

## Notes on Occupation Number Formalism for Fermions

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As I hope I amply demonstrated in class, Slater determinants are a very cumbersome way to write out many-electron (or many fermion) wave functions. The occupation number formalism is simply an elegant shorthand notation for writing such wave functions. All manipulations are reduced to linear algebra instead of unpleasant multiple integrals and explicit evaluation of determinants, and it is all automatic. Once you are familiar with the rules (and accept them) you don't have to think about the manipulations any more.

In these notes, I will simply state some of the basic rules - I won't prove many of them but you can do most of that yourselves, given the anticommutation rules.

We start by assuming that we have a complete orthonormal set of single-particle states which I will denote  $u_i(\vec{x})$ . Here  $\vec{x}$  is a shorthand for space and spin coordinates (i.e.  $\vec{x}$  means  $\vec{r}, s$  where  $\vec{r}$  are the three space coordinates and  $s$  ( $= +1/2$  or  $-1/2$ ) are the two spin coordinates for a spin-1/2 particle). Similarly,  $i$  denotes the quantum numbers for a single particle state. Orthonormality means

$$\int u_i^\dagger(\vec{x})u_j(\vec{x})d\vec{x} = \delta_{ij}. \quad (1)$$

If we have  $N$  particles, we can put each of them in one of the states  $u_i$ . We can then form a Slater determinant to get a properly antisymmetrized wave function. We will now describe these Slater determinants in a simple way using “fermion creation and annihilation operators”  $c_i^\dagger$  and  $c_i$ .

First we define a vacuum state, denoted  $|0\rangle$ , which contains no fermions and is normalized, so that

$$\langle 0|0\rangle = 1. \quad (2)$$

Then  $c_i^\dagger$  is defined to create a fermion in the  $i^{\text{th}}$  single-particle state by

$$c_i^\dagger|0\dots 0\rangle = |0\dots 010\dots 0\rangle \quad (3)$$

where the numbers inside the ket indicate the occupation number of the various single-particle states, and the 1 is in the  $i^{\text{th}}$  state. Since we can't put two fermions in the same state, we also require

$$c_i^\dagger|0\dots 010\dots 0\rangle = 0. \quad (4)$$

From the previous equation this implies that  $c_i^\dagger c_i^\dagger = 0$  or

$$\{c_i^\dagger, c_i^\dagger\} = 0 \quad (5)$$

where  $\{, \}$  denotes the anticommutator:

$$\{A, B\} = AB + BA. \quad (6)$$

Likewise we define the destruction operator  $c_i$  so that

$$c_i|0\dots 010\dots 0\rangle = |0\dots 0\rangle \quad (7)$$

$$c_i|0\dots 0\rangle = 0. \quad (8)$$

Just as for creation operators, the second of these equations implies that  $c_i^2 = 0$  or

$$\{c_i, c_i\} = 0. \quad (9)$$

From the above properties we also have

$$\langle 0 | c_i^\dagger c_i | 0 \rangle = 0 \quad (10)$$

$$\langle 0 | c_i c_i^\dagger | 0 \rangle = 1 \quad (11)$$

$$\langle 0 \dots 010 \dots 0 | c_i^\dagger c_i | 0 \dots 010 \dots 0 \rangle = 1 \quad (12)$$

$$\langle 0 \dots 010 \dots 0 | c_i c_i^\dagger | 0 \dots 010 \dots 0 \rangle = 0. \quad (13)$$

These equations imply that

$$\{c_i, c_i^\dagger\} = c_i c_i^\dagger + c_i^\dagger c_i = 1. \quad (14)$$

So far we have defined anticommutation relations only for creation and annihilation operators of the  $i^{\text{th}}$  single-particle state. In order to construct Slater determinants, we generalize these by assuming that the operators for different states anticommute, so that

$$\{c_i, c_j^\dagger\} = \delta_{ij} \quad (15)$$

$$\{c_i, c_j\} = 0 \quad (16)$$

$$\{c_i^\dagger, c_j^\dagger\} = 0. \quad (17)$$

With these anticommutation relations, the state

$$c_1^\dagger c_2^\dagger \dots c_N^\dagger | 0 \rangle \quad (18)$$

is equivalent to a Slater determinant made up of N fermions, one each in states 1,...N. The state has all the properties we demand of Slater determinants, as was first proven by Jordan and Wigner. For example, we want the Slater determinant to change sign under interchange of two columns, say the  $i^{th}$  and  $j^{th}$ . In our notation, this is equivalent to interchanging the operators  $c_i^\dagger$  and  $c_j^\dagger$ . This interchange, one can convince oneself, always involves an odd number of permutations, and hence, by the anticommutation relations, produces a change of sign, as required. The state is also automatically normalized. For example, consider the normalization of the two-fermion state:

$$\langle 0|c_j c_i c_i^\dagger c_j^\dagger|0 \rangle = \langle 0|c_j c_j^\dagger c_i c_i^\dagger|0 \rangle \quad (19)$$

$$= \langle 0|(1 - c_j^\dagger c_j)(1 - c_i^\dagger c_i)|0 \rangle \quad (20)$$

$$= \langle 0|(1 - c_j^\dagger c_j)|0 \rangle = 1. \quad (21)$$

It can be shown that the operator  $n_i \equiv c_i^\dagger c_i$  is the number operator for state i. That is, the expectation value of  $n_i$  in a given Slater determinant is 1 if the  $i^{th}$  single-particle state is occupied in that determinant, and 0 otherwise.

Note also that two N-fermion Slater determinants are orthogonal if they don't correspond to exactly the same occupation numbers. E. g. , consider the expectation value

$$\langle 0|c_1 c_3 c_2^\dagger c_1^\dagger|0 \rangle. \quad (22)$$

This is the overlap between two Slater determinants, one in which single-

particle states 1 and 2 are occupied, and one in which states 1 and 3 are occupied. Since  $c_3$  appears without a balancing  $c_3^\dagger$ , it can be permuted through to the right (with a change of sign each time) till it operates on the state  $|0\rangle$ , giving 0. Hence this expectation value is zero.

Note also that if the  $u_i$ 's are a complete set of orthonormal single particle states, then the N-fermion Slater determinants formed from them are a complete set of orthonormal N-fermion states. Any N particle state can therefore be formed as a linear combination of Slater determinants.

Now that we have described the states, we want to describe Hamiltonians so that we can calculate energies. Such a description is needed to discuss superconductivity, for example, and will be used next quarter.

First, we introduce another operator,

$$\psi(\vec{x}) = \sum_i u_i(\vec{x})c_i \quad (23)$$

and its hermitean conjugate

$$\psi^\dagger(\vec{x}) = \sum_i u_i^\dagger(\vec{x})c_i^\dagger. \quad (24)$$

I claim that the operator

$$n(\vec{x}) = \psi^\dagger(\vec{x})\psi(\vec{x}) \quad (25)$$

gives the density of fermions at point  $\vec{x}$ .

This is actually easy to prove. We write

$$n(\vec{x}) = \sum_{i,j} u_i^\dagger(\vec{x})u_j(\vec{x})c_i^\dagger c_j. \quad (26)$$

If we sandwich this operator between a bra and a ket representing the same Slater determinant, and calculate

$$\langle 0|c_N\dots c_1n(\vec{x})c_1^\dagger c_2^\dagger\dots c_N^\dagger|0\rangle, \quad (27)$$

only the diagonal terms ( $i = j$ ) in the sum above survive. This is because the expectation value of any operator of the form  $\langle 0| \times$  (product of creation and annihilation operators)  $\times |0\rangle$  vanishes unless in that product the creation and annihilation operators for each state  $i$  appear an equal number of times (i. e. in pairs). (This is an exercise for the reader.) Hence the expectation value of  $n(\vec{x})$  is just

$$\sum_i u_i^\dagger(\vec{x})u_i(\vec{x})n_i \quad (28)$$

where  $n_i$  is the expectation value of the number operator  $c_i^\dagger c_i$  in the Slater determinant. But the expression in eq. (28) is the density at point  $\vec{x}$ , and so the theorem is proved.

Now we use this to write out the Hamiltonian. Let us assume that the single particle states  $u(\vec{x})$  satisfy a Schrödinger equation of the form

$$H_1(\vec{x})u_i(\vec{x}) \equiv \left(-\frac{\hbar^2}{2m}\nabla^2 + V_1(\vec{x})\right)u_i(\vec{x}) = \epsilon_i u_i(\vec{x}) \quad (29)$$

and that the total Hamiltonian for our  $N$ -fermion system is

$$H = \sum_i H_1(\vec{x}_i) + \sum_{i>j} V_2(\vec{x}_i - \vec{x}_j). \quad (30)$$

If the density of particles is  $n(\vec{x})$ , then the Hamiltonian operator is

$$H = \int \psi^\dagger(\vec{x}) H_1(\vec{x}) \psi(\vec{x}) d\vec{x} + (1/2) \int d\vec{x} \int d\vec{x}' \psi^\dagger(\vec{x}) \psi^\dagger(\vec{x}') V_2(\vec{x} - \vec{x}') \psi(\vec{x}') \psi(\vec{x}). \quad (31)$$

The only thing that might puzzle us about the interaction term in (31) is the order of the  $\psi$ 's and  $\psi^\dagger$ 's. But the various operators are anticommutated through, it is found that this order is just equivalent to writing the interaction term as  $\int \int V_2(\vec{x} - \vec{x}') n(\vec{x}) n(\vec{x}')$  as we require. Thus the order is correct.

If we now substitute the forms for  $\psi$  and  $\psi^\dagger$  and use the orthonormality relations for the single-particle wave functions, we can rewrite H in so-called second-quantized form:

$$H = \sum_i \epsilon_i c_i^\dagger c_i + \sum_{ijkl} V_{ijkl} c_i^\dagger c_j^\dagger c_k c_l \quad (32)$$

where

$$V_{ijkl} = \int d\vec{x} \int d\vec{x}' u_i^\dagger(\vec{x}) u_j^\dagger(\vec{x}') V_2(\vec{x} - \vec{x}') u_k(\vec{x}') u_l(\vec{x}). \quad (33)$$

It might seem perverse to call the integral in (33)  $V_{ijkl}$  rather than  $V_{ijkl}$ . This convention insures that the Coulomb and exchange energies appear with aesthetically pleasing notation, as will be seen in the next paragraph.

What is the virtue of writing H in this elegant but obscure-looking notation? It is now very easy, by using the operator algebra of the  $c_i$ 's, to calculate the expectation value of H in a given Slater determinantal state. I

will just state the answer; it is

$$\langle H \rangle = \sum_i \epsilon_i n_i + \sum_{i>j} [V_{ij;ij} - V_{ij;ji}] n_i n_j. \quad (34)$$

The first term is just the sum of the single-particle energies. The second is the sum of the Coulomb and the exchange energies ( $V_{ij;ij}$  and  $V_{ij;ji}$  respectively) as I discussed in class. The notation  $\langle H \rangle$  just means the expectation value of  $H$  in a Slater determinant

$$\langle H \rangle \equiv \langle 0 | c_N \dots c_1 H c_1^\dagger \dots c_N^\dagger | 0 \rangle. \quad (35)$$

We can more or less understand the structure of the interaction term from looking at the integrals involved in (35). As stated earlier, all such terms vanish unless the creation and annihilation operators for each state  $i$  appear in pairs. With the product  $c_i^\dagger c_j^\dagger c_k c_l$  this can happen in only two ways: (1)  $i = j = k = l$ ; and (2)  $i = k, j = l$ . The first gives the Coulomb (or “direct”) energy; the second gives the exchange energies. You can also show that terms such that  $i = j = k = l$  vanish identically.

The Hartree-Fock approximation basically consists of finding the set of single-particle states which minimizes  $\langle H \rangle$ . The equations for this are discussed in Ashcroft and Mermin.

Note that the same occupation number formalism can be carried directly over to Bose particles instead of Fermi particles. In this case, the wave functions must be symmetric rather than antisymmetric under interchange

of coordinates of particles  $i$  and  $j$ . This leads to the requirement that the Bose creation and annihilation operators commute rather than anticommute. We have already an example of this with the occupation number representation for phonons, which are Bose particles.