Week 37: Wick's generalized theorem, particle hole-formalism and diagrammatic representation of operators

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Week 37

Topics to be covered

1. Thursday: Discussion of Wick's theorem, Wick's generalized theorem and examples with discussion of exercises for week 37. Introduction of the particle-hole formalism. Definition of new reference state, normal ordering of operators
2. Friday: Particle-hole formalism
3. Lecture Material: These slides, handwritten notes and chapter 3 of Shavitt and Bartlett covers most of the material discussed this week.
4. Fourth exercise set at https://github.com/ManyBodyPhysics/FYS4480/blob/master/doc/Exercises/2025/ExercisesWeek37.pdf
5. Answers to exercises from last week at https://github.com/ManyBodyPhysics/FYS4480/blob/master/doc/Exercises/2025/AnswersWeek36.pdf

Reminder from last week on Wick's theorem (standard and generalized), more on diagrammatic notation and examples

See notes from last week (week 36) and whiteboard notes for this week and last week.

Particle-hole formalism

Second quantization is a useful and elegant formalism for constructing many-body states and quantum mechanical operators. One can express and translate many physical processes into simple pictures such as Feynman diagrams. Expecation values of many-body states are also easily calculated.
However, although the equations are seemingly easy to set up, from a practical point of view, that is the solution of Schroedinger's equation, there is no particular gain. The many-body equation is equally hard to solve, irrespective of representation. The cliche that there is no free lunch brings us down to earth again. Note however that a transformation to a particular basis, for cases where the interaction obeys specific symmetries, can ease the solution of Schroedinger's equation.

Redefining the reference state

But there is at least one important case where second quantization comes to our rescue. It is namely easy to introduce another reference state than the pure vacuum $|0\rangle$, where all single-particle states are active. With many particles present it is often useful to introduce another reference state than the vacuum state$|0\rangle$. We will label this state $|c\rangle$ (c for core) and as we will see it can reduce considerably the complexity and thereby the dimensionality of the many-body problem. It allows us to sum up to infinite order specific many-body correlations. The particle-hole representation is one of these handy representations.

New operators

In the original particle representation these states are products of the creation operators $a^\dagger_{\alpha_i}$ acting on the true vacuum $|0\rangle$. We have

$$
\begin{aligned}
|\alpha_1\alpha_2\dots\alpha_{n-1}\alpha_n\rangle &= a^\dagger_{\alpha_1}a^\dagger_{\alpha_2}\dots a^\dagger_{\alpha_{n-1}}a^\dagger_{\alpha_n}|0\rangle && (1)\\
|\alpha_1\alpha_2\dots\alpha_{n-1}\alpha_n\alpha_{n+1}\rangle &= a^\dagger_{\alpha_1}a^\dagger_{\alpha_2}\dots a^\dagger_{\alpha_{n-1}}a^\dagger_{\alpha_n}a^\dagger_{\alpha_{n+1}}|0\rangle && (2)\\
|\alpha_1\alpha_2\dots\alpha_{n-1}\rangle &= a^\dagger_{\alpha_1}a^\dagger_{\alpha_2}\dots a^\dagger_{\alpha_{n-1}}|0\rangle && (3)
\end{aligned}
$$

Reference states

If we use Eq. (1) as our new reference state, we can simplify considerably the representation of this state

$$|c\rangle \equiv |\alpha_1\alpha_2\dots\alpha_{n-1}\alpha_n\rangle = a^\dagger_{\alpha_1}a^\dagger_{\alpha_2}\dots a^\dagger_{\alpha_{n-1}}a^\dagger_{\alpha_n}|0\rangle \tag{4}$$

The new reference states for the $n+1$ and $n-1$ states can then be written as

$$|\alpha_1\alpha_2\dots\alpha_{n-1}\alpha_n\alpha_{n+1}\rangle = (-1)^n a^\dagger_{\alpha_{n+1}}|c\rangle \equiv (-1)^n|\alpha_{n+1}\rangle_c \tag{5}$$

$$|\alpha_1\alpha_2\dots\alpha_{n-1}\rangle = (-1)^{n-1} a_{\alpha_n}|c\rangle \equiv (-1)^{n-1}|\alpha_{n-1}\rangle_c \tag{6}$$

Hole and particle states

The first state has one additional particle with respect to the new vacuum state $|c\rangle$ and is normally referred to as a one-particle state or one particle added to the many-body reference state. The second state has one particle less than the reference vacuum state $|c\rangle$ and is referred to as a one-hole state. When dealing with a new reference state it is often convenient to introduce new creation and annihilation operators since we have from Eq. (6)

$$a_\alpha|c\rangle \neq 0 \tag{7}$$

since α is contained in $|c\rangle$, while for the true vacuum we have $a_\alpha|0\rangle = 0$ for all α.

Redefinition of creation and annihilation operators

The new reference state leads to the definition of new creation and annihilation operators which satisfy the following relations

$$b_\alpha|c\rangle = 0 \tag{8}$$

$$\{b_\alpha^\dagger, b_\beta^\dagger\} = \{b_\alpha, b_\beta\} = 0$$

$$\{b_\alpha^\dagger, b_\beta\} = \delta_{\alpha\beta} \tag{9}$$

We assume also that the new reference state is properly normalized

$$\langle c|c\rangle = 1 \tag{10}$$

Physical interpretation

The physical interpretation of these new operators is that of so-called quasiparticle states. This means that a state defined by the addition of one extra particle to a reference state $|c\rangle$ may not necesseraly be interpreted as one particle coupled to a core. We define now new creation operators that act on a state α creating a new quasiparticle state

$$b_\alpha^\dagger|c\rangle = \left\{ \begin{array}{ll} a_\alpha^\dagger|c\rangle = |\alpha\rangle, & \alpha > F \\ \\ a_\alpha|c\rangle = |\alpha^{-1}\rangle, & \alpha \leq F \end{array} \right. \tag{11}$$

where F is the Fermi level representing the last occupied single-particle orbit of the new reference state $|c\rangle$.

Annihilation operator

The annihilation is the hermitian conjugate of the creation operator

$$b_\alpha = (b_\alpha^\dagger)^\dagger,$$

resulting in

$$b_\alpha^\dagger = \begin{cases} a_\alpha^\dagger & \alpha > F \\ \\ a_\alpha & \alpha \leq F \end{cases} \qquad b_\alpha = \begin{cases} a_\alpha & \alpha > F \\ \\ a_\alpha^\dagger & \alpha \leq F \end{cases} \tag{12}$$

Introducing the concept of quasiparticle states

With the new creation and annihilation operator we can now construct many-body quasiparticle states, with one-particle-one-hole states, two-particle-two-hole states etc in the same fashion as we previously constructed many-particle states. We can write a general particle-hole state as

$$|\beta_1\beta_2\dots\beta_{n_p}\gamma_1^{-1}\gamma_2^{-1}\dots\gamma_{n_h}^{-1}\rangle \equiv \underbrace{b_{\beta_1}^\dagger b_{\beta_2}^\dagger \dots b_{\beta_{n_p}}^\dagger}_{>F} \underbrace{b_{\gamma_1}^\dagger b_{\gamma_2}^\dagger \dots b_{\gamma_{n_h}}^\dagger}_{\leq F} |c\rangle \tag{13}$$

We can now rewrite our one-body and two-body operators in terms of the new creation and annihilation operators.

Number operator

The number operator becomes

$$\hat{N} = \sum_{\alpha} a_\alpha^\dagger a_\alpha = \sum_{\alpha > F} b_\alpha^\dagger b_\alpha + n_c - \sum_{\alpha \leq F} b_\alpha^\dagger b_\alpha \tag{14}$$

where n_c is the number of particle in the new vacuum state $|c\rangle$.
The action of $\hat{N}$ on a many-body state results in

$$N|\beta_1\beta_2\dots\beta_{n_p}\gamma_1^{-1}\gamma_2^{-1}\dots\gamma_{n_h}^{-1}\rangle = (n_p+n_c-n_h)|\beta_1\beta_2\dots\beta_{n_p}\gamma_1^{-1}\gamma_2^{-1}\dots\gamma_{n_h}^{-1} \tag{15}$$

More manipulations

Here $n = n_p + n_c - n_h$ is the total number of particles in the quasi-particle state of Eq. (13). Note that $\hat{N}$ counts the total number of particles present

$$N_{qp} = \sum_{\alpha} b_{\alpha}^{\dagger} b_{\alpha}, \tag{16}$$

gives us the number of quasi-particles as can be seen by computing

$$N_{qp} = |\beta_1 \beta_2 \dots \beta_{n_p} \gamma_1^{-1} \gamma_2^{-1} \dots \gamma_{n_h}^{-1}\rangle = (n_p + n_h) |\beta_1 \beta_2 \dots \beta_{n_p} \gamma_1^{-1} \gamma_2^{-1} \dots \gamma_{n_h}^{-} \tag{17}$$

where $n_{qp} = n_p + n_h$ is the total number of quasi-particles.

Onebody operator

We express the one-body operator $\hat{H}_0$ in terms of the quasi-particle creation and annihilation operators, resulting in

$$\hat{H}_0 = \sum_{\alpha\beta > F} \langle\alpha|\hat{h}_0|\beta\rangle b_\alpha^\dagger b_\beta + \sum_{\alpha > F, \beta \leq F} \left[\langle\alpha|\hat{h}_0|\beta\rangle b_\alpha^\dagger b_\beta^\dagger + \langle\beta|\hat{h}_0|\alpha\rangle b_\beta b_\alpha\right] + \sum_{\alpha \leq F} \langle\alpha|\hat{h}_0|\alpha\rangle - \sum_{\alpha\beta \leq F} \langle\beta|\hat{h}_0|\alpha\rangle b_\alpha^\dagger b_\beta \quad (18)$$

The first term gives contribution only for particle states, while the last one contributes only for holestates. The second term can create or destroy a set of quasi-particles and the third term is the contribution from the vacuum state $|c\rangle$.

New notations

Before we continue with the expressions for the two-body operator, we introduce a nomenclature we will use for the rest of this text. It is inspired by the notation used in quantum chemistry. We reserve the labels $i, j, k, \dots$ for hole states and $a, b, c, \dots$ for states above F, viz. particle states. This means also that we will skip the constraint $\leq F$ or $> F$ in the summation symbols. Our operator $\hat{H}_0$ reads now

$$
\begin{aligned}
\hat{H}_0 = & \sum_{ab} \langle a|\hat{h}|b\rangle b_a^\dagger b_b + \sum_{ai} \left[\langle a|\hat{h}|i\rangle b_a^\dagger b_i^\dagger + \langle i|\hat{h}|a\rangle b_i b_a \right] \\
+ & \sum_{i} \langle i|\hat{h}|i\rangle - \sum_{ij} \langle j|\hat{h}|i\rangle b_i^\dagger b_j
\end{aligned}
\tag{19}
$$

Two-particle operator

The two-particle operator in the particle-hole formalism is more complicated since we have to translate four indices $\alpha\beta\gamma\delta$ to the possible combinations of particle and hole states. When performing the commutator algebra we can regroup the operator in five different terms

$$\hat{H}_I = \hat{H}_I^{(a)} + \hat{H}_I^{(b)} + \hat{H}_I^{(c)} + \hat{H}_I^{(d)} + \hat{H}_I^{(e)} \quad (20)$$

Using anti-symmetrized matrix elements, bthe term $\hat{H}_I^{(a)}$ is

$$\hat{H}_I^{(a)} = \frac{1}{4}\sum_{abcd} \langle ab|\hat{V}|cd\rangle b_a^\dagger b_b^\dagger b_d b_c \quad (21)$$

More rewriting

The next term $\hat{H}_I^{(b)}$ reads

$$\hat{H}_I^{(b)} = \frac{1}{4}\sum_{abci}\left(\langle ab|\hat{V}|ci\rangle b_a^\dagger b_b^\dagger b_i^\dagger b_c + \langle ai|\hat{V}|cb\rangle b_a^\dagger b_i b_b b_c\right) \tag{22}$$

This term conserves the number of quasiparticles but creates or removes a three-particle-one-hole state. For $\hat{H}_I^{(c)}$ we have

$$\begin{aligned}\hat{H}_I^{(c)} = \quad & \frac{1}{4}\sum_{abij}\left(\langle ab|\hat{V}|ij\rangle b_a^\dagger b_b^\dagger b_j^\dagger b_i^\dagger + \langle ij|\hat{V}|ab\rangle b_a b_b b_j b_i\right) + \\ & \frac{1}{2}\sum_{abij}\langle ai|\hat{V}|bj\rangle b_a^\dagger b_j^\dagger b_b b_i + \frac{1}{2}\sum_{abi}\langle ai|\hat{V}|bi\rangle b_a^\dagger b_b.\end{aligned} \tag{23}$$

More terms

The first line stands for the creation of a two-particle-two-hole state, while the second line represents the creation to two one-particle-one-hole pairs while the last term represents a contribution to the particle single-particle energy from the hole states, that is an interaction between the particle states and the hole states within the new vacuum state.
The fourth term reads

$$
\begin{aligned}
\hat{H}_I^{(d)} = \quad & \frac{1}{4}\sum_{aijk}\left(\langle ai|\hat{V}|jk\rangle b_a^\dagger b_k^\dagger b_j^\dagger b_i + \langle ji|\hat{V}|ak\rangle b_k^\dagger b_j b_i b_a\right) + \\
& \frac{1}{4}\sum_{aij}\left(\langle ai|\hat{V}|ji\rangle b_a^\dagger b_j^\dagger + \langle ji|\hat{V}|ai\rangle - \langle ji|\hat{V}|ia\rangle b_j b_a\right). \qquad (24)
\end{aligned}
$$

Last expressions

The terms in the first line stand for the creation of a particle-hole state interacting with hole states, we will label this as a two-hole-one-particle contribution. The remaining terms are a particle-hole state interacting with the holes in the vacuum state. Finally we have

$$\hat{H}_I^{(e)} = \frac{1}{4}\sum_{ijkl}\langle kl|\hat{V}|ij\rangle b_i^\dagger b_j^\dagger b_l b_k + \frac{1}{2}\sum_{ijk}\langle ij|\hat{V}|kj\rangle b_k^\dagger b_i + \frac{1}{2}\sum_{ij}\langle ij|\hat{V}|ij\rangle \tag{25}$$

The first terms represents the interaction between two holes while the second stands for the interaction between a hole and the remaining holes in the vacuum state. It represents a contribution to single-hole energy to first order. The last term collects all contributions to the energy of the ground state of a closed-shell system arising from hole-hole correlations.

Summarizing and defining a normal-ordered Hamiltonian, part I

$$\Phi_{AS}(\alpha_1,\dots,\alpha_N;x_1,\dots x_N)=\frac{1}{\sqrt{A}}\sum_{\hat{P}}(-1)^P\hat{P}\prod_{i=1}^{A}\psi_{\alpha_i}(x_i),$$

which is equivalent with $|\alpha_1\dots\alpha_N\rangle = a_{\alpha_1}^{\dagger}\dots a_{\alpha_N}^{\dagger}|0\rangle$. We have also

$$a_p^{\dagger}|0\rangle = |p\rangle, \quad a_p|q\rangle = \delta_{pq}|0\rangle$$

$$\delta_{pq}=\left\{a_p, a_q^{\dagger}\right\},$$

and

$$0=\left\{a_p^{\dagger}, a_q\right\}=\left\{a_p, a_q\right\}=\left\{a_p^{\dagger}, a_q^{\dagger}\right\}$$

$$|\Phi_0\rangle = |\alpha_1\dots\alpha_N\rangle, \quad \alpha_1,\dots,\alpha_N\leq\alpha_F$$

Summarizing and defining a normal-ordered Hamiltonian, part II

$$\left\{a_p^\dagger, a_q\right\} = \delta_{pq}, p, q \le \alpha_F$$

$$\left\{a_p, a_q^\dagger\right\} = \delta_{pq}, p, q > \alpha_F$$

with $i, j, \ldots \le \alpha_F, \quad a, b, \ldots > \alpha_F, \quad p, q, \ldots - \mathrm{any}$

$$a_i|\Phi_0\rangle = |\Phi_i\rangle, \qquad a_a^\dagger|\Phi_0\rangle = |\Phi^a\rangle$$

and

$$a_i^\dagger|\Phi_0\rangle = 0 \qquad a_a|\Phi_0\rangle = 0$$

Summarizing and defining a normal-ordered Hamiltonian, part III

The one-body operator is defined as

$$\hat{F} = \sum_{pq} \langle p|\hat{f}|q\rangle a_p^\dagger a_q$$

while the two-body opreator is defined as

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

where we have defined the antisymmetric matrix elements

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

Summarizing and defining a normal-ordered Hamiltonian, part III

We can also define a three-body operator

$$\hat{V}_3 = \frac{1}{36}\sum_{pqrstu}\langle pqr|\hat{v}_3|stu\rangle_{AS} a_p^\dagger a_q^\dagger a_r^\dagger a_u a_t a_s$$

with the antisymmetrized matrix element

$$\langle pqr|\hat{v}_3|stu\rangle_{AS} = \langle pqr|\hat{v}_3|stu\rangle + \langle pqr|\hat{v}_3|tus\rangle + \langle pqr|\hat{v}_3|ust\rangle - \langle pqr|\hat{v}_3|su \tag{26}$$