}}$. The *excitation energy* $\epsilon_\psi = E_\psi - E_{\text{gnd}}$ is

$$\epsilon_\psi = E_{N+1} - E_N \geq 0 \quad (1.196)$$

1.11 Construction of the Physical Hilbert Space

It is apparent that, instead of using the empty state $|0\rangle$ for reference state, it is physically more reasonable to use instead the filled Fermi sea $|\text{gnd}\rangle$ as the physical reference state or *vacuum state*. Thus this state is a vacuum in the sense of *absence of excitations*. These arguments motivate the introduction of the *particle-hole transformation*.

Let us introduce the fermion operators b_α such that

$$\hat{b}_\alpha = \hat{a}_\alpha^\dagger \quad \text{for } \alpha \leq N \quad (1.197)$$

Since $\hat{a}_\alpha^\dagger|\text{gnd}\rangle = 0$ (for $\alpha \leq N$) the operators \hat{b}_α annihilate the ground state $|\text{gnd}\rangle$, *i.e.*,

$$\hat{b}_\alpha|\text{gnd}\rangle = 0 \quad (1.198)$$

The following anticommutation relations hold

$$\begin{aligned} \{\hat{a}_\alpha, \hat{a}'_\alpha\} &= \{\hat{a}_\alpha, \hat{b}_\beta\} = \{\hat{b}_\beta, \hat{b}'_\beta\} = \{\hat{a}_\alpha, \hat{b}_\beta^\dagger\} = 0 \\ \{\hat{a}_\alpha, \hat{a}'_{\alpha'}\} &= \delta_{\alpha\alpha'} \quad \{\hat{b}_\beta, \hat{b}'_{\beta'}\} = \delta_{\beta\beta'} \end{aligned} \quad (1.199)$$

where $\alpha, \alpha' > N$ and $\beta, \beta' \leq N$. Thus, relative to the state $|\text{gnd}\rangle$, \hat{a}_α^\dagger and \hat{b}_β^\dagger behave like creation operators. An arbitrary excited state has the form

$$|\alpha_1 \dots \alpha_m, \beta_1 \dots \beta_n; \text{gnd}\rangle \equiv \hat{a}_{\alpha_1}^\dagger \dots \hat{a}_{\alpha_m}^\dagger \hat{b}_{\beta_1}^\dagger \dots \hat{b}_{\beta_n}^\dagger |\text{gnd}\rangle \quad (1.200)$$

This state has m particles (in the single-particle states $\alpha_1, \dots, \alpha_m$) and n holes (in the single-particle states β_1, \dots, β_n). The ground state is annihilated by the operators \hat{a}_α and \hat{b}_β

$$\hat{a}_\alpha|\text{gnd}\rangle = \hat{b}_\beta|\text{gnd}\rangle = 0 \quad (\alpha > N \beta \leq N) \quad (1.201)$$

The Hamiltonian \hat{H} is normal ordered relative to the empty state $|0\rangle$, *i. e.* $\hat{H}|0\rangle = 0$, but is not normal ordered relative to the actual ground state $|\text{gnd}\rangle$. The particle-hole transformation enables us to normal order \hat{H} relative to $|\text{gnd}\rangle$.

$$\hat{H} = \sum_\alpha E_\alpha \hat{a}_\alpha^\dagger \hat{a}_\alpha = \sum_{\alpha \leq N} E_\alpha + \sum_{\alpha > N} E_\alpha \hat{a}_\alpha^\dagger \hat{a}_\alpha - \sum_{\beta \leq N} E_\beta \hat{b}_\beta^\dagger \hat{b}_\beta \quad (1.202)$$

Thus

$$\hat{H} = E_{\text{gnd}} + : \hat{H} : \quad (1.203)$$

where

$$E_{\text{gnd}} = \sum_{\alpha=1}^N E_\alpha \quad (1.204)$$

is the ground state energy, and the normal ordered Hamiltonian is

$$: \hat{H} : = \sum_{\alpha > N} E_\alpha \hat{a}_\alpha^\dagger \hat{a}_\alpha - \sum_{\beta \leq N} \hat{b}_\beta^\dagger \hat{b}_\beta E_\beta \quad (1.205)$$

The number operator \hat{N} is not normal-ordered relative to $|\text{gnd}\rangle$ either. Thus, we write

$$\hat{N} = \sum_\alpha \hat{a}_\alpha^\dagger \hat{a}_\alpha = N + \sum_{\alpha > N} \hat{a}_\alpha^\dagger \hat{a}_\alpha - \sum_{\beta \leq N} \hat{b}_\beta^\dagger \hat{b}_\beta \quad (1.206)$$

We see that particles raise the energy while holes reduce it. However, if we deal with Hamiltonians which conserve the particle number \hat{N} (*i.e.*, $[\hat{N}, \hat{H}] = 0$) for

every particle that is removed a hole must be created. Hence particles and holes can only be created in *pairs*. A particle-hole state $|\alpha, \beta \text{ gnd}\rangle$ is

$$|\alpha, \beta \text{ gnd}\rangle \equiv \hat{a}_\alpha^\dagger \hat{b}_\beta^\dagger |\text{gnd}\rangle \quad (1.207)$$

It is an eigenstate with an energy

$$\begin{aligned} \hat{H}|\alpha, \beta \text{ gnd}\rangle &= (E_{\text{gnd}} + \hat{H}) \hat{a}_\alpha^\dagger \hat{b}_\beta^\dagger |\text{gnd}\rangle \\ &= (E_{\text{gnd}} + E_\alpha - E_\beta) |\alpha, \beta \text{ gnd}\rangle \end{aligned} \quad (1.208)$$

This state has exactly N particles since

$$\hat{N}|\alpha, \beta \text{ gnd}\rangle = (N + 1 - 1) |\alpha, \beta \text{ gnd}\rangle = N |\alpha, \beta \text{ gnd}\rangle \quad (1.209)$$

Let us finally notice that the field operator $\hat{\psi}^\dagger(x)$ in position space is

$$\hat{\psi}^\dagger(\vec{x}) = \sum_\alpha \langle \vec{x} | \alpha \rangle \hat{a}_\alpha^\dagger = \sum_{\alpha > N} \phi_\alpha(\vec{x}) \hat{a}_\alpha^\dagger + \sum_{\beta \leq N} \phi_\beta(\vec{x}) \hat{b}_\beta \quad (1.210)$$

where $\{\phi_\alpha(\vec{x})\}$ are the single particle wave functions.

The procedure of normal ordering allows us to define the physical Hilbert space. The physical meaning of this approach becomes more transparent in the *thermodynamic limit* $N \rightarrow \infty$ and $V \rightarrow \infty$ at *constant density* ρ . In this limit, the space of Hilbert space is the set of states which is obtained by acting with creation and annihilation operators *finitely* on the ground state. The spectrum of states that results from this approach consists on the set of states with *finite* excitation energy. Hilbert spaces which are built on reference states with *macroscopically* different number of particles are effectively *disconnected* from each other. Thus, the normal ordering of a Hamiltonian of a system with an infinite number of degrees of freedom amounts to a choice of the Hilbert space. This restriction becomes of fundamental importance when interactions are taken into account.

1.12 The Free Fermi Gas

Let us consider the case of free spin one-half electrons moving in free space. The Hamiltonian for this system is

$$\tilde{H} = \int d^d x \sum_{\sigma=\uparrow, \downarrow} \hat{\psi}_\sigma^\dagger(\vec{x}) \left[-\frac{\hbar^2}{2m} \nabla^2 - \mu \right] \hat{\psi}_\sigma(\vec{x}) \quad (1.211)$$

where the label $\sigma = \uparrow, \downarrow$ indicates the z -projection of the spin of the electron. The value of the chemical potential μ will be determined once we satisfy that the electron *density* is equal to some fixed value $\bar{\rho}$.

In momentum space, we get

$$\hat{\psi}_\sigma(\vec{x}) = \int \frac{d^d p}{(2\pi\hbar)^d} \hat{\psi}_\sigma(\vec{p}) e^{-i\frac{\vec{p}\cdot\vec{x}}{\hbar}} \quad (1.212)$$

where the operators $\hat{\psi}_\sigma(\vec{p})$ and $\hat{\psi}_\sigma^\dagger(\vec{p})$ satisfy

$$\begin{aligned} \left\{ \hat{\psi}_\sigma(\vec{p}), \hat{\psi}_{\sigma'}^\dagger(\vec{p}') \right\} &= (2\pi\hbar)^d \delta_{\sigma\sigma'} \delta^d(\vec{p} - \vec{p}') \\ \left\{ \hat{\psi}_\sigma^\dagger(\vec{p}), \hat{\psi}_{\sigma'}^\dagger(\vec{p}') \right\} &= \left\{ \hat{\psi}_\sigma(\vec{p}), \hat{\psi}_{\sigma'}(\vec{p}') \right\} = 0 \end{aligned} \quad (1.213)$$

The Hamiltonian has the very simple form

$$\tilde{H} = \int \frac{d^d p}{(2\pi\hbar)^d} \sum_{\sigma=\uparrow,\downarrow} (\epsilon(\vec{p}) - \mu) \hat{\psi}_\sigma^\dagger(\vec{p}) \hat{\psi}_\sigma(\vec{p}) \quad (1.214)$$

where $\epsilon(\vec{p})$ is given by

$$\epsilon(\vec{p}) = \frac{\vec{p}^2}{2m} \quad (1.215)$$

For this simple case, $\epsilon(\vec{p})$ is independent of the spin orientation.

It is convenient to measure the energy relative to the chemical potential (or *Fermi energy*) $\mu = E_F$. The relative energy $E(\vec{p})$ is

$$E(\vec{p}) = \epsilon(\vec{p}) - \mu \quad (1.216)$$

i. e. $E(\vec{p})$ is the excitation energy measured from the Fermi energy $E_F = \mu$. The energy $E(\vec{p})$ does not have a definite sign since there are states with $\epsilon(\vec{p}) > \mu$ as well as states with $\epsilon(\vec{p}) < \mu$. Let us define by p_F the value of $|\vec{p}|$ for which

$$E(p_F) = \epsilon(p_F) - \mu = 0 \quad (1.217)$$

This is the *Fermi momentum*. Thus, for $|\vec{p}| < p_F$, $E(\vec{p})$ is *negative* while for $|\vec{p}| > p_F$, $E(\vec{p})$ is *positive*.

We can construct the ground state of the system by finding the state with lowest energy at fixed μ . Since $E(\vec{p})$ is negative for $|\vec{p}| \leq p_F$, we see that by filling up all of those states we get the *lowest* possible energy. It is then natural to normal order the system relative to a state in which all one-particle states with $|\vec{p}| \leq p_F$ are occupied. Hence we make the particle-hole transformation

$$\begin{aligned} \hat{b}_\sigma(\vec{p}) &= \hat{\psi}_\sigma^\dagger(\vec{p}) \quad \text{for } |\vec{p}| \leq p_F \\ \hat{a}_\sigma(\vec{p}) &= \hat{\psi}_\sigma(\vec{p}) \quad \text{for } |\vec{p}| > p_F \end{aligned} \quad (1.218)$$

In terms of the operators \hat{a}_σ and \hat{b}_σ , the Hamiltonian is

$$\tilde{H} = \sum_{\sigma=\uparrow,\downarrow} \int \frac{d^d p}{(2\pi\hbar)^d} [E(\vec{p})\theta(|\vec{p}| - p_F)\hat{a}_\sigma^\dagger(\vec{p})\hat{a}_\sigma(\vec{p}) + \theta(p_F - |\vec{p}|)E(\vec{p})\hat{b}_\sigma(\vec{p})\hat{b}_\sigma^\dagger(\vec{p})] \quad (1.219)$$

where $\theta(x)$ is the step function

$$\theta(x) = \begin{cases} 1 & x > 0 \\ 0 & x \leq 0 \end{cases} \quad (1.220)$$

Using the anticommutation relations in the last term we get

$$\tilde{H} = \sum_{\sigma=\uparrow,\downarrow} \int \frac{d^d p}{(2\pi\hbar)^d} E(\vec{p}) [\theta(|\vec{p}| - p_F) \hat{a}_\sigma^\dagger(\vec{p}) \hat{a}_\sigma(\vec{p}) - \theta(p_F - |\vec{p}|) \hat{b}_\sigma^\dagger(\vec{p}) \hat{b}_\sigma(\vec{p})] + \tilde{E}_{\text{gnd}} \quad (1.221)$$

where \tilde{E}_{gnd} , the ground state energy measured from the chemical potential μ , is given by

$$\tilde{E}_{\text{gnd}} = \sum_{\sigma=\uparrow,\downarrow} \int \frac{d^d p}{(2\pi\hbar)^d} \theta(p_F - |\vec{p}|) E(\vec{p}) (2\pi)^d \delta^d(0) = E_{\text{gnd}} - \mu N \quad (1.222)$$

Recall that $(2\pi\hbar)^d \delta(0)$ is equal to

$$(2\pi\hbar)^d \delta^d(0) = \lim_{\vec{p} \rightarrow 0} (2\pi\hbar)^d \delta^{(d)}(\vec{p}) = \lim_{\vec{p} \rightarrow 0} \int d^d x e^{i\vec{p} \cdot \vec{x}/\hbar} = V \quad (1.223)$$

where V is the *volume* of the system. Thus, \tilde{E}_{gnd} is extensive

$$\tilde{E}_{\text{gnd}} = V \tilde{\epsilon}_{\text{gnd}} \quad (1.224)$$

and the ground state energy density $\tilde{\epsilon}_{\text{gnd}}$ is

$$\tilde{\epsilon}_{\text{gnd}} = 2 \int_{|\vec{p}| \leq p_F} \frac{d^d p}{(2\pi\hbar)^d} E(\vec{p}) = \epsilon_{\text{gnd}} - \mu \bar{\rho} \quad (1.225)$$

where the factor of 2 comes from the two spin orientations. Putting everything together we get

$$\tilde{\epsilon}_{\text{gnd}} = 2 \int_{|\vec{p}| \leq p_F} \frac{d^d p}{(2\pi\hbar)^d} \left(\frac{\vec{p}^2}{2m} - \mu \right) = 2 \int_0^{p_F} dp p^{d-1} \frac{S_d}{(2\pi\hbar)^d} \left(\frac{p^2}{2m} - \mu \right) \quad (1.226)$$

where S_d is the area of the d -dimensional hypersphere. Our definitions tell us that the chemical potential is $\mu = \frac{p_F^2}{2m} \equiv E_F$ where E_F , is the Fermi energy. Thus the ground state energy density ϵ_{gnd} (measured from the empty state) is equal to

$$E_{\text{gnd}} = \frac{1}{m} \frac{S_d}{(2\pi\hbar)^d} \int_0^{p_F} dp p^{d+1} = \frac{p_F^{d+2}}{m(d+2)} \frac{S_d}{(2\pi\hbar)^d} = 2E_F \frac{p_F^d S_d}{(d+2)(2\pi\hbar)^d} \quad (1.227)$$

How many particles does this state have? To find that out we need to look at the number operator. The number operator can also be normal-ordered with

respect to this state

$$\begin{aligned}\hat{N} &= \int \frac{d^d p}{(2\pi\hbar)^d} \sum_{\sigma=\uparrow,\downarrow} \hat{\psi}_\sigma^\dagger(\vec{p}) \hat{\psi}_\sigma(\vec{p}) = \\ &= \int \frac{d^d p}{(2\pi\hbar)^d} \sum_{\sigma=\uparrow,\downarrow} \{ \theta(|\vec{p}| - p_F) \hat{a}_\sigma^\dagger(\vec{p}) \hat{a}_\sigma(\vec{p}) + \theta(p_F - |\vec{p}|) \hat{b}_\sigma(\vec{p}) \hat{b}_\sigma^\dagger(\vec{p}) \}\end{aligned}\quad (1.228)$$

Hence, \hat{N} can also be written in the form

$$\hat{N} = : \hat{N} : + N \quad (1.229)$$

where the normal-ordered number operator $: \hat{N} :$ is

$$: \hat{N} : = \int \frac{d^d p}{(2\pi\hbar)^d} \sum_{\sigma=\uparrow,\downarrow} [\theta(|\vec{p}| - p_F) \hat{a}_\sigma^\dagger(\vec{p}) \hat{a}_\sigma(\vec{p}) - \theta(p_F - |\vec{p}|) \hat{b}_\sigma^\dagger(\vec{p}) \hat{b}_\sigma(\vec{p})] \quad (1.230)$$

and N , the number of particles in the reference state $|\text{gnd}\rangle$, is

$$N = \int \frac{d^d p}{(2\pi\hbar)^d} \sum_{\sigma=\uparrow,\downarrow} \theta(p_F - |\vec{p}|) (2\pi\hbar)^d \delta^d(0) = \frac{2}{d} p_F^d \frac{S_d}{(2\pi\hbar)^d} V \quad (1.231)$$

Therefore, the particle density $\bar{\rho} = \frac{N}{V}$ is

$$\bar{\rho} = \frac{2}{d} \frac{S_d}{(2\pi\hbar)^d} p_F^d \quad (1.232)$$

This equation determines the *Fermi momentum* p_F in terms of the density $\bar{\rho}$. Similarly we find that the ground state energy *per particle* is $\frac{E_{\text{gnd}}}{N} = \frac{d}{d+2} E_F$.

The Excited states can be constructed in a similar fashion. The state $|+, \sigma, \vec{p}\rangle$

$$|+, \sigma, \vec{p}\rangle = \hat{a}_\sigma^\dagger(\vec{p}) |\text{gnd}\rangle \quad (1.233)$$

is a state which represents an *electron* with spin σ and momentum \vec{p} while the state $|-, \sigma, \vec{p}\rangle$

$$|-, \sigma, \vec{p}\rangle = \hat{b}_\sigma^\dagger(\vec{p}) |\text{gnd}\rangle \quad (1.234)$$

represents a *hole* with spin σ and momentum \vec{p} . From our previous discussion we see that *electrons* have momentum \vec{p} with $|\vec{p}| > p_F$ while *holes* have momentum \vec{p} with $|\vec{p}| < p_F$. The excitation energy of a one-electron state is $E(\vec{p}) \geq 0$ (for $|\vec{p}| > p_F$), while the excitation energy of a one-hole state is $-E(\vec{p}) \geq 0$ (for $|\vec{p}| < p_F$).

Similarly, an electron-hole *pair* is a state of the form

$$|\sigma\vec{p}, \sigma'\vec{p}'\rangle = \hat{a}_\sigma^\dagger(\vec{p}) \hat{b}_{\sigma'}^\dagger(\vec{p}') |\text{gnd}\rangle \quad (1.235)$$

with $|\vec{p}| > p_F$ and $|\vec{p}'| < p_F$. This state has excitation energy $E(\vec{p}) - E(\vec{p}')$, which is positive. Hence, states which are obtained from the ground state without changing the density, can only increase the energy. This proves that $|\text{gnd}\rangle$ is indeed the ground state. However, if the density is allowed to change, we can always construct states with energy less than E_{gnd} by creating a number of holes without creating an equal number of particles.

1.13 Free Bose and Fermi Gases at $T > 0$

We will now quickly review the properties of free Fermi and Bose gases and Bose condensation, and their thermodynamic properties. We'll work in the Grand Canonical Ensemble in which particle number is not exactly conserved, *i.e.* we couple the system to a bath at temperature T and fixed chemical potential μ . The Grand Partition Function at fixed T and μ is

$$Z_G = e^{-\beta\Omega} = \text{tr } e^{\beta(\hat{H} - \mu\hat{N})} \quad (1.236)$$

where \hat{H} is the Hamiltonian, \hat{N} is the total particle number operator, $\beta = (kT)^{-1}$, where T is the temperature and k is the Boltzmann constant, and Ω is the thermodynamic potential $\Omega = \Omega(T, V, \mu)$.

For a free particle system the total Hamiltonian H is a sum of one-particle Hamiltonians,

$$H = \sum_{\ell} \epsilon_{\ell} \hat{a}_{\ell}^{\dagger} \hat{a}_{\ell} \quad (1.237)$$

where $\ell = 0, 1, \dots$ labels the states of the complete set of single-particle states $\{|\ell\rangle\}$, and $\{\epsilon_{\ell}\}$ are the eigenvalues of the single-particle Hamiltonian.

The Grand Partition Function Z_G can be computed easily in the occupation number representation of the eigenstates of H :

$$Z_G = \sum_{n_1 \dots n_k \dots} \langle n_1 \dots n_k \dots | e^{\beta \sum_{\ell} (\mu - \epsilon_{\ell}) n_{\ell}} | n_1 \dots n_k \dots \rangle \quad (1.238)$$

where n_{ℓ} is the occupation number of the ℓ -th single particle state. The allowed values of the occupation numbers n_{ℓ} for fermions and bosons is

$$\begin{aligned} n_{\ell} = 0, 1 & \quad \text{fermions} \\ n_{\ell} = 0, 1, \dots & \quad \text{bosons} \end{aligned} \quad (1.239)$$

Thus, the Grand Partition Function is

$$Z_G = \prod_{\ell=0}^{\infty} \sum_{n_{\ell}} \langle n_{\ell} | e^{\beta(\mu - \epsilon_{\ell}) n_{\ell}} | n_{\ell} \rangle \quad (1.240)$$

For *fermions* we get

$$Z_G^F = e^{-\beta\Omega_G^F} = \prod_{\ell=0}^{\infty} \sum_{n_{\ell}=0,1} e^{\beta(\mu - \epsilon_{\ell}) n_{\ell}} = \prod_{\ell=0}^{\infty} [1 + e^{\beta(\mu - \epsilon_{\ell})}] \quad (1.241)$$

or, what is the same, the thermodynamic potential for a system of free fermions Ω_G^F at fixed T and μ is given by an expression of the form

$$\boxed{\Omega_G^F = -kT \sum_{\ell=0}^{\infty} \ln [1 + e^{\beta(\mu - \epsilon_{\ell})}]} \quad \text{Fermions} \quad (1.242)$$

For *bosons* we find instead,

$$Z_G^B = e^{-\beta\Omega_G^B} = \prod_{\ell=0}^{\infty} \sum_{n_{\ell}=0}^{\infty} e^{\beta(\mu-\epsilon_{\ell})} = \prod_{\ell=0}^{\infty} \frac{1}{1 - e^{\beta(\mu-\epsilon_{\ell})}} \quad (1.243)$$

Hence, the thermodynamic potential Ω_G^B for a system of free bosons at fixed T and μ is

$$\boxed{\Omega_G^B = kT \sum_{\ell=0}^{\infty} \ln [1 - e^{\beta(\mu-\epsilon_{\ell})}]} \quad \text{Bosons} \quad (1.244)$$

The average number of particles $\langle N \rangle$ is

$$\langle N \rangle = \frac{\text{tr} \hat{N} e^{-\beta(\hat{H}-\mu\hat{N})}}{\text{tr} e^{-\beta(\hat{H}-\mu\hat{N})}} = \frac{1}{\beta} \frac{1}{Z_G} \frac{\partial Z_G}{\partial \mu} = \frac{1}{\beta} \frac{\partial}{\partial \mu} \ln Z_G \quad (1.245)$$

$$\langle N \rangle = \rho V = \frac{1}{\beta} \frac{\partial}{\partial \mu} [-\beta\Omega_G] = - \frac{\partial \Omega_G}{\partial \mu} \quad (1.246)$$

where ρ is the particle density and V is the volume.

For bosons $\langle N \rangle$ is

$$\langle N \rangle = \frac{1}{\beta} \sum_{\ell=0}^{\infty} \frac{1}{1 - e^{\beta(\mu-\epsilon_{\ell})}} (-1) e^{\beta(\mu-\epsilon_{\ell})} \beta \quad (1.247)$$

Hence,

$$\boxed{\langle N \rangle = \sum_{\ell=0}^{\infty} \frac{1}{e^{\beta(\epsilon_{\ell}-\mu)} - 1}} \quad \text{Bosons} \quad (1.248)$$

Whereas for fermions we find,

$$\boxed{\langle N \rangle = \sum_{\ell=0}^{\infty} \frac{1}{e^{\beta(\epsilon_{\ell}-\mu)} + 1}} \quad \text{Fermions} \quad (1.249)$$

In general the average number of particles $\langle N \rangle$ is

$$\langle N \rangle = \sum_{\ell=0}^{\infty} \langle n_{\ell} \rangle = \sum_{\ell=0}^{\infty} \frac{1}{e^{\beta(\epsilon_{\ell}-\mu)} \pm 1} \quad (1.250)$$

where $+$ holds for *fermions* and $-$ holds for *bosons*.

The internal energy U of the system is

$$U = \langle H \rangle = \langle H - \mu N \rangle + \mu \langle N \rangle \quad (1.251)$$

where

$$\langle H - \mu N \rangle = - \frac{1}{Z_G} \frac{\partial Z_G}{\partial \beta} = - \frac{\partial \ln Z_G}{\partial \beta} = \frac{\partial}{\partial \beta} (\beta \Omega_G) \quad (1.252)$$

Hence,

$$U = \frac{\partial}{\partial \beta} (\beta \Omega_G) + \mu \langle N \rangle \quad (1.253)$$

As usual, we will need to find the value of the chemical potential μ in terms of the average number of particles $\langle N \rangle$ (or in terms of the average density ρ) at fixed temperature T and volume V . Once this is done we can compute the thermodynamic variables of the systems, such as the pressure P and the entropy S by using standard thermodynamic relations, *e.g.*

Pressure: $P = -\frac{\partial \Omega_G}{\partial V} \Big|_{\mu, T}$

Entropy: $S = -\frac{\partial \Omega_G}{\partial T} \Big|_{\mu, V}$

The following integrals will be helpful below

$$I(a, b) = \int_{-\infty}^{+\infty} e^{-\frac{a}{2}x^2 - bx} \frac{dx}{\sqrt{2\pi}} = \frac{1}{\sqrt{a}} e^{\frac{b^2}{2a}} \quad (1.254)$$

and

$$I_n(a) = \begin{cases} \frac{n!}{(n/2)! 2^{n/2}} a^{-(n+1)/2} & \text{for } n \text{ even} \\ 0 & \text{for } n \text{ odd} \end{cases} \quad (1.255)$$

1.13.1 Bose Case

Let $\epsilon_0 = 0$, $\epsilon_\ell \geq 0$, and $\mu \leq 0$. The thermodynamic potential for bosons Ω_G^B is

$$\Omega_G^B = kT \sum_{\ell=0}^{\infty} \ln \left[1 - e^{\beta(\mu - \epsilon_\ell)} \right] \quad (1.256)$$

The number of modes in the box of volume V with momenta in the infinitesimal region d^3p is $sV \frac{d^3k}{(2\pi\hbar)^3}$, and for bosons of spin S we have set $s = 2S + 1$. Thus for spin-1 bosons there are 3 states. (However, in the case of photons $S = 1$ but have only 2 polarization states and hence $s = 2$.)

The single-particle energies $\epsilon(\vec{p})$ are

$$\epsilon(\vec{p}) = \frac{p^2}{2m} \quad (1.257)$$

where we have approximated the discrete levels by a continuum. In these terms, Ω_G^B becomes

$$\Omega_G^B = kT sV \int \frac{d^3p}{(2\pi\hbar)^3} \ln \left[1 - e^{\beta(\mu - \frac{p^2}{2m})} \right] \quad (1.258)$$

and $\rho = \langle N \rangle / V$ is given by

$$\rho = \frac{\langle N \rangle}{V} = -\frac{1}{V} \frac{\partial \Omega}{\partial \mu} = s \int \frac{e^{-\frac{\beta p^2}{2m}} e^{\beta \mu}}{1 - e^{-\frac{\beta p^2}{2m} + \beta \mu}} \frac{d^3p}{(2\pi\hbar)^3} \quad (1.259)$$

It is convenient to introduce the fugacity z and the variable x

$$z = e^{\beta\mu} \quad x^2 = \frac{\beta p^2}{2m} \quad (1.260)$$

in terms of which the volume element of momentum space becomes

$$\frac{d^3p}{(2\pi\hbar)^3} \rightarrow \frac{4\pi p^2}{(2\pi\hbar)^3} dp = \frac{x^2}{2\pi^2\hbar^3} \left(\frac{2m}{\beta}\right)^{3/2} dx \quad (1.261)$$

where we have carried out the angular integration. The density ρ is

$$\begin{aligned} \rho &= s \int_0^\infty \frac{ze^{-x^2}}{1 - ze^{-x^2}} \left[\frac{x^2}{2\pi^2\hbar^3} \left(\frac{2m}{\beta}\right)^{3/2} \right] dx \\ &= \frac{s}{4\pi^2\hbar^3} \left(\frac{2m}{\beta}\right)^{3/2} \int_{-\infty}^{+\infty} dx \sum_{n=0}^{\infty} z^{n+1} e^{-(n+1)x^2} x^2 \\ &= \frac{s}{4\pi^2\hbar^3} \left(\frac{2m}{\beta}\right)^{3/2} \sum_{n=1}^{\infty} \int_{-\infty}^{+\infty} dx z^n x^2 e^{-nx^2} = \\ &= \frac{s}{4\pi^2\hbar^3} \left(\frac{2m}{\beta}\right)^{3/2} \sum_{n=1}^{\infty} \frac{z^n}{n^{3/2}} \int_{-\infty}^{+\infty} dy y^2 e^{-y^2} \\ &= \frac{s}{4\pi^2\hbar^3} \left(\frac{2m}{\beta}\right)^{3/2} \sum_{n=1}^{\infty} \frac{z^n}{n^{3/2}} \frac{\sqrt{\pi}}{2} \end{aligned} \quad (1.262)$$

We now introduce the (generalized) Riemann ζ -function, $\zeta_r(z)$

$$\zeta_r(z) = \sum_{n=1}^{\infty} \frac{z^n}{n^r} \quad (1.263)$$

(which is well defined for $r > 0$ and $\text{Re } z > 0$) in terms of which the expression for the density takes the more compact form

$$\rho = s \left(\frac{mkT}{2\pi\hbar^2}\right)^{3/2} \zeta_{3/2}(z), \quad \text{where } z = e^{\beta\mu} \quad (1.264)$$

This equation must be inverted to determine $\mu(\rho)$.

Likewise, the internal energy U can also be written in terms of a Riemann ζ -function:

$$U = \frac{\partial}{\partial\beta} (\beta\Omega_G) + \mu V \rho = s \frac{3}{2} kT \left(\frac{mkT}{2\pi\hbar^2}\right)^{3/2} V \zeta_{5/2}(z) \quad (1.265)$$

If ρ is low and T high (or $\frac{\rho}{T^{3/2}}$ low) $\Rightarrow \zeta_{3/2}(z)$ is small and can be approximated by a few terms of its power series expansion

$$\zeta_{3/2}(z) = \frac{z}{1} + \frac{z^2}{2^{3/2}} + \dots \Rightarrow z \text{ small (i.e. } \mu \text{ large)} \quad (1.266)$$

Hence, in the low density (or high temperature) limit we can approximate

$$\zeta_{3/2}(z) \approx z \text{ and } \zeta_{5/2}(z) \approx z \quad (1.267)$$

and, in this limit, the internal energy density is

$$\frac{U}{V} = \epsilon \simeq \frac{3}{2} kT\rho, \quad (1.268)$$

which is the classical result.

Conversely if $\frac{\rho}{T^{3/2}}$ is large, *i.e.* large ρ and low T , the fugacity z is no longer small. Furthermore the function $\zeta_r(z)$ has a singularity at $|z| = 1$. For $r = \frac{3}{2}, \frac{5}{2}$ the $\zeta_r(1)$ -function takes the finite values

$$\begin{aligned} \zeta_{3/2}(1) &= 2.612\dots \\ \zeta_{5/2}(1) &= 1.341\dots \end{aligned} \quad (1.269)$$

although the derivatives $\zeta'_{3/2}(1)$ and $\zeta''_{5/2}(1)$ diverge.

Let us define the *critical temperature* T_c as the temperature at which the fugacity takes the value 1

$$z(T_c) = 1 \quad (1.270)$$

In other terms, at $T = T_c$ the expressions are at the radius of convergence of the ζ -function. Since

$$\rho = s \left(\frac{mkT_c}{2\pi\hbar^2} \right)^{3/2} \zeta_{3/2}(1) \quad (1.271)$$

we find the T_c is given by

$$\boxed{T_c = \frac{2\pi\hbar^2}{mk} \left(\frac{\rho/s}{\zeta_{3/2}(1)} \right)^{2/3}} \quad \text{Critical Temperature} \quad (1.272)$$

Our results work only for $T \geq T_c$.

Why do we have a problem for $T < T_c$? Let's reexamine the sum

$$\rho = -\frac{\partial\Omega}{\partial\mu} = \sum_{\ell=0}^{\infty} \frac{1}{e^{-\beta(\mu-\epsilon_\ell)} - 1} \quad (1.273)$$

For small z , $e^{-\beta\mu} = e^{+\beta|\mu|}$ is large, and each term has a small contribution. But for $|z| \rightarrow 1$ the first few terms may have a large contribution. In particular

$$\langle n_1 \rangle = \frac{1}{e^{\beta(\epsilon_1-\mu)} - 1} \ll \frac{1}{e^{\beta(\epsilon_0-\mu)} - 1} = \langle n_0 \rangle \quad (1.274)$$

If we now set $\epsilon_0 = 0$, we find that

$$\langle n_0 \rangle = \frac{1}{e^{-\beta\mu} - 1} \Rightarrow \mu = -kT \ln \left[1 + \frac{1}{\langle n_0 \rangle} \right] \approx \frac{-kT}{\langle n_0 \rangle} \quad (1.275)$$

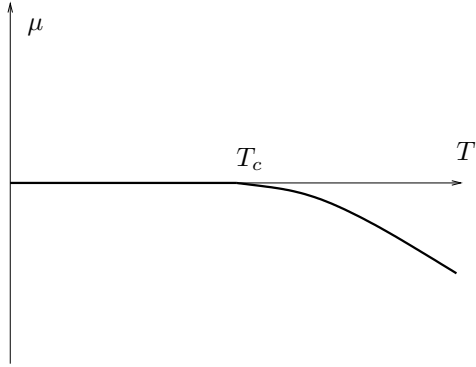


Figure 1.5: The chemical potential as a function of temperature in a free Bose gas. Here T_c is the Bose-Einstein condensation temperature.

for $\langle n_0 \rangle \gg 1$. For low T , μ approaches zero as $N \rightarrow \infty$ (at fixed ρ), and $\epsilon_\ell - \mu \approx \epsilon_\ell$, for $\ell > 0$. Hence, the number of particles \tilde{N} which are not in the lowest energy state $\epsilon_0 = 0$ is

$$\begin{aligned} \tilde{N} &= \langle N - n_0 \rangle = \sum_{\ell=1}^{\infty} \frac{1}{e^{\beta\epsilon_\ell} - 1} \\ &\simeq sV \int \frac{d^3p}{(2\pi\hbar)^3} \frac{1}{e^{\beta p^2/2m} - 1} \\ &= sV \left(\frac{mkT}{2\pi\hbar^2} \right)^{3/2} \zeta_{3/2}(1) \end{aligned} \quad (1.276)$$

Hence,

$$\tilde{N} = \langle N \rangle \left(\frac{T}{T_c} \right)^{3/2} \quad (1.277)$$

and

$$\langle n_0 \rangle = \langle N \rangle - \tilde{N} = \langle N \rangle \left[1 - \left(\frac{T}{T_c} \right)^{3/2} \right] \quad (1.278)$$

Then, the average number of particles in the “single-particle ground state” $|0\rangle$ is

$$\langle n_0(T) \rangle = \langle N \rangle \left[1 - \left(\frac{T}{T_c} \right)^{3/2} \right] \quad (1.279)$$

and their density (the “condensate fraction”) is

$$\rho_0(T) = \begin{cases} \rho \left[1 - \left(\frac{T}{T_c} \right)^{3/2} \right] & T < T_c \\ 0 & T \geq T_c \end{cases} \quad (1.280)$$

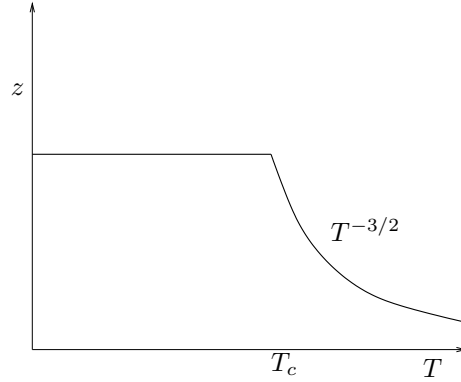


Figure 1.6: The fugacity as a function of temperature in a free Bose gas. T_c is the Bose-Einstein condensation temperature.

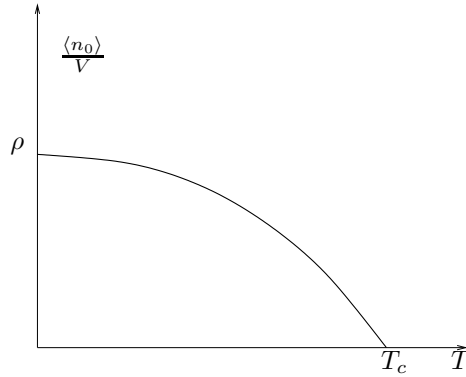


Figure 1.7: The condensate fraction $\langle n_0 \rangle / V$ a function of temperature in a free Bose gas.

This is a *phase transition* known as *Bose Condensation*. Thus, for $T < T_c$, the lowest energy state is macroscopically occupied, which is why this phenomenon is called Bose-condensation. It simply means that for a Bose system the ground state has finite *fraction* bosons in the same single-particle ground state.

Let us examine the behavior of the thermodynamic quantities near and below the phase transition. The total energy is

$$U = \frac{3}{2}kTs \left(\frac{mkT}{2\pi\hbar^2} \right)^{3/2} V \zeta_{5/2}(1) = \frac{3}{2}kT\tilde{N} \frac{\zeta_{5/2}(1)}{\zeta_{3/2}(1)} \quad (1.281)$$

Hence,

$$U = \frac{3}{2}kT \frac{\zeta_{5/2}(1)}{\rho_{3/2}(1)} \langle N \rangle \left(\frac{T}{T_c} \right)^{3/2} \propto T^{5/2} \quad (1.282)$$

The specific heat at constant volume (and particle number) C_v is

$$C_v = \left(\frac{\partial U}{\partial T} \right)_{V,N} \propto \left(\frac{T}{T_c} \right)^{3/2}, \quad \text{for } T < T_c \quad (1.283)$$

On the other hand, since for $T > T_c$

$$\langle N \rangle = \left(\frac{mkT}{2\pi\hbar^2} \right)^{3/2} \zeta_{3/2}(z) sV \quad (1.284)$$

we find that the internal energy above T_c is

$$U = \frac{3}{2}kT \langle N \rangle \frac{\zeta_{5/2}(z)}{\zeta_{3/2}(z)} \quad (1.285)$$

To use this expression we must determine first $z = z(T)$ at fixed density ρ .

How do the thermodynamic quantities of a Bose system behave near T_c ? From the above discussion we see that at T_c there must be a *singularity* in most thermodynamic quantities. However it turns out that while the *free* Bose gas does have a phase transition at T_c , the behavior near T_c is dominated by *critical fluctuations* which are governed by inter-particle interactions which are not included in a system of free bosons. Thus, while the specific heat C_v of a real system of bosons has a *divergence* as $T \rightarrow T_c$ (both from above and from below), a system of free bosons has a mild singularity in the form of a jump in the slope of $C_v(T)$ at T_c . The study of the behavior of singularities at critical points is the subject of the theory of Critical Phenomena.

The free Bose gas is also pathological in other ways. Below T_c a free Bose gas exhibits Bose condensation but it is not a *superfluid*. We will discuss this issue later on this semester. For now we note that there are no true *free* Bose gases in nature since all atoms interact with each other however weakly. These interactions govern the superfluid properties of the Bose *fluid*.

1.13.2 Fermi Case

In the case of fermions, due to the Pauli Principle there is no condensation in a single-particle state. In the presence of interactions the ground state of a system of fermions may be in a highly non-trivial phase including superconductivity, charge density waves and other more exotic possibilities. Contrary to the case of a free Bose system, a system of free fermions does not have a phase transition at any temperature.

The thermodynamic potential for *free* fermions $\Omega_G^F(T, V, \mu)$ is

$$\Omega_G^F(T, V, \mu) = -kT \sum_{\ell=0}^{\infty} \ln \left(1 + e^{-\beta(\epsilon_{\ell} - \mu)} \right) \quad (1.286)$$

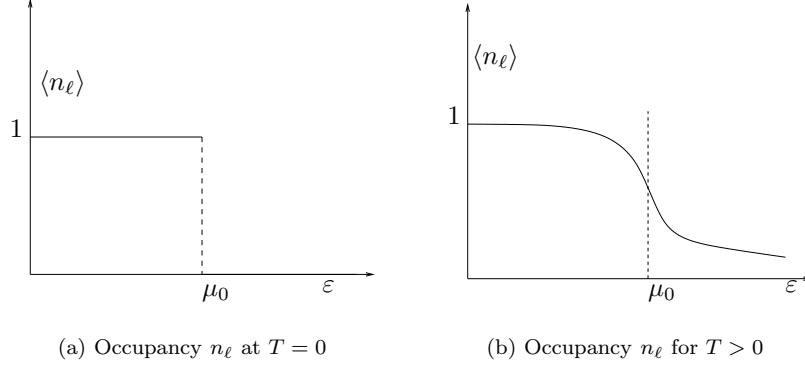


Figure 1.8: The occupation number of eigenstate $|\ell\rangle$ in a free Fermi gas, (a) at $T = 0$ and (b) for $T > 0$. Here, $\mu_0 = E_F$ is the Fermi energy.

where, once again, the integers $\ell = 0, 1, \dots$ label a complete set of one-particle states. No restriction on the sign of μ is now necessary since the argument of the logarithm is now positive as all terms are manifestly positive. Thus there are no vanishing denominators in the expressions for the thermodynamic quantities as in the Bose case. Thus, in the case of (free) fermions we can take the thermodynamic limit without difficulty, and use the integral expressions right away.

For spin S fermions, $s = 2S + 1$, the thermodynamic potential is

$$\Omega_G^F = -kT s V \int \frac{d^3p}{(2\pi\hbar)^3} \ln \left[1 + e^{-\beta\left(\frac{p^2}{2m} - \mu\right)} \right] \quad (1.287)$$

and the density ρ is given by

$$\rho = \frac{\langle N \rangle}{V} = -\frac{1}{V} \frac{\partial \Omega}{\partial \mu} = s \int \frac{d^3p}{(2\pi\hbar)^3} \frac{e^{-\frac{\beta p^2}{2m}} e^{\beta\mu}}{1 + e^{-\frac{\beta p^2}{2m}} e^{\beta\mu}} \quad (1.288)$$

The average occupation number of a general one-particle state $|\ell\rangle$ is

$$\langle n_\ell \rangle = \frac{\partial \Omega}{\partial \epsilon_\ell} = \frac{e^{-\beta(\epsilon_\ell - \mu)}}{1 + e^{-\beta(\epsilon_\ell - \mu)}} = \frac{1}{e^{\beta(\epsilon_\ell - \mu)} + 1} \quad (1.289)$$

which is the Fermi-Dirac distribution function.

Most of the expressions of interest for fermions involve the the Fermi function $f(x)$

$$f(x) = \frac{1}{e^x + 1} \quad (1.290)$$

In particular, if we introduce the one-particle density of states $N_0(\epsilon)$,

$$N_0(\epsilon) = s \frac{2\pi(2m)^{3/2}}{(2\pi\hbar)^3} \sqrt{\epsilon} \quad (1.291)$$

the expression for the particle density ρ can be written in the more compact form

$$\rho = s \int_0^\infty d\epsilon N_0(\epsilon) f(\beta(\epsilon - \mu)) \quad (1.292)$$

where we have assumed that the one-particle spectrum begins at $\epsilon_0 = 0$.

Similarly, the internal energy density for a system of free fermions of spin S is

$$\begin{aligned} u = \frac{U}{V} &= \frac{1}{V} \left(\frac{\partial \beta \Omega_G^F}{\partial \beta} + \mu N \right) = s \int \frac{d^3 p}{(2\pi\hbar)^3} \frac{p^2}{2m} \frac{e^{-\beta(\frac{p^2}{2m} - \mu)}}{1 + e^{-\beta(\frac{p^2}{2m} - \mu)}} \\ &\equiv s \int_0^\infty d\epsilon \epsilon N_0(\epsilon) f(\beta(\epsilon - \mu)) \end{aligned} \quad (1.293)$$

In particular, at $T = 0$ we get

$$u(0) = \frac{3}{5} E_F \rho \quad (1.294)$$

The pressure P at temperature T is obtained from the thermodynamic relation

$$P = - \left(\frac{\partial \Omega_G^F}{\partial V} \right)_{T, \mu} \quad (1.295)$$

For a free Fermi system we obtain

$$P = kTs \int_0^\infty d\epsilon N_0(\epsilon) \ln \left(1 + e^{-\beta(\epsilon - \mu)} \right) \quad (1.296)$$

This result implies that there is a non-zero pressure P_0 in a Fermi gas at $T = 0$ even in the absence of interactions:

$$P_0 = \lim_{T \rightarrow 0} P(T, \mu, V) = \int_0^{\mu_0} d\epsilon N_0(\epsilon) (\mu_0 - \epsilon) = \mu_0 \rho - u(0) = \frac{2}{5} E_F \rho > 0 \quad (1.297)$$

which is known as the *Fermi pressure*. Thus, the pressure of a system of free fermions is non-zero (and positive) even at $T = 0$ due to the effects of the Pauli Principle which keeps fermions from occupying the same single-particle state.

For a free Fermi gas at $T = 0$, $\mu_0 = E_F$. Hence, at $T = 0$ all states with $\epsilon_\ell < \mu_0$ are occupied and all other states are empty. At low temperatures $kT \ll E_F$, most of the states below E_F will remain occupied while most of the states above E_F will remain empty, and only a small fraction of states with single particle energies close to the Fermi energy will be affected by thermal fluctuations. This observation motivates the Sommerfeld expansion which is useful to determine the low temperature behavior of a free Fermi system. Consider an expression of the form

$$I = \int_0^\infty d\epsilon f(\beta(\epsilon - \mu)) g(\epsilon) \quad (1.298)$$

where $g(\epsilon)$ is a smooth function of the energy. Eq.(1.298) can be written in the equivalent form

$$I = \int_{\mu}^{\infty} d\epsilon \frac{g(\epsilon)}{e^{\beta(\epsilon - \mu)} + 1} - \int_0^{\mu} d\epsilon \frac{g(\epsilon)}{e^{-\beta(\epsilon - \mu)} + 1} + \int_0^{\mu} d\epsilon g(\epsilon) \quad (1.299)$$

If we now make the change of variables $x = \beta(\epsilon - \mu)$ in the first integral of eq.(1.299) and $x = -\beta(\epsilon - \mu)$ in the second integral of Eq.(1.299), we get

$$I = \int_0^{\mu} d\epsilon g(\epsilon) + kT \int_0^{\infty} dx \frac{g(\mu + x/\beta)}{e^x + 1} - kT \int_0^{\beta\mu} dx \frac{g(\mu - x/\beta)}{e^x + 1} \quad (1.300)$$

Since the function $g(x)$ is a smooth differentiable function of its argument we can approximate

$$g(\mu \pm \frac{x}{\beta}) = g(\mu) \pm g'(\mu) \frac{x}{\beta} + \dots \quad (1.301)$$

At low temperatures $\beta\mu \gg 1$, or $kT \ll \mu$, with exponential precision we can extend the upper end of the integral in the last term of Eq.(1.300) to infinity, and obtain the asymptotic result

$$I = \int_0^{\mu} d\epsilon g(\epsilon) + \frac{2}{\beta^2} g'(\mu) \int_0^{\infty} \frac{x}{e^x + 1} dx + \dots = \int_0^{\mu} d\epsilon g(\epsilon) + \frac{\pi^2}{6} (kT)^2 g'(\mu) + \dots \quad (1.302)$$

where we have neglected terms $\mathcal{O}(e^{-\beta\mu})$ and $\mathcal{O}((kT)^4)$, and used the integral:

$$\int_0^{\infty} dx \frac{x}{e^x + 1} = \frac{\pi^2}{12} \quad (1.303)$$

Using these results we can now determine the low temperature behavior of all thermodynamic quantities of interest. Thus we obtain

$$\mu(T) = \mu_0 \left(1 - \frac{\pi^2}{12} \left(\frac{kT}{\mu_0} \right)^2 + \dots \right) \quad (1.304)$$

$$u(T) = u(0) + \gamma T^2 + \dots \quad (1.305)$$

where

$$\gamma = \frac{2\pi(2m)^{3/2}}{(2\pi\hbar)^3} s \frac{\pi^2}{6} \sqrt{\mu_0} k^2 \quad (1.306)$$

from where we find that the low-temperature specific heat C_v for *free* fermions is

$$C_v = 2\gamma T + \dots \quad (1.307)$$

A similar line of argument shows that the thermodynamic potential Ω_G^F at low temperatures, $kT \ll \mu$, is

$$\begin{aligned} \frac{\Omega_G^F}{V} &= u(0) - \mu\rho - s \frac{\pi^2}{6} N_0(E_F)(kT)^2 + \dots \\ &= \frac{\Omega_G^F(0)}{V} - \frac{\pi^2}{6} (kT)^2 \frac{\rho}{E_F} + \mathcal{O}((kT)^4) \end{aligned} \quad (1.308)$$

There is a simple and intuitive way to understand the T^2 dependence (or *scaling*) of the thermodynamic potential. First we note that the thermal fluctuations only affect a small number of single particle states all contained within a range of the order of kT around the Fermi energy, E_F , multiplied by the density of single particle states, $N_0(E_F)$. This number is thus $kTN_0(E_F)$. On the other hand, the temperature dependent part of the thermodynamic potential has a factor of kT in front. Thus, we obtain the scaling $N_0(E_F)(kT)^2$. Similar considerations apply to all other quantities.