Second Quantization - The Quantization of the Schrödinger Field.

Selected chapter of lecture notes on Quantum Mechanics

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1 Introduction

Let us consider the Schrödinger equation for a free particle

$$i\hbar\frac{\partial\psi(\mathbf{r},\mathrm{t})}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r},\mathrm{t}) \tag{1}$$

and regard it as equation for a classical field $\psi(\mathbf{r},t)$ just like we regarded the Maxwell equations for the electromagnetic field. To remind - the Maxwell field after the quantization describes free quanta - photons - which behave like quantum particles. Their energy-momentum relation $\epsilon = c|\mathbf{p}|$ is determined by the classical dispersion relation $\omega = c|\mathbf{k}|$ of the free EM waves supplemented with the basic QM particle-wave relations $\epsilon = \hbar\omega$ and $\mathbf{p} = \hbar\mathbf{k}$.

For the free Schrödinger field the dispersion relation is read off the equation (1) as

$$\hbar\omega = \frac{\hbar^2|\mathbf{k}|^2}{2m}$$

which suggests that the quantization of this field will lead to the description of free quanta with the energy-momentum relation

$$\epsilon = \frac{\mathbf{p}^2}{2m}$$

i.e. that of non relativistic particles. This procedure is called *second quantization* for obvious reasons.

We will start by confirming this picture and then extending it to describe particles moving in an external potential and also interacting between themselves. In the process of doing this we will discover that the formalism describes identical particles obeying boson statistics. We will then understand how to extend the formalism to describe particle obeying fermion statistics.

2 Free Schrödinger field. Quantization

The Schrödinger field $\psi(\mathbf{r}, t)$ is a scalar field and in that it is simpler than the vector EM field. It is however complex valued unlike the real valued EM field. The last feature means that actually the equation (1) should be considered as a pair of equations for real and imaginary parts or equivalently for $\psi(\mathbf{r})$ and its complex conjugate $\psi^*(\mathbf{r})$

$$i\hbar\frac{\partial\psi(\mathbf{r},\mathrm{t})}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r},\mathrm{t}) \quad ; \quad -i\hbar\frac{\partial\psi^*(\mathbf{r},\mathrm{t})}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi^*(\mathbf{r},\mathrm{t}) \; . \tag{2}$$

Following the motivation outlined in the Introduction we consider the quantization of this field. We follow the standard quantization procedure and start by identifying the hamiltonian structure and the canonical conjugate pairs of the Schrödinger field.

We note that the pair of equations (2) can be regarded as the Hamiltonian pair of equations with the Hamiltonian

$$H = \frac{\hbar^2}{2m}\int d^3r|\nabla\psi(\mathbf{r})|^2 \tag{3}$$

Indeed, the variation of this expression gives

$$\begin{aligned}\delta H &= \frac{\hbar^2}{2m}\int d^3r\,[\nabla\psi^*(\mathbf{r})\cdot\nabla\delta\psi(\mathbf{r}) + \nabla\delta\psi^*(\mathbf{r})\cdot\nabla\psi(\mathbf{r})] = \\ &= -\frac{\hbar^2}{2m}\int d^3r\left\{[\nabla^2\psi^*(\mathbf{r})]\delta\psi(\mathbf{r}) + [\nabla^2\psi(\mathbf{r})]\,\delta\psi^*(\mathbf{r})\right\}\end{aligned} \tag{4}$$

Now regarding $\delta\psi(\mathbf{r})$ and $\delta\psi^*(\mathbf{r})$ as **independent** we read off that

$$\frac{\delta H}{\delta\psi(\mathbf{r})} = -\frac{\hbar^2}{2m}\nabla^2\psi^*(\mathbf{r}) \quad ; \quad \frac{\delta H}{\delta\psi^*(\mathbf{r})} = -\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r}) \tag{5}$$

This shows that the pair (2) is indeed the Hamiltonian pair provided one considers $\psi(\mathbf{r})$ and $i\hbar\psi^*(\mathbf{r})$ (i.e. their values at every space point $\mathbf{r}$) as respectively **canonically conjugate coordinates and momenta**,

$$\frac{\partial\psi(\mathbf{r},t)}{\partial t} = \frac{\delta H}{\delta(i\hbar\psi^*(\mathbf{r},t))} \quad , \quad \frac{\partial(i\hbar\psi^*(\mathbf{r},t))}{\partial t} = -\frac{\delta H}{\delta\psi(\mathbf{r},t)} \tag{6}$$

2.1 Separating the real and imaginary parts

The complex valuedness of ψ and $i\hbar\psi^*$ presents a slight problem in applying the standard rules of the canonical quantization procedure. A possible way to avoid this problem is to transforms to the real and imaginary parts

$$\psi = \mathrm{Re}\psi + i\mathrm{Im}\psi \quad ; \quad \psi^* = \mathrm{Re}\psi - i\mathrm{Im}\psi \tag{7}$$

We will proceed with this for a little while and use it to learn how to quantize using the original ψ and $i\hbar\psi^*$. As we will see it will be a more convenient (and conventional) option.

One must take care that the transformation (7) is canonical to make sure that the transformed variables also form a canonical pair. This is achieved by

$$\psi(\mathbf{r}) = \frac{1}{\sqrt{2\hbar}}[\phi(\mathbf{r}) + i\pi(\mathbf{r})] \quad ; \quad \psi^*(\mathbf{r}) = \frac{1}{\sqrt{2\hbar}}[\phi(\mathbf{r}) - i\pi(\mathbf{r})] \tag{8}$$

with real ϕ and π. To verify that ϕ and π are canonical let us use the known property[1] that time independent canonical transformation from a set p_k, q_k to P_k, Q_k obeys

$$\sum_k p_k dq_k = \sum_k P_k dQ_k + dF$$

where dF is a total differential. In our case the sum over k is the integral over $\mathbf{r}$ so that

$$\int i\hbar\psi^*(\mathbf{r})d\psi(\mathbf{r})d\mathbf{r} = \int i\hbar\frac{1}{2\hbar}\left[\phi(\mathbf{r})d\phi(\mathbf{r}) + i\phi(\mathbf{r})d\pi(\mathbf{r}) - i\pi(\mathbf{r})d\phi(\mathbf{r}) + \right.$$
$$\left. + \pi(\mathbf{r})d\pi(\mathbf{r})\right]d\mathbf{r} = \int \pi(\mathbf{r})d\phi(\mathbf{r})d\mathbf{r} + d\int \frac{i}{4}\left[\phi^2(\mathbf{r}) + \pi^2(\mathbf{r}) + 2i\phi(\mathbf{r})\pi(\mathbf{r})\right]d\mathbf{r}$$

showing that indeed ϕ and π are canonical i.e. difference of the symplectic forms in the old and the new canonical variables is a complete differential.

Inserting (8) into the equations (2) we obtain

$$\frac{\partial\phi(\mathbf{r},\mathrm{t})}{\partial t} = -\frac{\hbar}{2m}\nabla^2\pi(\mathbf{r},\mathrm{t}) \quad ; \quad \frac{\partial\pi(\mathbf{r},\mathrm{t})}{\partial t} = \frac{\hbar}{2m}\nabla^2\phi(\mathbf{r},\mathrm{t})\ . \tag{9}$$

The Hamiltonian becomes

$$H = \frac{\hbar^2}{2m}\int d^3r|\nabla\psi(\mathbf{r})|^2 = \frac{\hbar}{4m}\int d^3r\left[(\nabla\pi(\mathbf{r}))^2 + (\nabla\phi(\mathbf{r}))^2\right] \tag{10}$$

[1]cf, L. Landau and E. Lifshitz, Mechanics, Sec.45, Elsevier Ltd. 1976

Its variation

$$\delta H = \frac{\hbar}{2m}\int d^3r\,[\nabla\pi(\mathbf{r})\cdot\nabla\delta\pi(\mathbf{r}) + \nabla\phi(\mathbf{r})\cdot\nabla\delta\phi(\mathbf{r})] = \\ = -\frac{\hbar}{2m}\int d^3r\,\left[\nabla^2\pi(\mathbf{r})\delta\pi(\mathbf{r}) + \nabla^2\phi(\mathbf{r})\delta\phi(\mathbf{r})\right] \tag{11}$$

so that

$$\frac{\delta H}{\delta\phi(\mathbf{r})} = -\frac{\hbar}{2m}\nabla^2\phi(\mathbf{r}) \quad , \quad \frac{\delta H}{\delta\pi(\mathbf{r})} = -\frac{\hbar}{2m}\nabla^2\pi(\mathbf{r}) \tag{12}$$

Thus we see that Eqs. (9) indeed are in the Hamiltonian form

$$\frac{\partial\phi(\mathbf{r},\mathrm{t})}{\partial t} = \frac{\delta H}{\delta\pi(\mathbf{r},t)} \quad , \quad \frac{\partial\pi(\mathbf{r},\mathrm{t})}{\partial t} = -\frac{\delta H}{\delta\phi(\mathbf{r},t)}\ . \tag{13}$$

with $\phi(\mathbf{r})$ as coordinates and $\pi(\mathbf{r})$ as momenta. These are real and we can quantize the theory in the usual way by introducing wave functionals $\Psi[\phi(\mathbf{r})]$ and operators which act on them

$$\hat{\phi}(\mathbf{r})\Psi[\phi(\mathbf{r})] = \phi(\mathbf{r})\Psi[\phi(\mathbf{r})]\ ;\ \hat{\pi}(\mathbf{r})\Psi[\phi(\mathbf{r})] = -i\hbar\frac{\delta}{\delta\phi(\mathbf{r})}\Psi[\phi(\mathbf{r})]\ . \tag{14}$$

with the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\Psi[\phi(\mathbf{r}),t] = H_{op}\Psi[\phi(\mathbf{r}),t] \tag{15}$$

where the Hamiltonian operator is given by the expression (10) with $\phi(\mathbf{r})$ and $\pi(\mathbf{r})$ replaced by the corresponding operators

$$H_{op} = \frac{\hbar}{4m}\int d^3r\,\left[(\nabla\hat{\pi}(\mathbf{r}))^2 + (\nabla\hat{\phi}(\mathbf{r}))^2\right] \tag{16}$$

We note that the commutation relations for the operators $\hat{\phi}(\mathbf{r})$ and $\hat{\pi}(\mathbf{r})$ are

$$[\hat{\phi}(\mathbf{r}),\hat{\phi}(\mathbf{r}')] = [\hat{\pi}(\mathbf{r}),\hat{\pi}(\mathbf{r}')] = 0$$

$$[\hat{\pi}(\mathbf{r}),\hat{\phi}(\mathbf{r}')] = \hat{\pi}(\mathbf{r})\,\hat{\phi}(\mathbf{r}') - \hat{\phi}(\mathbf{r}')\,\hat{\pi}(\mathbf{r}) = -i\hbar\frac{\delta\phi(\mathbf{r}')}{\delta\phi(\mathbf{r})} = -i\hbar\delta(\mathbf{r}-\mathbf{r}') \tag{17}$$

2.2 Back to the complex valued field

As was already stated it is more convenient to work with complex valued field. Using (8) we introduce non hermitian combinations of the operators $\phi(\hat{\mathbf{r}})$ and $\hat{\pi}(\mathbf{r}))$

$$\hat{\psi}(\mathbf{r}) = \frac{1}{\sqrt{2\hbar}}[\hat{\phi}(\mathbf{r}) + i\hat{\pi}(\mathbf{r})] \quad ; \quad \hat{\psi}^+(\mathbf{r}) = \frac{1}{\sqrt{2\hbar}}[\hat{\phi}(\mathbf{r}) - i\hat{\pi}(\mathbf{r})] \tag{18}$$

We note here a clear analogy with the familiar operators $\hat{a}$ and $\hat{a}^+$

$$\hat{a} = \frac{1}{\sqrt{2\hbar}}[\hat{x} + i\hat{p}] \quad , \quad \hat{a}^+ = \frac{1}{\sqrt{2\hbar}}[\hat{x} - i\hat{p}] \ ,$$

the non hermitian combinations of coordinate and momentum operators for a single degree of freedom.

In our case we have such combinations (18) for every $\mathbf{r}$, i.e. for ∞^3 coordinate-momentum pairs.

From the commutation relations (17) we have

$$[\hat{\psi}(\mathbf{r}), \hat{\psi}^+(\mathbf{r}')] = \delta(\mathbf{r} - \mathbf{r}') \quad , \quad [\hat{\psi}(\mathbf{r}), \hat{\psi}(\mathbf{r}')] = 0 = [\hat{\psi}^+(\mathbf{r}), \hat{\psi}^+(\mathbf{r}')] \tag{19}$$

Looking back at (6) we observe that had we postulated the usual commutation relations for the operators corresponding to the complex field canonical coordinates and momenta $\psi(\mathbf{r})$ and $i\hbar\psi(\mathbf{r})$

$$[\hat{\psi}(\mathbf{r}), i\hbar\hat{\psi}^+(\mathbf{r}')] = i\hbar\delta(\mathbf{r} - \mathbf{r}') \tag{20}$$

we would have arrived at the same result Eq. (19).

As we will soon see the commutation relations (19) will be essentially all (well almost all) we will need to know about the operators $\hat{\psi}(\mathbf{r})$ and $\hat{\psi}^+(\mathbf{r})$ in order to understand how they act on any wave function.

2.3 The Hamiltonian of the free Schrödinger field

The Hamiltonian operator is directly obtained from Eq. (3) by replacing $\psi(\mathbf{r})$ and $\psi^*(\mathbf{r})$ with the operators $\hat{\psi}(\mathbf{r})$ and $\hat{\psi}^+(\mathbf{r})$. One usually finds two expressions in the literature

$$H_{op} = \frac{\hbar^2}{2m}\int d^3r \nabla\hat{\psi}^+(\mathbf{r})\nabla\hat{\psi}(\mathbf{r}) \tag{21}$$

or

$$H_{op} = \int d^3r \hat{\psi}^+(\mathbf{r}) \left(-\frac{\hbar^2\nabla^2}{2m}\right) \hat{\psi}(\mathbf{r}) = -\frac{\hbar^2}{2m}\int d^3r \hat{\psi}^+(\mathbf{r})\nabla^2\hat{\psi}(\mathbf{r}) \tag{22}$$

The difference is obviously just a "surface term" at large distances. This is an operator valued term so disregarding this difference means the requirement that all the wave functions of the field will produce zero when acted upon by such "surface" operators.

Note also the order of the operators chosen in the above expression for H_{op} with $\hat{\psi}^{+}(\mathbf{r})$ acting after $\hat{\psi}(\mathbf{r})$. As will become clear below this order of operators (called "normal ordering") assures that the vacuum of the theory has zero energy.

2.4 The eigenstates. Field quanta are free non relativistic particles

Having established the form of the Hamiltonian operator of the theory we should proceed to solve the Schrödinger equation of the theory

$$i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle = H_{op}|\Psi(t)\rangle \tag{23}$$

Note - to solve the Schrödinger equation for the quantum Schrödinger field!

2.4.1 The normal modes

Since H_{op} is time independent we can solve the above equation in a standard way by first finding the eigenfunctions of the Schrödinger field Hamiltonian i.e. solutions of

$$H_{op}\Psi = E\Psi \tag{24}$$

To this end we will go to the normal modes of the field. As we know from the systems with finite number of degrees of freedom quadratic Hamiltonians become sums of independent terms when the original degrees of freedom are transformed to the normal modes.

To find the normal modes let us recall that they are special solutions of the classical equations in which all the degrees of freedom of the physical system oscillate with the same frequency. Classical equations in the present case are just the field equations (2). Their solutions with a given frequency $\psi(\mathbf{r},t) = u(\mathbf{r})\exp(-i\omega t)$ satisfy

$$\frac{\hbar^2}{2m}\nabla^2 u(\mathbf{r}) + \hbar\omega\, u(\mathbf{r}) = 0 \tag{25}$$

and can be chosen as plane waves

$$u_{\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{\Omega}}e^{i\mathbf{k}\cdot\mathbf{r}} \;\text{ with }\; \hbar\omega = \frac{\hbar^2k^2}{2m} \tag{26}$$

where we assumed the usual periodic boundary condition in a very large volume Ω

$$\mathbf{k} = \frac{2\pi}{\Omega^{1/3}}(n_x, n_y.n_z) \quad \text{with} \;\; n_x, n_y, n_z = 0, \pm 1, \pm 2, ...$$

We now expand the field operators using these normal modes

$$\begin{aligned} \hat{\psi}(\mathbf{r}) &= \sum_{\mathbf{k}} \hat{a}_{\mathbf{k}} u_{\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{\Omega}} \sum_{\mathbf{k}} \hat{a}_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} \\ \hat{\psi}^{+}(\mathbf{r}) &= \sum_{\mathbf{k}} \hat{a}^{+}_{\mathbf{k}} u^{*}_{\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{\Omega}} \sum_{\mathbf{k}} \hat{a}^{+}_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{r}} \end{aligned} \tag{27}$$

The coefficients $\hat{a}_{\mathbf{k}}$ and $\hat{a}^{+}_{\mathbf{k}}$ in the above expansions of the field operators are obviously operators. This expansion must be viewed as a transformation from a canonical set of $2 \times \infty^3$ operators $\hat{\psi}(\mathbf{r})$, $\hat{\psi}^{+}(\mathbf{r})$ to another canonical set of $2 \times \infty^3$ operators $\hat{a}_{\mathbf{k}}$, $\hat{a}^{+}_{\mathbf{k}}$. Using orthonormality of $u_{\mathbf{k}}$'s it is easy to invert (27)

$$\hat{a}_{\mathbf{k}} = \frac{1}{\sqrt{\Omega}} \int d^3r \, \hat{\psi}(\mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r}} \quad , \quad \hat{a}^{+}_{\mathbf{k}} = \frac{1}{\sqrt{\Omega}} \int d^3r \, \hat{\psi}^{+}(\mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{r}}$$

Using the commutations (19) one can then find the commutation relations between $\hat{a}_{\mathbf{k}}$'s and $\hat{a}^{+}_{\mathbf{k}'}$'s,

$$[\hat{a}_{\mathbf{k}} \, , \, \hat{a}^{+}_{\mathbf{k}'}] = \delta_{\mathbf{k}\mathbf{k}'} \quad , \quad [\hat{a}_{\mathbf{k}} \, , \, \hat{a}_{\mathbf{k}'}] = 0 = [\hat{a}^{+}_{\mathbf{k}} \, , \, \hat{a}^{+}_{\mathbf{k}'}] \tag{28}$$

which of course express the harmonic oscillator character of the normal modes for each $\mathbf{k}$ and their independence for different $\mathbf{k}$'s.

2.4.2 Diagonalizing the field Hamiltonian

Inserting the expansions (27) into the Hamiltonian Eq. (22) we obtain a sum of independent (commuting) oscillators

$$H_{op} = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} \hat{a}^{+}_{\mathbf{k}} \hat{a}_{\mathbf{k}} \tag{29}$$

where we have denoted the energies of the oscillator quanta

$$\epsilon_{\mathbf{k}} = \frac{\hbar^2 \mathbf{k}^2}{2m} \tag{30}$$

Based on this it is trivial to find the eigenfunctions and eigenenergies of each term. Clearly the eigenstates of this H_{op} are products of the familiar harmonic oscillator-like states (cf., Appendix, Eq. (159))

$$|\{n_{\mathbf{k}}\}\rangle = \prod_{\mathbf{k}} |n_{\mathbf{k}}\rangle = \prod_{\mathbf{k}} \frac{(\hat{a}^+_{\mathbf{k}})^{n_{\mathbf{k}}}}{\sqrt{n_{\mathbf{k}}!}} |0\rangle \tag{31}$$

with eigenvalues which are

$$E_{\{n_{\mathbf{k}}\}} = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}}\, n_{\mathbf{k}} \quad \text{with each} \;\; n_{\mathbf{k}} = 0, 1, 2, \ldots \tag{32}$$

So the eigenenergies of the free Schrödinger field are sums over the modes $u_{\mathbf{k}}(\mathbf{r})$ of integer numbers $n_{\mathbf{k}}$ of quanta with energies $\epsilon_{\mathbf{k}}$. To understand the physics of these quanta it is useful to ask/determine what are their momenta. For this one must find the corresponding operator. We deal with this in the next section.

We note that the ground state corresponds to all $n_{\mathbf{k}} = 0$, i.e. it is the vacuum state $|0\rangle$. Its energy is equal to zero which was assured by the normal ordered form of H_{op}, Eq. (22), which we have adopted. Let us also note that in this formulation the only properties we will ever need of the vacuum state are that it gives zero when acted upon with anyone of the operators $\hat{a}_{\mathbf{k}}$ and that it is normalized

$$\hat{a}_{\mathbf{k}}|0\rangle = 0 \;\; , \;\; \langle 0|0\rangle = 1 \tag{33}$$

Let us also note that the most general states of the theory are linear combinations of the eigenstates (31)

$$|\Psi\rangle = \sum_{\{n_{\mathbf{k}}\}} C_{\{n_{\mathbf{k}}\}} |\{n_{\mathbf{k}}\}\rangle \tag{34}$$

They may appear e.g. as solutions of the time dependent Schrödinger equation of the field

$$i\hbar \frac{\partial |\Psi(t)\rangle}{\partial t} = H_{op}|\Psi(t)\rangle \tag{35}$$

with coefficients depending on time via the usual

$$C_{\{n_{\mathbf{k}}\}}(t) = C_{\{n_{\mathbf{k}}\}}(0) \exp(-iE_{\{n_{\mathbf{k}}\}} t/\hbar)$$

We note that the number of particles in the above expressions for $C_{\{n_{\mathbf{k}}\}}$ is given by

$$N = \sum_{\mathbf{k}} n_{\mathbf{k}}$$

It is important to note that nowhere in the formalism there appears a requirement that N is fixed, i.e. has the same value in the e.g. expression for the general wave function $|\Psi\rangle$. The formalism in principle allows to have states with coherent combinations of different particle numbers. We will address this issue in the last section.

2.4.3 Degeneracy of the normal modes. Spherical waves

The normal modes Eq. (26) are clearly infinitely degenerate having the same frequency ω for all $\mathbf{k}$ with the same $k = |\mathbf{k}|$. This of course follows from the degeneracy of the solutions of the (free Schrödinger) equation (25). This degeneracy means that other sets can be chosen for a given k. The familiar spherical or cylindrical waves rather than the plane waves would supply examples of such sets.

Let us consider the spherical waves set of solutions

$$u_{klm}(\mathbf{r}) = R_{kl}(r)Y_{lm}(\theta,\phi)$$

with l, m the angular momentum and its projection (for a free particle) and $R_{kl}(r)$ and $Y_{lm}(\theta,\phi)$ the radial and angular parts[2]. We can expand the field operators using such normal modes[3]

$$\begin{aligned} \hat{\psi}(\mathbf{r}) &= \sum_{klm} \hat{a}_{klm}\, u_{klm}(r,\theta,\phi) \\ \hat{\psi}^{+}(\mathbf{r}) &= \sum_{klm} \hat{a}^{+}_{klm}\, u^{*}_{klm}(r,\theta,\phi) \end{aligned} \tag{36}$$

with the operators

$$\hat{a}_{klm} = \int d^3r \hat{\psi}(\mathbf{r})\, u^{*}_{klm}(r,\theta,\phi) \;\; , \;\; \hat{a}^{+}_{klm} = \int d^3r \hat{\psi}^{+}(\mathbf{r})\, u_{klm}(r,\theta,\phi)$$

and (as can be easily checked) the commutation relations equivalent to Eq. (28) with $\mathbf{k}$ and $\mathbf{k}'$ indices replaced by klm and $k'l'm'$.

Inserting the expansions (36) into the Hamiltonian Eq. (22) we obtain

$$H_{op} = \sum_{klm} \epsilon_{klm} \hat{a}^{+}_{klm} \hat{a}_{klm} \tag{37}$$

[2]Recall the solutions of the stationary Schrödinger equation for a free particle in spherical coordinates, cf., Sakurai, Modern Quantum Mechanics, Sec.3.7, Addison-Wesley, 1994.

[3]For convenience we assume that k values are made discrete by imposing boundary condition in a large spherical box

As with the plane waves it is a sum of independent (commuting) oscillators with quanta energies depending only on k

$$\epsilon_{klm} = \frac{\hbar^2 k^2}{2m}$$

i.e. equal to the energy of the plane wave quanta - reflecting the degeneracy of the normal modes.

2.5 Momentum and angular momentum

2.5.1 Field momentum

We now discuss the total (mechanical) momentum of the Schrödinger field. To find its expression we could go back to the classical fields and use the Noether theorem. We prefer to find it by considering the generator of the translations $\mathbf{r} \to \mathbf{r} + \mathbf{a}$ with a constant vector $\mathbf{a}$. The field operators change as $\hat{\psi}(\mathbf{r}) \to \hat{\psi}(\mathbf{r} + \mathbf{a})$ and $\hat{\psi}^+(\mathbf{r}) \to \hat{\psi}^+(\mathbf{r} + \mathbf{a})$. So we are looking for the operator $\mathbf{P}_{op}$ with which

$$e^{-i\mathbf{a}\cdot\mathbf{P}_{op}/\hbar} \left\{ \begin{array}{c} \hat{\psi}(\mathbf{r}) \\ \hat{\psi}^+(\mathbf{r}) \end{array} \right\} e^{i\mathbf{a}\cdot\mathbf{P}_{op}/\hbar} = \left\{ \begin{array}{c} \hat{\psi}(\mathbf{r} + \mathbf{a}) \\ \hat{\psi}^+(\mathbf{r} + \mathbf{a}) \end{array} \right\} \tag{38}$$

For infinitesimal $\mathbf{a}$ this is

$$(1 - i\mathbf{a} \cdot \mathbf{P}_{op}/\hbar) \left\{ \begin{array}{c} \hat{\psi}(\mathbf{r}) \\ \hat{\psi}^+(\mathbf{r}) \end{array} \right\} (1 + i\mathbf{a} \cdot \mathbf{P}_{op}/\hbar) = \left\{ \begin{array}{c} (1 + \mathbf{a} \cdot \nabla)\hat{\psi}(\mathbf{r}) \\ (1 + \mathbf{a} \cdot \nabla)\hat{\psi}^+(\mathbf{r}) \end{array} \right\}$$

which means that must have the commutator

$$\left[\mathbf{P}_{op} \, , \left\{ \begin{array}{c} \hat{\psi}(\mathbf{r}) \\ \hat{\psi}^+(\mathbf{r}) \end{array} \right\} \right] = \left\{ \begin{array}{c} i\hbar\nabla\hat{\psi}(\mathbf{r}) \\ i\hbar\nabla\hat{\psi}^+(\mathbf{r}) \end{array} \right\}$$

This is achieved with the expression

$$\mathbf{P}_{op} = \int d^3r' \hat{\psi}^+(\mathbf{r}')(-i\hbar\nabla_{\mathbf{r}'})\hat{\psi}(\mathbf{r}') \tag{39}$$

Indeed

$$\left[\mathbf{P}_{op}, \left\{ \begin{array}{c} \hat{\psi}(\mathbf{r}) \\ \hat{\psi}^+(\mathbf{r}) \end{array} \right\} \right] = \int d^3r' \left[\begin{array}{c} \hat{\psi}^+(\mathbf{r}')(-i\hbar\nabla_{\mathbf{r}'})\hat{\psi}(\mathbf{r}') \, , \, \hat{\psi}(\mathbf{r}) \\ \hat{\psi}^+(\mathbf{r}')(-i\hbar\nabla_{\mathbf{r}'})\hat{\psi}(\mathbf{r}') \, , \, \hat{\psi}^+(\mathbf{r}) \end{array} \right] =$$

$$= \int d^3r' \left\{ \begin{array}{c} \delta(\mathbf{r} - \mathbf{r}')i\hbar\nabla_{\mathbf{r}'}\hat{\psi}(\mathbf{r}') \\ \hat{\psi}^+(\mathbf{r}')(-i\hbar\nabla_{\mathbf{r}'})\delta(\mathbf{r} - \mathbf{r}') \end{array} \right\} = \left\{ \begin{array}{c} i\hbar\nabla_{\mathbf{r}}\hat{\psi}(\mathbf{r}) \\ i\hbar\nabla_{\mathbf{r}}\hat{\psi}^+(\mathbf{r}) \end{array} \right\}$$

where in the second line of the last equality we used integration by parts.

2.5.2 Field quanta are free nonrelativistic particles

The momentum $\mathbf{P}_{op}$ commutes with the Hamiltonian H_{op}, Eq. (22)

$$[H_{op}, \mathbf{P}_{op}] = 0 \tag{40}$$

Verifying this explicitly with H_{op} and $\mathbf{P}_{op}$ written in terms of the field operators $\hat{\psi}(\mathbf{r})$ and $\hat{\psi}^+(\mathbf{r})$ is a good exercise which is left to the reader. Physically this is the result of the invariance of H_{op} under the translation.

Let us write $\mathbf{P}_{op}$ in terms of the normal modes operators $\hat{a}_{\mathbf{k}}$'s and $\hat{a}^+_{\mathbf{k}'}$'s. Using the expansions (27) in (39) we obtain

$$\mathbf{P}_{op} = \sum_{\mathbf{k}} \hbar\mathbf{k}\; \hat{a}^+_{\mathbf{k}'}\hat{a}_{\mathbf{k}'} \tag{41}$$

This expression compared to Eq. (29) trivially shows that indeed $\mathbf{P}_{op}$ commutes with H_{op}. It has the same eigenfunctions (31) and its eigenvalues are

$$\mathbf{P}_{\{n_{\mathbf{k}}\}} = \sum_{\mathbf{k}} \hbar\mathbf{k}\; n_{\mathbf{k}} \tag{42}$$

This shows that each field quantum with energy $\epsilon_{\mathbf{k}}$ carry momentum $p_{\mathbf{k}} = \hbar\mathbf{k}$. The energy momentum relation $\epsilon(\mathbf{p})$ follows from the explicit dependence of $\epsilon_{\mathbf{k}} = \hbar^2\mathbf{k}^2/2m$ on $\mathbf{k}$

$$\epsilon_{\mathbf{k}}(\mathbf{p}) = \frac{|\mathbf{p}_{\mathbf{k}}|^2}{2m} \tag{43}$$

which is the familiar energy-momentum relation of non relativistic particles. This indicates that quanta of the free Schrödinger field behave like such particles.

2.5.3 Field angular momentum

In analogy with the field momentum one can find the expression for the operator of the field angular momentum by considering infinitesimal rotations $\mathbf{r} \to \mathbf{r} + \delta\phi\, \mathbf{n} \times \mathbf{r}$ with $\delta\phi$ - angle of rotation and $\mathbf{n}$ - unit vector along the rotation axis (with the usual "right hand rule" convention). As with the momentum we should look for the operator $\mathbf{L}_{op}$ for which

$$e^{-i\delta\phi\mathbf{n}\cdot\mathbf{L}_{op}/\hbar} \left\{ \begin{array}{c} \hat{\psi}(\mathbf{r}) \\ \hat{\psi}^+(\mathbf{r}) \end{array} \right\} e^{i\delta\phi\mathbf{n}\cdot\mathbf{L}_{op}/\hbar} = \left\{ \begin{array}{c} \hat{\psi}(\mathbf{r} + \delta\phi\mathbf{n} \times \mathbf{r}) \\ \hat{\psi}^+(\mathbf{r} + \delta\phi\mathbf{n} \times \mathbf{r}) \end{array} \right\} \tag{44}$$

For infinitesimal $\delta\phi$ it is straightforward to conclude that $\mathbf{L}_{op}$ must satisfy

$$\left[\mathbf{n}\cdot\mathbf{L}_{op}\,,\left\{\begin{array}{c}\hat{\psi}(\mathbf{r})\\ \hat{\psi}^{+}(\mathbf{r})\end{array}\right\}\right]=\left\{\begin{array}{c}i\hbar(\mathbf{n}\times\mathbf{r})\cdot\nabla\hat{\psi}(\mathbf{r})\\ i\hbar(\mathbf{n}\times\mathbf{r})\cdot\nabla\hat{\psi}^{+}(\mathbf{r})\end{array}\right\}=\left\{\begin{array}{c}i\hbar\mathbf{n}\cdot(\mathbf{r}\times\nabla)\hat{\psi}(\mathbf{r})\\ i\hbar\mathbf{n}\cdot(\mathbf{r}\times\nabla)\hat{\psi}^{+}(\mathbf{r})\end{array}\right\}$$

This is achieved with the expression

$$\mathbf{L}_{op}=\int d^3r'\hat{\psi}^{+}(\mathbf{r}')[\mathbf{r}'\times(-i\hbar\nabla_{\mathbf{r}'})]\hat{\psi}(\mathbf{r}') \tag{45}$$

Indeed

$$\begin{aligned}\left[\mathbf{L}_{op},\left\{\begin{array}{c}\hat{\psi}(\mathbf{r})\\ \hat{\psi}^{+}(\mathbf{r})\end{array}\right\}\right]&=\int d^3r'\left[\begin{array}{c}\hat{\psi}^{+}(\mathbf{r}')[\mathbf{r}'\times(-i\hbar\nabla_{\mathbf{r}'})]\hat{\psi}(\mathbf{r}')\,,\ \hat{\psi}(\mathbf{r})\\ \hat{\psi}^{+}(\mathbf{r}')[\mathbf{r}'\times(-i\hbar\nabla_{\mathbf{r}'})]\hat{\psi}(\mathbf{r}')\,,\ \hat{\psi}^{+}(\mathbf{r})\end{array}\right]=\\ =\quad\int d^3r'\left\{\begin{array}{c}\delta(\mathbf{r}-\mathbf{r}')i\hbar(\mathbf{r}'\times\nabla_{\mathbf{r}'})\hat{\psi}(\mathbf{r}')\\ \hat{\psi}^{+}(\mathbf{r}')[-i\hbar(\mathbf{r}'\times\nabla_{\mathbf{r}'})]\delta(\mathbf{r}-\mathbf{r}')\end{array}\right\}&=\left\{\begin{array}{c}i\hbar(\mathbf{r}\times\nabla_{\mathbf{r}})\hat{\psi}(\mathbf{r})\\ i\hbar(\mathbf{r}\times\nabla_{\mathbf{r}})\hat{\psi}^{+}(\mathbf{r})\end{array}\right\}\end{aligned} \tag{46}$$

where in the second line of the last equality we used integration by parts.

The angular momentum operator commutes with the free field Hamiltonian, Eq. (22)

$$[H_{op},\mathbf{L}_{op}]=0 \tag{47}$$

The reader is advised to carry out this calculation the result of which essentially follows from the commutativity of the "first quantized" $h_0=-\hbar^2\nabla^2/2m$ and $\mathbf{l}=\mathbf{r}\times(-i\hbar\nabla)$ which enter the expressions of these operators. Physically of course it reflects the invariance of the free field H_{op} under rotations. Another useful calculation for the reader to work out is to verify the validity of the standard commutation relations for the components of $\mathbf{L}_{op}$

$$[L_{op,i}\,,\,L_{op,j}]=i\hbar\sum_n\epsilon_{ijn}\,L_{op,n} \tag{48}$$

Here again the corresponding commutators of $\mathbf{l}_i=[\mathbf{r}\times(-i\hbar\nabla)]_i$'s which enter the expressions of $L_{op,i}$'s are the "cause" of this result.

Following the experience of transforming the field momentum operator $\mathbf{P}_{op}$ to the plane wave basis it is instructive to consider transforming the field operators in the field angular momentum operator $\mathbf{L}_{op}$, Eq. (45) to the spherical wave normal modes basis $u_{klm}(\mathbf{r})$ as given in Eq. (36). In contrast to $\mathbf{P}_{op}$ the non commutativity of different components of $\mathbf{L}_{op}$ leads to different forms of the expressions for different $L_{op,j}$'s. The simplest is for $L_{op,z}$

$$L_{op,z}=\sum_{klm}\hbar m\,\hat{a}^{+}_{klm}\hat{a}_{klm}$$

The expressions for $L_{op,x}$ and $L_{op,y}$ will contain non diagonal $m\to m\pm1$ terms. We leave for the reader to work this out explicitly.

3 Adding external potential

So the conclusions at this stage are that the quantized free Schrödinger field describes a collection of quanta which behave like free moving non interacting non relativistic quantum particles. We also note that these particles are identical (see longer discussion of this aspect in the following sections). It is therefore natural to ask how to include interactions of the particles and how to account for their statistics?

3.1 The Hamiltonian

We begin by considering the Schrödinger field in the presence of an external potential. The field equation is the familiar

$$i\hbar \frac{\partial \psi(\mathbf{r},t)}{\partial t} = \left(-\frac{\hbar^2}{2m}\nabla^2 + U(\mathbf{r}) \right) \psi(\mathbf{r},t) \equiv h\psi(\mathbf{r},t) \tag{49}$$

with h defined as

$$h = -\frac{\hbar^2}{2m}\nabla^2 + U(\mathbf{r}) \tag{50}$$

Following what we did in the case of the free field, cf., Eq.(2) we consider this equation and its complex conjugate as the pair of Hamilton equations with $\psi(\mathbf{r})$ and $i\hbar\psi^*(\mathbf{r})$ as canonical variables and the following Hamiltonian

$$H = \int d^3r \left[\frac{\hbar^2}{2m} |\nabla\psi(\mathbf{r})|^2 + U(\mathbf{r})|\psi(\mathbf{r})|^2 \right] \tag{51}$$

Indeed from

$$\begin{aligned} \delta H \;\; &= \;\; \int d^3r \left[\frac{\hbar^2}{2m} \left(\nabla\psi^*(\mathbf{r})\nabla\delta\psi(\mathbf{r}) + \nabla\delta\psi^*(\mathbf{r})\nabla\psi(\mathbf{r}) \right) + \right. \\ &\quad \left. + U(\mathbf{r}) \left(\psi^*(\mathbf{r})\delta\psi(\mathbf{r}) + \delta\psi^*(\mathbf{r})\psi(\mathbf{r}) \right) \right] \end{aligned}$$

we find that Hamilton equations for $i\hbar\psi^*(\mathbf{r})$ and $\psi(\mathbf{r})$

$$\begin{aligned} \frac{\partial\psi(\mathbf{r})}{\partial t} = \frac{\delta H}{\delta[i\hbar\psi^*(\mathbf{r})]} \;\; &= \;\; \frac{1}{i\hbar}\left[-\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r}) + U(\mathbf{r})\psi(\mathbf{r}) \right] \\ \frac{\partial[i\hbar\psi^*(\mathbf{r})]}{\partial t} = -\frac{\delta H}{\delta\psi(\mathbf{r})} \;\; &= \;\; -\left[-\frac{\hbar^2}{2m}\nabla^2\psi^*(\mathbf{r}) + U(\mathbf{r})\psi^*(\mathbf{r}) \right] \end{aligned}$$

reproduce correctly the field equation (49) and its complex conjugate.

On this basis we will quantize this field following the by now familiar pattern

$$\psi(\mathbf{r}) \to \hat{\psi}(\mathbf{r}) \quad , \quad \psi^*(\mathbf{r}) \to \hat{\psi}^+(\mathbf{r}) \tag{52}$$

with commutation relations (19) and the Hamiltonian operator

$$H_{op} = \int d^3r \left[\frac{\hbar^2}{2m} \nabla \hat{\psi}^+(\mathbf{r}) \cdot \nabla \hat{\psi}(\mathbf{r}) + U(\mathbf{r}) \hat{\psi}^+(\mathbf{r}) \hat{\psi}(\mathbf{r}) \right]$$

or in an equivalent form (cf., the remark after Eq. (22))

$$H_{op} = \int d^3r\ \hat{\psi}^+(\mathbf{r}) \left[-\frac{\hbar^2}{2m} \nabla^2 + U(\mathbf{r}) \right] \hat{\psi}(\mathbf{r}) \equiv \int d^3r\ \hat{\psi}^+(\mathbf{r}) h \hat{\psi}(\mathbf{r}) \tag{53}$$

with h defined above in Eq. (50). As in the case of the free field the general goal of the theory is to solve the Schrödinger equation (35) but with the Hamiltonian operator given by (53). As always the general method of doing this is to find the eigenfunctions of this operator.

Before this let us note that the Heisenberg equation for the field operators calculated with the Hamiltonian H_{op}, Eq. (53) coincides in form (as they should) with the wave equation (49) which we have quantized

$$i\hbar \frac{\partial \hat{\psi}(\mathbf{r}, t)}{\partial t} = \left[\hat{\psi}(\mathbf{r}, t), H_{op} \right] = h \hat{\psi}(\mathbf{r}, t)$$

with h defined in Eq. (50). The calculation of the commutator in this equation can be efficiently done by commuting the operator $\hat{\psi}(\mathbf{r}, t)$ through the elements of the expression $\int d^3r'\ \hat{\psi}^+(\mathbf{r}', t) h \hat{\psi}(\mathbf{r}', t)$ for H_{op}. Since the only non zero commutator of $\hat{\psi}(\mathbf{r}, t)$ is with $\hat{\psi}^+(\mathbf{r}', t)$ we get

$$\left[\hat{\psi}(\mathbf{r}, t), H_{op} \right] = \int d^3r'\ \delta(\mathbf{r} - \mathbf{r}') h \hat{\psi}(\mathbf{r}', t) = h \hat{\psi}(\mathbf{r}, t)$$

The Heisenberg equation for $\hat{\psi}^+(\mathbf{r}, t)$ coincides in form with complex conjugate of Eq. (49).

3.2 The eigenstates. Field quanta are particles in the external potential

To find the eigenfunctions of the above Hamiltonian

$$H_{op} \Psi = E \Psi$$

we use the experience with the free field and look for the basis $u_i(\mathbf{r})$ to expand the field operators $\hat{\psi}(\mathbf{r})$ in which H_{op} will become a sum of decoupled commuting terms like Eq. (29) for the free field Hamiltonian. Before doing this let us briefly consider the general aspects of changing basis.

3.2.1 Changing basis

The transformation from $\hat{\psi}(\mathbf{r})$ and $\hat{\psi}^+(\mathbf{r})$ to $\hat{a}_{\mathbf{k}}$ and $\hat{a}^+_{\mathbf{k}}$ can be viewed as a particular example of a more general operator transformation

$$\hat{\psi}(\mathbf{r}) = \sum_i \hat{a}_i u_i(\mathbf{r}) \quad , \quad \hat{\psi}^+(\mathbf{r}) = \sum_i \hat{a}^+_i u^*_i(\mathbf{r}) \tag{54}$$

with $\{u_i(\mathbf{r})\}$ - any complete orthonormal basis, i.e. set of functions which obey

$$\begin{aligned} \int d^3r\, u^*_i(\mathbf{r}) u_j(\mathbf{r}) &= \delta_{ij} \quad \text{orthonormality} \\ \sum_i u_i(\mathbf{r}) u^*_i(\mathbf{r}') &= \delta(\mathbf{r}-\mathbf{r}') \quad \text{completeness} \end{aligned} \tag{55}$$

Inverting the transformation

$$\hat{a}_i = \int d^3r\, \hat{\psi}(\mathbf{r}) u^*_i(\mathbf{r}) \quad , \quad \hat{a}^+_i = \int d^3r \hat{\psi}^+(\mathbf{r}) u_i(\mathbf{r}) \tag{56}$$

and using the commutation relations (19) for the field operators $\hat{\psi}(\mathbf{r})$ and $\hat{\psi}^+(\mathbf{r})$ and orthogonality of the basis set $\{u_i(\mathbf{r})\}$ one finds that the commutations of the $\hat{a}_i, \hat{a}^+_i$ set remain canonical

$$[\hat{a}_i, \hat{a}^+_j] = \delta_{ij} \quad , \quad [\hat{a}_i, \hat{a}_j] = 0 = [\hat{a}^+_i, \hat{a}^+_j] \tag{57}$$

Let us note a useful view of the expansion (54) as transforming "vectors" of operators from one basis to another. E.g. a vector $\hat{\psi}_{\mathbf{r}}$ (i.e the set $\{\hat{\psi}_{\mathbf{r}}\}$with $\mathbf{r}$ regarded as an index) in the operator valued Hilbert space of functions of $\mathbf{r}$ gets transformed to the vector $\{\hat{a}_i\}$ in this space with the use of the transformation matrix $\{u_{\mathbf{r},i}\}$ (with $\mathbf{r}$ in $u_i(\mathbf{r})$ regarded as index). The orthogonality and completeness relations (55) of the set $\{u_i(\mathbf{r})\}$ are just the expressions of the unitarity of the matrix $\{u_{\mathbf{r},i}\}$. In Appendix we review the properties of the operators $\hat{a}_j$ and $\hat{a}^+_i$ for a general basis set $\{u_i(\mathbf{r})\}$ and the quantum states which they generate.

Using the expansions Eq. (54) in the expression Eq. (53) for H_{op}, we obtain

$$H_{op} = \sum_{ij} h_{ij} \hat{a}^+_i \hat{a}_j \tag{58}$$

where

$$h_{ij} \equiv \int d^3r\, u_i^*(\mathbf{r}) h u_j(\mathbf{r})$$

are matrix elements of h in the basis $u_i(\mathbf{r})$.

3.2.2 The normal modes

We now choose $u_i(\mathbf{r})$'s to be solutions of

$$h u_i(\mathbf{r}) = \epsilon_i u_i(\mathbf{r}) \tag{59}$$

These solutions are obviously the normal modes of the field described by the linear equation (49). Indeed in a trivial way the field configurations $\psi(\mathbf{r}, t) = u_i(\mathbf{r}) \exp(-i\epsilon_i t/\hbar)$ solve the (classical) field equation (49), i.e. in each of these configurations all the field degrees of freedom (indexed by $\mathbf{r}$) oscillate with the same frequency $\epsilon_i/\hbar$.

We note that in the non interacting limit $U(\mathbf{r}) = 0$ the operator h reduces to

$$h_0 = -\frac{\hbar^2}{2m}\nabla^2$$

and $u_i(\mathbf{r})$'s become the plane waves $u_{\mathbf{k}}(\mathbf{r})$, Eq.(26).

It is important to observe that h_0 and h appear as operators acting on functions of $\mathbf{r}$. As such they are very different from the operator H_{op} which acts on the states of the field $\hat{\psi}$, like e.g. the states Eq. (34). As was already noted the field operators are on the one hand operators in the space of the states of the field (and in this role $\mathbf{r}$ is just an index labelling these operators) and on the other hand they are functions of $\mathbf{r}$ on which the operator h acts. Perhaps a helpful analogy is the quantized EM field in which the components of $\mathbf{E}_{op}(\mathbf{r})$ and $\mathbf{B}_{op}(\mathbf{r})$ are both operators and functions of $\mathbf{r}$. In the present context for reasons which will become clear in the sections below operators like h_0 and h will often be called single particle operators and the bases of functions like $u_{\mathbf{k}}(\mathbf{r})$ or $u_i(\mathbf{r})$ - single particle bases.

In the basis of the eigenstates of h we have

$$h_{ij} = \epsilon_i \delta_{ij}$$

so that as in the free field case H_{op} is a sum of independent (commuting) oscillators

$$H_{op} = \sum_i \epsilon_i \hat{a}_i^+ \hat{a}_i \tag{60}$$

corresponding to the "vibrations" of amplitudes of the normal modes Eq. (59). The eigenfunctions of H_{op} are products of eigenstates $|n_i\rangle$ of these field oscillators, i.e eigenstates of the operators

$$\hat{n}_i = \hat{a}_i^+ \hat{a}_i \tag{61}$$

cf., Appendix, Eq. (159) while the eigenenergies are the corresponding sums

$$|\Psi_{\{n_i\}}\rangle \equiv |n_1, n_2, \ldots, n_i, \ldots\rangle = \prod_i |n_i\rangle = \prod_i \frac{(\hat{a}_i^+)^{n_i}}{\sqrt{n_i!}}|0\rangle \quad , \quad E_{\{n_i\}} = \sum_i \epsilon_i n_i \tag{62}$$

To conclude, the quantization of the Schrödinger field in the presence of an external potential, Eq.(49) describes collections of independent quanta of the normal modes given by the solutions of the equation (59). Since this equation is just a Schrödinger equation for a single particle in the potential $U(\mathbf{r})$ we therefore obtained a description of systems of such particles in this potential occupying its eigenstates $u_i(\mathbf{r})$.

3.2.3 The particle number operator. $U(1)$ symmetry

We note that the operators $\hat{n}_i$, Eq. (61) "count" the number of particles n_i in each single particle state $u_i(\mathbf{r})$. We had similar operators $\hat{n}_{\mathbf{k}}$ in the free field case, cf., Eq. (29). It is useful and important to introduce the total number of particles operator

$$N_{op} = \sum_i \hat{n}_i \tag{63}$$

which "measures" the sum of all n_i's

$$N_{op}|\Psi_{\{n_i\}}\rangle = N_{op}|n_1, n_2, \ldots, n_i, \ldots\rangle = N|n_1, n_2, \ldots, n_i, \ldots\rangle \text{ with } N = \sum_i n_i \tag{64}$$

This operator has the same form in any complete orthonormal basis

$$N_{op} = \sum_i \hat{a}_i^+ \hat{a}_i = \sum_{\mathbf{k}} \hat{a}_{\mathbf{k}}^+ \hat{a}_{\mathbf{k}} = \int d^3r\, \hat{\psi}^+(\mathbf{r})\hat{\psi}(\mathbf{r}) \tag{65}$$

as can be verified by inserting the expansions (54) with different sets $u_i(\mathbf{r})$ in the last integral.

The result that the eigenfunctions (62) of the Hamiltonian (60) are also eigenfunctions of the number operator (63) is linked to the fact that N_{op} commutes with the Hamiltonian

$$[H_{op}, N_{op}] = 0 \tag{66}$$

so that the particle number is a conserved quantum number in this theory, not a fixed quantity prescribed from "outside".

Let us note that H_{op} commutes with the individual mode number operators $\hat{n}_i$, Eq. (61). This however is only for the eigenmodes of the field, i.e. for the single particle states Eq. (59). The conservation of N_{op} is a much more general property independent of the basis, cf. Eq. (65). It is intuitively related to the manner in which the operators $\hat{a}_j$ and $\hat{a}_i^+$ enter the general Hamiltonian Eq. (58) and can be traced to the way the field Hamiltonian Eq. (53) contains the field operators $\hat{\psi}^+$ and $\hat{\psi}$. Formally this is reflected in the invariance of the expression (53) under a global (coordinate independent) phase transformation

$$\hat{\psi}(\mathbf{r}) \;\to\; e^{i\alpha}\hat{\psi}(\mathbf{r}) \quad , \quad \hat{\psi}^+(\mathbf{r}) \;\to\; e^{-i\alpha}\hat{\psi}^+(\mathbf{r}) \tag{67}$$

In a more general context such a transformation is called a global $U(1)$ gauge transformation and the operator N_{op} is its generator. This means that

$$e^{-i\alpha N_{op}}\hat{\psi}(\mathbf{r})e^{i\alpha N_{op}} = e^{i\alpha}\hat{\psi}(\mathbf{r}) \;\; , \;\; e^{-i\alpha N_{op}}\hat{\psi}^+(\mathbf{r})e^{i\alpha N_{op}} = e^{-i\alpha}\hat{\psi}^+(\mathbf{r}) \tag{68}$$

As usual to prove this it is sufficient to consider an infinitesimal α. It is enough to do this for $\hat{\psi}(\mathbf{r})$ since the relation for $\hat{\psi}^+(\mathbf{r})$ is just the hermitian conjugate. We have

$$(1 - i\alpha N_{op})\hat{\psi}(\mathbf{r})(1 + i\alpha N_{op}) = (1 + i\alpha)\hat{\psi}(\mathbf{r}) \;\to\; [N_{op}, \hat{\psi}(\mathbf{r})] = -\hat{\psi}(\mathbf{r}) \tag{69}$$

Simple calculation supplies the proof

$$[N_{op}, \hat{\psi}(\mathbf{r})] = \int d^3r'[\hat{\psi}^+(\mathbf{r}')\hat{\psi}(\mathbf{r}'), \hat{\psi}(\mathbf{r})] = -\int d^3r'\delta(\mathbf{r}' - \mathbf{r})\hat{\psi}(\mathbf{r}') = -\hat{\psi}(\mathbf{r})$$

Using Eq. (68), the invariance of H_{op} under (67) and denoting

$$U_{op}(\alpha) \equiv e^{-i\alpha N_{op}}$$

one has

$$\begin{aligned} U_{op}(\alpha)H_{op}U_{op}^+(\alpha) &= U_{op}(\alpha)\left[\int d^3r\; \hat{\psi}^+(\mathbf{r})h\hat{\psi}(\mathbf{r})\right]U_{op}^+(\alpha) = \\ &= \int d^3r\; U_{op}(\alpha)\hat{\psi}^+(\mathbf{r})U_{op}^+(\alpha)\; h\; U_{op}(\alpha)\hat{\psi}(\mathbf{r})U_{op}^+(\alpha) = H_{op} \end{aligned}$$

For infinitesimal α

$$U_{op}(\alpha)H_{op}U_{op}^+(\alpha) \to (1 - i\alpha N_{op})H_{op}(1 + i\alpha N_{op}) = (H_{op} - i\alpha[N_{op}, H_{op}]) \tag{70}$$

and to have it equal to H_{op} must have Eq. (66).

Going back to the eigenfunctions and eigenvalues of H_{op} we note that the general solution of the Schrödinger equation (35) with this H_{op} is a familiar linear combination

$$|\Psi(t)\rangle = \sum_{\{n_i\}} C_{\{n_i\}} |\Psi_{\{n_i\}}\rangle e^{-E_{\{n_i\}} t/\hbar} \tag{71}$$

with (as always) the coefficients $C_{\{n_i\}}$ determined by the initial condition for $|\Psi(t)\rangle$ at $t = 0$. And we note that the formalism in principle allows to have states with coherent combinations of different particle numbers $N = \sum_i n_i$. The choice to have a fixed N, i.e. to have it the same for all components in the above solution is in the freedom of setting the appropriate initial condition supported (conserved in time) by the commutativity of H_{op} with N_{op}.

3.3 Working with the field operators

The last equality in the expressions (65) for N_{op} in terms of the field operators represents N_{op} as a sum (integral) over particle number operators $d\hat{n}(\mathbf{r}) = \hat{\psi}^+(\mathbf{r})\hat{\psi}(\mathbf{r})d^3r$ in the infinitesimal volume d^3r situated at $\mathbf{r}$. This suggest that

$$\hat{\rho}(\mathbf{r}) = \hat{\psi}^+(\mathbf{r})\hat{\psi}(\mathbf{r}) \tag{72}$$

is the particle density operator. This also explains what is the physical meaning of the field operators $\hat{\psi}^+(\mathbf{r})$. Indeed let us consider a state

$$|\mathbf{r}'\rangle \equiv const\, \hat{\psi}^+(\mathbf{r}')|0\rangle \tag{73}$$

where we introduced a multiplicative constant for normalization, see below. Let us act on this state with the operator $\hat{\rho}(\mathbf{r})$

$$\hat{\rho}(\mathbf{r})|\mathbf{r}'\rangle = const\, \hat{\psi}^+(\mathbf{r})\hat{\psi}(\mathbf{r})\hat{\psi}^+(\mathbf{r}')|0\rangle = const\, \delta(\mathbf{r}-\mathbf{r}')\hat{\psi}^+(\mathbf{r}')|0\rangle = \delta(\mathbf{r}-\mathbf{r}')|\mathbf{r}'\rangle \tag{74}$$

where we commuted $\hat{\psi}(\mathbf{r})$ with $\hat{\psi}^+(\mathbf{r}')$to its right and then used $\hat{\psi}(\mathbf{r})|0\rangle = 0$. The result shows that $\hat{\psi}^+(\mathbf{r})$ acting on the vacuum state creates a particle at the position $\mathbf{r}$. More precisely it creates delta like particle density at this position.

What happens if several $\hat{\psi}^+$'s act on the vacuum? E.g. consider the state

$$|\mathbf{r}_1, \ldots, \mathbf{r}_N\rangle = const_N\, \hat{\psi}^+(\mathbf{r}_1) \ldots \hat{\psi}^+(\mathbf{r}_N)|0\rangle \tag{75}$$

Let us act on this state with $\hat{\rho}(\mathbf{r})$. As in the one particle case we find the result by first commuting $\hat{\psi}(\mathbf{r})$ through $\hat{\psi}^+(\mathbf{r}_a)$'s to its right all the way to the vacuum. This calculation will appear in several places below so we show it in details

$$\begin{aligned}
&\hat{\psi}(\mathbf{r}) \prod_{a=1}^{N} \hat{\psi}^+(\mathbf{r}_a)|0\rangle = [\delta(\mathbf{r}-\mathbf{r}_1) + \hat{\psi}^+(\mathbf{r}_1)\hat{\psi}(\mathbf{r})] \prod_{a\neq 1}^{N} \hat{\psi}^+(\mathbf{r}_a)|0\rangle = \\
&= \delta(\mathbf{r}-\mathbf{r}_1) \prod_{a\neq 1}^{N} \hat{\psi}^+(\mathbf{r}_a) + \hat{\psi}^+(\mathbf{r}_1)[\delta(\mathbf{r}-\mathbf{r}_2) + \hat{\psi}^+(\mathbf{r}_2)\hat{\psi}(\mathbf{r})] \prod_{a=3}^{N} \hat{\psi}^+(\mathbf{r}_a)]|0\rangle = \\
&= \delta(\mathbf{r}-\mathbf{r}_1) \prod_{a\neq 1}^{N} \hat{\psi}^+(\mathbf{r}_a) + \delta(\mathbf{r}-\mathbf{r}_2) \prod_{a\neq 2}^{N} \hat{\psi}^+(\mathbf{r}_a) + \ldots + \\
&+ \prod_{a=1}^{N-1} \hat{\psi}^+(\mathbf{r}_a)[\delta(\mathbf{r}-\mathbf{r}_N) + \hat{\psi}^+(\mathbf{r}_N)\hat{\psi}(\mathbf{r})]|0\rangle = \\
&\qquad = \left[\sum_{b=1}^{N} \delta(\mathbf{r}-\mathbf{r}_b) \prod_{a\neq b}^{N} \hat{\psi}^+(\mathbf{r}_a)\right] |0\rangle \qquad (76)
\end{aligned}$$

Acting on this with $\hat{\psi}^+(\mathbf{r})$ and using the delta function in each term to replace $\mathbf{r} \to \mathbf{r}_b$ in it we get

$$\hat{\rho}(\mathbf{r})|\mathbf{r}_1, \ldots, \mathbf{r}_N\rangle = [\sum_{a=1}^{N} \delta(\mathbf{r}-\mathbf{r}_a)]|\mathbf{r}_1, \ldots, \mathbf{r}_N\rangle$$

i.e. have N particles (delta like particle densities) at the positions $\mathbf{r}_a, a = 1, \ldots, N$. In the same manner one can show that $\hat{\psi}^+(\mathbf{r})$ creates a particle at $\mathbf{r}$ when it acts on any general state (discussed below). We also note that the result (76) shows that $\hat{\psi}(\mathbf{r})$ destroys (annihilates) a particle if its coordinates coincide with $\mathbf{r}$.

It is important to notice that $\hat{\psi}^+$ and $\hat{\psi}$ create and annihilate particles only when they act to the right. Acting to the left they produce an opposite result - they correspondingly annihilate and create particles. For example the state $\langle\mathbf{r}_1, \ldots, \mathbf{r}_N|$ is the hermitian conjugate of $|\mathbf{r}_1, \ldots, \mathbf{r}_N\rangle$ so

$$\langle\mathbf{r}_1, \ldots, \mathbf{r}_N| = [const_N\ \hat{\psi}^+(\mathbf{r}_1)\ldots\hat{\psi}^+(\mathbf{r}_N)|0\rangle]^+ = \langle 0|\hat{\psi}(\mathbf{r}_N)\ldots\hat{\psi}(\mathbf{r}_1)(const_N)^* \qquad (77)$$

since $[\hat{\psi}^+]^+ = \hat{\psi}$. Thus the state $\langle\mathbf{r}_1, \ldots, \mathbf{r}_N|$ is the result of acting with N $\hat{\psi}$'s to the left on the vacuum $\langle 0|$.

What is the norm of $|\mathbf{r}_1, \ldots, \mathbf{r}_N\rangle$? Take as an example one particle state Eq. (73) and calculate

$$\langle\mathbf{r}'|\mathbf{r}\rangle = |const|^2\langle 0|\hat{\psi}(\mathbf{r}')\hat{\psi}^+(\mathbf{r})|0\rangle = |const|^2\delta(\mathbf{r}-\mathbf{r}')$$

The result shows that such a state is non normalizable. This should not be surprising as one has a continuum of states labeled by $\mathbf{r}$. Just as with more familiar momentum states labeled by $\mathbf{p}$. Also the momentum states are non normalizable. The common regularization is to make $\mathbf{p}$ discrete by introducing very large but finite volume, i.e. to introduce an infrared cutoff. In the same way one can make $\mathbf{r}$ discrete by introducing a lattice of discrete $\mathbf{r}$'s. If this is not done - then one can normalize as convenient.

As we will see in the next section the most common use of the states $|\mathbf{r}\rangle$ or their N particle generalization $|\mathbf{r}_1, \ldots, \mathbf{r}_N\rangle$, Eq. (75), makes it convenient to choose the normalization of these states as

$$const_N = \frac{1}{\sqrt{N!}}$$

4 Wave functions. Operators. Comparison with the first quantized description

The quantization of the Schrödinger field is (for obvious reasons) called the second quantization. For the field governed by Eq.(49) this seems to result in an alternative description of quantum non interacting particles in the external potential $U(\mathbf{r})$.

Here we want to understand if this description is indeed complete and how it is related to the standard quantum mechanical description of say N particles with the wave function $\Phi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N, t)$ obeying the N particle Schrödinger equation

$$i\hbar \frac{\partial \Phi(\mathbf{r}_1, ..., \mathbf{r}_N, t)}{\partial t} = \sum_{a=1}^{N} \left[-\frac{\hbar^2}{2m} \nabla_a^2 + U(\mathbf{r}_a) \right] \Phi(\mathbf{r}_a, ..., \mathbf{r}_N, t) \tag{78}$$

4.1 Wave functions in the second quantization

4.1.1 Coordinate representation. Second vs first quantization

The states $|\mathbf{r}_1, \ldots, \mathbf{r}_N\rangle$ introduced in the previous section, cf., Eq. (75), form a very convenient basis to represent a general N particles wave function in the second quantization

$$|\Phi\rangle = \int \prod_{a=1}^{N} d^3 r_a \; \Phi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N) |\mathbf{r}_1, \ldots, \mathbf{r}_N\rangle \tag{79}$$

The interpretation of this expression is quite clear - we have a linear combination of N particles in different coordinate positions $\mathbf{r}_1, \ldots, \mathbf{r}_N$ weighted each with the probability amplitude $\Phi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N)$. These amplitudes form the wave function

$|\Phi\rangle$ in the coordinate representation and clearly are equivalent to this wave function in the first quantization formalism. We will see this equivalence even more explicitly in the discussions below of how physical operators of particle observables act on $|\Phi\rangle$.

As discussed in the Appendix in order to have both $|\Phi\rangle$ and $\Phi(\mathbf{r}_1, \ldots, \mathbf{r}_N)$ normalized to unity, i.e. to have

$$\int d^3r_1 \ldots d^3r_N |\Phi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N)|^2 = 1 \quad \text{and} \quad \langle\Phi|\Phi\rangle = 1 \tag{80}$$

one must choose the normalization $const_N = 1/\sqrt{N!}$ in the definition (75) of the states $|\mathbf{r}_1, \ldots, \mathbf{r}_N\rangle$ as they appear in the relation (79) between $|\Phi\rangle$ and $\Phi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N)$. We thus have

$$|\Phi\rangle = \frac{1}{\sqrt{N!}} \int \prod_{a=1}^{N} d^3r_a \; \Phi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N) \hat{\psi}^+(\mathbf{r}_1)\hat{\psi}^+(\mathbf{r}_2) \ldots \hat{\psi}^+(\mathbf{r}_N)|0\rangle \tag{81}$$

4.1.2 Permutation symmetry

The commutativity properties of the field operators $\hat{\psi}^+(\mathbf{r})$ imply that the coordinate probability amplitudes $\Phi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N)$ in Eq. (81) can not be arbitrary. These functions must be symmetric under all possible permutations of the particles' coordinates.

Let us demonstrate this for the simplest case of two particles

$$|\Phi\rangle \equiv \frac{1}{\sqrt{2}} \int d^3r_1 d^3r_2 \Phi(\mathbf{r}_1, \mathbf{r}_2) \hat{\psi}^+(\mathbf{r}_1)\hat{\psi}^+(\mathbf{r}_2)|0\rangle \tag{82}$$

Functions of two variables can belong to one of the two symmetry representations - symmetric or antisymmetric,

$$\Phi_S(\mathbf{r}_1, \mathbf{r}_2) = \Phi_S(\mathbf{r}_2, \mathbf{r}_1) \;\; \text{and} \;\; \Phi_A(\mathbf{r}_1, \mathbf{r}_2) = -\Phi_A(\mathbf{r}_2, \mathbf{r}_1)$$

and in general have

$$\Phi(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{2}[\Phi(\mathbf{r}_1, \mathbf{r}_2) + \Phi(\mathbf{r}_2, \mathbf{r}_1)] + \frac{1}{2}[\Phi(\mathbf{r}_1, \mathbf{r}_2) - \Phi(\mathbf{r}_2, \mathbf{r}_1)] \equiv \Phi_S(\mathbf{r}_1, \mathbf{r}_2) + \Phi_A(\mathbf{r}_1, \mathbf{r}_2)$$

It is straightforward to show that $|\Phi\rangle_A$ obtained with $\Phi_A(\mathbf{r}_1, \mathbf{r}_2)$ in Eq. (82) vanishes identically. Have

$$|\Phi\rangle_A = \frac{1}{\sqrt{2}} \int d^3r_1 d^3r_2 \Phi_A(\mathbf{r}_1, \mathbf{r}_2) \hat{\psi}^+(\mathbf{r}_1)\hat{\psi}^+(\mathbf{r}_2)|0\rangle =$$

$$= -\frac{1}{\sqrt{2}} \int d^3 r_1 d^3 r_2 \Phi_A(\mathbf{r}_2, \mathbf{r}_1) \hat{\psi}^+(\mathbf{r}_1) \hat{\psi}^+(\mathbf{r}_2)|0\rangle =$$
$$= -\frac{1}{\sqrt{2}} \int d^3 r_1 d^3 r_2 \Phi_A(\mathbf{r}_2, \mathbf{r}_1) \hat{\psi}^+(\mathbf{r}_2) \hat{\psi}^+(\mathbf{r}_1)|0\rangle =$$
$$= -\frac{1}{\sqrt{2}} \int d^3 r_1 d^3 r_2 \Phi_A(\mathbf{r}_1, \mathbf{r}_2) \hat{\psi}^+(\mathbf{r}_1) \hat{\psi}^+(\mathbf{r}_2)|0\rangle = -|\Phi\rangle_A$$

where in the 3rd line we commuted $\hat{\psi}^+(\mathbf{r}_1)\hat{\psi}^+(\mathbf{r}_2) = \hat{\psi}^+(\mathbf{r}_2)\hat{\psi}^+(\mathbf{r}_1)$ and in the 4th line have interchanged the integration variables $\mathbf{r}_1 \leftrightarrow \mathbf{r}_2$. So we have proved that $|\Phi\rangle_A = -|\Phi\rangle_A$ which means that $|\Phi\rangle_A = 0$.

The same proof obviously holds for any pair of coordinates in a general wave function $\Phi(\mathbf{r}_1, \ldots, \mathbf{r}_N)$. Thus only $\Phi(\mathbf{r}_1, \ldots, \mathbf{r}_N)$'s which are symmetric with respect to permutation of any two particles produce non zero result in Eq. (81). This means that this is true also for $\Phi(\mathbf{r}_1, \ldots, \mathbf{r}_N)$'s which are symmetric under permutations of any number of particles. Indeed (as is simple to understand[4] and can be proved by induction) any such permutation can be decomposed into a product of permutations of two particles (transpositions).

The above symmetry under permutations of the wave functions is one of the most important features of the second quantization formalism. Together with the symmetry of the physical observables as represented by the operators as discussed below this property means that the quanta of the theory are bosons, i.e. identical particles obeying Bose statistics. We will provide more details to this discussion in Section 4.3.

4.1.3 Occupation number representation

Expanding the field operators in Eq. (81) in an arbitrary complete and orthonormal single particle basis, cf., Eq. (54), we obtain

$$|\Phi\rangle = \sum_{i_1,\ldots,i_N} C_{i_1,\ldots,i_N} \hat{a}^+_{i_1} \ldots \hat{a}^+_{i_N} |0\rangle \tag{83}$$

with

$$C_{i_1,\ldots,i_N} = \frac{1}{\sqrt{N!}} \int \prod_{a=1}^{N} d^3 r_a \; \Phi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N) u^*_{i_1}(\mathbf{r}_1) \ldots u^*_{i_N}(\mathbf{r}_N)$$

[4] Cf, Messiah, Quantum Mechanics (Dover Books in Physics), Ch. XIV. Denote for example by (1532476) a permutation $1 \to 5 \to 3 \to 2 \to 4 \to 7 \to 6 \to 1$. It can clearly be written as an ordered product (15)(53)(32)(24)(47)(76) of transpositions (with right to left order)

The coefficients $C_{i_1,...,i_N}$ represent the function $|\Phi\rangle$ in the basis of products of the single particle states $u_i(\mathbf{r})$. As we discussed in the previous Section the functions $\Phi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N)$ are symmetric with respect to permutations of the particle coordinates $\mathbf{r}_a$'s. One can use this to replace the products of $u_i(\mathbf{r})$'s in the above expression for $C_{i_1,...,i_N}$'s by symmetrized products

$$u^*_{i_1}(\mathbf{r}_1)\ldots u^*_{i_N}(\mathbf{r}_N) \to const \sum_P u^*_{i_1}(\mathbf{r}_{p_1})\ldots u^*_{i_N}(\mathbf{r}_{p_N})$$

with P denoting the permutations of particle coordinates $\mathbf{r}_1, ..., \mathbf{r}_N \to \mathbf{r}_{p_1}, ..., \mathbf{r}_{p_N}$, the normalization constant

$$const = \sqrt{n_1!...n_N!/N!}$$

and appropriate adjustment of the expansion constants $C_{i_1,...,i_N}$. It is a useful exercise to work this out starting with the simple $N = 2$ case, writing $u^*_{i_1}(\mathbf{r}_1)u^*_{i_2}(\mathbf{r}_2)$ as a sum of symmetric and antisymmetric products, with the antisymmetric part vanishing in the integral of its product and the symmetric $\Phi(\mathbf{r}_1, \mathbf{r}_2)$.

It is useful and conventional to write the expansion (83) using the notation of Eq. (62) with the occupation numbers n_i of the single particle states. In this representation the state $|\Phi\rangle$ will be written as

$$|\Phi\rangle = \sum_{n_1,...,n_i,...;\text{with} \sum_i n_i = N} C_{n_1,...,n_i,...}|n_1, n_1, ..., n_i, ...\rangle \tag{84}$$

with appropriate adjustment of the coefficients $C_{n_1,...,n_i,...}$. Such representation of the N particles wave functions is called **occupation number representation**. It emphasizes the fact that we are dealing with identical quanta (particles) so that all one needs is their numbers n_i in each single particle state. Note that in this representation one must "supply" infinite (actually ∞^3) set of (positive) integers n_i. But since they are subject to the constraint $\sum_i = N$ only $\leq N$ of them are not zero.

4.2 Operators in the second quantization

In this section we want to establish how the operators of the physical observables act on wave functions in the second quantization formalism. In this way we will also understand much better the connection with the first quantization.

4.2.1 The one body Hamiltonian

We will start with the discussion of the action on $|\Phi\rangle$ by the Hamiltonian (53). Let us write it as a sum of two terms - kinetic and potential

$$H_{op} = K_{op} + U_{op} \tag{85}$$

$$K_{op} \;=\; \int d^3r\; \hat{\psi}^+(\mathbf{r})\left(-\frac{\hbar^2}{2m}\nabla^2\right)\hat{\psi}(\mathbf{r}) \quad , \quad U_{op} = \int d^3r \hat{\psi}^+(\mathbf{r})U(\mathbf{r})\hat{\psi}(\mathbf{r})$$

and let us consider first the action on $|\Phi\rangle$ of the potential part

$$U_{op}|\Phi\rangle = \frac{1}{\sqrt{N!}}\int\prod_{a=1}^{N} d^3r_a\Phi(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N)\int d^3r\hat{\psi}^+(\mathbf{r})U(\mathbf{r})\hat{\psi}(\mathbf{r})\;\prod_{a=1}^{N}\hat{\psi}^+(\mathbf{r}_a)|0\rangle \quad (86)$$

Using the result Eq. (76), multiplying it by $U(\mathbf{r})$ and $\hat{\psi}^+(\mathbf{r})$ and doing the d^3r integral with the help of the δ-functions we get

$$\int d^3r\hat{\psi}^+(\mathbf{r})U(\mathbf{r})\hat{\psi}(\mathbf{r})\;\prod_{a=1}^{N}\hat{\psi}^+(\mathbf{r}_a)|0\rangle = \left[\sum_{b=1}^{N}U(\mathbf{r}_b)\right]\prod_{a=1}^{N}\hat{\psi}^+(\mathbf{r}_a)|0\rangle \quad (87)$$

so that

$$U_{op}|\Phi\rangle = \frac{1}{\sqrt{N!}}\int\prod_{a=1}^{N} d^3r_a\Phi'(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N)\prod_{a=1}^{N}\hat{\psi}^+(\mathbf{r}_a)|0\rangle \quad (88)$$

with

$$\Phi'(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N) = \left[\sum_{a=1}^{N}U(\mathbf{r}_a)\right]\Phi(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N) \quad (89)$$

We see that the action of the second quantized operator U_{op} on $|\Phi\rangle$ is equivalent to the action of the first quantized $\sum_a U(\mathbf{r}_a)$ on $\Phi(\mathbf{r}_1,\ldots,\mathbf{r}_N)$ i.e. on the first quantized partner of $|\Phi\rangle$.

To calculate the action of K_{op} on $|\Phi\rangle$ is a bit more involved but straightforward. The details are given in the Appendix 7.3 with the result

$$K_{op}|\Phi\rangle = \frac{1}{\sqrt{N!}}\int\prod_{a=1}^{N} d^3r_a\Phi'(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N)\prod_{a}\hat{\psi}^+(\mathbf{r}_a)|0\rangle \quad (90)$$

with

$$\Phi'(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N) = \left[\sum_{b=1}^{N}\left(-\frac{\hbar^2}{2m}\nabla^2_{\mathbf{r}_b}\right)\right]\Phi(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N) \quad (91)$$

As in the U_{op} case we see that the action of K_{op} on $|\Phi\rangle$ is equivalent to the action of the first quantized kinetic energy operator

$$\sum_{a=1}^{N}\left(-\frac{\hbar^2}{2m}\nabla^2_{\mathbf{r}_b}\right)$$

on the first quantized partner $\Phi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N)$ of $|\Phi\rangle$

Combining these results we find that

$$H_{op}|\Phi\rangle = (K_{op} + U_{op})|\Phi\rangle = \frac{1}{\sqrt{N!}} \int \prod_{a=1}^{N} d^3 r_a \left[\sum_{a=1}^{N} h_a \right] \Phi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N) \prod_a^N \hat{\psi}^+(\mathbf{r}_a)|0\rangle \tag{92}$$

with the single particle hamiltonian h given by Eq. (50)

4.2.2 Other one body operators

The operators K_{op}, U_{op} and H_{op} discussed above are all of the type which in the first quantization formulation have the form

$$\hat{F}^{(1)} = \sum_{a=1}^{N} f_a^{(1)} \tag{93}$$

with each $f_a^{(1)}$ being a function of $\mathbf{r}_a$ and $\mathbf{p}_a = -i\hbar\nabla_a$. Such operators act on wave functions of N particles but at one particle at a time. They are called one-body operators and the subscript which we attached to $\hat{F}^{(1)}$ and $f^{(1)}$ serves to make this distinction.

On the basis of our above discussion of the operators K_{op}, U_{op} and H_{op} we can make a general statement that in the second quantization one body operators have the form

$$F_{op}^{(1)} = \int d^3 r \hat{\psi}^+(\mathbf{r}) f^{(1)} \hat{\psi}(\mathbf{r}) \tag{94}$$

where $f^{(1)}$ in the last expression is one (any) of the operators in the sum (93) and it is acting on $\hat{\psi}(\mathbf{r})$ as a function of $\mathbf{r}$. E.g. angular momentum

$$\mathbf{L} = \sum_{a=1}^{N} \mathbf{l}_a \equiv \sum_{a=1}^{N} \mathbf{r}_a \times (-i\hbar\nabla_{\mathbf{r}_a}) \tag{95}$$

becomes

$$\mathbf{L}_{op} = \int d^3 r \hat{\psi}^+(\mathbf{r})[\mathbf{r} \times (-i\hbar\nabla_{\mathbf{r}})]\hat{\psi}(\mathbf{r}) \tag{96}$$

in the second quantization formalism.

It is important to observe that the particle number N which appears in the operators in the 1st quantization Eq. (93) is a part of their definition while the corresponding operators in the second quantization do not contain any information about N. It is the wave functions on which these operators act, like $|\Psi\rangle$ in the previous section which depend on N. The second quantization $F_{op}^{(1)}$'s "are ready to act" on $|\Psi\rangle$ with any value of N including a linear combination with different N's (see the section below on the general Fock space). At the same time these particular type of operators do not change N since they contain an equal number of creation and annihilation operators - one of each type. But nothing intrinsically in the formalism prevents having operators which change N. In fact the elementary ones $\hat{\psi}(\mathbf{r})$ and $\hat{\psi}^+(\mathbf{r})$ do just that.

Formally the conserving N property of the operators $F_{op}^{(1)}$ is expressed by their commutativity with the particle number operator $N_{op} = \int d^3r \hat{\psi}^+(\mathbf{r})\hat{\psi}(\mathbf{r})$,

$$[F_{op}^{(1)}, N_{op}] = 0 \tag{97}$$

which as in the case of H_{op}, Eq. (66) follows from the invariance of Eq. (94) with respect to the global $U(1)$ transformation Eq. (67).

From our derivations in the previous section it should also be clear in details the "mechanics" of how the one body second quantized operators act on functions like $|\Psi\rangle$. Pictorially one can say that first the destruction operator $\hat{\psi}(\mathbf{r})$ acts on $|\Psi\rangle$ "seeking out" all the particles at their position $\mathbf{r}_a$, $a = 1, \ldots, N$ and "annihilating" them one at a time. The result depends on the coordinates of the particle positions. The operator $\hat{f}$ then acts on these coordinates and then the operator $\hat{\psi}^+(\mathbf{r})$ puts the particles back ("creates" them) where they originally were. All this gets weighted with the probability amplitude $\Phi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N)$ and integrated over all possible $\mathbf{r}_a$'s.

4.2.3 Particle interactions. Two body operators

Let us now understand how do we write in the second quantization the operators which represent interactions between particles. The most common such operators are potential energy which is a sum of all pairwise interactions (e.g. Coulomb interaction). Their form in the first quantization is

$$V = \frac{1}{2} \sum_{a,b=1, a\neq b}^{N} V(\mathbf{r}_a - \mathbf{r}_b) \tag{98}$$

As we see this is a sum of operators with each acting on two particles at a time. Such operators are called two body operators.

Based on the experience of the previous sections it is not difficult to guess that the following corresponding expression holds in the second quantization

$$V_{op} = \frac{1}{2} \int d^3r d^3r' \hat{\psi}^+(\mathbf{r})\hat{\psi}^+(\mathbf{r}')V(\mathbf{r} - \mathbf{r}')\hat{\psi}(\mathbf{r}')\hat{\psi}(\mathbf{r}) \tag{99}$$

To verify this guess let us do what we did with one body operators - let us act with this expression on the general N particle wave function in Eq. (81).

$$\begin{aligned} V_{op}|\Phi\rangle &= \frac{1}{\sqrt{N!}}\int\prod_{a=1}^{N} d^3r_a \Phi(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N)\times \\ &\times\frac{1}{2}\int d^3r d^3r' \hat{\psi}^+(\mathbf{r})\hat{\psi}^+(\mathbf{r}')V(\mathbf{r}-\mathbf{r}')\hat{\psi}(\mathbf{r}')\hat{\psi}(\mathbf{r})\prod_{a=1}^{N}\hat{\psi}^+(\mathbf{r}_a)|0\rangle \end{aligned} \tag{100}$$

To evaluate this we use the relation Eq. (76), act on it with $\hat{\psi}(\mathbf{r}')$ and obtain

$$\hat{\psi}(\mathbf{r}')\hat{\psi}(\mathbf{r})\prod_{a=1}^{N}\hat{\psi}^+(\mathbf{r}_a)|0\rangle = \left[\sum_{b\neq c}^{N}\delta(\mathbf{r}'-\mathbf{r}_c)\delta(\mathbf{r}-\mathbf{r}_b)\prod_{a\neq b,c}^{N}\hat{\psi}^+(\mathbf{r}_a)\right]|0\rangle$$

Using this we find

$$\begin{aligned} &\frac{1}{2}\int d^3r d^3r' \hat{\psi}^+(\mathbf{r})\hat{\psi}^+(\mathbf{r}')V(\mathbf{r}-\mathbf{r}')\hat{\psi}(\mathbf{r}')\hat{\psi}(\mathbf{r})\prod_{a=1}^{N}\hat{\psi}^+(\mathbf{r}_a)|0\rangle = \\ &\frac{1}{2}\int d^3r d^3r' \hat{\psi}^+(\mathbf{r})\hat{\psi}^+(\mathbf{r}')V(\mathbf{r}-\mathbf{r}')\left[\sum_{b,c=1,b\neq c}^{N}\delta(\mathbf{r}'-\mathbf{r}_c)\delta(\mathbf{r}-\mathbf{r}_b)\prod_{a\neq b,c}^{N}\hat{\psi}^+(\mathbf{r}_a)\right]|0\rangle = \\ &\qquad = \frac{1}{2}\sum_{b,c=1,b\neq c}^{N} V(\mathbf{r}_b-\mathbf{r}_c)\prod_{a=1}^{N}\hat{\psi}^+(\mathbf{r}_a)|0\rangle \end{aligned}$$

and therefore

$$V_{op}|\Phi\rangle = \frac{1}{\sqrt{N!}}\int\prod_{a=1}^{N} d^3r_a\left[\frac{1}{2}\sum_{b,c=1,b\neq c}^{N} V(\mathbf{r}_b-\mathbf{r}_c)\right]\Phi(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N)\prod_{a=1}^{N}\hat{\psi}^+(\mathbf{r}_a)|0\rangle \tag{101}$$

So indeed the action of V_{op} on $|\Phi\rangle$ is equivalent to/results in the action of the first quantized V, Eq. (98) on $\Phi(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N)$

The intuitive understanding of the expression (99) is similar to what we saw in the one body operators case - the operators $\hat{\psi}(\mathbf{r}')\hat{\psi}(\mathbf{r})$ "search" to annihilate two particles (as $\mathbf{r}$ and $\mathbf{r}'$ are integrated over) and thereby "reveal" their position. The function $V(\mathbf{r}-\mathbf{r}')$ weighs the result while the operators $\hat{\psi}^+(\mathbf{r})\hat{\psi}^+(\mathbf{r})$ put the particles back. All this is integrated over all possible positions $\mathbf{r}$ and $\mathbf{r}'$.

The general form of the two body operator in the first quantization is

$$\hat{F}^{(2)} = \frac{1}{2}\sum_{a,b=1,a\neq b}^{N} f_{ab}^{(2)} \tag{102}$$

with the second quantized counterpart

$$F_{op}^{(2)} = \frac{1}{2} \int d^3r d^3r' \hat{\psi}^+(\mathbf{r}) \hat{\psi}^+(\mathbf{r}') f^{(2)} \hat{\psi}(\mathbf{r}') \hat{\psi}(\mathbf{r}) \tag{103}$$

with $f^{(2)}$ in general being a function of $\mathbf{r}, \mathbf{r}'$ and $\hat{\mathbf{p}} = -i\hbar\nabla_{\mathbf{r}}, \hat{\mathbf{p}}' = -i\hbar\nabla_{\mathbf{r}'}$.

It is important to observe that also here as with the one body operators the second quantized operators do not contain any information about the number N of the particles which is encoded in the wave functions on which these operators act. Also here the operators $F_{op}^{(2)}$ do not change the value of N and commute with the particle number operator

$$[F_{op}^{(2)}, N_{op}] = 0 \tag{104}$$

which is a consequence of the $U(1)$ unitary symmetry Eq. (67) which the operators $F_{op}^{(2)}$ posses.

4.2.4 Changing the single particle basis

The one and two body operators discussed above were expressed in terms of the basic field operators $\hat{\psi}(\mathbf{r})$ and $\hat{\psi}^+(\mathbf{r})$. It is easy and instructive to express them using the expansion (54) of these operators in a general single particle basis $\{u_i(\mathbf{r})\}$. Inserting (54) into the expressions (94) and (103) we obtain

$$F_{op}^{(1)} = \sum_{ij} \langle i|f^{(1)}|j\rangle \hat{a}_i^+ \hat{a}_j \tag{105}$$

$$F_{op}^{(2)} = \sum_{ijkl} \langle ij|f^{(2)}|kl\rangle \hat{a}_i^+ \hat{a}_j^+ \hat{a}_l \hat{a}_k \tag{106}$$

where we used the notation for the matrix elements of elementary one and two body operators

$$\langle i|f^{(1)}|j\rangle = \int d^3r u_i^*(\mathbf{r}) f^{(1)} u_j(\mathbf{r}) \tag{107}$$

$$\langle ij|f^{(2)}|kl\rangle = \int d^3r d^3r' u_i^*(\mathbf{r}) u_j^*(\mathbf{r}') f^{(2)} u_k(\mathbf{r}) u_l(\mathbf{r}') \tag{108}$$

We draw attention to the "logic" of how the operators $F_{op}^{(1)}$ and $F_{op}^{(2)}$ in a general single particle basis act on a wave function in this basis as written in the occupation number representation of Eq. (84). In the one body $F_{op}^{(1)}$ one starts with the operator $\hat{a}_j$ annihilating a particle in a (single particle basis) state u_j reducing the corresponding n_j occupation to n_j-1. This is "weighted" with a corresponding amplitude to find this

n_j as encoded in the coefficients $C_{n_1,...,n_j,...}$ of the occupation number representation. The following action of the operator $\hat{a}_i^+$ creates (puts back) a particle in the state u_i and the result gets multiplied by the transition matrix element $\langle i|f^{(1)}|j\rangle$. At the end one sums over all such transitions. The two body $F_{op}^{(2)}$ operates in a similar fashion but with two particles annihilation and creation and the sum over all two particle transitions.

4.3 Second quantization via commutators describes identical bosons

The following important features of the above formalism must be observed at this stage. The first quantization operators which are counterparts of the operators in the second quantization are always *symmetric sums* over all the particles or their pairs etc in the wave functions on which they act.

The symmetry of these sums follows since all their terms are identical in acting on different particles. They have the same functional dependence on the coordinates and momenta with the same parameters - masses, charges, etc., e.g. same kinetic energy, same external potential, same inter-particle interactions, etc. This is seen in the formal correspondence Eq. (93) $\rightarrow$ Eq. (94) and Eq. (102) $\rightarrow$ Eq. (103) and in the explicit examples in Eqs. (89, 91, 95, 98). There is no possibility to have second quantized operators representing observables distinguishing a particular particle, say $f_5^{(1)}$ or sets of particular particles, e.g $f_7^{(1)} + f_{15}^{(1)}$. This is a general feature of quantum systems of identical particles.

Let us also recall that as we discovered in Section 4.1.2 the first quantization wave functions $\Phi(\mathbf{r}_1, ..., \mathbf{r}_N)$ which are counterparts of the second quantization $|\Phi\rangle$ are symmetric under the permutation of all the particles coordinates. This confirms the particle being identical and moreover obeying the spin-statistics theorem requirements for systems of bosons.

Let us remind that the spin-statistics theorem, proved by Pauli, states (in its first part) that the wave functions of a system of identical integer-spin particles must be symmetric under the exchange of the coordinates of any two particles. Such particles are bosons obeying the Bose-Einstein statistics.

In our case of the identical particles without spin the symmetry requirement dictated by the Pauli theorem is an additional rule which is imposed in the first quantization formalism on selecting the wave function solutions of the Schrödinger equation (78). As we have seen it is automatically fulfilled in the second quantization wave functions Eqs. (79,81).

The second part of the spin-statistics theorem concerns wave functions of system of identical half-integer spin particles. The theorem states that they must be anti-symmetric under any pair of particle exchange. Such particles are fermions obeying the Fermi-Dirac statistics. We will discuss in the next Chapter how the second quantization allows for a simple and straightforward modification to be extended to the descriptions of fermions.

Concerning the proof of the spin-statistics theorem - as Feynman states in his Lectures on Physics: "...An explanation has been worked out by Pauli from complicated arguments of QFT and relativity...but we haven't found a way of reproducing his arguments on an elementary level..."[5].

4.4 Self interacting Schrödinger field.

4.4.1 Summing up. Interacting Hamiltonian

To summarize we learned how to translate the wave functions and physical operators into the second quantization formalism. The N particle wave function of N bosons $\Phi(\mathbf{r}_1, ..., \mathbf{r}_N)$ should be symmetric and becomes the amplitude of the $|\mathbf{r}_1, ..., \mathbf{r}_N\rangle$ state in the expression (79) or the more explicit (81).

Dealing with operators one should first determine to which type they belong - one body, two body, etc. Examples of one body operators are momentum, density, current, etc

$$\begin{aligned}
\mathbf{P} &= \sum_{a=1}^{N} \mathbf{p}_a = \sum_{a=1}^{N}(-i\hbar\nabla_{\mathbf{r}_a}) \ , \ \rho(\mathbf{r}) = \sum_{a=1}^{N}\delta(\mathbf{r}-\mathbf{r}_a) \\
\mathbf{j}(\mathbf{r}) &= \frac{1}{2m}\sum_{a=1}^{N}[\delta(\mathbf{r}-\mathbf{r}_a)(-i\hbar\nabla_{\mathbf{r}_a}) + (-i\hbar\nabla_{\mathbf{r}_a})\delta(\mathbf{r}-\mathbf{r}_a)]
\end{aligned}$$

Note that identical particles imply that any such operator is a sum of identical operators acting on each particle. So one takes one member of the sum and uses it in the expression (94) to find the corresponding 2nd quantized operator. If one prefers a general basis $\{u_i\}$ rather than the coordinate representation of the field operators one needs to calculate the matrix elements between all possible pairs of u_i's and use them in the expression (105). The number N of particles appears explicitly in the operators of the first quantized formalism but not in the 2nd quantization.

[5] cf., I. Duck and E. Sudarshan, Towards an understanding of the spin-statistics theorem, Am. J. Phys., 66 (4) 1998

There are not too many examples of two body operators. Beside the two body interaction (98) there are various correlators like density-density or current-current, etc

$$\rho_{op}(\mathbf{r})\rho_{op}(\mathbf{r}') = \sum_{a,b=1}^{N} \delta(\mathbf{r}-\mathbf{r}_a)\delta(\mathbf{r}'-\mathbf{r}_b) \quad \text{, etc}$$

As in the one body case one must take one term in such a double sum and either use it in the expression (103) with field operators or calculate all its two particle matrix elements in a chosen basis of the single particle states u_i's. One should then form an expression (106) using these matrix elements.

As a rule it is extremely rare to find 3 body operator but it is straightforwardly clear how to extend what we have learned to such cases.

Let us follow the above rules to write the full 2nd quantization Hamiltonian of a many body interacting system. Consider its (most common) expression in the 1st quantization

$$\hat{H} = \sum_{a=1}^{N} \left[\frac{\hat{\mathbf{p}}_a^2}{2m} + U(\mathbf{r}_a) \right] + \frac{1}{2} \sum_{a,b=1,a\neq b}^{N} V(\mathbf{r}_a - \mathbf{r}_b) \quad , \quad \hat{\mathbf{p}}_a = -i\hbar\nabla_a \tag{109}$$

with externally fixed number N of the particles. Assuming that the particles are bosons their particles statistics must be imposed "by hand" allowing only symmetric wave functions.

The 2nd quantized version of the above Hamiltonian is

$$H_{op} = \int d^3r \hat{\psi}^+(\mathbf{r})\, h\, \hat{\psi}(\mathbf{r}) + \frac{1}{2} \int d^3r d^3r' \hat{\psi}^+(\mathbf{r})\hat{\psi}^+(\mathbf{r}')V(\mathbf{r}-\mathbf{r}')\hat{\psi}(\mathbf{r}')\hat{\psi}(\mathbf{r}) \tag{110}$$

with

$$h = -\frac{\hbar^2}{2m}\nabla^2 + U(\mathbf{r})$$

In a general single particle basis this Hamiltonian is written

$$H_{op} = \sum_{ij} \langle i|\, h\, |j\rangle \hat{a}_i^+ \hat{a}_j + \frac{1}{2} \sum_{ijkl} \langle ij|V|kl\rangle \hat{a}_i^+ \hat{a}_j^+ \hat{a}_l \hat{a}_k \tag{111}$$

If one knows the solutions of the one body part, i.e. knows the eigenfunctions $u_i(\mathbf{r})$ and the eigenenergies ϵ_i of h, Eq. (59) one can "incorporate" this knowledge in the above expression for H_{op}. Using the set $\{u_i\}$ as the basis one has $\langle i|\, h\, |j\rangle = \epsilon_i \delta_{ij}$ and

$$H_{op} = \sum_{i} \epsilon_i \hat{a}_i^+ \hat{a}_i + \frac{1}{2} \sum_{ijkl} \langle ij|V|kl\rangle \hat{a}_i^+ \hat{a}_j^+ \hat{a}_l \hat{a}_k \tag{112}$$

In the Mean Field Approximations chapter of this course we shall discuss and give examples of even more optimal ways to choose the single particle basis which incorporate on the average the effect of the interaction term in many body systems.

4.4.2 Heisenberg equations. Classical limits - field vs particles

Let us consider the Heisenberg equations for the field operators $\hat{\psi}(\mathbf{r})$ and $\hat{\psi}^+(\mathbf{r})$ and the general interacting Hamiltonian (110). We have

$$i\hbar\frac{\partial}{\partial t}\left(\begin{array}{c}\hat{\psi}(\mathbf{r},t)\\ \hat{\psi}^+(\mathbf{r},t)\end{array}\right)=\left[\left(\begin{array}{c}\hat{\psi}(\mathbf{r},t)\\ \hat{\psi}^+(\mathbf{r},t)\end{array}\right),H_{op}\right]$$

Straightforward calculations produce Hermitian conjugate equations

$$\begin{aligned} i\hbar\frac{\partial\hat{\psi}(\mathbf{r},t)}{\partial t} &= \left[-\frac{\hbar^2}{2m}\nabla^2+U(\mathbf{r})\right]\hat{\psi}(\mathbf{r},t)+\int V(\mathbf{r}-\mathbf{r}')\hat{\psi}^+(\mathbf{r}',t)\hat{\psi}(\mathbf{r}',t)\,d^3r'\;\hat{\psi}(\mathbf{r},t) \\ &\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad (113) \\ -i\hbar\frac{\partial\hat{\psi}^+(\mathbf{r},t)}{\partial t} &= \left[-\frac{\hbar^2}{2m}\nabla^2+U(\mathbf{r})\right]\hat{\psi}^+(\mathbf{r},t)+\hat{\psi}^+(\mathbf{r},t)\int V(\mathbf{r}-\mathbf{r}')\hat{\psi}^+(\mathbf{r}',t)\hat{\psi}(\mathbf{r}',t)\,d^3r' \end{aligned}$$

These equations find many uses in the theory of many-particle systems. The Green's functions method provides a good example[6].

Here we want to point out a simple but conceptually important aspect - their classical limit. Like in other quantum systems this limit is intuitively obtained by replacing coordinate and momentum operators by the corresponding classical functions of time turning Heisenberg equations into classical Hamilton equations. In the above equations (113) this means replacing $\hat{\psi}(\mathbf{r},t)$ and $\hat{\psi}^+(\mathbf{r},t)$ by the c-number (classical, commuting) functions $\psi(\mathbf{r},t)$ and $\psi^*(\mathbf{r},t)$. In the non interacting limit $V=0$ the resulting wave equations bring us back to where we started, cf., the Schrödinger equation (49). The classical limit of the fully interacting case leads to a non linear Schrödinger equation with cubic non linear term controlled by the interaction.

Let us add two more remarks.

a) Our intuitive "derivation" of the classical limit of Eq. (113) requires formal justification which will be discussed in the Chapter "Mean Field Approximations for Many Body Problems". On the intuitive level the classical limit of the quantum field corresponds to physical processes in which very large number of quanta (particles) are "condensed" in the same wave mode, i.e the same single particle state.

[6]cf., Quantum Theory of Many-Particle Systems, A. Fetter and J. Walecka, Dover, 2003

b) The classical limit referred to above is different from the common classical limit for the N particle Hamiltonian Eq. (109). The latter is given by replacing the operators for the particle coordinates and momenta by the classical variables in the corresponding Heisenberg equations. It is easy to show that this results in the classical Hamilton equations

$$\frac{d\mathbf{r}_a}{dt} = \frac{\partial H}{\partial \mathbf{p}_a} \quad , \quad \frac{d\mathbf{p}_a}{dt} = -\frac{\partial H}{\partial \mathbf{r}_a} \quad , \quad a = 1, ..., N \tag{114}$$

We therefore have two classical limits - the "field" classical limit for the fields $\psi(\mathbf{r}, t)$ and $\psi^*(\mathbf{r}, t)$ vs the more familiar "particle" classical limit for the particle coordinates $\mathbf{r}_a$'s and momenta $\mathbf{p}_a$'s. The latter classical limit is the limit of $\hbar \to 0$ while the former is achieved for the large number $N_0 \gg 1$ of condensed quanta (i.e. the boson particles) of the theory.

5 Fermions – another alternative of the second quantization

As we have learned so far the quantization of the Schrödinger field leads to a very efficient and elegant description of many particle bosonic systems in all their aspects. A natural question is if this treatment can be extended to systems of fermions.

5.1 Quantization via anticommutators

A clear hint towards a positive answer can be found in our discussions in Section 4.1.2. There we saw that the symmetry of the bosonic wave functions was assured by the most basic property of the field operators $\psi^+(\mathbf{r}_a)$'s creating the particles - their commutativity. As we will now show there is a consistent way of quantizing the Schrödinger field by postulating anticommutativity of the basic operators. This single change of the quantization postulate will lead to a description of many fermion systems similar to the second quantized formalism for many bosons.

Dealing with fermions one must introduce spin variable together with position coordinates in order to describe the particles of the theory. Accordingly we start with the classical field which is described by functions

$$\psi_\sigma(\mathbf{r}) \quad \text{and} \quad \psi^*_\sigma(\mathbf{r}) \tag{115}$$

with the spin projection index $\sigma = \pm 1/2$ (we assume spin 1/2 fermions as by far the most common). It is often useful to write/view these functions in the explicit spinor form as

$$\begin{pmatrix} \psi_{1/2}(\mathbf{r}) \\ \psi_{-1/2}(\mathbf{r}) \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} \psi^*_{1/2}(\mathbf{r}) \\ \psi^*_{-1/2}(\mathbf{r}) \end{pmatrix}$$

We quantize this field by introducing two sets of operators

$$\hat{\psi}_\sigma(\mathbf{r}) \;\; \text{and} \;\; \hat{\psi}^+_\sigma(\mathbf{r})$$

with $\mathbf{r}$ and $\sigma = \pm 1/2$ labelling each set. We need to define the space of states on which these $2 \times \infty^3$ operators act and the results of their action. We have seen with the bosonic field $\psi(\mathbf{r})$ treated above that to achieve this it was sufficient to define an abstract vacuum state $|0\rangle$ and the commutation relations between the field operators. Following this we could define the basis of the space of states on which the operators act and calculate any matrix element for any given operator.

Following this experience we start by defining the vacuum state $|0\rangle$ with the properties

$$\begin{aligned} &a) \qquad \langle 0|0\rangle = 1 \\ &b) \qquad \hat{\psi}_\sigma(\mathbf{r})|0\rangle = 0 \quad \text{for all values of } \mathbf{r} \text{ and } \sigma \end{aligned} \tag{116}$$

This we supplement with imposing (posulating) the anticommutation relations as follows

$$\begin{aligned} &\hat{\psi}_\sigma(\mathbf{r})\hat{\psi}^+_{\sigma'}(\mathbf{r}') + \hat{\psi}^+_{\sigma'}(\mathbf{r}')\hat{\psi}_\sigma(\mathbf{r}) \equiv \{\hat{\psi}_\sigma(\mathbf{r}), \hat{\psi}^+_{\sigma'}(\mathbf{r}')\} = \delta_{\sigma\sigma'}\delta(\mathbf{r}-\mathbf{r}') \\ &\hat{\psi}_\sigma(\mathbf{r})\hat{\psi}_{\sigma'}(\mathbf{r}') + \hat{\psi}_{\sigma'}(\mathbf{r}')\hat{\psi}_\sigma(\mathbf{r}) \equiv \{\hat{\psi}_\sigma(\mathbf{r}), \hat{\psi}_{\sigma'}(\mathbf{r}')\} = 0 \\ &\hat{\psi}^+_\sigma(\mathbf{r})\hat{\psi}^+_{\sigma'}(\mathbf{r}') + \hat{\psi}^+_{\sigma'}(\mathbf{r}')\hat{\psi}^+_\sigma(\mathbf{r}) = \{\hat{\psi}^+_\sigma(\mathbf{r})\, \hat{\psi}^+_{\sigma'}(\mathbf{r}')\} = 0 \end{aligned} \tag{117}$$

where the curly brackets $\{\ ,\ \}$ define anticommutators.

As we will demonstrate below these two definitions are sufficient to define a quantum mechanical fermion field with any dynamics. We note that while the definition of the vacuum is the same as in the bosonic case the anticommutation relations define a new quantization "paradigm" which is different from the familiar canonical quantization via the commutators.

5.2 Fermions in external potential

In order to understand the consequences of the new quantization scheme defined above we start by considering a simple example - particles in an external potential.

5.2.1 The field equations and the Hamiltonian

The dynamical equation for the field (115) in an external potential is a generalization of the Eq. (49) to include the spin

$$i\hbar\frac{\partial\psi_\sigma(\mathbf{r},t)}{\partial t}=\sum_{\sigma'}h_{\sigma\sigma'}\psi_{\sigma'}(\mathbf{r},t) \tag{118}$$

As an example we consider the following $h_{\sigma\sigma'}$

$$h_{\sigma\sigma'}=\delta_{\sigma\sigma'}\left(-\frac{\hbar^2}{2m}\right)\nabla^2+U_{\sigma\sigma'}(\mathbf{r}) \tag{119}$$

We assumed a spin dependent external potential, like for instance the interaction of the spin with an inhomogeneous magnetic field (e.g. in the Stern-Gerlach experiment)

$$U_{\sigma\sigma'}(\mathbf{r})=-\gamma\mathbf{B}(\mathbf{r})\cdot\mathbf{s}_{\sigma\sigma'}$$

with a constant γ and vector $\mathbf{s}$ of spin 1/2 matrices.

Using our experience with the spinless field and appropriately generalizing it we consider the equation (118) and its complex conjugate as the pair of Hamilton equations with $\psi_\sigma(\mathbf{r})$ and $i\hbar\psi^*_\sigma(\mathbf{r})$ as canonical variables and the following classical Hamiltonian function

$$H=\sum_{\sigma\sigma'}\int d^3r\left[\delta_{\sigma\sigma'}\frac{\hbar^2}{2m}|\nabla\psi_\sigma(\mathbf{r})|^2+U_{\sigma\sigma'}(\mathbf{r})\psi^*_\sigma(\mathbf{r})\psi_{\sigma'}(\mathbf{r})\right] \tag{120}$$

Indeed from

$$\begin{aligned}\delta H &= \sum_{\sigma\sigma'}\int d^3r\left\{\delta_{\sigma\sigma'}\frac{\hbar^2}{2m}\left[\nabla\psi^*_\sigma(\mathbf{r})\nabla\delta\psi_{\sigma'}(\mathbf{r})+\nabla\delta\psi^*_\sigma(\mathbf{r})\nabla\psi_{\sigma'}(\mathbf{r})\right]+\right.\\ &\quad\left.+U_{\sigma\sigma'}(\mathbf{r})\left[\psi^*_\sigma(\mathbf{r})\delta\psi_{\sigma'}(\mathbf{r})+\delta\psi^*_\sigma(\mathbf{r})\psi_{\sigma'}(\mathbf{r})\right]\right\}\end{aligned}$$

we find

$$\frac{\partial\psi_\sigma(\mathbf{r})}{\partial t}=\frac{\delta H}{\delta[i\hbar\psi^*_\sigma(\mathbf{r})]}=\frac{1}{i\hbar}\sum_{\sigma\sigma'}\left[-\delta_{\sigma\sigma'}\frac{\hbar^2}{2m}\nabla^2\psi_{\sigma'}(\mathbf{r})+U_{\sigma\sigma'}(\mathbf{r})\psi_{\sigma'}(\mathbf{r})\right]$$

$$\frac{\partial[i\hbar\psi^*_\sigma(\mathbf{r})]}{\partial t}=-\frac{\delta H}{\delta\psi_\sigma(\mathbf{r})}=-\sum_{\sigma\sigma'}\left[-\delta_{\sigma\sigma'}\frac{\hbar^2}{2m}\nabla^2\psi^*_{\sigma'}(\mathbf{r})+U_{\sigma\sigma'}(\mathbf{r})\psi^*_{\sigma'}(\mathbf{r})\right]$$

which reproduce correctly the field equation (118) and its complex conjugate.

On this basis we quantize this spinor field by replacing it with the field operators

$$\psi_\sigma(\mathbf{r}) \to \hat{\psi}_\sigma(\mathbf{r}) \quad , \quad \psi^*_\sigma(\mathbf{r}) \to \hat{\psi}^+_\sigma(\mathbf{r}) \tag{121}$$

with the anticommutation relations (117) and the Hamiltonian operator

$$H_{op} = \sum_{\sigma\sigma'} \int d^3r \left[\delta_{\sigma\sigma'} \frac{\hbar^2}{2m} \nabla \hat{\psi}^+_\sigma(\mathbf{r}) \cdot \nabla \hat{\psi}_{\sigma'}(\mathbf{r}) + U_{\sigma\sigma'}(\mathbf{r}) \hat{\psi}^+_\sigma(\mathbf{r}) \hat{\psi}_{\sigma'}(\mathbf{r}) \right] \tag{122}$$

or in an equivalent form (cf., the remark after Eq. (22))

$$H_{op} = \sum_{\sigma\sigma'} \int d^3r \; \hat{\psi}^+_\sigma(\mathbf{r}) \left[-\delta_{\sigma\sigma'} \frac{\hbar^2}{2m} \nabla^2 + U_{\sigma\sigma'}(\mathbf{r}) \right] \hat{\psi}_{\sigma'}(\mathbf{r}) = \sum_{\sigma\sigma'} \int d^3r \; \hat{\psi}^+_{\sigma'}(\mathbf{r}) h_{\sigma'\sigma} \hat{\psi}_\sigma(\mathbf{r}) \tag{123}$$

5.2.2 Transforming to the normal modes

Let us now solve the quantum mechanical problem defined by the Hamiltonian (123). This is not hard since it is quadratic. We need to find its normal modes. Following a very similar route as in dealing with (53) we consider a single particle equation

$$\sum_{\sigma'} h_{\sigma\sigma'} u_i(\mathbf{r}, \sigma) = \epsilon_i u_i(\mathbf{r}, \sigma) \tag{124}$$

The set $\{u_i(\mathbf{r}, \sigma)\}$ is complete and orthonormal in the space of functions of $\mathbf{r}, \sigma$

$$\sum_\sigma \int d^3 u^*_i(\mathbf{r}, \sigma) u_j(\mathbf{r}, \sigma) = \delta_{ij} \quad , \quad \sum_i u_i(\mathbf{r}, \sigma) u^*_i(\mathbf{r}', \sigma') = \delta_{\sigma\sigma'} \delta(\mathbf{r} - \mathbf{r}') \tag{125}$$

We expand the field operators using this set

$$\hat{\psi}_\sigma(\mathbf{r}) = \sum_i \hat{a}_i u_i(\mathbf{r}, \sigma) \quad , \quad \hat{\psi}^+_\sigma(\mathbf{r}) = \sum_i \hat{a}^+_i u^*_i(\mathbf{r}, \sigma) \tag{126}$$

The operators $\hat{a}_i$ and $\hat{a}^+_i$ can be expressed as

$$\hat{a}_i = \sum_\sigma \int d^3r \, \hat{\psi}_\sigma(\mathbf{r}) u^*_i(\mathbf{r}, \sigma) \quad , \quad \hat{a}^+_i = \sum_\sigma \int d^3r \, \hat{\psi}^+_\sigma(\mathbf{r}) u_i(\mathbf{r}, \sigma) \tag{127}$$

Using the anticommutators (117) and the completeness of the set $\{u_i(\mathbf{r}, \sigma)\}$ it is easy to see that $\hat{a}_i$'s and $\hat{a}^+_i$'s satisfy anticommutation relations too

$$\{\hat{a}_i, \hat{a}^+_j\} = \delta_{ij} \quad , \quad \{\hat{a}_i, \hat{a}_j\} = 0 = \{\hat{a}^+_i, \hat{a}^+_j\} \tag{128}$$

Inserting the expansions (126) in the Hamiltonian (123) we obtain

$$H_{op} = \sum_i \epsilon_i \hat{a}_i^+ \hat{a}_i \tag{129}$$

exactly as in the bosonic case but with the operators obeying the anticommutation relations.

5.2.3 The eigenstates. Working with anticommiting $\hat{a}$'s and $\hat{a}^+$'s

The Hamiltonian (129) is a sum of commuting parts. Indeed as is easy to verify that

$$[\hat{n}_i, \hat{n}_j] = 0 \tag{130}$$

where we denoted

$$\hat{n}_i = \hat{a}_i^+ \hat{a}_i \tag{131}$$

We need to find the eigenfunctions of $\hat{n}_i$'s. We follow the same construction as in the bosonic case, cf., Sec.7.1. We note that from Eqs.(127) it follows that the vacuum state $|0\rangle$ defined in (116) is annihilated by all $\hat{a}_i$'s

$$\hat{a}_i|0\rangle = 0 \quad \text{for} \quad \text{all} \;\; i'\text{s} \tag{132}$$

Since it is also annihilated by all $\hat{n}_i$'s it is clearly an eigenstate of the Hamiltonian (129) with zero energy eigenvalue.

We now define one particle states

$$|1_i\rangle \equiv \hat{a}_i^+|0\rangle$$

for any i. We note the following properties of such states

$$\begin{aligned}
\langle 1_i|1_i\rangle &= \langle 0|\hat{a}_i\hat{a}_i^+|0\rangle = \langle 0|1 - \hat{a}_i^+\hat{a}_i|0\rangle = 1 \\
\langle 0|1_i\rangle &= \langle 0|\hat{a}_i^+|0\rangle = 0 \quad , \quad \hat{a}_i^+|1_i\rangle = (\hat{a}_i^+)^2|0\rangle = 0
\end{aligned} \tag{133}$$

In the 1st equality we used the anticomutation relation $\{\hat{a}_i, \hat{a}_i^+\} = 1$ and

$$\langle 1_i| \equiv [\hat{a}_i^+|0\rangle]^+ = \langle 0|[\hat{a}_i^+]^+ = \langle 0|\hat{a}_i$$

In the 2nd equality we used

$$\langle 0|\hat{a}_i^+ = [\hat{a}_i|0\rangle]^+ = 0$$

In the 3rd we used the anticommutator

$$\{\hat{a}_i^+, \hat{a}_i^+\} = 2[\hat{a}_i^+]^2 = 0$$

Remarkably this last relation is the expression of the Pauli exclusion principle that two (or more) identical fermions cannot occupy the same quantum state - in this case the state u_i.

The most relevant for us property of the states $|1_i\rangle$ is that they are eigenstates of $\hat{n}_i$ with eigenvalue $n_i = 1$

$$\hat{n}_i|1_i\rangle = \hat{a}_i^+\hat{a}_i\hat{a}_i^+|0\rangle = \hat{a}_i^+[1 - \hat{a}_i^+\hat{a}_i]|0\rangle = \hat{a}_i^+|0\rangle = |1_i\rangle \tag{134}$$

The last relation in Eq. (133) means that there are only two eigenstates of each $\hat{n}_i$ - $|0\rangle$ and $|1_i\rangle$ with respective eigenvalues $n_i = 0$ and $n_i = 1$.

It follows then that the eigenfunctions of the Hamiltonian (129) are the products of all possible eigenstates of $\hat{n}_i$

$$|\Psi_{\{n_i\}}\rangle = |n_1, n_2, \ldots, n_i, \ldots\rangle = \prod_i |n_i\rangle = \prod_i [\hat{a}_i^+]^{n_i}|0\rangle \quad \text{with} \quad n_i = 0 \text{ or } 1$$

and with the corresponding eigenenergies

$$E_{\{n_i\}} = \sum_i \epsilon_i n_i \quad \text{with} \quad n_i = 0 \text{ or } 1 \;\; ; \;\; N = \sum_i n_i$$

The restriction of the occupations n_i to 0 or 1 is of course another expression of the Pauli principle and is a direct result of the anti-commutation relations which we assumed in the process of the quantization.

As is the bosonic case the total number of particles N is an eigenvalue of the total particle number operator

$$N_{op} = \sum_i \hat{n}_i \tag{135}$$

which commutes with the Hamiltonian H_{op}, Eq.(129). We will expand on this below in Section 5.2.5.

So to summarize - the solution of this problem amounts to solving the single particle Schrödinger equation (124) and then populating (filling in) the resulting single particle states u_i with N particles according to the Pauli principe. This solution is of course identical to what we would obtain in the 1st quantization formalism for N fermions with the difference that there N was a fixed, given parameter of the problem while it is a quantum number and can take any value in the 2nd quantization formalism.

5.2.4 Spin independent potential

Let us discuss an important limiting case of the single particle hamiltonian in Eq.(118) which is spin-independent, i.e. diagonal in spin indices

$$h_{\sigma\sigma'} = \delta_{\sigma\sigma'} h \quad \text{with} \quad h = -\frac{h^2}{2m}\nabla^2 + U(\mathbf{r})$$

and correspondingly

$$H_{op} = \sum_{\sigma} \int d^3r \, \hat{\psi}_{\sigma}^{+}(\mathbf{r}) h \hat{\psi}_{\sigma}(\mathbf{r})$$

The normal modes are then products of space and spin parts

$$u_i(\mathbf{r}, \sigma) = u_k(\mathbf{r}) \chi_s(\sigma)$$

with $u_k(\mathbf{r})$ solving

$$h u_k(\mathbf{r}) = \epsilon_k u_k(\mathbf{r})$$

and $\chi_s(\sigma), \; s = \pm 1/2$ being just two orthogonal space independent spinors, e.g.

$$\chi_{1/2} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad , \quad \chi_{-1/2} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

The single particle energies ϵ_k are now spin degenerate and the expansion in normal modes has the form

$$\hat{\psi}_{\sigma}(\mathbf{r}) = \sum_{ks} \hat{a}_{ks} u_k(\mathbf{r}) \chi_s(\sigma) \;\; , \;\; \hat{\psi}_{\sigma}^{+}(\mathbf{r}) = \sum_{ks} \hat{a}_{ks}^{+} u_k^{*}(\mathbf{r}) \chi_s^{*}(\sigma)$$

with the commutation relations

$$\{\hat{a}_{ks}, \hat{a}_{k's'}^{+}\} = \delta_{kk'} \delta_{ss'} \;\; , \;\; \{\hat{a}_{ks}, \hat{a}_{k's'}\} = 0 = \{\hat{a}_{ks}^{+}, \hat{a}_{k's'}^{+}\}$$

The Hamiltonian is expressed as

$$H_{op} = \sum_{ks} \epsilon_k \hat{a}_{ks}^{+} \hat{a}_{ks} = \sum_{ks} \epsilon_k \hat{n}_{ks}$$

The number operators $\hat{n}_{ks}$ commute and their eigenfunctions are easily found as before to be $|0\rangle$ and $|1_{ks}\rangle \equiv \hat{a}_{ks}^{+}|0\rangle$ with corresponding eigenvalies $n_{ks} = 0$ and 1. The eigenfunctions of H_{op} are then

$$|\Psi_{\{n_{ks}\}}\rangle = |n_1, n_2, \ldots, n_{ks}, \ldots\rangle = \prod_{ks} |n_{ks}\rangle = \prod_{ks} [\hat{a}_{ks}^{+}]^{n_{ks}} |0\rangle \quad \text{with} \quad n_{ks} = 0 \;\text{ or }\; 1$$

and with the corresponding eigenenergies

$$E_{\{n_{ks}\}} = \sum_{ks} \epsilon_k n_{ks} \quad \text{with} \quad n_{ks} = 0 \;\text{ or }\; 1 \;\; ; \;\; N = \sum_{ks} n_{ks}$$

5.2.5 The particle number operator

As in the bosonic case it is useful to express the total particle number operator N_{op} in terms of the field operators. Using (127) in the expression (135) we obtain

$$N_{op} = \sum_\sigma \int d^3r \hat{\psi}^+_\sigma(\mathbf{r})\hat{\psi}_\sigma(\mathbf{r})$$

As in the bosonic case this operator is the generator of the global $U(1)$ gauge transformation, the analogue of Eq. (67 for the fermion field

$$\hat{\psi}_\sigma(\mathbf{r}) \;\to\; e^{i\alpha}\hat{\psi}_\sigma(\mathbf{r}) \quad , \quad \hat{\psi}^+_\sigma(\mathbf{r}) \;\to\; e^{-i\alpha}\hat{\psi}^+_\sigma(\mathbf{r}) \tag{136}$$

It is indeed easy to check that "despite" the anticommutation relations for the fermion field operators the relation Eq. (69) holds for each spin component

$$[N_{op}, \hat{\psi}_\sigma(\mathbf{r})] = -\hat{\psi}_\sigma(\mathbf{r})$$

and therefore so is the corresponding generalization of Eq. (68)

$$e^{-i\alpha N_{op}}\hat{\psi}_\sigma(\mathbf{r})e^{i\alpha N_{op}} = e^{i\alpha}\hat{\psi}_\sigma(\mathbf{r}) \;\; , \;\; e^{-i\alpha N_{op}}\hat{\psi}^+_\sigma(\mathbf{r})e^{i\alpha N_{op}} = e^{-i\alpha}\hat{\psi}^+_\sigma(\mathbf{r})$$

Since the Hamiltonian Eq. (123) is invariant under this transformation it commutes with N_{op}.

5.2.6 Working with the fermion field operators

The expression for the particle number operator shows that

$$\hat{\rho}_\sigma(\mathbf{r}) = \hat{\psi}^+_\sigma(\mathbf{r})\hat{\psi}_\sigma(\mathbf{r})$$

is the density operator of particles with the spin projection σ. Let us consider a state

$$|\mathbf{r}, \sigma\rangle \equiv \hat{\psi}^+_\sigma(\mathbf{r})|0\rangle \tag{137}$$

and let us act on it with the operator $\hat{\rho}_{\sigma'}(\mathbf{r}')$. Using the anticommutation relations (117) to commute $\hat{\psi}_{\sigma'}(\mathbf{r}')$ towards $|0\rangle$ and using Eq. (116) we find

$$\hat{\rho}_{\sigma'}(\mathbf{r}')|\mathbf{r}, \sigma\rangle = \hat{\psi}^+_{\sigma'}(\mathbf{r}')\hat{\psi}_{\sigma'}(\mathbf{r}')\hat{\psi}^+_\sigma(\mathbf{r})|0\rangle = \delta_{\sigma\sigma'}\delta(\mathbf{r}-\mathbf{r}')\hat{\psi}^+_{\sigma'}(\mathbf{r}')|0\rangle = \delta_{\sigma\sigma'}\delta(\mathbf{r}-\mathbf{r}')|\mathbf{r}, \sigma\rangle \tag{138}$$

which shows that $\hat{\psi}^+_\sigma(\mathbf{r})$ creates a particle at the position $\mathbf{r}$ with spin projection σ. More precisely it creates delta like particle density of particles with spin projection σ at this position.

Continuing as we did in the boson case let us consider the state

$$|\mathbf{r}_1\sigma_1,\dots,\mathbf{r}_N\sigma_N\rangle = const_N\,\hat{\psi}^+_{\sigma_1}(\mathbf{r}_1)\dots\hat{\psi}^+_{\sigma_N}(\mathbf{r}_N)|0\rangle \tag{139}$$

where we introduced a multiplicative constant for normalization, see below. Acting on this state with the operator $\hat{\psi}_\sigma(\mathbf{r})$, commuting it towards $|0\rangle$ and using Eq. (116) we get

$$\hat{\psi}_\sigma(\mathbf{r})|\mathbf{r}_1\sigma_1,\dots,\mathbf{r}_N\sigma_N\rangle = const_N\sum_{a=1}^{N}(-1)^{P_a}\delta_{\sigma\sigma_a}\delta(\mathbf{r}-\mathbf{r}_a)\prod_{b\neq a}^{N}\hat{\psi}^+_{\sigma_b}(\mathbf{r}_b)|0\rangle \tag{140}$$

where P_a is the parity of the number of permutations one needs to make in order to move $\hat{\psi}_\sigma(\mathbf{r})$ to the right of $\hat{\psi}^+_{\sigma_a}(\mathbf{r}_a)$. The result (140) means that $\hat{\psi}_\sigma(\mathbf{r})$ destroys (annihilates) one particle if its coordinates coincide with $\mathbf{r}$ and its spin projection with σ. In doing this it also changes the sign of the resulting part of the wave function if the permutation number P_a is odd. In this way it's action is sensitive to the order of the destroyed particle in the wave function.

We can use the above result to act on the state (139) with the operator $\hat{\rho}_\sigma(\mathbf{r})$. We obtain in the same manner as in the boson case (cf., Eq.(76))

$$\hat{\rho}_\sigma(\mathbf{r})|\mathbf{r}_1,\dots,\mathbf{r}_N\rangle = [\sum_{a=1}^{N}\delta_{\sigma\sigma_a}\delta(\mathbf{r}-\mathbf{r}_a)]|\mathbf{r}_1,\dots,\mathbf{r}_N\rangle$$

showing that this state describes N particles (delta like particle densities) with spin projections σ_a at the positions $\mathbf{r}_a,\ a=1,\dots,N$.

5.3 Relation to the first quantization

In this Section we follow a similar development as in the boson case but with the additional spin index in the field operators and anti-commutation instead of the commutation relations.

5.3.1 The wave functions

Consider the fermionic version of the N particles wave function in the second quantization

$$|\Phi\rangle = \frac{1}{\sqrt{N!}}\sum_{\sigma_1,\dots\sigma_N}\int\prod_{a=1}^{N}d^3r_a\;\Phi(\mathbf{r}_1\sigma_1,\mathbf{r}_2\sigma_2,\dots,\mathbf{r}_N\sigma_N)\hat{\psi}^+_{\sigma_1}(\mathbf{r}_1)\dots\hat{\psi}^+_{\sigma_N}(\mathbf{r}_N)|0\rangle \tag{141}$$

The interpretation of this expression is quite clear - we have a linear combination of N particles in positions $\mathbf{r}_1, \ldots, \mathbf{r}_N$ with spin projections $\sigma_1, ..., \sigma_N$ weighted each by the probability amplitude $\Phi(\mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2, \ldots, \mathbf{r}_N\sigma_N)$. The anticommutation of $\hat{\psi}^+_\sigma(\mathbf{r})$'s assures that this amplitude is antisymmetric with respect to the exchange of any pair of $(\mathbf{r}, \sigma)$'s[7]. This amplitude is clearly the first quantization partner of the wave function $|\Phi\rangle$

As in the bosonic case the normalization of $|\Phi\rangle$ assures that it is normalized, i.e. $\langle\Phi|\Phi\rangle = 1$ provided the amplitude $\Phi(\mathbf{r}_1\sigma_1, \ldots, \mathbf{r}_N\sigma_N)$ is

$$\sum_{\sigma_1,\ldots,\sigma_N} \int \prod_{a=1}^{N} d^3r_a |\Phi(\mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2, \ldots, \mathbf{r}_N\sigma_N)|^2 = 1$$

In the arbitrary single particle basis $u_i(\mathbf{r}, \sigma)$ the above wave function looks exactly as in the boson case

$$|\Phi\rangle = \sum_{i_1,\ldots,i_N} C_{i_1,\ldots,i_N} \hat{a}^+_{i_1} \ldots \hat{a}^+_{i_N}|0\rangle \tag{142}$$

with the "only" difference that the operators $\hat{a}^+_i$'s are anticommuting.

As in the bosonic case it is useful and practical to work with the wave functions in the **occupation number representation**, cf., Eq (84),

$$|\Phi\rangle = \sum_{n_1,\ldots,n_i,\ldots;\text{with } n_i=0 \text{ or } 1\,,\, \sum_i n_i=N} C_{n_1,\ldots,n_i,\ldots}|n_1, n_1, \ldots, n_i, \ldots\rangle \tag{143}$$

with the "only" difference that the fermionic occupations n_i's are restricted to be zero or one.

5.3.2 The operators

As in the bosonic case the operators in the 1st quantized formulation of fermions are classified as one-body, two-body, etc.

One body operators

To remind - these operators act on wave functions of identical particles one particle at a time and have a general form given by the expression (93). The difference in the present fermion case is that each $f^{(1)}_a$ operator in addition to being a function of $\mathbf{r}_a$, $\hat{\mathbf{p}}_a = -i\hbar\nabla_a$ may also depend on the spin matrices $\mathbf{s}_a$. This means that in general $f^{(1)}_a$'s are 2×2 spinor matrices with matrix elements depending on $\mathbf{r}_a$ and $\hat{\mathbf{p}}_a$, cf., the example of $h_{\sigma\sigma'}$ in Eq.(118).

[7] As was already discussed in the bosonic case one can prove that any permutation of N objects can be achieved by a an ordered "product" (sequence) of pairwise transpositions.

In a very similar way as in the bosonic case one can show (cf., Appendix 7.4) that in the second quantization one body operators have the form

$$F_{op}^{(1)} = \sum_{\sigma\sigma'} \int d^3r \hat{\psi}_{\sigma'}^{+}(\mathbf{r}) f_{\sigma'\sigma}^{(1)} \hat{\psi}_{\sigma}(\mathbf{r}) \tag{144}$$

where $f_{\sigma\sigma'}^{(1)}$ is one (any) of the operators in the sum (93) generalized to include the spin dependence. It is acting on $\hat{\psi}_{\sigma}(\mathbf{r})$ as a spinor function of $\mathbf{r}$. The expression (123) for the Hamiltonian in an external potential provides a good example of such an operator.

Two body operators

The two body operators for identical particles with spins in the 1st quantization have the same form (102) as in the bosonic case but with the elementary operators $f_{ab}^{(2)}$ in general depending in addition to $\mathbf{r}_a, \mathbf{r}_b, \hat{\mathbf{p}}_a$ and $\hat{\mathbf{p}}_b$ also on the spin matrices $\mathbf{s}_a, \mathbf{s}_b$. An example is given by the so called spin exchange term in a (phenomenological) two particle interaction

$$\frac{1}{2} \sum_{a,b=1;a\neq b}^{N} \left[V(\mathbf{r}_a - \mathbf{r}_b) + W(\mathbf{r}_a - \mathbf{r}_b)\left(\hat{\mathbf{s}}_a \cdot \hat{\mathbf{s}}_b\right)\right]$$

For simplicity we will consider only spin independent $f_{ab}^{(2)}$. One can show that such two body operators in the fermionic 2nd quantization have a form similar to the bosonic expression (103) with the addition of the spin indices in the field operators

$$F_{op}^{(2)} = \frac{1}{2} \sum_{\sigma\sigma'} \int d^3r d^3r' \hat{\psi}_{\sigma}^{+}(\mathbf{r}) \hat{\psi}_{\sigma'}^{+}(\mathbf{r}') f^{(2)} \hat{\psi}_{\sigma'}(\mathbf{r}') \hat{\psi}_{\sigma}(\mathbf{r})$$

with $f^{(2)}$ being a function of $\mathbf{r}, \mathbf{r}'$ and $\hat{\mathbf{p}} = -i\hbar\nabla_{\mathbf{r}}, \hat{\mathbf{p}'} = -i\hbar\nabla_{\mathbf{r}'}$ [8]. Note the relative order of the field operators. Since they anticommute it is important to keep it.

[8]The general spin dependent two body $F_{op}^{(2)}$ will have the pairwise $f^{(2)}$'s depending in addition on the spin operators $\hat{\mathbf{s}}, \hat{\mathbf{s}'}$ of the particles' pairs. This means they will be four index matrices $f_{\sigma\sigma',\sigma"\sigma'''}^{(2)}$ and the expression for $F_{op}^{(2)}$ will be

$$F_{op}^{(2)} = \frac{1}{2} \sum_{\sigma\sigma'\sigma''\sigma'''} \int d^3r d^3r' \hat{\psi}_{\sigma}^{+}(\mathbf{r}) \hat{\psi}_{\sigma'}^{+}(\mathbf{r}') f_{\sigma\sigma',\sigma''\sigma'''}^{(2)} \hat{\psi}_{\sigma'''}(\mathbf{r}') \hat{\psi}_{\sigma''}(\mathbf{r})$$

with the corresponding generalization of the expression (145)

$$\langle ij|f^{(2)}|kl\rangle = \sum_{\sigma\sigma'\sigma''\sigma'''} \int d^3r d^3r' u_i^*(\mathbf{r},\sigma) u_j^*(\mathbf{r}',\sigma') f_{\sigma\sigma',\sigma''\sigma'''}^{(2)} u_k(\mathbf{r},\sigma'') u_l(\mathbf{r}',\sigma''')$$

General single particle basis

To obtain the expression for $F_{op}^{(1)}$ and $F_{op}^{(2)}$ in a general basis $u_i(\mathbf{r},\sigma)$ one just has to expand the field operators in their expressions in this basis, cf., Eq.(126). The result has identical form to the bosonic expressions (105) and (106) but the matrix elements have spin summations in addition to space coordinates integrals

$$\begin{aligned}
\langle i|f^{(1)}|j\rangle &= \sum_{\sigma\sigma'}\int d^3r u_i^*(\mathbf{r},\sigma')f^{(1)}_{\sigma'\sigma}u_j(\mathbf{r},\sigma) \\
\langle ij|f^{(2)}|kl\rangle &= \sum_{\sigma\sigma'}\int d^3rd^3r'u_i^*(\mathbf{r},\sigma)u_j^*(\mathbf{r}',\sigma')f^{(2)}u_k(\mathbf{r},\sigma)u_l(\mathbf{r}',\sigma') \qquad (145)
\end{aligned}$$

where for the two-body operator we write only for the simple (but very common) case of the spin independent $f^{(2)}$.

5.4 Interacting fermions

5.4.1 Hamiltonian

The most common Hamiltonian of interacting fermions has the form

$$\begin{aligned}
H_{op} &= \sum_{\sigma\sigma'}\int d^3r\hat{\psi}^+_{\sigma'}(\mathbf{r})\,h_{\sigma'\sigma}\,\hat{\psi}_\sigma(\mathbf{r}) + \qquad (146) \\
&\quad +\frac{1}{2}\sum_{\sigma\sigma'}\int d^3rd^3r'\hat{\psi}^+_\sigma(\mathbf{r})\hat{\psi}^+_{\sigma'}(\mathbf{r}')V(\mathbf{r}-\mathbf{r}')\hat{\psi}_{\sigma'}(\mathbf{r}')\hat{\psi}_\sigma(\mathbf{r})
\end{aligned}$$

with

$$h_{\sigma'\sigma} = -\delta_{\sigma'\sigma}\frac{\hbar^2}{2m}\nabla^2 + U_{\sigma'\sigma}(\mathbf{r})$$

and a spin independent two body interaction. In a general single particle basis this Hamiltonian is

$$H_{op} = \sum_{ij}\langle i|\,h\,|j\rangle\hat{a}_i^+\hat{a}_j + \frac{1}{2}\sum_{ijkl}\langle ij|V|kl\rangle\hat{a}_i^+\hat{a}_j^+\hat{a}_l\hat{a}_k \qquad (147)$$

As in the boson case if the solutions of the non interacting part are known, i.e. if one knows the eigenfunctions of the single particle Hamiltonian h, cf. Eq. (124) (e.g. Coulomb wave functions in atoms) one can use the operators $\hat{a}_i^+$, $\hat{a}_j$ in this basis. The matrix $\langle i|\,h\,|j\rangle$ is then diagonal making the first term in H_{op} trivial

$$H_{op} = \sum_i \epsilon_i\hat{a}_i^+\hat{a}_i + \frac{1}{2}\sum_{ijkl}\langle ij|V|kl\rangle\hat{a}_i^+\hat{a}_j^+\hat{a}_l\hat{a}_k \qquad (148)$$

and helping to "focus attention" on the particle interactions.

5.4.2 Heisenberg equations. No classical limit

Despite anticommutation relations of the fermion field operators $\hat{\psi}_\sigma(\mathbf{r})$ and $\hat{\psi}^+_\sigma(\mathbf{r})$ the Heisenberg equations for these operators

$$i\hbar\frac{\partial}{\partial t}\left(\begin{array}{c}\hat{\psi}_\sigma(\mathbf{r},t)\\ \hat{\psi}^+_\sigma(\mathbf{r},t)\end{array}\right)=\left[\left(\begin{array}{c}\hat{\psi}_\sigma(\mathbf{r},t)\\ \hat{\psi}^+_\sigma(\mathbf{r},t)\end{array}\right),H_{op}\right]$$

for the general interacting Hamiltonian (146) have the same formal appearance as for bosons apart of the presence of the spin indices. It is a useful exercise for the reader to work this out explicitly. The equation for $\hat{\psi}_\sigma(\mathbf{r})$ is

$$i\hbar\frac{\partial\hat{\psi}_\sigma(\mathbf{r},t)}{\partial t}=\sum_{\sigma'}h_{\sigma\sigma'}\hat{\psi}_{\sigma'}(\mathbf{r},t)+\int V(\mathbf{r}-\mathbf{r}')\sum_{\sigma'}\hat{\psi}^+_{\sigma'}(\mathbf{r}',t)\hat{\psi}_{\sigma'}(\mathbf{r}',t)d^3r'\,\hat{\psi}_\sigma(\mathbf{r},t) \quad (149)$$

and the Hermitian conjugate of this equation for $\hat{\psi}^+_\sigma(\mathbf{r},t)$. We note that unlike the boson case these equations do not have classical limit. This for the obvious reason that Pauli principle and formally the anti commutation relations of the field operators prevent having more than one fermion in any given field mode[9].

5.4.3 Mean field approximation

Let us assume for simplicity the spin independent $U(\mathbf{r})$) and write the Heisenberg equation (149) in the following form

$$i\hbar\frac{\partial\hat{\psi}_\sigma(\mathbf{r},t)}{\partial t}=\left[-\frac{\hbar^2}{2m}\nabla^2+U(\mathbf{r})+\int V(\mathbf{r}-\mathbf{r}')\hat{\rho}(\mathbf{r}',t)d^3r'\right]\hat{\psi}_\sigma(\mathbf{r},t) \quad (150)$$

with

$$\hat{\rho}(\mathbf{r},t)=\sum_\sigma\hat{\psi}^+_\sigma(\mathbf{r},t)\hat{\psi}_\sigma(\mathbf{r},t)$$

[9]The so called anticommuting c-numbers (Grassman variables) are often related to the classical limit of fermionic second quantized operators. In a very crude way they are obtained by setting to zero all the anticommutators in Eq. (117),

$$\{\hat{\psi}_\sigma(\mathbf{r}),\hat{\psi}^+_{\sigma'}(\mathbf{r}')\}=\{\hat{\psi}_\sigma(\mathbf{r}),\hat{\psi}_{\sigma'}(\mathbf{r}')\}=\{\hat{\psi}^+_\sigma(\mathbf{r})\,\hat{\psi}^+_{\sigma'}(\mathbf{r}')\}=0$$

This is in (again a crude) analogy with the classical limit of the bosonic case in which all the canonical commutators vanish, cf., Berezin, F. A., "The Method of Second Quantization," Academic Press, 1965.

The Grassman variables are most often used in constructing functional integrals for femionic systems, cf., Negele, J. W., and Orland, H., "Quantum Many-Particle Systems," Perseus Books Group, 1998, pp.25-37

The potential $U(\mathbf{r})$ in these equations is formally modified by the last term which is a convolution of the two body interaction $V(\mathbf{r}-\mathbf{r}')$ and the operator of the particle density $\hat{\rho}(\mathbf{r}',t)$. For a classical particle density function $\rho(\mathbf{r},t)$ this term would have a natural meaning of the potential which the particles of the system induce[10]. In quantum mechanic context one can qualitatively think of $\hat{\rho}(\mathbf{r},t)$ as a random variable the probability amplitude distribution of which is determined by the wave function $|\Phi\rangle$ of the many fermion system under consideration.

Given $|\Phi\rangle$ one can write

$$\hat{\rho}(\mathbf{r}) = \langle\Phi|\hat{\rho}(\mathbf{r})|\Phi\rangle + \delta\hat{\rho}(\mathbf{r})$$

separating the average and the fluctuations of $\hat{\rho}(\mathbf{r},t)$. It is natural to ask if neglecting the fluctuations would be a good approximation. This would certainly greatly simplify the problem. It would also be in line with similar approximations known in other fields under the name "mean field approximation"[10]. In the many-fermion systems such mean field approximations were first introduced in atomic physics by Hartree and then supplemented by Fock to result in the Hatree-Fock method. We will address these developments in a separate chapter. Mean mean approximation and its extensions play a very important role in theoretical treatment of such many fermion systems as atoms, nuclei and solids.

6 The Fock space.

In the first quantization formalism we encountered the notion of the Hilbert space. For N particles this was the space of all functions of N variables

$$\begin{aligned}
&\Phi(x_1, x_2, ..., x_N) \qquad \text{with} \\
&x_a = \mathbf{r}_a \ , \ a = 1, ..., N, \ \text{symmetrized for spinless bosons} \ , \\
&x_a = \mathbf{r}_a, \sigma_a \ , \ a = 1, ..., N, \ \text{antisymmetrized for fermions}
\end{aligned}$$

The operators acting on such functions didn't change the particle number N. The situation is different in the second quantization formulation. Here already the most

[10] There is an important aspect which must be addressed first. This is related to the fact that $\hat{\rho}(\mathbf{r},t)$ and therefore its average includes all the particles in the system while the mean field potential acting on any given particle

$$\int V(\mathbf{r}-\mathbf{r}')\rho(\mathbf{r}',t)d^3r'$$

must exclude this particular particle. This problem is elegantly solved in the Hartree-Fock method described in the Mean Field Approximations chapter elementary operators $\hat{\psi}(\mathbf{r})$, $\hat{\psi}^{+}(\mathbf{r})$, $\hat{a}_i$, $\hat{a}_i^+$, etc., change the particle number and the most general wave function should be a linear combination of functions like Φ_N with different N's and including the vacuum

$$\begin{aligned}|\Phi\rangle &= C^{(0)}|0\rangle + \sum_i C_i^{(1)} \hat{a}_i^+|0\rangle + \sum_{ij} C_{ij}^{(2)} \hat{a}_i^+ \hat{a}_j^+|0\rangle + ... + \\ &+ \sum_{i_1 i_2 ..} C^{(2)}_{i_1 i_2 ... i_N} \hat{a}^+_{i_1} \hat{a}^+_{i_2} ... \hat{a}^+_{i_N}|0\rangle + ...\end{aligned} \tag{151}$$

The Hilbert space of all such functions is called the Fock space and is a direct sum

$$\begin{aligned}&(\text{vacuum}) \bigoplus (\text{1 particle Hilbert space}) \bigoplus (\text{2 particle Hilbert space}) \bigoplus \ ... \\ &... \bigoplus (\text{N particle Hilbert space}) \bigoplus \ ...\end{aligned} \tag{152}$$

7 Appendix

7.1 Bosons - reviewing the properties of $\hat{a}$' s and $\hat{a}^+$'s

7.1.1 The vacuum state

Let us defined a special state denoted $|0\rangle$. We shall call this state a vacuum state. The only properties we will ever need of this state are that it gives zero when acted upon with anyone of the operators $\hat{a}_i$ and that it is normalized

$$\begin{aligned}\hat{a}_i|0\rangle &= 0 \quad i = 1, 2, ... \\ \langle 0|0\rangle &= 1\end{aligned} \tag{153}$$

7.1.2 Single mode

We start by considering the pair $\hat{a}_i, \hat{a}_i^+$ of operators with a fixed index i. We will call them operators of a single mode $u_i(\mathbf{r})$. We then define the state (following an analogy with the oscillator ladder operators)

$$|1_i\rangle \equiv \hat{a}_i^+|0\rangle \tag{154}$$

As is easy to see this state is normalized. Indeed using the commutation relations and the properties of $|0\rangle$ find

$$\langle 1_i|1_i\rangle = \langle 0|\hat{a}_i \hat{a}_i^+|0\rangle = \langle 0|1 + \hat{a}_i^+ \hat{a}_i|0\rangle = \langle 0|0\rangle = 1$$

Also have orthogonality

$$\langle 1_i|0\rangle = \langle 0|\hat{a}_i|0\rangle = 0$$

In the same way we define

$$|2_i\rangle = \text{const}\ \hat{a}_i^+|1_i\rangle = \frac{1}{\sqrt{2}}\ \hat{a}_i^+|1_i\rangle \tag{155}$$

The normalization constant is found as $const = 1/\sqrt{2}$ by calculating the norm

$$\begin{aligned}\langle 2_i|2_i\rangle &= |const|^2\langle 1_i|\hat{a}_i\hat{a}_i^+|1_i\rangle = |const|^2\langle 1_i|\hat{a}_i\hat{a}_i^+\hat{a}_i^+|0\rangle = \\ &= |const|^2\langle 1_i|(1+\hat{a}_i^+\hat{a}_i)\hat{a}_i^+|0\rangle = |const|^2[\langle 1_i|\hat{a}_i^+|0\rangle + \\ &+ \langle 1_i|\hat{a}_i^+(1+\hat{a}_i^+\hat{a}_i)|0\rangle] = 2|const|^2\langle 1_i|1_1\rangle = 2|const|^2\end{aligned}$$

We have orthogonality

$$\langle 2_i|1_i\rangle = \frac{1}{\sqrt{2}}\langle 1_i|\hat{a}_i|1_i\rangle = \frac{1}{\sqrt{2}}\langle 1_i|\hat{a}_i\hat{a}_i^+|0_i\rangle = \frac{1}{\sqrt{2}}\langle 1_i|1+\hat{a}_i^+\hat{a}_i|0_i\rangle = \frac{1}{\sqrt{2}}\langle 1_i|0_i\rangle = 0$$

and even more trivially

$$\langle 2_i|0_i\rangle = \frac{1}{\sqrt{2}}\langle 1_i|\hat{a}_i|0\rangle = 0$$

By iterating we define

$$|n_i\rangle = \frac{1}{\sqrt{n_i}}\hat{a}_i^+|n_i-1\rangle = \frac{1}{\sqrt{n_i(n_i-1)}}(\hat{a}_i^+)^2|n_i-2\rangle = \ldots = \frac{1}{\sqrt{n_i!}}(\hat{a}_i^+)^{n_i}|0\rangle \tag{156}$$

One can prove that the resulting states $|n_i\rangle$ form orthogonal set

$$\langle m_i|n_i\rangle = 0 \quad \text{for} \quad m_i \neq n_i$$

Indeed writing

$$\langle m_i|n_i\rangle = \frac{1}{\sqrt{m_i n_i}}\langle 0|(\hat{a}_i)^{m_i}(\hat{a}_i^+)^{n_i}|0\rangle$$

and commuting each $\hat{a}_i$'s to the right all the way to $|0\rangle$ one proves this to vanish for $m_i \neq n_i$.

We also have

$$\begin{aligned}\hat{a}_i^+|n_i\rangle &= \hat{a}_i^+\frac{1}{\sqrt{n_i!}}(\hat{a}_i^+)^{n_i}|0\rangle = \sqrt{n_i+1}\frac{1}{\sqrt{(n_i+1)!}}(\hat{a}_i^+)^{n_i+1}|0\rangle \\ \hat{a}_i|n_i\rangle &= \hat{a}_i\frac{1}{\sqrt{n_i!}}(\hat{a}_i^+)^{n_i}|0\rangle = n_i\frac{1}{\sqrt{n_i!}}(\hat{a}_i^+)^{n_i-1}|0\rangle = \sqrt{n_i}\frac{1}{\sqrt{(n_i-1)!}}(\hat{a}_i^+)^{n_i-1}|0\rangle\end{aligned}$$

where the factor n_i in the second equality of the second line results from commuting $\hat{a}_i$ through n operators in $(\hat{a}_i^+)^{n_i}$ to get it acting on $|0\rangle$. The above calculation shows that

$$\hat{a}_i^+|n_i\rangle = \sqrt{n_i+1}|n_i+1\rangle \quad , \quad \hat{a}_i|n_i\rangle = \sqrt{n_i}|n_i-1\rangle \tag{157}$$

Note also that by hermitian conjugation

$$\langle n_i|\hat{a}_i = \sqrt{n_i+1}\langle n_i+1| \quad , \quad \langle n_i|\hat{a}_i^+ = \sqrt{n_i}\langle n_i-1| \tag{158}$$

The last two sets of equalities define the action of the operators $\hat{a}_i$ and $\hat{a}_i^+$ on any state "belonging" to the mode $u_i(\mathbf{r})$. Indeed for any such state $|\xi_i\rangle$ we can determine the result of acting on it with $\hat{a}_i$ or $\hat{a}_i^+$ by writing it as a linear combination $|\xi_i\rangle = \sum_{n_i} c_{n_i}|n_i\rangle$ of the basis states $|n_i\rangle$.

Let us now consider the operator $\hat{n}_i = \hat{a}_i^+\hat{a}_i$. The basis states $|n_i\rangle$, Eq. (156) are its eigenstates

$$\hat{n}_i|n_i\rangle = \hat{a}_i^+\hat{a}_i|n_i\rangle = \sqrt{n_i}\,\hat{a}_i^+|n_i-1\rangle = n_i|n_i\rangle \tag{159}$$

This operator is the i-th mode number operator.

7.1.3 Many modes

We now generalize the above single mode construction to all modes of the complete set $u_i(\mathbf{r})$. This is easily done mostly because pairs of $\hat{a}_i$ and $\hat{a}_i^+$ commute for different i's. The general multimode analogue of the states $|n_i\rangle$ is

$$|\{n_i\}\rangle \equiv |n_1, n_2, \ldots, n_k, \ldots\rangle = \prod_i |n_i\rangle = \prod_i \frac{1}{\sqrt{n_i!}}(\hat{a}_i^+)^{n_i}|0\rangle \tag{160}$$

The operators $\hat{a}_i$ and $\hat{a}_i^+$ act on these states as

$$\begin{aligned} \hat{a}_i^+|n_1, \ldots, n_i, \ldots\rangle &= \sqrt{n_i+1}|n_1, \ldots, n_i+1, \ldots\rangle \\ \hat{a}_i|n_1, \ldots, n_i, \ldots\rangle &= \sqrt{n_i}\,|n_1, \ldots, n_i-1, \ldots\rangle \end{aligned} \tag{161}$$

and have number operators for all modes

$$\hat{n}_i|n_1, \ldots, n_i, \ldots\rangle = \hat{a}_i^+\hat{a}_i|n_1, \ldots, n_i, \ldots\rangle = n_i|n_1, \ldots, n_i, \ldots\rangle \tag{162}$$

It is useful and important to introduce the total particle number operator

$$N_{op} = \sum_i \hat{n}_i = \sum_i \hat{a}_i^+\hat{a}_i \tag{163}$$

which "measures" the sum of all n_i's

$$N_{op}|n_1, n_2, \ldots, n_i, \ldots\rangle = \left(\sum_i n_i\right)|n_1, n_2, \ldots, n_i, \ldots\rangle \tag{164}$$

7.2 Bosons - wave function normalization

Let us consider the norm of the wave function Eq. (79)

$$\begin{aligned}\langle\Phi|\Phi\rangle &= \qquad\qquad (165)\\ &= \int\int\prod_{a,b=1}^{N} d^3r_a d^3r'_b\ \Phi^*(\mathbf{r}'_1,\mathbf{r}'_2,\ldots,\mathbf{r}'_N)\Phi(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N)\langle\mathbf{r}'_1,\ldots,\mathbf{r}'_N|\mathbf{r}_1,\ldots,\mathbf{r}_N\rangle\end{aligned}$$

We need to evaluate the overlap $\langle\mathbf{r}'_1,\ldots,\mathbf{r}'_N|\mathbf{r}_1,\ldots,\mathbf{r}_N\rangle$. In a straightforward way by commuting $\hat{\psi}(\mathbf{r}'_a)$'s to the right all the way to the vacuum state $|0\rangle$ we obtain

$$\begin{aligned}\langle\mathbf{r}'_1,\ldots,\mathbf{r}'_N|\mathbf{r}_1,\ldots,\mathbf{r}_N\rangle &= |const_N|^2\langle 0|\hat{\psi}(\mathbf{r}'_N),\ldots\hat{\psi}(\mathbf{r}'_1)\hat{\psi}^+(\mathbf{r}_1)\ldots\hat{\psi}^+(\mathbf{r}_N)|0\rangle =\\ &= |const_N|^2\langle 0|\hat{\psi}(\mathbf{r}'_N),\ldots\hat{\psi}(\mathbf{r}'_2)\sum_{a=1}^{N}\delta(\mathbf{r}'_1-\mathbf{r}_a)\prod_{b\neq a}^{N}\hat{\psi}^+(\mathbf{r}_b)|0\rangle =\\ &= |const_N|^2\langle 0|\hat{\psi}(\mathbf{r}'_N),\ldots\hat{\psi}(\mathbf{r}'_3)\sum_{a=1}^{N}\delta(\mathbf{r}'_1-\mathbf{r}_a)\sum_{b=1,b\neq a}^{N}\delta(\mathbf{r}'_2-\mathbf{r}_b)\prod_{c=1,c\neq a,b}^{N}\hat{\psi}^+(\mathbf{r}_c)|0\rangle =\\ &= \ldots = |const_N|^2\sum_{a=1}^{N}\delta(\mathbf{r}'_1-\mathbf{r}_a)\sum_{b=1,b\neq a}^{N}\delta(\mathbf{r}'_2-\mathbf{r}_b)\sum_{d=1,d\neq a,b,c}^{N}\delta(\mathbf{r}'_3-\mathbf{r}_d)..\langle 0|0\rangle =\\ &= |const_N|^2\sum_P\prod_{a=1}^{N}\delta(\mathbf{r}'_a-\mathbf{r}_{Pa}) \qquad\qquad (166)\end{aligned}$$

where P stands for permutations of the particle indices $a = 1, 2, .., N$. There are $N!$ permutations of N indices and therefore $N!$ terms in the last sum.

Using this result in Eq. (165) one can use the delta functions to reduce the norm $\langle\Phi|\Phi\rangle$ to a sum of integrals

$$\langle\Phi|\Phi\rangle = |const_N|^2\sum_P\int\prod_{a=1}^{N} d^3r_a\Phi^*(\mathbf{r}_{P1},\mathbf{r}_{P2},\ldots,\mathbf{r}_{PN})\Phi(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N)$$

Since $\Phi(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N)$ is symmetric with respect to the permutations of its arguments the above $N!$ integrals are identical

$$\langle\Phi|\Phi\rangle = N!|const_N|^2\int\prod_{a=1}^{N} d^3r_a|\Phi(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N)|^2$$

which leads to the consistent normalization conditions to unity of both first and second quantization wave functions Eq. (80) for the choice of the const as

$$const_N = \frac{1}{\sqrt{N!}}$$

7.3 Bosons - calculating $K_{op}|\Phi\rangle$

As with $U_{op}|\Psi\rangle$ we start by considering

$$\int d^3r\ \hat{\psi}^+(\mathbf{r})\left(-\frac{\hbar^2}{2m}\nabla^2_{\mathbf{r}}\right)\hat{\psi}(\mathbf{r})\prod_{a=1}^{N}\hat{\psi}^+(\mathbf{r}_a)|0\rangle$$

Using in this expression the result (76) and

$$\nabla^2_{\mathbf{r}}\delta(\mathbf{r}-\mathbf{r}_b) = -\nabla_{\mathbf{r}}\nabla_{\mathbf{r}_b}\delta(\mathbf{r}-\mathbf{r}_b) = \nabla^2_{\mathbf{r}_b}\delta(\mathbf{r}-\mathbf{r}_b)$$

we get it in the form

$$\int d^3r\ \hat{\psi}^+(\mathbf{r})\left[\sum_{b=1}^{N}\left(-\frac{\hbar^2}{2m}\nabla^2_{\mathbf{r}_b}\right)\delta(\mathbf{r}-\mathbf{r}_b)\prod_{a\neq b}^{N}\hat{\psi}^+(\mathbf{r}_a)\right]|0\rangle$$

Therefore

$$K_{op}|\Phi\rangle = \frac{1}{\sqrt{N!}}\int\prod_{a=1}^{N}d^3r_a\Phi(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N)\int d^3r\ \hat{\psi}^+(\mathbf{r})\left(-\frac{\hbar^2}{2m}\nabla^2_{\mathbf{r}}\right)\hat{\psi}(\mathbf{r})\prod_{a=1}^{N}\hat{\psi}^+(\mathbf{r}_a)|0\rangle =$$

$$= \frac{1}{\sqrt{N!}}\int\prod_{a=1}^{N}d^3r_a\Phi(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N)\int d^3r\ \hat{\psi}^+(\mathbf{r})\left[\sum_{b=1}^{N}\left(-\frac{\hbar^2}{2m}\nabla^2_{\mathbf{r}_b}\right)\delta(\mathbf{r}-\mathbf{r}_b)\prod_{a\neq b}^{N}\hat{\psi}^+(\mathbf{r}_a)\right]|0\rangle =$$

$$= \frac{1}{\sqrt{N!}}\int d^3r\ \hat{\psi}^+(\mathbf{r})\int\prod_{a=1}^{N}d^3r_a\left[\sum_{b=1}^{N}\left(-\frac{\hbar^2}{2m}\nabla^2_{\mathbf{r}_b}\right)\Phi(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N)\delta(\mathbf{r}-\mathbf{r}_b)\prod_{a\neq b}^{N}\hat{\psi}^+(\mathbf{r}_a)\right]|0\rangle$$

in the last line we changed the order of integration and then did integration by parts (twice) to free the delta functions and transfer $\nabla^2_{\mathbf{r}_b}$ to act on $\Phi(\mathbf{r}_1,\ldots,\mathbf{r}_N)$.

Changing the order of integrations back again and using the delta functions we obtain

7.4 Fermions - calculating $F_{op}|\Phi\rangle$

Deriving the action of the operator $F^{(1)}_{op}$, Eq. (144) on the many fermion wave function Eq. (141) let us start by applying the part $\hat{\psi}^+_{\sigma'}(\mathbf{r})f^{(1)}_{\sigma'\sigma}$ of $F^{(1)}_{op}$ to the expression (140), with the result

$$const_N\sum_{a=1}^{N}f^{(1)}_{\sigma'\sigma}(\mathbf{r})\delta_{\sigma\sigma_a}\delta(\mathbf{r}-\mathbf{r}_a)\prod_{b<a}\hat{\psi}^+_{\sigma_b}(\mathbf{r}_b)\hat{\psi}^+_{\sigma'}(\mathbf{r})\prod_{b>a}\hat{\psi}^+_{\sigma_b}(\mathbf{r}_b)|0\rangle \tag{167}$$

Here we for simplicity assumed that $f^{(1)}_{\sigma'\sigma}$ is a function of $\mathbf{r}$ only so that we could bring $\hat{\psi}^+_{\sigma'}(\mathbf{r})$ "through it" and commute to where $\hat{\psi}^+_{\sigma_a}(\mathbf{r}_a)$ was. This commuting generated additional the factor $(-1)^{P_a}$ giving overall unity when combined with the same factor in Eq. (140). We note that for $f^{(1)}_{\sigma'\sigma}$ depending on $-i\hbar\nabla_{\mathbf{r}}$ one should use the intermediate integration by parts in analogy with what we did in the kinetic energy case with bosons, cf., Appendix 7.3.

To finish the calculation let us sum the result (167) over σ and σ' and integrate over $\mathbf{r}$. Using $\delta_{\sigma\sigma_a}$ to perform the sum over σ and $\delta(\mathbf{r}-\mathbf{r}_a)$ to do the integral we obtain

$$F^{(1)}_{op}\prod_{a=1}^{N}\hat{\psi}^+_{\sigma_a}(\mathbf{r}_a)|0\rangle = \sum_{a=1}^{N}\sum_{\sigma'} f^{(1)}_{\sigma'\sigma_a}(\mathbf{r}_a)\prod_{b<a}\hat{\psi}^+_{\sigma_b}(\mathbf{r}_b)\hat{\psi}^+_{\sigma'}(\mathbf{r}_a)\prod_{b>a}\hat{\psi}^+_{\sigma_b}(\mathbf{r}_b)|0\rangle$$

This gives

$$\begin{aligned}
F^{(1)}_{op}|\Phi\rangle &= \frac{1}{\sqrt{N!}}\sum_{\sigma_1,\ldots\sigma_N}\int\prod_{a=1}^{N} d^3r_a\ \Phi(\mathbf{r}_1\sigma_1,\mathbf{r}_2\sigma_2,\ldots,\mathbf{r}_N\sigma_N)F^{(1)}_{op}\prod_{a=1}^{N}\hat{\psi}^+_{\sigma_a}(\mathbf{r}_a)|0\rangle = \\
&= \frac{1}{\sqrt{N!}}\sum_{\sigma_1,\ldots\sigma_N}\int\prod_{b=1}^{N} d^3r_b\ \Phi(\mathbf{r}_1\sigma_1,\mathbf{r}_2\sigma_2,\ldots,\mathbf{r}_a\sigma_a,\ldots,\mathbf{r}_N\sigma_N)\times \\
&\qquad\times\sum_{a=1}^{N}\sum_{\sigma'} f^{(1)}_{\sigma'\sigma_a}(\mathbf{r}_a)\prod_{b<a}\hat{\psi}^+_{\sigma_b}(\mathbf{r}_b)\hat{\psi}^+_{\sigma'}(\mathbf{r}_a)\prod_{b>a}\hat{\psi}^+_{\sigma_b}(\mathbf{r}_b)|0\rangle = \\
&= \frac{1}{\sqrt{N!}}\sum_{\sigma_1,\ldots\sigma_N}\int\prod_{b=1}^{N} d^3r_b\ \sum_{a=1}^{N}\sum_{\sigma'} f^{(1)}_{\sigma_a\sigma'}(\mathbf{r}_a)\Phi(\mathbf{r}_1\sigma_1,\mathbf{r}_2\sigma_2,\ldots,\mathbf{r}_a\sigma',\ldots,\mathbf{r}_N\sigma_N)\times \\
&\qquad\times\prod_{b<a}\hat{\psi}^+_{\sigma_b}(\mathbf{r}_b)\hat{\psi}^+_{\sigma_a}(\mathbf{r}_a)\prod_{b>a}\hat{\psi}^+_{\sigma_b}(\mathbf{r}_b)|0\rangle
\end{aligned}$$

where after the last equality sign we have used the presence of sums over both σ_a and σ' and interchanged notation of their summation variables $\sigma_a \leftrightarrow \sigma'$. This finally gives

$$F^{(1)}_{op}|\Phi\rangle = \frac{1}{\sqrt{N!}}\sum_{\sigma_1,\ldots\sigma_N}\int\prod_{a=1}^{N} d^3r_a\ \Phi'(\mathbf{r}_1\sigma_1,\mathbf{r}_2\sigma_2,\ldots,\mathbf{r}_N\sigma_N)\prod_{a=1}^{N}\hat{\psi}^+_{\sigma_a}(\mathbf{r}_a)|0\rangle$$

with

$$\Phi'(\mathbf{r}_1\sigma_1,\mathbf{r}_2\sigma_2,\ldots,\mathbf{r}_N\sigma_N) = \left[\sum_{a=1}^{N}\sum_{\sigma'} f^{(1)}_{\sigma_a\sigma'}(\mathbf{r}_a)\right]\Phi(\mathbf{r}_1\sigma_1,\mathbf{r}_2\sigma_2,\ldots,\mathbf{r}_a\sigma',\ldots,\mathbf{r}_N\sigma_N)$$