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Lecture notes for FYS610 Many particle Quantum Mechanics

Note 5, 24.1 2017

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. 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 in the same one-particle state $|\, i\rangle$, we can, of course, write the wavefunction as

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

where $\psi_i(\mathbf{r}_j) = \langle \mathbf{r}_j | i \rangle$ is a one-particle wavefunction, which is not too bad. But already if we have n_1 particles in state $|\, i\rangle$ and $n_2 = N - n_1$ in state $|\, j\rangle$, things start to get unwieldy:

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

where $\binom{N}{n_1} = \frac{N!}{n_1! n2_!}$ 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.

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 eigenstates of H are discrete and ordered so that we can assume that i can be taken to be the natural numbers, and that:

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

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 state $i = 1$ etc. The symmetry condition id fulfilled per definition. The state of lowest energy, the *ground state* or *vacuum*, is the state without any particles at all:

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

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 it. Since the particles are non-interacting, the energy of a state with n_1 particle in the state $i = 1$, n_2 in that with i_2 etc is evidently:

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

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

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

We can now use 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):

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

Thus this creation operator leaves all particles in states $|\,j\rangle \neq |\,i\rangle$ unchanged. This definition leads to:

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

The matrix element of a_i follows like before:

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

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:

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

and the algebra:

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

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

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, may look like a particular implementation of the bra-ket formalism for a many-particle system. Indeed for non-interacting particles it is, since 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. But for this purpose the basis we have constructed is far too large, it suffices to restrict oneself to the subspace of a fixed $N = n$. The only drawback of this is that the expression for H in this basis becomes a bit cumbersome:

$$H = \sum_n H_n \,, \qquad H_n = \sum_{i;\, \sum_j N_j = n} \epsilon_i N_i + E_0^i \,, \tag{5.14}$$

where $E_0 = \sum_i E_0^i$. We note that $\epsilon_1 < \epsilon_i$ for all $i > 1$, then the state $|\, n, 0, 0, \ldots \rangle$ is the unique state of lowest energy. $E_{n,0,0,\ldots}$, for n particles, *i.e.* the ground state in H_n.

Both in condensed matter physics and in quantum field theory, we are interested in the 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 it is a basis for a much larger Hilbert space, as it allows for the existence of an arbitrary number of particles. Of course, unless $\epsilon_0 = 0$, a state with infinitely many particles cannot be realized 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, $\mathcal{H}_\backslash$. 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 traditionally it was 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 of dealing with this is to introduce a *regularization*. We imagine our initially infinite system 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 the x-direction first. 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 these condition. But since the Hamiltonian of a free particle is invariant under a parity transformation, $x \leftrightarrow -x$, 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 condition, does. The constants in this equation have been chosen so that $\psi(0) = 0$ is fulfilled. In order also to have $\psi(L) = 0$, we must require the *quantization condition*:

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

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 ψ is real. Thus no particle leaves or enters the box. Indeed, we recognize this ψ_p as the stationary wavefunction of a particle constrained to move within the box $0 \le x \le L$.

To obtain a solution describing a particle moving with 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 boundary condition 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 the same 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.

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

Thus one can chose $N_p = 1/\sqrt{L}$. In 3 dimensions the normalized momentum eigenstates are then:

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

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

$$\delta(\mathbf{r}-\mathbf{r}') = \sum_{\mathbf{p}} \langle \mathbf{r}'|\mathbf{p}\rangle\langle \mathbf{p}|\mathbf{r}\rangle = \frac{1}{V}\sum_{\mathbf{p}} e^{-\mathrm{i}\mathbf{p}\cdot(\mathbf{r}-\mathbf{r}')} \,. \tag{5.18}$$

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

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

Thus, we find the transition between the discrete and continuous description is obtained simply by the prescription:

$$\frac{1}{V}\sum_{\mathbf{p}} \qquad \Longleftrightarrow \qquad \frac{1}{(2\pi)^3}\int_{-\infty}^{\infty} \mathrm{d}^3\mathbf{p} \,. \tag{5.19}$$

We shall come back to the normalization conventions for the momentum eigenstates, because it is convenient to do this differently for non-relativistic and relativistic theories.