UNIVERSITETET I STAVANGER
Institutt for matematikk og naturvitenskap

# Lecture notes for FYS610 Many particle Quantum Mechanics

**Note 5, 18.1 2018**

**Additions and comments to *Quantum Field Theory and the Standard Model* by Matthew D. Schwartz (2014)**

## Second quantization of bosons

Since it is impossible in quantum mechanics to distinguish *identical particles*, there is really no point of having a notation that keeps track of particle identities. In the following, we shall only consider non-interacting particles, which suffices to give us a suitable basis for the many-particle Hilbert space. This note is an extension of sec. 2.3 on *Schwartz*. Here, and in the following notes, we shall use units such that $\hbar = 1$ and $c = 1$, see appendix A.1 of *Schwartz*,

If we have $N$ non-interacting bosons, all in the same one-particle state $|\, i \,\rangle$, we can write the wavefunction for the entire system as:

$$\psi_{\underbrace{i,\, i,\, \ldots i}_{N}}(\mathbf{r}_1,\, \ldots \mathbf{r}_N) = \prod_{k=1}^{N} \psi_i(\mathbf{r}_k)\,, \tag{5.1}$$

where $\psi_i(\mathbf{r}_j) = \langle \mathbf{r}_j | i \rangle$ is a one-particle wavefunction. This is simple enough. But already if we have $n_1$ particles in state $|\, i \,\rangle$ and $n_2 = N - n_1$ in a different state $|\, j \,\rangle$, things start to get unwieldy, because if the particles are truly identical, we have no way of telling *which* particle is in which state. We therefore have to symmetrize the wavefunction over all possible permutations:

$$\psi_{\underbrace{i,\, \ldots i}_{n_1}\underbrace{j \ldots j}_{n_2}}(\mathbf{r}_1, \ldots \mathbf{r}_N) = \frac{1}{\binom{N}{n_1}} \left[ \prod_{k=1}^{n_1} \psi_i(\mathbf{r}_k) \prod_{l=n_1+1}^{N} \psi_j(\mathbf{r}_l) + (\text{permutations}) \right], \tag{5.2}$$

where $\binom{N}{n_1} = \frac{N!}{n_1! n_2!}$ is the number ow ways one can split $N$ particles into two groups of sizes $n_1$ and $n_2$. The permutations are only those where we interchange particles between the two groups. This construction can be further extended to states with particles in even more different states, but the expressions for the wavefunctions become increasingly unwieldy.

By using the Dirac formalism with some further conventions, we obtain a much more compact notation. To do that, we assume that the one-particle states are energy eigenstates of a single-particle Hamiltonian, $h$:

$$h|\, i \,\rangle = \epsilon_i |\, i \,\rangle\,. \tag{5.3}$$

Furthermore, the notation can be simplified if we assume that the single particle eigenstates are discrete, and are labelled by natural numbers such that:

$$\epsilon_1 \leq \epsilon_2 \leq \epsilon_3 \leq \ldots\,. \tag{5.4}$$

We then define the state:

$$|\, n_1, n_2, n_3, \dots\ n_i, \dots \rangle \tag{5.5}$$

as the state with $n_1$ bosons in the one-particle state $|\, 1 \rangle$, $n_2$ in the state $|\, 2 \rangle$, etc. The symmetry condition shall be assumed to be fulfilled per definition. The state of lowest energy, the *ground state*, or *vacuum*, is the state without any particles at all:

$$|\, 0 \rangle = |\, 0, 0, \dots \rangle\,. \tag{5.6}$$

It would be physically reasonable if the energy of this state would be $E_0 = 0$, but it will turn out that this is not always automatically the case, so we shall keep $E_0$. Since the particles are non-interacting, the energy of a state with $n_1$ particles in the state $|\, 1 \rangle$, $n_2$ in $|\, 2 \rangle$ etc. is clearly:

$$E_{n_1,n_2,\dots} = E_0 + n_1\epsilon_1 + n_2\epsilon_2 + \dots\,, \tag{5.7}$$

Obviously, $E \to \infty$ if the number of particles, $N = \sum_i n_i \to \infty$, so states with infinitely many particles are not physically realizable. Since the energy of any physical state is the eigenvalue of the many-particle Hamiltonian, $H$, we have:

$$H\,|\, n_1, n_2, \dots \rangle = E_{n_1,n_2,\dots}|\, n_1, n_2, \dots \rangle\,. \tag{5.8}$$

We can now adapt the construction of *creation* and *annihilation* operators from the end of note 4, with one important difference: We introduce a separate pair of these operators for *each* one-particle state $|\, i \rangle$. They have matrix elements in the many-particle basis analogous to eq. (4.16a):

$$\langle m_1, m_2, \dots\ m_i, \dots |a_i^\dagger|\, n_1, n_2, \dots\ n_i, \dots \rangle = \sqrt{n_i + 1}\,\delta_{m_1,n_1}\delta_{m_2,n_2}\dots\delta_{m_i,n_i+1}\dots\,. \tag{4.16$'a$}$$

Thus $a_i^\dagger$ leaves all particles in states $|\, j \rangle \neq |\, i \rangle$ unchanged. This definition leads to:

$$\begin{aligned} &a_i^\dagger|\, n_1, n_2, \dots\ n_i, \dots \rangle \\ &\quad= \sum_{m_1,m_2,\dots} |\, m_1, m_2, \dots\ m_i, \dots \rangle\langle m_1, m_2, \dots\ m_i, \dots |a_i^\dagger|\, n_1, n_2, \dots\ n_i, \dots \rangle \\ &\quad= \sqrt{n_i + 1}\,|\, n_1, n_2, \dots\ n_i + 1, \dots \rangle\,. \end{aligned} \tag{4.16$'b$}$$

The matrix element of $a_i$ follows in a similar manner:

$$\begin{aligned} \langle m_1, m_2, \dots\ m_i, \dots |a_i|\, n_1, n_2, \dots\ n_i, \dots \rangle &= \sqrt{n_i}\,\delta_{m_1,n_1}\delta_{m_2,n_2}\dots\delta_{m_i,n_i-1}\dots \\ a_i|\, n_1, n_2, \dots\ n_i, \dots \rangle &= \sqrt{n_i}\,|\, n_1, n_2, \dots\ n_i - 1, \dots \rangle\,. \end{aligned} \tag{4.17$'$}$$

With $N_i = a_i^\dagger a_i$ (no sum over $i$) as the operator counting the number of particles in state $|\, i \rangle$, one easily verifies:

$$N_i|\, n_1, n_2, \dots\ n_i, \dots \rangle = n_i|\, n_1, n_2, \dots\ n_i, \dots \rangle \tag{5.9}$$

and the algebra:

$$[a_i, a_j] = 0\,, \qquad [a_i^\dagger, a_j^\dagger] = 0\,, \qquad [a_i, a_j^\dagger] = \delta_{i,j} \tag{5.10$a$}$$

$$[N_i, a_j^\dagger] = \delta_{i,j}\,a_i^\dagger\,, \qquad [N_i, a_j] = -\delta_{i,j}\,a_i \tag{5.10$b$}$$

The total number of particles is evidently:

$$N = \sum_i N_i = \sum_i a_i^\dagger a_i \,. \tag{5.11}$$

so

$$N|\, n_1, n_2, \ldots\rangle = \left(\sum_i n_i\right) |\, n_1, n_2, \ldots\rangle \,. \tag{5.12}$$

Similarly we see that we can write the energy operator, *i.e.* the Hamiltonian of a system of non-interacting particles, as:

$$\begin{aligned} H &= \sum_i \epsilon_i N_i + E_0 \,, \\ H|\, n_1, n_2, \ldots\rangle &= \left(\sum_i \epsilon_i n_i\right) |\, n_1, n_2, \ldots\rangle = E_{n_1,n_2,\ldots}|\, n_1, n_2, \ldots\rangle \,. \end{aligned} \tag{5.13}$$

The above construction, called the *occupation number formalism* for obvious reasons, is an implementation of the bra-ket formalism for a bosonic many-particle system. For non-interacting particles the particle number, $N$, is conserved, $[N, H] = 0$, as one easily verifies. This remains true for interacting systems with a *fixed* number of bosons, like a gas of helium atoms, with energies low enough for ionization to be impossible. For such systems the basis we have constructed is actually far too large. It suffices to restrict oneself to the subspace with a fixed $N = n$. The only drawback of this is that the expression for $H$ in this basis is a bit cumbersome:

$$H = \sum_{n=1}^{\infty} H_n \,, \qquad H_n = \sum_{i;\; n=\sum_j N_j} \left(\epsilon_i N_i + E_0^i\right) \,, \tag{5.14}$$

We note that if $\epsilon_1 < \epsilon_i$ for all $i > 1$, then the state $|\, n, 0, 0, \ldots\rangle$ is the unique state of lowest energy. $E_{n,0,0,\ldots} = n\epsilon_1$, for $n$ particles, *i.e.* the ground state for the $n$-particle Hamiltonian $H_n$.

Both in condensed matter physics and in quantum field theory, we are interested in cases where the number of particles, or more generally "pseudo-particles", is not conserved. The basis constructed above is perfectly suitable also for this purpose. But this results in a much larger Hilbert space, allowing for the description of states with an indefinite, and even arbitrarily large, number of particles. Of course, unless $\epsilon_1 = 0$, a state with infinitely many particles cannot be realized physically, because it would have infinite energy, but there is no fixed upper limit to the value of $n$. The basis we have constructed is the basis of the bosonic **Fock space**, $\mathcal{F}$, which is the direct sum of the Hilbert spaces of fixed numbers, $n$, of particles, $\mathcal{H}_n$. This can be written (cf *Schwartz*, sec. 2.3).

$$\mathcal{F} = \oplus_n \mathcal{H}_n \,. \tag{$S$ 2.67}$$

This is just a way of expressing that any physical state can be described as a superposition of states with a fixed number of particles. This formalism goes beyond that of traditional non-relativistic quantum mechanics, where it is taken as a postulate that one cannot realize states which are superpositions of states with a different number of

particles. This postulate is not obeyed by relativistic quantum fields, and indeed not even by excitations in non-relativistic many-body systems.

It remains to consider the case of states labelled by a continuous variable, like the momentum eigenstates, which are not only used as the standard basis in relativistic quantum field theory, but also in non-relativistic scattering theory. If $i \to \mathbf{p}$, we have for a free particle of mass $m$: $e_i \to e(\mathbf{p}) = \mathbf{p}^2/2m$ in the non-relativistic case and $e_i \to \omega(\mathbf{p}) = \sqrt{\mathbf{p}^2 + m^2}$ in the relativistic case. It is not quite obvious how to handle the notation of eq. (5.4) in this case. The standard way is to introduce a *regularization*. We imagine that our initially infinite system is placed in a cubical box of side length $L$, so the volume is $V = L^3$ (in 3 dimensions). To find the wavefunction of a free boson in this volume, we have to define the boundary conditions. These depend on the physical situation we want to describe.

Let us concentrate on motion in a single direction. A free particle moving in the $x$ direction has a wavefunction:

$$\psi_p(x) = \langle x|p\rangle = N_p e^{\mathrm{i}px}\,, \tag{5.15}$$

both for non-relativistic and relativistic particles, where $N_p$ is a normalization factor. If we take the box boundaries to be at $x = 0$ and $x = L$, and implement the boundary conditions $\psi(0) = \psi(L) = 0$, no wavefunction of the form of eq. (5.15) satisfy the conditions. But since the Hamiltonian of a free particle is invariant under a parity transformation, $x \longleftrightarrow -x$, a linear combination of such wavefunctions of the form:

$$\psi(x) = \psi_p(x) - \psi_p(-x) = A_p \sin(px)\,,$$

where $A_p$ is a normalization factor, does. The constants in this equation have been chosen so that $\psi(0) = 0$. In order also to have $\psi(L) = 0$, we must require the *quantization condition*:

$$\psi(L) = A_p \sin(pL) = 0 \qquad \Longleftrightarrow \qquad p = \frac{n\pi}{L}\,, \quad n \text{ an integer}\,. \tag{5.16}$$

But this is not a scattering solution, as can be seen in several ways. Thus if we calculate the probability current from *BJ* eq. (2.50), we find:

$$j_x = \frac{1}{2m\mathrm{i}}\left(\psi^*\frac{\partial\psi}{\partial x} - \frac{\partial\psi^*}{\partial x}\psi\right) = 0\,,$$

since $\psi$ is real. Thus no particle leaves or enters the box. Indeed, we recognize this $\psi(x)$ as the stationary wavefunction of a particle constrained to move back and forth within the box $0 \le x \le L$.

To obtain a solution, $\psi_p(x)$, describing a particle moving along with a conserved momentum $p$, we use a standard trick. We imagine that our box is one of an infinite set of identical boxes, and that the particle can move from box to box, but in such a manner that the value of the wavefunction *on each boundary* is the same. This condition is called the *periodic boundary condition*, and reads in one dimension:

$$\psi_p(L) = \psi_p(0) \qquad \Longleftrightarrow \qquad p = \frac{2\pi n}{L}\,, \quad n \text{ an integer}\,. \tag{5.17}$$

Thus we arrive at only a slightly modified quantization condition, but the probability current density becomes:

$$j_x = \frac{p}{m}|N_p|^2\,,$$

as expected. Thus eqs. (5.15) with the boundary condition (5.17) does indeed describe a particle travelling through the box with momentum $p$. It remains to determine the normalization constant $N_p$. Since the values of $p$ are discrete, one finds, using the quantization condition.

$$\delta_{p,p'} = \langle p'|p\rangle = \int_0^L \mathrm{d}x\,\psi^*_{p'}(x)\psi_p(x) = N_{p'}N_p\int_0^L \mathrm{d}x\,e^{i(p-p')x} = \begin{cases} |N_p|^2 L, & \text{if } p = p'\,; \\ 0 & p \neq p'\,. \end{cases}$$

Thus choosing $N_p = 1/\sqrt{L}$ results in the standard normalization of the wavefunctions. The corresponding normalized momentum eigenstates in 3 dimensions are then:

$$\psi_{\mathbf{p}}(\mathbf{r}) = \langle \mathbf{r}|\mathbf{p}\rangle = \frac{1}{\sqrt{V}}e^{\mathrm{i}\mathbf{p}\cdot\mathbf{r}}\,, \tag{5.18}$$

both for non-relativistic and relativistic particles. This leads to the resolution of the unit operator in the coordinate representation:

$$\delta(\mathbf{r}-\mathbf{r}') = \sum_{\mathbf{p}}\langle \mathbf{r}'|\mathbf{p}\rangle\langle\mathbf{p}|\mathbf{r}\rangle = \frac{1}{V}\sum_{\mathbf{p}} e^{-\mathrm{i}\mathbf{p}\cdot(\mathbf{r}-\mathbf{r}')}\,. \tag{5.19}$$

The sum over $\mathbf{p}$ here is over the positive and negative integers $n_x, n_y$ and $n_z$ (not including 0), such that $p_i = 2\pi n_i/L$. On the other hand, in the continuum limit we have the well-known integral representation of the $\delta$-function:

$$\delta(\mathbf{r}-\mathbf{r}') = \frac{1}{(2\pi)^3}\int_{-\infty}^{\infty}\mathrm{d}^3\mathbf{p}\,e^{-\mathrm{i}\mathbf{p}\cdot(\mathbf{r}-\mathbf{r}')}\,.$$

For the normalization based on periodic boundary condition to reproduce the standard normalization conditions, the transition between the discrete and continuous noralization is obtained by the simple prescription:

$$\frac{1}{V}\sum_{\mathbf{p}} \qquad \Longleftrightarrow \qquad \frac{1}{(2\pi)^3}\int_{-\infty}^{\infty}\mathrm{d}^3\mathbf{p}\,. \tag{5.20}$$

We shall come back to the normalization conventions for the momentum eigenstates, because it turns out to be convenient to modify them slightly for relativistic theories.