Second Quantization*

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May 19, 2016

1 The harmonic oscillator: raising and lowering operators

Lets first reanalyze the harmonic oscillator with potential

$$V(x) = \frac{m\omega^2}{2}x^2 \tag{1}$$

where ω is the frequency of the oscillator. One of the numerous approaches we use to solve this problem is based on the following representation of the momentum and position operators:

$$\begin{aligned} \widehat{x} &= \sqrt{\frac{\hbar}{2m\omega}}\left(\widehat{a}^{\dagger} + \widehat{a}\right) \\ \widehat{p} &= i\sqrt{\frac{m\hbar\omega}{2}}\left(\widehat{a}^{\dagger} - \widehat{a}\right). \end{aligned} \tag{2}$$

From the canonical commutation relation

$$[\widehat{x}, \widehat{p}] = i\hbar \tag{3}$$

follows

$$\begin{aligned} \left[\widehat{a}, \widehat{a}^{\dagger}\right] &= 1 \\ [\widehat{a}, \widehat{a}] &= \left[\widehat{a}^{\dagger}, \widehat{a}^{\dagger}\right] = 0. \end{aligned} \tag{4}$$

Inverting the above expression yields

$$\begin{aligned} \widehat{a} &= \sqrt{\frac{m\omega}{2\hbar}}\left(\widehat{x} + \frac{i}{m\omega}\widehat{p}\right) \\ \widehat{a}^{\dagger} &= \sqrt{\frac{m\omega}{2\hbar}}\left(\widehat{x} - \frac{i}{m\omega}\widehat{p}\right) \end{aligned} \tag{5}$$

demonstrating that $\widehat{a}^\dagger$ is indeed the operator adjoined to $\widehat{a}$. We also defined the operator

$$\widehat{N} = \widehat{a}^\dagger \widehat{a} \tag{6}$$

which is Hermitian and thus represents a physical observable. It holds

$$\begin{aligned} \widehat{N} &= \frac{m\omega}{2\hbar}\left(\widehat{x} - \frac{i}{m\omega}\widehat{p}\right)\left(\widehat{x} + \frac{i}{m\omega}\widehat{p}\right) \\ &= \frac{m\omega}{2\hbar}\widehat{x}^2 + \frac{1}{2m\hbar\omega}\widehat{p}^2 - \frac{i}{2\hbar}\left[\widehat{p}, \widehat{x}\right] \\ &= \frac{1}{\hbar\omega}\left(\frac{\widehat{p}^2}{2m} + \frac{m\omega^2}{2}\widehat{x}^2\right) - \frac{1}{2}. \end{aligned} \tag{7}$$

We therefore obtain

$$\widehat{H} = \hbar\omega\left(\widehat{N} + \frac{1}{2}\right). \tag{8}$$

Since the eigenvalues of $\widehat{H}$ are given as $E_n = \hbar\omega\left(n + \frac{1}{2}\right)$ we conclude that the eigenvalues of the operator $\widehat{N}$ are the integers n that determine the eigenstates of the harmonic oscillator.

$$\widehat{N}\left|n\right\rangle = n\left|n\right\rangle. \tag{9}$$

Using the above commutation relation $\left[\widehat{a}, \widehat{a}^\dagger\right] = 1$ we were able to show that

$$\begin{aligned} \widehat{a}\left|n\right\rangle &= \sqrt{n}\left|n-1\right\rangle \\ \widehat{a}^\dagger\left|n\right\rangle &= \sqrt{n+1}\left|n+1\right\rangle \end{aligned} \tag{10}$$

The operator $\widehat{a}^\dagger$ and $\widehat{a}$ raise and lower the quantum number (i.e. the number of quanta). For these reasons, these operators are called creation and annihilation operators.

2 second quantization of noninteracting bosons

While the above results were derived for the special case of the harmonic oscillator there is a similarity between the result

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right) \tag{11}$$

for the oscillator and our expression

$$E_{\{n_{\mathbf{p}}\}} = \sum_{\mathbf{p}} \varepsilon_{\mathbf{p}} n_{\mathbf{p}} \tag{12}$$

for the energy of a many body system, consisting of non-interacting indistinguishable particles. While n in case of the oscillator is the quantum number label, we may alternatively argue that it is the *number of oscillator quanta in the oscillator.* Similarly we can consider the many body system as a collection of a set of harmonic oscillators labelled by the single particle quantum number $\mathbf{p}$ (more generally by $\mathbf{p}$ and the spin). The state of the many body system was characterized by the set $\{n_{\mathbf{p}}\}$ of occupation numbers of the states (the number of particles in this single particle state). We the generalize the wave function $|n\rangle$ to the many body case

$$|\{n_{\mathbf{p}}\}\rangle = |n_1, n_2, ..., n_{\mathbf{p}}, ...\rangle \tag{13}$$

and introduce operators

$$\begin{aligned} \widehat{a}_{\mathbf{p}} |n_1, n_2, ..., n_{\mathbf{p}}, ...\rangle &= \sqrt{n_{\mathbf{p}}} |n_1, n_2, ..., n_{\mathbf{p}} - 1, ...\rangle \\ \widehat{a}^{\dagger}_{\mathbf{p}} |n_1, n_2, ..., n_{\mathbf{p}}, ...\rangle &= \sqrt{n_{\mathbf{p}} + 1} |n_1, n_2, ..., n_{\mathbf{p}} + 1, ...\rangle \end{aligned} \tag{14}$$

That obey

$$\left[\widehat{a}_{\mathbf{p}}, \widehat{a}^{\dagger}_{\mathbf{p}'}\right] = \delta_{\mathbf{p},\mathbf{p}'}. \tag{15}$$

It is obvious that these operators commute if $\mathbf{p} \neq \mathbf{p}'$. For $\mathbf{p} = \mathbf{p}'$ follows

$$\begin{aligned} \widehat{a}_{\mathbf{p}}\widehat{a}^{\dagger}_{\mathbf{p}} |n_1, n_2, ..., n_{\mathbf{p}}, ...\rangle &= \sqrt{n_{\mathbf{p}} + 1}\widehat{a}_{\mathbf{p}} |n_1, n_2, ..., n_{\mathbf{p}} + 1, ...\rangle \\ &= (n_{\mathbf{p}} + 1) |n_1, n_2, ..., n_{\mathbf{p}}, ...\rangle \end{aligned} \tag{16}$$

and

$$\begin{aligned} \widehat{a}^{\dagger}_{\mathbf{p}}\widehat{a}_{\mathbf{p}} |n_1, n_2, ..., n_{\mathbf{p}}, ...\rangle &= \sqrt{n_{\mathbf{p}}}\widehat{a}^{\dagger}_{\mathbf{p}} |n_1, n_2, ..., n_{\mathbf{p}} - 1, ...\rangle \\ &= n_{\mathbf{p}} |n_1, n_2, ..., n_{\mathbf{p}}, ...\rangle \end{aligned} \tag{17}$$

which gives $\widehat{a}_{\mathbf{p}}\widehat{a}^{\dagger}_{\mathbf{p}} - \widehat{a}^{\dagger}_{\mathbf{p}}\widehat{a}_{\mathbf{p}} = 1$. Thus the commutation relation follow even if the operators are not linear combinations of position and momentum. It also follows

$$\widehat{n}_{\mathbf{p}} = \widehat{a}^{\dagger}_{\mathbf{p}}\widehat{a}_{\mathbf{p}} \tag{18}$$

for the operator of the number of particles with single particle quantum number $\mathbf{p}$. The total number operator is $\widehat{N} = \sum_{\mathbf{p}} \widehat{a}^{\dagger}_{\mathbf{p}}\widehat{a}_{\mathbf{p}}$. Similarly, the Hamiltonian in this representation is given as

$$\widehat{H} = \sum_{\mathbf{p}} \varepsilon_{\mathbf{p}}\widehat{a}^{\dagger}_{\mathbf{p}}\widehat{a}_{\mathbf{p}} \tag{19}$$

which gives the correct matrix elements.

We generalize the problem and analyze a many body system of particles with single particle Hamiltonian

$$\widehat{h} = \frac{\widehat{\mathbf{p}}^2}{2m} + U\left(\widehat{\mathbf{r}}\right) \tag{20}$$

which is characterized by the single particle eigenstates

$$\widehat{h} |\phi_{\alpha}\rangle = \varepsilon_{\alpha} |\phi_{\alpha}\rangle . \tag{21}$$

α is the label of the single particle quantum number. We can then introduce the occupation number representation with

$$|n_1, n_2, ..., n_\alpha, ...\rangle \tag{22}$$

and corresponding creation and destruction operators $\left[\widehat{a}_\alpha, \widehat{a}^\dagger_{\alpha'}\right] = \delta_{\alpha,\alpha'}$. We can then perform a unitary transformation among the states

$$|\beta\rangle = \sum_\alpha U_{\beta\alpha} |\alpha\rangle = \sum_\alpha |\alpha\rangle \langle\alpha|\beta\rangle \tag{23}$$

The states $|\beta\rangle$ are in general not the eigenstates of the single particle Hamiltonian (they only are if $U_{\beta\alpha} = \langle\alpha|\beta\rangle = \delta_{\alpha\beta}$). We can nevertheless introduce creation and destruction operators of these states, that are most naturally defined as:

$$\widehat{a}_\beta = \sum_\alpha \langle\beta|\alpha\rangle \widehat{a}_\alpha \tag{24}$$

and the corresponding adjoined equation

$$\widehat{a}^\dagger_\beta = \sum_\alpha \langle\beta|\alpha\rangle^* \widehat{a}^\dagger_\alpha. \tag{25}$$

This transformation preserves the commutation relation (see below for an example).

We can for example chose the basis β as the eigenbasis of the potential. Then holds in second quantization

$$\widehat{U} = \sum_\beta \langle\beta |U(\mathbf{r})| \beta\rangle a^\dagger_\beta a_\beta \tag{26}$$

and we can transform the result as

$$\begin{aligned} \widehat{U} &= \sum_{\beta,\alpha,\alpha'} \langle\alpha|\beta\rangle \langle\beta |U(\mathbf{r})| \beta\rangle \langle\beta|\alpha'\rangle \widehat{a}^\dagger_\alpha \widehat{a}_{\alpha'} \\ &= \sum_{\alpha,\alpha'} \langle\alpha |U(\mathbf{r})| \alpha'\rangle \widehat{a}^\dagger_\alpha \widehat{a}_{\alpha'} \end{aligned} \tag{27}$$

It holds of course $\langle\alpha |U(\mathbf{r})| \alpha'\rangle = \int d^3r \phi_\alpha(\mathbf{r}) U(\mathbf{r}) \phi_{\alpha'}(\mathbf{r})$.

In particular, we can chose $|\beta\rangle = |\mathbf{r}\rangle$ such that $\langle\beta|\alpha\rangle = \langle\mathbf{r}|\alpha\rangle = \phi_\alpha(\mathbf{r})$. In this case we use the notation $\widehat{a}_\mathbf{r} = \widehat{\psi}(\mathbf{r})$ and our unitary transformations are

$$\begin{aligned} \widehat{\psi}(\mathbf{r}) &= \sum_\alpha \phi_\alpha(\mathbf{r}) \widehat{a}_\alpha \\ \widehat{\psi}^\dagger(\mathbf{r}) &= \sum_\alpha \phi^*_\alpha(\mathbf{r}) \widehat{a}^\dagger_\alpha \end{aligned} \tag{28}$$

The commutation relation is then $\delta_{\alpha,\alpha'}$

$$\begin{aligned}\left[\widehat{\psi}(\mathbf{r}),\widehat{\psi}(\mathbf{r}')\right] &= \sum_{\alpha,\alpha'}\phi_\alpha(\mathbf{r})\,\phi^*_{\alpha'}(\mathbf{r}')\left[\widehat{a}_\alpha,\widehat{a}^\dagger_{\alpha'}\right] \\ &= \sum_\alpha \phi_\alpha(\mathbf{r})\,\phi^*_\alpha(\mathbf{r}') = \sum_\alpha \langle\mathbf{r}|\alpha\rangle\,\langle\alpha|\mathbf{r}'\rangle \\ &= \langle\mathbf{r}|\mathbf{r}'\rangle = \delta(\mathbf{r}-\mathbf{r}') \end{aligned} \tag{29}$$

and it follows

$$\widehat{U} = \int d^3r U(\mathbf{r})\,\widehat{\psi}^\dagger(\mathbf{r})\,\widehat{\psi}(\mathbf{r}) \tag{30}$$

Similarly holds for the kinetic energy

$$\begin{aligned}\widehat{T} &= -\frac{\hbar^2}{2m}\int d^3r d^3r' \left\langle\mathbf{r}\left|\nabla^2\right|\mathbf{r}'\right\rangle \widehat{\psi}^\dagger(\mathbf{r})\,\widehat{\psi}(\mathbf{r}') \\ &= -\frac{\hbar^2}{2m}\int d^3r d^3r' \widehat{\psi}^\dagger(\mathbf{r})\,\nabla^2\delta(\mathbf{r}-\mathbf{r}')\,\widehat{\psi}(\mathbf{r}') \\ &= -\frac{\hbar^2}{2m}\int d^3r \widehat{\psi}^\dagger(\mathbf{r})\,\nabla^2\widehat{\psi}(\mathbf{r}) \end{aligned} \tag{31}$$

Thus we find

$$\begin{aligned} H &= \sum_\alpha \varepsilon_\alpha \widehat{a}^\dagger_\alpha \widehat{a}_\alpha \\ &= \int d^3r \widehat{\psi}^\dagger(\mathbf{r})\left(-\frac{\hbar^2\nabla^2}{2m} + U(\mathbf{r})\right)\widehat{\psi}(\mathbf{r}) \end{aligned} \tag{32}$$

With the help of the field operators $\widehat{\psi}(\mathbf{r})$ and $\widehat{\psi}^\dagger(\mathbf{r})$ is it possible to bring the many body Hamiltonian in occupation number representation into the same form as the Hamiltonian of a single particle.

2.1 Example 1: a single particle

We consider the most general wave function of a single spinless boson:

$$|\psi_\alpha\rangle = \int d^3r \phi_\alpha(\mathbf{r})\,\widehat{\psi}^\dagger(\mathbf{r})\,|0\rangle \tag{33}$$

where $|0\rangle$ is the completely empty system. Let the Hamiltonian be

$$H = \int d^3r \widehat{\psi}^\dagger(\mathbf{r})\left(-\frac{\hbar^2\nabla^2_{\mathbf{r}}}{2m} + U(\mathbf{r})\right)\widehat{\psi}(\mathbf{r}) \tag{34}$$

It follows

$$\begin{aligned} H|\psi_\alpha\rangle &= \int d^3r \int d^3r' \widehat{\psi}^\dagger(\mathbf{r})\left(-\frac{\hbar^2\nabla^2_{\mathbf{r}}}{2m} + U(\mathbf{r})\right)\phi_\alpha(\mathbf{r}')\,\widehat{\psi}(\mathbf{r})\,\widehat{\psi}^\dagger(\mathbf{r}')\,|0\rangle \\ &= \int d^3r \int d^3r' \widehat{\psi}^\dagger(\mathbf{r})\left(-\frac{\hbar^2\nabla^2_{\mathbf{r}}}{2m} + U(\mathbf{r})\right)\phi_\alpha(\mathbf{r}')\,\widehat{\psi}^\dagger(\mathbf{r}')\,\widehat{\psi}(\mathbf{r})\,|0\rangle \\ &+ \int d^3r \int d^3r' \widehat{\psi}^\dagger(\mathbf{r})\left(-\frac{\hbar^2\nabla^2_{\mathbf{r}}}{2m} + U(\mathbf{r})\right)\phi_\alpha(\mathbf{r}')\,\delta(\mathbf{r}-\mathbf{r}')\,|0\rangle \end{aligned} \tag{35}$$

The first term disappears since $\widehat{\psi}(\mathbf{r})|0\rangle = 0$ for the empty state. Performing the integration over $\mathbf{r}'$ gives

$$\begin{aligned} H|\psi_\alpha\rangle &= \int d^3r \widehat{\psi}^\dagger(\mathbf{r}) \left(-\frac{\hbar^2\nabla_\mathbf{r}^2}{2m} + U(\mathbf{r})\right)\phi_\alpha(\mathbf{r})|0\rangle \\ &= \int d^3r \left[\left(-\frac{\hbar^2\nabla_\mathbf{r}^2}{2m} + U(\mathbf{r})\right)\phi_\alpha(\mathbf{r})\right]\widehat{\psi}^\dagger(\mathbf{r})|0\rangle \end{aligned} \tag{36}$$

Thus, we need to find the eigenvalue of and eigenfunction of

$$\left(-\frac{\hbar^2\nabla^2}{2m} + U(\mathbf{r})\right)\phi_\alpha(\mathbf{r}) = \varepsilon_\alpha\phi_\alpha(\mathbf{r}) \tag{37}$$

to obtain

$$H|\psi_\alpha\rangle = \varepsilon_\alpha \int d^3r phi_\alpha(\mathbf{r})\widehat{\psi}^\dagger(\mathbf{r})|0\rangle = \varepsilon_\alpha|\psi_\alpha\rangle. \tag{38}$$

Thus, for a single particle problem we recover the original formulation of the "first quantization". The function $\phi(\mathbf{r})$ in Eq.33 is therefore the wave function of the single particle problem.

Using $\widehat{\psi}^\dagger(\mathbf{r}) = \sum_\alpha \phi_\alpha^*(\mathbf{r})\widehat{a}_\alpha^\dagger$ follows $\widehat{a}_\alpha^\dagger = \int d^3r\phi_\alpha(\mathbf{r})\widehat{\psi}^\dagger(\mathbf{r})$ and our above wave function is nothing but

$$|\psi_\alpha\rangle = \widehat{a}_\alpha^\dagger|0\rangle \tag{39}$$

Applying the Hamiltonian to the wave function in this basis is obviously giving the same answer.

$$H|\psi_\alpha\rangle = \sum_{\alpha'} \varepsilon_{\alpha'}\widehat{a}_{\alpha'}^\dagger\widehat{a}_{\alpha'}\widehat{a}_\alpha^\dagger|0\rangle = \varepsilon_a|\psi_\alpha\rangle \tag{40}$$

3 Second quantization of interacting bosons

Next we analyze the formulation of particle-particle interactions within the second quantization. We consider a two body interaction $\widehat{V}$ that has, by definition, matrix elements that depend on the states of two particles. Thus the expression for a single particle where

$$\widehat{U} = \sum_{\alpha,\alpha'} \langle\alpha|U|\alpha'\rangle\widehat{a}_\alpha^\dagger\widehat{a}_{\alpha'} \tag{41}$$

will be determined by a matrix elements of the kind:

$$\langle\alpha\gamma|V|\alpha'\gamma'\rangle = \int d^3r d^3r' \phi_\alpha^*(\mathbf{r})\phi_\gamma^*(\mathbf{r}')V(\mathbf{r},\mathbf{r}')\phi_{\alpha'}(\mathbf{r}')\phi_{\gamma'}(\mathbf{r}). \tag{42}$$

In general there will be a two particle basis $|\alpha\gamma\rangle$ where the interaction is diagonal

$$\widehat{V}|\alpha\gamma\rangle = V_{\alpha\gamma}|\alpha\gamma\rangle \tag{43}$$

where $V_{\alpha\gamma} = \langle \alpha\gamma | V | \alpha\gamma \rangle$. In this basis we can proceed just like for the interaction $\widehat{U}$, where the operator was given by $\sum_\alpha \langle \alpha | U | \alpha \rangle \widehat{a}_\alpha^\dagger \widehat{a}_\alpha$. In case of a two particle interaction we have contributions if there are two particles, one in state α the other in state γ. This the interaction must be

$$\widehat{V} = \frac{1}{2} \sum_{\alpha\gamma} V_{\alpha\gamma} \widehat{P}_{\alpha\gamma} \tag{44}$$

where $\widehat{P}_{\alpha\beta}$ is the operator which counts the number of pairs of particles in the states $|\alpha\rangle$ and $|\gamma\rangle$. The prefactor $\frac{1}{2}$ takes into account that each pair is considered only once.

If $|\alpha\rangle = |\gamma\rangle$, the number of pairs is $n_\alpha (n_\alpha - 1)$, while for $|\alpha\rangle \neq |\gamma\rangle$ it is $n_\alpha n_\gamma$, where the n_α are the occupation numbers of those states. It follows

$$\begin{aligned} \widehat{P}_{\alpha\gamma} &= \widehat{n}_\alpha \widehat{n}_\gamma - \delta_{\alpha\gamma} \widehat{n}_\alpha \\ &= a_\alpha^\dagger a_\gamma^\dagger a_\alpha a_\gamma = a_\alpha^\dagger a_\gamma^\dagger a_\gamma a_\alpha \end{aligned} \tag{45}$$

and we find

$$\widehat{V} = \frac{1}{2} \sum_{\alpha\gamma} V_{\alpha\gamma} a_\alpha^\dagger a_\gamma^\dagger a_\gamma a_\alpha = \frac{1}{2} \sum_{\alpha\gamma} \langle \alpha\gamma | V | \alpha\gamma \rangle a_\alpha^\dagger a_\gamma^\dagger a_\gamma a_\alpha \tag{46}$$

Transforming this expression into an arbitrary basis $|\mu\rangle = \sum\limits_\alpha |\alpha\rangle \langle \alpha | \mu \rangle$, we insert the operators in the new basis

$$\begin{aligned} \widehat{a}_\alpha^\dagger &= \sum_\lambda \langle \lambda | \alpha \rangle \widehat{a}_\lambda^\dagger \\ \widehat{a}_\alpha &= \sum_\lambda \langle \alpha | \lambda \rangle \widehat{a}_\lambda \end{aligned} \tag{47}$$

and it follows

$$\widehat{V} = \frac{1}{2} \sum_{\alpha\gamma, \lambda\mu\rho\nu} \langle \lambda | \alpha \rangle \langle \mu | \gamma \rangle \langle \alpha\gamma | V | \alpha\gamma \rangle \langle \alpha | \rho \rangle \langle \gamma | \nu \rangle a_\lambda^\dagger a_\mu^\dagger a_\rho a_\nu \tag{48}$$

which simplifies to:

$$\widehat{V} = \frac{1}{2} \sum_{\lambda\mu\rho\nu} \langle \lambda\mu | V | \rho\nu \rangle a_\lambda^\dagger a_\mu^\dagger a_\rho a_\nu \tag{49}$$

If for example

$$\langle \mathbf{r}, \mathbf{r}' | V | \mathbf{r}'' \mathbf{r}''' \rangle = v(\mathbf{r} - \mathbf{r}') \delta(\mathbf{r}'' - \mathbf{r}') \delta(\mathbf{r}''' - \mathbf{r}) \tag{50}$$

for an interaction that only depends on the distance between the two particles, it follows

$$\widehat{V} = \frac{1}{2} \int d^3r d^3r' v(\mathbf{r} - \mathbf{r}') \widehat{\psi}^\dagger(\mathbf{r}) \widehat{\psi}^\dagger(\mathbf{r}') \widehat{\psi}(\mathbf{r}') \widehat{\psi}(\mathbf{r}). \tag{51}$$

4 Second quantization of noninteracting fermions

4.1 The fermionic "harmonic oscillator"

When we introduced the second quantized representation for bosons we took advantage of the fact that the eigenstates of a free bose system

$$E = \sum_{\alpha} \varepsilon_{\alpha} n_{\alpha} \tag{52}$$

could be expressed in terms of the set $\{n_{\alpha}\}$ of occupation numbers. In case of bosons these occupation numbers were allowed to take all integer values $n_a = 0, 1, \cdots, \infty$, reminiscent of the quantum number of the harmonic oscillator. The latter then led to the introduction of creation and annihilation operators of the bosons, where the occupation number operator of a given state was $\widehat{n}_{\alpha} = \widehat{a}_{\alpha}^{\dagger} \widehat{a}_{a}$. The Hamiltonian was then written as

$$\widehat{H} = \sum_{\alpha} \varepsilon_{\alpha} \widehat{n}_{\alpha} \tag{53}$$

Obviously, this approach cannot be used to describe fermions where $n_{\alpha} = 0$ or 1. In case of fermions, the single particle quantum state always includes the spin, for example $\alpha = (\mathbf{k}, \sigma)$.

We need to find the fermion analog to the harmonic oscillator, i.e. a state that only allows for the two occupations $n_{\alpha} = 0$ or 1. We want to express the Hamiltonian for a single quantum state as

$$\widehat{h} = \varepsilon \widehat{n} \tag{54}$$

This is easily done with the help of a (2×2) matrix representation (note, these matrices have nothing to do with the spin of the system). If we introduce

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{55}$$

for the empty and occupied state, it holds

$$\widehat{n} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \tag{56}$$

We can equally introduce lowering and raising operators

$$\widehat{a}\,|0\rangle = 0 \quad \text{and}\ \widehat{a}\,|1\rangle = |0\rangle \tag{57}$$

as well as

$$\widehat{a}^{\dagger}\,|1\rangle = 0 \quad \text{and}\ \widehat{a}^{\dagger}\,|0\rangle = |1\rangle\,. \tag{58}$$

It follows easily that this is accomplished by

$$\widehat{a} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \quad \text{and} \quad \widehat{a}^{\dagger} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}\,. \tag{59}$$

As in case of bosons, $\widehat{a}^\dagger$ is the adjoined operator of $\widehat{a}$.

The action of these operators of a state with arbitrary occupation is then

$$\begin{aligned} \widehat{a}\,|n\rangle &= n\,|n-1\rangle = n\,|1-n\rangle \\ \widehat{a}^\dagger\,|n\rangle &= (1-n)\,|n+1\rangle = (1-n)\,|1-n\rangle \end{aligned} \tag{60}$$

If we now determine $a^\dagger a$ it follows

$$\widehat{a}^\dagger\widehat{a} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \tag{61}$$

and we have, just as for bosons,

$$\widehat{n} = \widehat{a}^\dagger\widehat{a}. \tag{62}$$

However, an important difference is of course that now holds

$$\widehat{a}\widehat{a}^\dagger + \widehat{a}^\dagger\widehat{a} = 1 \tag{63}$$

in addition we immediately see

$$\widehat{a}^\dagger\widehat{a}^\dagger = \widehat{a}\widehat{a} = 0 \tag{64}$$

Fermionic creation and annihilation operators do not commute, they anticommute:

$$\begin{aligned} \left[\widehat{a}, \widehat{a}^\dagger\right]_+ &= 1 \\ \left[\widehat{a}^\dagger, \widehat{a}^\dagger\right]_+ &= \left[\widehat{a}, \widehat{a}\right]_+ = 0. \end{aligned} \tag{65}$$

Note, we could have introduced equally

$$\widehat{a} = -\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \quad \text{and} \quad \widehat{a}^\dagger = -\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}. \tag{66}$$

with the only change that now $\widehat{a}\,|1\rangle = -\,|0\rangle$ and $\widehat{a}^\dagger\,|0\rangle = -\,|1\rangle$ and all other results remain unchanged.

4.2 Many fermi states

To generalize the single fermi result to many fermions we the any body wave function in occupation number representation

$$|n_1, n_2, \ldots, n_\alpha, \ldots\rangle \tag{67}$$

We then need to analyze the creation and annihilation operators $\widehat{a}_\alpha^\dagger$ and $\widehat{a}_a$for the individual states, respectively.

At first glance it is natural to introduce$(1-n)\,|n+1\rangle$

$$\begin{aligned} \widehat{a}_a\,|n_1, n_2, \ldots, n_\alpha, \ldots\rangle &= n_\alpha\,|n_1, n_2, \ldots, n_\alpha - 1, \ldots\rangle \\ \widehat{a}_a^\dagger\,|n_1, n_2, \ldots, n_\alpha, \ldots\rangle &= (1-n_\alpha)\,|n_1, n_2, \ldots, n_\alpha + 1, \ldots\rangle \end{aligned} \tag{68}$$

(**Note, these equations will turn out to be incorrect!**)

This implies however that

$$\left[\widehat{a}_\alpha, \widehat{a}_\alpha^\dagger\right]_+ = 1 \qquad (69)$$

while for different states $\alpha \neq \alpha'$ follows

$$\left[\widehat{a}_\alpha, \widehat{a}_{\alpha'}^\dagger\right]_+ = 2\widehat{a}_\alpha \widehat{a}_{\alpha'}^\dagger \qquad (70)$$

a result that follows from $\left[\widehat{a}_\alpha, \widehat{a}_{\alpha'}^\dagger\right] = 0$ for $\alpha \neq \alpha'$. If we now want to transform from one basis to another, with

$$|l\rangle = \sum_\alpha |\alpha\rangle \langle\alpha|l\rangle \qquad (71)$$

Just like in case of bosons the new operators should be linear combinations of the old ones, which yields

$$\widehat{a}_l = \sum_\alpha \langle l|\alpha\rangle \, \widehat{a}_\alpha \qquad (72)$$

and the corresponding adjoined equation

$$\widehat{a}_l^\dagger = \sum_\alpha \langle l|\alpha\rangle^* \, \widehat{a}_\alpha^\dagger. \qquad (73)$$

We now require

$$\left[\widehat{a}_l, \widehat{a}_l^\dagger\right]_+ = 1 \qquad (74)$$

which leads to

$$1 = \sum_{\alpha,\alpha'} \langle l|\alpha\rangle \langle\alpha'|l\rangle \left[\widehat{a}_\alpha, \widehat{a}_{\alpha'}^\dagger\right]_+ \qquad (75)$$

For a complete set of states $\langle l|\alpha\rangle$ this is only possible if

$$\left[\widehat{a}_\alpha, \widehat{a}_{\alpha'}^\dagger\right]_+ = \delta_{\alpha,\alpha'} \qquad (76)$$

i.e. for $\alpha \neq \alpha'$ the anticommutator and not the commutator must vanish. We conclude that Eq.68 cannot be correct.

Jordan and Wigner realized that a small change in the definition of these operators can fix the problem. To proceed we need to order the quantum numbers in some arbitrary but fixed way. We then introduce

$$\nu_\alpha = \sum_{\alpha'=1}^{\alpha-1} n_\alpha \qquad (77)$$

as the number of occupied states that precede the α-th state. We can then introduce

$$\widehat{a}_\alpha = (-1)^{\nu_\alpha} \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \quad \text{and} \quad \widehat{a}^\dagger = (-1)^{\nu_\alpha} \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \qquad (78)$$

The matrix acts on the occupation of the α-th state. As shown above, a prefactor -1 in the definition of these operators causes no problem. It then follows

$$\begin{aligned}
\widehat{a}_a \left|n_1, n_2, \ldots, n_\alpha, \ldots\right\rangle &= (-1)^{\nu_\alpha} n_\alpha \left|n_1, n_2, \ldots, n_\alpha - 1, \ldots\right\rangle \\
&= (-1)^{\nu_\alpha} n_\alpha \left|n_1, n_2, \ldots, 1 - n_\alpha, \ldots\right\rangle \\
\widehat{a}_a^\dagger \left|n_1, n_2, \ldots, n_\alpha, \ldots\right\rangle &= (-1)^{\nu_\alpha} (1 - n_\alpha) \left|n_1, n_2, \ldots, n_\alpha + 1, \ldots\right\rangle \\
&= (-1)^{\nu_\alpha} (1 - n_\alpha) \left|n_1, n_2, \ldots, 1 - n_\alpha, \ldots\right\rangle \qquad (79)
\end{aligned}$$

It obviously holds that

$$\left[\widehat{a}_\alpha, \widehat{a}_\alpha^\dagger\right]_+ = 1 \qquad (80)$$

We next analyze (assume α' prior to α)

$$\begin{aligned}
\widehat{a}_{a'} \widehat{a}_a^\dagger \left|n_1, \ldots, n_{\alpha'}, \ldots, n_\alpha, \ldots\right\rangle &= (-1)^{\nu_\alpha} (1 - n_\alpha) \widehat{a}_{a'} \left|n_1, \ldots, n_{\alpha'}, \ldots, 1 - n_\alpha, \ldots\right\rangle \\
&= (-1)^{\nu_\alpha + \nu_{\alpha'}} n_{\alpha'} (1 - n_\alpha) \left|n_1, \ldots, 1 - n_{\alpha'}, \ldots, 1 - n_\alpha, \ldots\right\rangle
\end{aligned}$$

On the other hand:

$$\begin{aligned}
\widehat{a}_a^\dagger \widehat{a}_{a'} \left|n_1, \ldots, n_{\alpha'}, \ldots, n_\alpha, \ldots\right\rangle &= (-1)^{\nu_{\alpha'}} n_{\alpha'} \widehat{a}_a^\dagger \left|n_1, \ldots, 1 - n_{\alpha'}, \ldots, n_\alpha, \ldots\right\rangle \\
&= (-1)^{\nu_\alpha + \nu_{\alpha'} - 1} n_{\alpha'} (1 - n_\alpha) \left|n_1, \ldots, 1 - n_{\alpha'}, \ldots, 1 - n_\alpha, \ldots\right\rangle
\end{aligned}$$

It then follows

$$\widehat{a}_{a'} \widehat{a}_a^\dagger + \widehat{a}_a^\dagger \widehat{a}_{a'} = (-1)^{\nu_\alpha + \nu_{\alpha'}} \left(n_{\alpha'} (1 - n_\alpha) - n_{\alpha'} (1 - n_\alpha)\right) = 0 \qquad (81)$$

The same holds of course if we assume α' to occur after α.

Thus, we find

$$\left[\widehat{a}_\alpha, \widehat{a}_{\alpha'}^\dagger\right]_+ = \delta_{\alpha,\alpha'} \qquad (82)$$

as desired, yielding after a unitary transformation

$$\left[\widehat{a}_l, \widehat{a}_{l'}^\dagger\right]_+ = \sum_{\alpha,\alpha'} \langle l|\alpha\rangle \langle\alpha'|l'\rangle \left[\widehat{a}_\alpha, \widehat{a}_{\alpha'}^\dagger\right]_+ = \delta_{l,l'} \qquad (83)$$

i.e. the anticommutation relation of fermionic operators is independent on the specific representation.

The Hamiltonian of noninteracting fermions is then

$$H = \sum_\alpha \varepsilon_\alpha \widehat{a}_\alpha^\dagger \widehat{a}_\alpha \qquad (84)$$

which in case of free particles reads

$$H = \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}} \widehat{a}_{\mathbf{k},\sigma}^\dagger \widehat{a}_{\mathbf{k},\sigma} \qquad (85)$$

where $\mathbf{k}$ goes over all momentum values and $\sigma = \pm\frac{1}{2}$.

5 Interacting fermions

To incorporate interaction effects is now rather similar to the case of bosons. We start from the two particle basis $|\alpha\gamma\rangle$ where the interaction is diagonal

$$\widehat{V}\,|\alpha\gamma\rangle = V_{\alpha\gamma}\,|\alpha\gamma\rangle\,. \tag{86}$$

Here $V_{\alpha\gamma} = \langle\alpha\gamma\,|V|\,\alpha\gamma\rangle$. In this basis we can proceed just like for bosons. In case of a two particle interaction we have contributions if there are two particles, one in state α the other in state γ. This the interaction must be

$$\widehat{V} = \frac{1}{2}\sum_{\alpha\gamma} V_{\alpha\gamma}\widehat{P}_{\alpha\gamma} \tag{87}$$

where $\widehat{P}_{\alpha\beta}$ is the operator which counts the number of pairs of particles in the states $|\alpha\rangle$ and $|\gamma\rangle$. The prefactor $\frac{1}{2}$ takes into account that each pair is considered only once. It follows again

$$\begin{aligned}
\widehat{P}_{\alpha\gamma} &= \widehat{n}_{\alpha}\widehat{n}_{\gamma} - \delta_{\alpha\gamma}\widehat{n}_{\alpha} \\
&= a_{\alpha}^{\dagger}a_{\alpha}a_{\gamma}^{\dagger}a_{\gamma} - \delta_{\alpha\gamma}a_{\alpha}^{\dagger}a_{\alpha} \\
&= -a_{\alpha}^{\dagger}a_{\gamma}^{\dagger}a_{\alpha}a_{\gamma} + a_{\alpha}^{\dagger}\delta_{\alpha\gamma}a_{\gamma} - \delta_{\alpha\gamma}a_{\alpha}^{\dagger}a_{\alpha} \\
&= a_{\alpha}^{\dagger}a_{\gamma}^{\dagger}a_{\alpha}a_{\gamma}
\end{aligned} \tag{88}$$

and we find

$$\widehat{V} = \frac{1}{2}\sum_{\alpha\gamma} V_{\alpha\gamma}a_{\alpha}^{\dagger}a_{\gamma}^{\dagger}a_{\gamma}a_{\alpha} \tag{89}$$

just as in case of bosons. Transforming this expression into an arbitrary basis $|\mu\rangle = \sum_{\alpha}|\alpha\rangle\langle\alpha|\mu\rangle$ where $\widehat{a}_{\mu} = \sum_{\alpha}\langle\mu|\alpha\rangle\,\widehat{a}_{\alpha}$ it holds

$$\widehat{V} = \frac{1}{2}\sum_{\lambda\mu\rho\nu}\langle\lambda\mu\,|V|\,\rho\nu\rangle\, a_{\lambda}^{\dagger}a_{\mu}^{\dagger}a_{\rho}a_{\nu} \tag{90}$$

If for example

$$\langle\mathbf{r},\mathbf{r}'\,|V|\,\mathbf{r}''\mathbf{r}'''\rangle = v\left(\mathbf{r}-\mathbf{r}'\right)\delta\left(\mathbf{r}''-\mathbf{r}'\right)\delta\left(\mathbf{r}'''-\mathbf{r}\right) \tag{91}$$

for an interaction that only depends on the distance between the two particles, it follows

$$\widehat{V} = \frac{1}{2}\int d^3r d^3r' v\left(\mathbf{r}-\mathbf{r}'\right)\widehat{\psi}^{\dagger}\left(\mathbf{r}\right)\widehat{\psi}^{\dagger}\left(\mathbf{r}'\right)\widehat{\psi}\left(\mathbf{r}'\right)\widehat{\psi}\left(\mathbf{r}\right). \tag{92}$$

5.1 Example 1: free electron gas

We want to derive the ground state wave function of the free electron gas. The Hamiltonian of an individual electron is

$$h = -\frac{\hbar^2\nabla^2}{2m} \tag{93}$$

which leads to the single particle eigenvalues

$$\varepsilon_{\mathbf{k}} = \frac{\hbar^2 k^2}{2m}. \tag{94}$$

The Hamiltonian of the many fermion system is then

$$H = \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}} \widehat{a}^\dagger_{\mathbf{k},\sigma} \widehat{a}_{\mathbf{k},\sigma}. \tag{95}$$

The ground state wave function is the state where all single particle states with energy

$$\varepsilon_{\mathbf{k}} < E_F \tag{96}$$

are occupied and all states above the Fermi energy are empty. ,

$$E_F = \frac{\hbar^2}{2m} \left(\frac{3\pi^2 \langle N \rangle}{V} \right)^{2/3} \tag{97}$$

was determined earlier. The ground state wave function is then

$$|\Psi_0\rangle = \prod_{\mathbf{k},\sigma(\varepsilon_{\mathbf{k}} < E_F)} \widehat{a}^\dagger_{\mathbf{k},\sigma} |0\rangle \tag{98}$$

This state is normalized:

$$\begin{aligned} \langle \Psi_0 | \Psi_0 \rangle &= \left\langle 0 \left| \prod_{\mathbf{k},\sigma(\varepsilon_{\mathbf{k}} < E_F)} \widehat{a}_{\mathbf{k},\sigma} \widehat{a}^\dagger_{\mathbf{k},\sigma} \right| 0 \right\rangle \\ &= \left\langle 0 \left| \prod_{\mathbf{k},\sigma(\varepsilon_{\mathbf{k}} < E_F)} \left(1 - \widehat{a}^\dagger_{\mathbf{k},\sigma} \widehat{a}_{\mathbf{k},\sigma} \right) \right| 0 \right\rangle \\ &= \prod_{\mathbf{k},\sigma(\varepsilon_{\mathbf{k}} < E_F)} \langle 0 | 0 \rangle = 1 \end{aligned} \tag{99}$$

and it is indeed the eigenstate of the problem

$$H |\Psi_0\rangle = \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}} \widehat{a}^\dagger_{\mathbf{k},\sigma} \widehat{a}_{\mathbf{k},\sigma} |\Psi_0\rangle \tag{100}$$

It follows immediately that

$$\widehat{a}^\dagger_{\mathbf{k},\sigma} \widehat{a}_{\mathbf{k},\sigma} \prod_{\mathbf{q},\sigma(\varepsilon_{\mathbf{q}} < E_F)} \widehat{a}^\dagger_{\mathbf{q},\sigma} |0\rangle = \theta\left(E_F - \varepsilon_{\mathbf{k}}\right) |\Psi_0\rangle . \tag{101}$$

Either $\mathbf{k}$ is among the states below the Fermi surface or it isn't. This yields

$$H |\Psi_0\rangle = E_0 |\Psi_0\rangle \tag{102}$$

with

$$E_0 = \sum_{\mathbf{k},\sigma} \theta\left(E_F - \varepsilon_{\mathbf{k}}\right) \varepsilon_{\mathbf{k}} \tag{103}$$

The states that contribute to the ground state energy are all those with an energy below E_F. Since $\varepsilon_{\mathbf{k}} = \frac{\hbar^2 k^2}{2m}$ is implies that the magnitude of the momentum must be smaller than a given value

$$\frac{\hbar^2 k^2}{2m} < \frac{\hbar^2 k_F^2}{2m} = E_F \tag{104}$$

Here k_F is the so called Fermi momentum. All momentum states inside the sphere of radius k_F are occupied. Those outside are empty. Our above result for the Fermi energy yields

$$k_F = \left(3\pi^2 \rho\right)^{1/3} \tag{105}$$

where $\rho = \langle N \rangle / V$ is the electron density.

5.2 Example 2: two particles

The natural state of two noninteracting particles is

$$|\psi_{\alpha,\alpha'}\rangle = \widehat{a}_{\alpha}^{\dagger} \widehat{a}_{\alpha'}^{\dagger} |0\rangle \tag{106}$$

Applying the Hamiltonian

$$H = \sum_{\alpha} \varepsilon_{\alpha} \widehat{a}_{\alpha}^{\dagger} \widehat{a}_{\alpha} \tag{107}$$

to this wave function gives

$$\begin{aligned} H|\psi_{\alpha,\alpha'}\rangle &= \sum_{\gamma} \varepsilon_{\gamma} \widehat{a}_{\gamma}^{\dagger} \widehat{a}_{\gamma} \widehat{a}_{\alpha}^{\dagger} \widehat{a}_{\alpha'}^{\dagger} |0\rangle \\ &= -\sum_{\gamma} \varepsilon_{\gamma} \widehat{a}_{\gamma}^{\dagger} \widehat{a}_{\alpha}^{\dagger} \widehat{a}_{\gamma} \widehat{a}_{\alpha'}^{\dagger} |0\rangle + \varepsilon_{\alpha} \widehat{a}_{\alpha}^{\dagger} \widehat{a}_{\alpha'}^{\dagger} |0\rangle \\ &= -\varepsilon_{\alpha'} \widehat{a}_{\alpha'}^{\dagger} \widehat{a}_{\alpha}^{\dagger} |0\rangle + \varepsilon_{\alpha} \widehat{a}_{\alpha}^{\dagger} \widehat{a}_{\alpha'}^{\dagger} |0\rangle \\ &= \left(\varepsilon_{\alpha} + \varepsilon_{\alpha'}\right) |\psi_{\alpha,\alpha'}\rangle \end{aligned} \tag{108}$$

The eigenvalue is $E_{\alpha,\alpha'} = \varepsilon_{\alpha} + \varepsilon_{\alpha'}$. The wave function can also be written as

$$|\psi_{\alpha,\alpha'}\rangle = \frac{1}{\sqrt{2}} \int d^3 r d^3 r' \phi_{\alpha}(\mathbf{r}) \phi_{\alpha'}(\mathbf{r}') \widehat{\psi}^{\dagger}(\mathbf{r}) \widehat{\psi}^{\dagger}(\mathbf{r}') |0\rangle \tag{109}$$

Since a labelling of the particles is not necessary within the second quantization, there is no need to symmetrize $\phi_{\alpha}(\mathbf{r}) \phi_{\alpha'}(\mathbf{r}')$ in this formulation.

To determine the wave function in real space we analyze

$$\Psi_{\alpha\alpha'}(\mathbf{r}, \mathbf{r}') = \langle \mathbf{r}, \mathbf{r}' | \psi_{\alpha,\alpha'} \rangle \tag{110}$$

It holds

$$|\mathbf{r},\mathbf{r}'\rangle = \widehat{\psi}^{\dagger}(\mathbf{r})\,\widehat{\psi}^{\dagger}(\mathbf{r}')\,|0\rangle \tag{111}$$

such that

$$\langle\mathbf{r},\mathbf{r}'| = \langle 0|\,\widehat{\psi}(\mathbf{r}')\,\widehat{\psi}(\mathbf{r}) \tag{112}$$

and we can analyze

$$\begin{aligned}
\langle\mathbf{r},\mathbf{r}'|\psi_{\alpha,\alpha'}\rangle &= \frac{1}{\sqrt{2}}\int d^3r''d^3r'''\phi_{\alpha}(\mathbf{r}'')\,\phi_{\alpha'}(\mathbf{r}''') && (113)\\
&\quad\times\langle 0|\,\widehat{\psi}(\mathbf{r}')\,\widehat{\psi}(\mathbf{r})\,\widehat{\psi}^{\dagger}(\mathbf{r}'')\,\widehat{\psi}^{\dagger}(\mathbf{r}''')\,|0\rangle && (114)
\end{aligned}$$

It holds

$$\begin{aligned}
\langle 0|\,\widehat{\psi}(\mathbf{r}')\,\widehat{\psi}(\mathbf{r})\,\widehat{\psi}^{\dagger}(\mathbf{r}'')\,\widehat{\psi}^{\dagger}(\mathbf{r}''')\,|0\rangle &= -\langle 0|\,\widehat{\psi}(\mathbf{r}')\,\widehat{\psi}^{\dagger}(\mathbf{r}'')\,\widehat{\psi}(\mathbf{r})\,\widehat{\psi}^{\dagger}(\mathbf{r}''')\,|0\rangle\\
&\quad+\delta(\mathbf{r}-\mathbf{r}'')\,\langle 0|\,\widehat{\psi}(\mathbf{r}')\,\widehat{\psi}^{\dagger}(\mathbf{r}''')\,|0\rangle\\
&= -\delta(\mathbf{r}-\mathbf{r}''')\,\langle 0|\,\widehat{\psi}(\mathbf{r}')\,\widehat{\psi}^{\dagger}(\mathbf{r}'')\,|0\rangle\\
&\quad+\delta(\mathbf{r}-\mathbf{r}'')\,\langle 0|\,\widehat{\psi}(\mathbf{r}')\,\widehat{\psi}^{\dagger}(\mathbf{r}''')\,|0\rangle\\
&= -\delta(\mathbf{r}-\mathbf{r}''')\,\delta(\mathbf{r}'-\mathbf{r}'')+\delta(\mathbf{r}-\mathbf{r}'')\,\delta(\mathbf{r}'-\mathbf{r}''')
\end{aligned}$$

Inserting this yields

$$\Psi_{\alpha\alpha'}(\mathbf{r},\mathbf{r}') = \frac{1}{\sqrt{2}}\left(\phi_{\alpha}(\mathbf{r})\,\phi_{\alpha'}(\mathbf{r}')-\phi_{\alpha}(\mathbf{r}')\,\phi_{\alpha'}(\mathbf{r})\right) \tag{115}$$

This is of course the correct result for the wave function of two indistinguishable fermions.