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Lecture notes for FYS610 Many particle Quantum Mechanics

Note 6, 25.1 2017

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

Second quantization of fermions

Consider a system of n non-interacting *fermions*, each in one particle state $|\, i_k\rangle$. Since two fermions cannot be in the same quantum state, according to the Pauli principle, all the i_k are different. Er can then write their antisymmetric n-particle wavefunction as:

$$\psi_{i_1,i_2\ldots\, i_n}(\mathbf{r}_1,\mathbf{r}_2,\ldots\,\mathbf{r}_n) = \frac{1}{n!}\sum_{\pi}(-1)^{P(\pi)}\prod_{k=1}^{n}\psi_{i_k}(\mathbf{r}_{\pi(k)})\,, \tag{6.1}$$

where π is a permutation of $\{1,2,\ldots\,n\}$, and $P(\pi)$ is the parity of the permutation. But this formula can be written as a determinant, the so-called *Slater determinant*:

$$\begin{aligned}\psi_{i_1,i_2\ldots\,,i_n}(\mathbf{r}_1,\mathbf{r}_2,\ldots\,\mathbf{r}_n) &= \frac{1}{n!}\begin{vmatrix}\psi_{i_1}(\mathbf{r}_1) & \psi_{i_1}(\mathbf{r}_2) & \ldots & \psi_{i_1}(\mathbf{r}_n)\\ \psi_{i_2}(\mathbf{r}_1) & \psi_{i_2}(\mathbf{r}_2) & \ldots & \psi_{i_2}(\mathbf{r}_n)\\ \vdots & \vdots & \ddots & \vdots\\ \psi_{i_n}(\mathbf{r}_1) & \psi_{i_n}(\mathbf{r}_2) & \ldots & \psi_{i_n}(\mathbf{r}_n)\end{vmatrix}\\ &= \frac{1}{n!}\begin{vmatrix}\psi_{i_1}(\mathbf{r}_1) & \psi_{i_2}(\mathbf{r}_1) & \ldots & \psi_{i_n}(\mathbf{r}_1)\\ \psi_{i_1}(\mathbf{r}_2) & \psi_{i_2}(\mathbf{r}_2) & \ldots & \psi_{i_n}(\mathbf{r}_2)\\ \vdots & \vdots & \ddots & \vdots\\ \psi_{i_1}(\mathbf{r}_n) & \psi_{i_2}(\mathbf{r}_n) & \ldots & \psi_{i_n}(\mathbf{r}_n)\end{vmatrix}\end{aligned} \tag{6.2}$$

where we have used that a determinant is unchanged under transposition. The slater determinants are actually much used in the atomic and nuclear theory to describe systems with a fixed number of fermions. When interactions are included, the wavefunction can no longer be expressed by a single determinant, but they are still very useful as forming a basis of antisymmetric n-particle wavefunctions. We see that the Pauli principle is automatically fulfilled, if either $i_m = i_n$ or $\mathbf{r}m = \mathbf{r_n}$ for $m \neq n$, the determinant vanishes, because two rows or two columns are equal.

But in spite of the fact that Slater determinants are a convenient basis for small fixed values of n, they become cumbersome for large n, and in particular for describing processes with a variable particle number. Fortunately, the Fock-space construction works at least as well for fermions as for bosons. Starting from the one-particle states $|\, i\rangle$, which we assume to be ordered according to increasing energy, ϵ_i, like in eq. (5.4), we define a general many-particle state as in eq. (5.5):

$$|\, n_1, n_2, n_3, \ldots\; n_i, \ldots\rangle\,. \tag{5.5}$$

The important difference is that for fermions all n_i are restricted to the values 0 and 1, in accordance with the Pauli principle. Eqs. (5.6-8) remain valid: The ground (vacuum) state is $|\,0\rangle = |\,0,0,\ldots\rangle$ and the energy eigenvalues are given by $H\,|\,n_1,n_2,\ldots\rangle = E_{n_1,n_2,\ldots}|\,n_1,n_2,\ldots\rangle$ with $E_{n_1,n_2,\ldots} = E_0 + n_1\epsilon_1 + n_2\epsilon_2 + \ldots$.

The crucial difference is the construction of the creation and annihilation operators so that the Pauli principle is respected. It is useful first to consider a *single state*, *i.e.* some fixed $|\,i\rangle$. In the fermionic case, this state may be either empty, which we can write $|\,0\rangle$, or it is occupied, $|\,1\rangle$. These to vectors form a complete orthonormal basis in a 2-dimensional subspace of $\mathcal{H}$, since we must have $\langle 0|1\rangle = 0$, since the probability must be zero to detect a particle in an empty state and no particle in an occupied state. An appropriate creation operator is defined by the following two relations, with corresponding matrix elements:

$$
\begin{gathered}
c^\dagger|\,0\rangle = |\,1\rangle\,, \qquad c^\dagger|\,1\rangle = 0\,, \\
\langle 0|c^\dagger|\,0\rangle = \langle 0|1\rangle = 0\,, \quad \langle 1|c^\dagger|\,0\rangle = \langle 1|1\rangle = 1\,, \quad \langle 0|c^\dagger|\,1\rangle = \langle 1|c^\dagger|\,0\rangle = 0\,.
\end{gathered} \tag{6.3}
$$

By demanding that the annihilation operator c is the Hermitean conjugate of $c^\dagger$, we have correspondingly:

$$
\begin{aligned}
\langle 0|c|\,0\rangle = \langle 0|c^\dagger|\,0\rangle^* = 0\,, \quad \langle 0|c|\,1\rangle = \langle 1|c^\dagger|\,0\rangle^* = 1\,, \\
\langle 1|c|\,0\rangle = \langle 0|c^\dagger|\,1\rangle^* = 0\,, \quad \langle 1|c|\,1\rangle = \langle 1|c^\dagger|\,1\rangle^* = 0\,.
\end{aligned} \tag{6.4}
$$

By using the resolution of the unit operator in the two-state subspace:

$$
\mathbb{I} = |\,0\rangle\langle 0| + |\,1\rangle\langle 1|\,, \tag{6.5}
$$

we then find:

$$
c|\,0\rangle = |\,0\rangle\langle 0|c|\,0\rangle + |\,1\rangle\langle 1|c|\,0\rangle = 0\,, \qquad c|\,1\rangle = |\,0\rangle\langle 0|c|\,1\rangle + |\,1\rangle\langle 1|c|\,0\rangle = |\,0\rangle\,. \tag{6.6a}
$$

This can be summarized as:

$$
c^\dagger|\,n\rangle = (1-n)|\,n-1\rangle\,, \qquad c|\,n\rangle = n|\,n-1\rangle\,, \tag{6.6b}
$$

with $n = 0,1$. The most noteworthy of these relations is $c^\dagger|\,1\rangle = 0$, which states that if one attempt to create a second fermion in an occupied state, the state vanishes. This is of course the essence of the Pauli principle. The other relations are actually the same as for bosonic operators applied to vacuum and one-particle states.

Using eqs. (6.3-6) we find:

$$
\begin{aligned}
c^2 &= cc\mathbb{I} = c(c|\,0\rangle\langle 0| + c|\,1\rangle\langle 1|) = c(0 + |\,0\rangle\langle 1|) = 0\,, \\
{c^\dagger}^2 &= c^\dagger c^\dagger\mathbb{I} == c^\dagger(c^\dagger|\,0\rangle\langle 0| + c^\dagger|\,1\rangle\langle 1|) = c^\dagger(|\,1\rangle\langle 0| + 0) = 0\,, \\
c^\dagger c &= c^\dagger c\mathbb{I} = c^\dagger(c|\,0\rangle\langle 0| + c|\,1\rangle\langle 1|) = c^\dagger(0 + |\,0\rangle\langle 1|) = |\,1\rangle\langle 1|\,, \\
cc^\dagger &= cc^\dagger\mathbb{I} = c(c^\dagger|\,0\rangle\langle 0| + c^\dagger|\,1\rangle\langle 1|) = c(|\,1\rangle\langle 0| + 0) = |\,0\rangle\langle 0|\,.
\end{aligned}
$$

Thus $N = c^\dagger c$ and $cc^\dagger$ are the projection operators on the occupied and empty subspaces, respectively. N also is the number operator, in the sense that it has eigenvalue 1 when applied to an occupied state, 0 if applied to an empty state.

If we introduce the **anti-commutator**, $\{A, B\}$, of any two operators A and B by the definition:

$$\{A, B\} = AB + BA = \{B, A\}\,, \tag{6.7}$$

we see that the *commutator relation* for bosonic creation and annihilation operators, eq. (4,5), is replaced by the *anti-commutator relations*:

$$\begin{aligned} \{c, c\} = cc + cc = 0 \qquad \{c^\dagger, c^\dagger\} = c^\dagger c^\dagger + c^\dagger c^\dagger = 0\,, \\ \{c, c^\dagger\} = cc^\dagger + c^\dagger c = |\,0\rangle\langle 0| + |\,1\rangle\langle 1| = \mathbb{I}\,. \end{aligned} \tag{6.8}$$

This is a basic result: The commutator algebra of bosons is replaced by an anti-commutator algebra for fermions. The anti-commutator, in addition to being symmetric instead of antisymmetric, satisfies the linearity conditions of eqs. (1.4c), but is not distributive, nor is there a Jacobi identity.

With the basic fermionic algebra established, we can return to the many-body case, with separate creation and annihilation operators, $c_i^\dagger$ and c_i, for each state $|\,i\rangle$, each obeying eq. (6.8). Starting with the many-particle vacuum, which we for simplicity also call $|\,0\rangle = |\,0, 0, \ldots\rangle$, we easily find an arbitrary one-particle state where the state labelled by i is the occupied one can be written:

$$|\,0_1, 0_2, \ldots\, 1_i, \ldots\rangle = c_i^\dagger |\,0\rangle \tag{6.9}$$

To keep track on *which* states that are occupied, and which not, we use indices on the occupation numbers. But when we come to the two-particle state, we have to be more careful. The reason is the minus-sign which appears when we interchange the two particles. From the Slater determinant formulation, eq. (6.2), we know that such a wavefunction in position space can be written:

$$\Psi_{i,j}(\mathbf{r}_i, \mathbf{r_2}) = \langle \mathbf{r_1}, \mathbf{r}_2 | 0_1, 0_2, \ldots\, i, \ldots\, j, \ldots\rangle = \frac{1}{2}\left(\psi_i(\mathbf{r_1})\psi_j(\mathbf{r}_2) - \psi_j(\mathbf{r_1})\psi_i(\mathbf{r}_2)\right)\,.$$

We would like to create th0is state as $|\,0_1, 0_2, \ldots\, i, \ldots\, j, \ldots\rangle = c_i^\dagger c_j^\dagger |\,0\rangle$. But what happens if we interchanges the two creation operators, what is the relation of $c_j^\dagger c_i^\dagger |\,0\rangle$ to $c_i^\dagger c_j^\dagger |\,0\rangle$? Although both represent the same physical state, interpreted as a ray in $\mathcal{H}$, we still have to distinguish the wavefunctions to have a consistent operator algebra. The notation indicates that in the state $c_j^\dagger c_i^\dagger |\,0\rangle$ one has in some sense "first" filled the state $|\,i\rangle$, then the state $|\,j\rangle$, while in the case of $c_i^\dagger c_j^\dagger |\,0\rangle$ the filling order is the opposite. Thus one has interchanged the particles, and the wavefunctions should have a relative minus sign. This intuitive analysis is indeed correct, the order of the operators matters, and the requirement of antisymmetry of the wavefunction with respect to interchange of particles is really a requirement regarding interchange of operator order. Thus we have to fix some convention to determine the (relative) signs of the wavefunctions. A workable convention is summarized in the following fermionic counterpart to eq. (4.16):

$$\begin{aligned} c_i^\dagger | \, n_1, n_2, \ldots \, n_i, \ldots \rangle &= (-1)^{\Sigma_i} (1 - n_i) | \, n_1, n_2, \ldots \, n_i + 1, \ldots \rangle \,, \\ c_i | \, n_1, n_2, \ldots \, n_i, \ldots \rangle &= (-1)^{\Sigma_i} n_i | \, n_1, n_2, \ldots \, n_i - 1, \ldots \rangle \,, \end{aligned} \tag{6.10}$$

where

$$(-1)^{\Sigma_i} = (-1)^{n_1 + n_2 + \ldots \, n_{i-1}} \,. \tag{6.11}$$

In words: We have a factor -1 for each occupied state standing to the left of the state i in the state vector. We note that it is not a problem in eq. (6.10) that the occupation numbers $n_i + 1$ and $n_i - 1$ appear even if $n_i = 1$, respectively $n_i = 0$, since the prefactors $(1 - n_i)$ and n_i cancels these wavefunctions anyhow.

With the definition of eq. (6.10) we have that $c_j c_i | \, 0 \rangle = -c_i c_j | \, 0 \rangle$, since one of the i and j must stand to the left of the other, and it does not matter which. Thus we have that the anti-commutation relations of eq. (6.8) generalizes to:

$$\{c_i, cj\} = 0 \qquad \{c_i^\dagger, c_j^\dagger\} = 0 \,, \qquad \{c_i, c_j^\dagger\} = \delta_{ij} \,. \tag{6.12}$$

Except for this crucial difference, the Fock-space formalism for fermions is quite similar to that of bosons.