Summary of lectures FYS4480 autumn 2018

October 22, 2018

Disclaimer

The purpose of this note is to summarize what has been covered so far in the course and provide a general overview over important results and methods. Statements are given without proof and one should consult the lecture notes for more in depth discussion of the various topics.

Introduction

Slater Determinants

Creation and annihilation operators

Definition 1 (Vacuum state). The state $|0\rangle$ represents the state containing no particles and is referred to as the vacuum state. Another common notation is to use $|-\rangle$. The vacuum state satisfies $\langle 0|0\rangle = 1$. It should be noted that $|0\rangle \neq 0$.

Definition 2 (The creation operator). We define the fermion creation operator $a_\alpha^\dagger$, creating a particle in the single-particle state ϕ_α, as

$$a_\alpha^\dagger |0\rangle \equiv |\alpha\rangle \tag{1}$$

and

$$a_\alpha^\dagger |\alpha_1\alpha_2\cdots\alpha_n\rangle = |\alpha\alpha_1\alpha_2\cdots\alpha_n\rangle, \tag{2}$$

if $\alpha \neq \alpha_i$ for all single-particle states in the determinant. Furthermore, insertion of α at position $j+1$ will induce a sign change $(-1)^j$

$$a_\alpha^\dagger |\alpha_1\alpha_2\cdots\alpha_j\alpha_{j+1}\cdots\alpha_n\rangle = (-1)^j |\alpha_1\alpha_2\cdots\alpha_j\alpha\alpha_{j+1}\cdots\alpha_n\rangle. \tag{3}$$

If $\alpha = \alpha_i$ for some single-particle state, then

$$a_\alpha^\dagger |\alpha_1\alpha_2\cdots\alpha_n\rangle = |\alpha\alpha_1\alpha_2\cdots\alpha_n\rangle = 0 \tag{4}$$

Definition 3 (The annihilation operator). The annihilation operator, a_α, is the Hermitian adjoint of $a_\alpha^\dagger$, i.e

$$a_\alpha \equiv (a_\alpha^\dagger)^\dagger. \tag{5}$$

The annihilation operator gives the zero result when acting on the vacuum state

$$a_\alpha |0\rangle = 0. \tag{6}$$

If $|\Phi\rangle = |\alpha_1\alpha_2\cdots\alpha_{i-1}\alpha_i\alpha_{i+1}\cdots\alpha_n\rangle$ is an arbitrary Slater determinant and $\alpha = \alpha_i$

$$a_\alpha |\alpha_1\alpha_2\cdots\alpha_{i-1}\alpha_i\alpha_{i+1}\cdots\alpha_n\rangle = (-1)^{i-1} |\alpha_1\alpha_2\cdots\alpha_{i-1}\alpha_{i+1}\cdots\alpha_n\rangle, \tag{7}$$

i.e it removes particle i from the determinant. Otherwise $a_\alpha |\Phi\rangle = 0$, that is if $\alpha \neq \alpha_i$ for all single-particle states in the determinant.

Definition 4 (Anticommutator of operators). The anticommutator of two operators $\hat{A}$ and $\hat{B}$ is defined as

$$\{\hat{A}, \hat{B}\} \equiv \hat{A}\hat{B} + \hat{B}\hat{A}. \tag{8}$$

Theorem 1 (The fundamental anticommutator relations). The creation and annihilation operators satisfy the so-called "fundamental anticommutator" relations

$$\{a_p^\dagger, a_q^\dagger\} = 0 \tag{9}$$

$$\{a_p, a_q\} = 0 \tag{10}$$

$$\{a_p, a_q^\dagger\} = \delta_{pq}. \tag{11}$$

$$\tag{12}$$

Representation of operators

The matrix representation of a one-body operator, relative to a single particle basis $\{\phi_i\}_{i=1}$, is given by

$$\langle \phi_p | \hat{h} | \phi_q \rangle \equiv \int \phi_p^*(\mathbf{r}) \hat{h} \phi_q(\mathbf{r}) d\mathbf{r}. \tag{13}$$

Common notations are $\langle \phi_p | \hat{h} | \phi_q \rangle = \langle p | \hat{h} | q \rangle = h_q^p$. The second quantized form a one-body operator is given by

$$\hat{H}_0 = \sum_{pq} \langle p | \hat{h} | q \rangle a_p^\dagger a_q. \tag{14}$$

Likewise the matrix representation of a two-body operator, typically the coulomb interaction, is given by

$$\langle \phi_p \phi_q | \hat{v} | \phi_r \phi_s \rangle = \int \phi_p^*(\mathbf{r_1}) \phi_q^*(\mathbf{r_2}) \hat{v}(\mathbf{r}_1, \mathbf{r}_2) \phi_q(\mathbf{r_1}) \phi_s(\mathbf{r_2}) d\mathbf{r_1} d\mathbf{r_2}. \tag{15}$$

It is common to write $\langle \phi_p \phi_q | \hat{v} | \phi_r \phi_s \rangle = \langle pq | \hat{v} | rs \rangle = v_{rs}^{pq}$. Furthermore, it is customary to introduce the *anti-symmetric* matrix element

$$\langle pq | \hat{v} | rs \rangle_{AS} \equiv \langle pq | \hat{v} | rs \rangle - \langle pq | \hat{v} | sr \rangle. \tag{16}$$

Here it should be noted that many sources drop the AS subscript, which can be a source of confusion. The second quantized form a two-body operator is given by

$$\hat{H}_I = \frac{1}{2} \sum_{pqrs} \langle pq | \hat{v} | rs \rangle a_p^\dagger a_q^\dagger a_s a_r \tag{17}$$

$$= \frac{1}{4} \sum_{pqrs} \langle pq | \hat{v} | rs \rangle_{AS} a_p^\dagger a_q^\dagger a_s a_r \tag{18}$$

Thus, the full Hamiltonian $\hat{H} = \hat{H}_0 + \hat{H}_I$, using anti-symmetric matrix elements is given by

$$\hat{H} = \sum_{pq} \langle p | \hat{h} | q \rangle a_p^\dagger a_q + \frac{1}{4} \sum_{pqrs} \langle pq | \hat{v} | rs \rangle_{AS} a_p^\dagger a_q^\dagger a_s a_r. \tag{19}$$

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Wicks theorem and related concepts

Definition 5 (Operator string). A sequence of creation and annihilation operators is called an operator string. Generally an operator string of n creation and annihilation operators are on the form

$$A_1 A_2 \cdots A_n, \quad A_i \in \{a_p, a_p^\dagger\}. \tag{20}$$

For example

$$A_1 A_2 A_3 A_4 = a_p a_q^\dagger a_r a_s^\dagger,$$

where $A_1 = a_p$, $A_2 = a_q^\dagger$, $A_3 = a_r$ and $A_4 = a_s^\dagger$.

Definition 6 (Vacuum expecatation value). The number

$$\langle -|A_1 A_2 \cdots A_n|-\rangle \tag{21}$$

is referred to as a vacuum expecatation value, where $A_1 A_2 \cdots A_n$ is an operator string.

Definition 7 (Normal ordered product). The normal-ordered product form of an operator string $A_1 A_2 \cdots A_n$ is defined as a rearrangement,

$$\{A_1 A_2 \cdots A_n\} \equiv (-1)^{|\sigma|} A_{\sigma(1)} A_{\sigma(2)} \cdots A_{\sigma(n)}, \tag{22}$$

where σ is a permutation such that all the creation operators in the operator string is to the left of all the annihilation operators, i.e.,

$$\{A_1 A_2 \cdots A_n\} \equiv (-1)^{|\sigma|}[\text{creation operators}] \cdot [\text{annihilation operators}]. \tag{23}$$

The permutation σ is in general not unique, since we may permute the creation and annihilation operators separately without affecting the total expression. For example,

$$\{a_p a_q^\dagger a_r^\dagger a_s\} = a_q^\dagger a_r^\dagger a_p a_s = -a_r^\dagger a_q^\dagger a_p a_s = a_r^\dagger a_q^\dagger a_s a_p = -a_q^\dagger a_r^\dagger a_s a_p \tag{24}$$

To find the permutation σ that normal-orders an operator product, it is usually simplest to count the number f of anticommutations necessary to achieve the rearrangement, and set $(-1)^{|\sigma|} = (-1)^f$. Note that the string $A_1 \cdots A_n \neq \{A_1 \cdots A_n\}$ in general, since by reordering creation and annihilation operators we neglect the extra terms arising from the Kronecker delta in the anticommutator relation $\{a_p, a_q^\dagger\} = \delta_{pq}$.

Definition 8 (Contraction). A contraction between two arbitrary creation and annihilation operators X and Y, is the number defined by

$$\overparen{XY} \equiv \langle -|XY|-\rangle. \tag{25}$$

We list the possible contractions, relative to the vacuum state $|-\rangle$,

$$\overparen{a_p^\dagger a_q^\dagger} = \langle -|a_p^\dagger a_q^\dagger|-\rangle = 0 \tag{26}$$

$$\overparen{a_p a_q} = \langle -|a_p a_q|-\rangle = 0 \tag{27}$$

$$\overparen{a_p^\dagger a_q} = \langle -|a_p^\dagger a_q|-\rangle = 0 \tag{28}$$

$$\overparen{a_p a_q^\dagger} = \langle -|a_p a_q^\dagger|-\rangle = \delta_{pq} \tag{29}$$

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Wick's theorem states that every string of creation and annihilation operators can be written as a sum of normal-ordered products where we perform every possible contraction.

Theorem 2 (Wicks theorem). Let $A_1 \cdots A_n$ be an operator string of creation and annihilation operators. Then,

$$A_1 A_2 \cdots A_n = \{A_1 A_2 \cdots A_n\} + \sum_{(1)} \{A_1 \overset{\sqcap}{\ldots\ldots\ldots} A_n\} \quad + \sum_{(2)} \{A_1 \overset{\sqcap\!\!\sqcap}{\ldots\ldots\ldots}\} + \cdots$$

$$+ \sum_{\lfloor \frac{n}{2} \rfloor} \underbrace{\{A_1 \ldots\ldots\ldots\ldots\ldots A_n\}}_{\lfloor \frac{n}{2} \rfloor \text{ contractions}}$$

The notation $\sum_{(m)}$ signifies that we sum over all combinations of m contractions. When n is even, the last sum signifies that we sum over $n/2$ contractions, i.e., all operators are contracted. If n is odd, there is one uncontracted operator left in each term of the last sum.

Evaluation of vacuum expecatation values are greatly simplified by Wicks theorem. First note that for any string with at least one factor

$$\langle -|\{A_1 \cdots A_n\}|-\rangle = 0, \tag{30}$$

because in the normal-order product, the annihilation operators are to the right, and the creation operators are on the left.

Theorem 3 (Wicks theorem for vacuum expecatation values). For odd n, Wicks theorem gives

$$\langle -|A_1 \cdots A_n|-\rangle = 0, \tag{31}$$

while for even n,

$$\langle -|A_1 \cdots A_n|-\rangle = \sum_{\lfloor \frac{n}{2} \rfloor} \underbrace{\{A_1 \ldots\ldots\ldots\ldots A_n\}}_{\text{all contracted}}. \tag{32}$$

Fact 1. A useful fact is that the sign of a fully contracted operator product is $(-1)^k$, where k is the number of contraction line crossings.

Consider an operator string on the form

$$\{A_1 A_2 \cdots A_p\}\{B_1 B_2 \cdots B_q\} \cdots \{Z_1 Z_2 \cdots Z_r\} \tag{33}$$

where each substring is normal ordered. Then the generalized Wicks theorem states that we only have to consider contractions between different substrings. That is, contractions involving two operators from the same substring -referred to as self contractions- do not contribute.

Theorem 4 (The generalized Wicks theorem). Let

$$\{A_1 A_2 \cdots A_p\}\{B_1 B_2 \cdots B_q\} \cdots \{Z_1 Z_2 \cdots Z_r\}$$

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be an operator string consisting of normal ordered substrings. Then,

$$\{A_1 A_2 \cdots A_p\}\{B_1 B_2 \cdots B_q\} \cdots \{Z_1 Z_2 \cdots Z_r\} = \{A_1 A_2 \cdots A_p \vdots B_1 B_2 \cdots B_q \vdots \cdots \vdots Z_1 Z_2 \cdots Z_r\}$$

$$+ \sum_{(1)}{}' \{A_1 \overset{\frown}{A_2 \cdots A_p \vdots B_1 B_2 \cdots B_q} \vdots \cdots \vdots Z_1 Z_2 \cdots Z_r\}$$

$$+ \sum_{(2)}{}' \{A_1 \overset{\frown}{A_2 \cdots A_p \vdots B_1} \overset{\frown}{B_2 \cdots B_q \vdots \cdots \vdots Z_1} Z_2 \cdots Z_r\}$$

$$+ \cdots$$

$$+ \sum_{\lfloor \frac{n}{2} \rfloor}{}' \underbrace{\{A_1 A_2 \cdots A_p \vdots B_1 B_2 \cdots B_q \vdots \cdots \vdots Z_1 Z_2 \cdots Z_r\}}_{\lfloor \frac{n}{2} \rfloor \text{ contractions}}$$

The notation $\sum'_{(m)}$ signifies that we sum over all combinations of m contractions that each involve operators from different substrings. The vertical dots are only a bookkeeping device to remind ourselves which operators belong to which substrings.

Particle-hole formalism

Consider a N-particle system and the single-particle functions $\{\phi_p\}_{p=1}^L$, with L denoting the number of single-particle functions. In particle-hole formalism we divide the single-particle functions into two sets. The first N single-particle functions, $\{\phi\}_{i=1}^N$, are referred to as particle/occupied-states/functions while the $N+1, \cdots, L$ states, $\{\phi\}_{a=N+1}^L$, are referred to as hole/unoccupied/virtual states. The indices $i, j, k, \cdots$ are reserved for particle states and indices $a, b, c, \cdots$ are reserved for hole states. General states, particle or hole, are indexed by $p, q, r, \cdots$.

Definition 9 (The reference state). We define the reference Slater determinant $|c\rangle$ to be the determinant constructed from the hole states, i.e

$$|c\rangle = \prod_{i=1}^N a_i^\dagger |0\rangle = |\phi_1 \phi_2 \cdots \phi_N\rangle. \tag{34}$$

Other common notations for the reference state are $|c\rangle = |\Phi_0\rangle = |\Phi\rangle_{\text{ref}}$.

Definition 10 (Excited determinants). From the reference determinant, we can construct excited determinants using the creation and annihilation operators, substituting one or more particle states with hole states.

$$|\Phi_i^a\rangle = a_a^\dagger a_i |c\rangle, \quad \text{single excitation}$$
$$|\Phi_{ij}^{ab}\rangle = a_b^\dagger a_j a_a^\dagger a_i |c\rangle, \quad \text{double excitation},$$
$$\vdots$$

Definition 11 (Quasiparticle creation and annihilation operators). Quasiparticle creation and annihilation operators $b_p, b_p^\dagger$ are defined as follows

$$b_i = a_i^\dagger, \quad b_a = a_a \tag{35}$$
$$b_i^\dagger = a_i, \quad b_a^\dagger = a_a^\dagger. \tag{36}$$

Thus, for hole indices, quasiparticle creation operators are the ordinary creation operators, but for particle states, creating a quasiparticle is the same as destroying a particle in a particle state. One says that $b_i^\dagger$ creates a hole, while $b_a^\dagger$ creates a particle.

Furthermore, the fundamental anticommutator relations are preserved for quasiparticle creation and annihilation operators

$$\{b_p^\dagger, b_q^\dagger\} = 0, \tag{37}$$

$$\{b_p, b_q\} = 0, \tag{38}$$

$$\{b_p, b_q^\dagger\} = \delta_{pq}. \tag{39}$$

Definition 12 (The new vacuum state). Making the observation that

$$b_p \ket{c} = 0 \text{ for all } p, \tag{40}$$

we see that the reference acts for quasiparticle creation/annihilation as the vacuum did for the ordinary creation/annihilation operators. Thus, we define the reference $\ket{c}$ to be vacuum state for the quasiparticle operators. We will often refer to $\ket{c}$ as the new vacuum state in the following.

Fact 2. The definition of normal-ordering, contractions, and ultimately Wick's theorem, depended only on the anticommutator relations and the property

$$a_p \ket{0} = .0$$

Thus, Wick's theorem is valid also for quasiparticles.

Notice that relative to the new vacuum state, there are now two non-zero contractions

$$\contraction{}{b}{{}_a}{b} b_a b_b^\dagger = \contraction{}{a}{{}_a}{a} a_a a_b^\dagger = \braket{c | a_a a_b^\dagger | c} = \delta_{ab} \tag{41}$$

$$\contraction{}{b}{{}_i}{b} b_i b_j^\dagger = \contraction{}{a}{{}_i^\dagger}{a} a_i^\dagger a_j = \braket{c | a_i^\dagger a_j | c} = \delta_{ij}. \tag{42}$$

$$\tag{43}$$

Normal ordering relative to the new vacuum state

If we normal order relative to the new vacuum $\ket{c}$ the one-body Hamiltonian can be written

$$\hat{H}_0 = H_0^{(1\text{-body})} + H_0^{(0\text{-body})} \tag{44}$$

where we have defined

$$H_0^{(0\text{-body})} \equiv \sum_i \braket{i | \hat{h} | i} \tag{45}$$

$$H_0^{(1\text{-body})} \equiv \sum_{pq} \braket{p | \hat{h} | q} \{a_p^\dagger a_q\}. \tag{46}$$

The notation $H^{n\text{-body}}$ means that the operator acts as a n-body operator, with 0-body being the same as a constant.

The two-body Hamiltonian can be written as

$$\hat{H}_I = \hat{H}_I^{(\text{2-body})} + \hat{H}_I^{(\text{1-body})} + \hat{H}_I^{(\text{0-body})} \tag{47}$$

$$\tag{48}$$

where

$$\hat{H}_I^{(\text{2-body})} = \frac{1}{4} \sum_{pqrs} \langle pq|\hat{v}|rs\rangle_{\text{AS}} \{a_p^\dagger a_q^\dagger a_s a_r\}, \tag{49}$$

$$\hat{H}_I^{(\text{1-body})} = \sum_{pqi} \langle pi|\hat{v}|qi\rangle_{\text{AS}} \{a_p^\dagger a_q\}, \tag{50}$$

$$\hat{H}_I^{(\text{0-body})} = \frac{1}{2} \sum_{ij} \langle ij|\hat{v}|ij\rangle_{\text{AS}} \tag{51}$$

We now define

$$E_0^{\text{ref}} \equiv H_0^{(\text{0-body})} + \hat{H}_I^{(\text{0-body})} = \sum_i \langle i|\hat{h}|i\rangle + \frac{1}{2} \sum_{ij} \langle ij|\hat{v}|ij\rangle_{\text{AS}}$$

$$\{\hat{F}\} \equiv H_0^{(\text{1-body})} + \hat{H}_I^{(\text{1-body})} = \sum_{pq} \langle p|\hat{f}|q\rangle \{a_p^\dagger a_q\}$$

$$\{\hat{H}_I\} \equiv \hat{H}_I^{(\text{2-body})}$$

where we defined the so-called fock matrix element

$$\langle p|\hat{f}|q\rangle = \langle p|\hat{h}|q\rangle + \sum_i \langle pi|\hat{v}|qi\rangle_{\text{AS}} \tag{52}$$

E_0^{ref} is referred to as the reference energy and $\{\hat{F}\}$ is the Fock-operator.

Thus, we can write the full Hamiltonian normal ordered relative to the new vacuum as

$$\hat{H} = E_0^{\text{ref}} + \{\hat{F}\} + \{\hat{H}_I\}. \tag{53}$$

When computing expectation values using the normal ordered Hamiltonian we can now use Wicks generalized theorem, considering only contractions between normal ordered substrings. Recall carefully, that there are two possible non-zero contractions relative to the new vacuum state.

Example 1. Consider the computation of the matrix element $\langle c|\{\hat{F}\}|\Phi_i^a\rangle$. By Wicks generalized theorem we have

$$\langle c|\{\hat{F}\}|\Phi_i^a\rangle = \sum_{\lfloor \frac{n}{2}\rfloor}' \langle c| \left(\sum_{pq} \langle p|\hat{f}|q\rangle \{a_p^\dagger a_q\} a_a^\dagger a_i \right) |c\rangle,$$

With $\sum_{\lfloor \frac{n}{2}\rfloor}'$ meaning that we sum over all possible contractions between different normal ordered substrings.

Note that $a_a^\dagger a_i$ already is on normal order form. The computation is also simplified by noting that there is only one possible way of contracting all operators and get a non-zero result, that is

$$\{\overline{a_p^\dagger \overline{a_q}\}a_a^\dagger} a_i = \delta_{pi}\delta_{qa} \tag{54}$$

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with a positive sign since there are two line crossings. Thus,

$$\langle c|\{\hat{F}\}|\Phi_i^a\rangle = \langle c|\left(\sum_{pq}\langle p|\hat{f}|q\rangle\delta_{pi}\delta_{qa}\right)|c\rangle$$
$$= \langle i|\hat{f}|a\rangle\langle c|c\rangle$$
$$= \langle i|\hat{f}|a\rangle.$$

Configuration Interaction Theory

Hartree-Fock theory

Many-body Perturbation Theory

Coupled Cluster Theory