3 Interacting electrons: Many-body methods

Helpful reading:

[Mar] M. P. Marder, Condensed Matter Physics (Appendix C on second quantization).

[AM] N. W. Ashcroft and N. D. Mermin, Solid State Physics (Chapter 17 on Hartree–Fock)

[PS2] Handwritten lecture notes from the course "Statistical Physics II" (parts 2 and 3 on second quantization, in French): `http://www.phys.ethz.ch/~ivanov/ps2/1011/`

[BR] J.-P. Blaizot et G. Ripka, "Quantum theory of finite systems" (diagonalization of quadratic Hamiltonians and Wick theoreom)

3.1 Second quantization and Wick theorem

3.1.1 Bosons and fermions

Indistinguishable quantum particles can be of two types: *bosons* (the wave function is fully symmetric with respect to the permutations of particles) and *fermions* (fully antisymmetric). [In terms of the irreducible representations of the permutation group, these states belong to the trivial and "parity" representations, respectively.]

Fully symmetric and antisymmetric states may be described in terms of Hilbert spaces. Given a *single-particle* Hilbert space $\mathcal{H}$, we can construct the space of symmetrized and antisymmetrized N-particle states as symmetrized and antisymmetrized products of N copies of $\mathcal{H}$: we denote such spaces $S_\pm \mathcal{H}^{\otimes N}$, respectively. If we add together all such spaces with all possible particle numbers, we construct the bosonic/fermionic *Fock space*:

$$\mathcal{F}_\pm(\mathcal{H}) = \bigoplus_{N=0}^{\infty} S_\pm \mathcal{H}^{\otimes N} \,. \tag{3.1.1}$$

Note that the sum starts with $N = 0$ (the vacuum state). In the case of fermions, if $\mathcal{H}$ has a finite dimension m, then the spaces $S_+\mathcal{H}^{\otimes N}$ vanish for $m > N$ (so the sum is actually limited to $N \leq m$).

The symmetrization/antisymmetrization of states can be defined as

$$S_\pm(\varphi_1 \otimes \ldots \otimes \varphi_N) = \frac{1}{N!} \sum_{\sigma}^{N!} \varphi_\sigma(1) \otimes \ldots \otimes \varphi_\sigma(N) \,, \tag{3.1.2}$$

where the sum is taken over all the permutations of N elements (N states). In our discussion below, we will assume that the states φ_α are chosen from an orthonormal basis (although many of the formulas may be simply generalized to a non-orthonormal case as well).

Since the ordering of the states φ_α in the (anti)symmetrized product (3.1.2) is irrelevant, the multi-particle state may be specified by the *occupation numbers* n_α: the multiplicity of each basis state φ_α in the product (3.1.2). For fermions, the occupation number n_α can take values 0 and 1. For bosons, it can take all non-negative integer values.

The states (3.1.2) for all possible sets of occupation numbers form a basis of the Fock space $\mathcal{F}_\pm(\mathcal{H})$.

The states (3.1.2) are not correctly normalized. Their normalization can be computed:

$$\|S_\pm(\varphi_1 \otimes \ldots \otimes \varphi_N)\|^2 = \frac{\prod_\alpha n_\alpha!}{N!}\,. \tag{3.1.3}$$

Therefore correctly normalized states can be defined as

$$|\varphi_1, \ldots, \varphi_N\rangle_\pm^{(n)} = \frac{\sqrt{N!}}{\prod_\alpha \sqrt{n_\alpha!}}\, S_\pm(\varphi_1 \otimes \ldots \otimes \varphi_N)\,. \tag{3.1.4}$$

This construction is completely parallel for bosons and fermions.

3.1.2 Operators of creation and annihilation

For interacting particles, one needs to operate with states in the many-particle space $S_\pm\mathcal{H}^{\otimes N}$. It turns out more practical to work with the full Fock space (3.1.1), even if the particle number N is conserved. The operators in the Fock space may be most conveninently expressed in terms of *creation* and *annihilation* operators. The creation operators are defined as (both for bosons and for fermions):

$$a_\alpha^+ |\varphi_1, \ldots, \varphi_N\rangle_\pm^{(n)} = \sqrt{n_\alpha + 1}\, |\varphi_\alpha, \varphi_1, \ldots, \varphi_N\rangle_\pm^{(n)} \tag{3.1.5}$$

in terms of the normalized states. Equivalently, the same operators may be written as

$$a_\alpha^+ S_\pm(\varphi_1 \otimes \ldots \otimes \varphi_N) = \sqrt{N+1}\, S_\pm(\varphi_\alpha \otimes \varphi_1 \otimes \ldots \otimes \varphi_N)\,. \tag{3.1.6}$$

The annihilation operators are defined as their Hermitian conjugates:

$$a_\alpha = \left(a_\alpha^+\right)^\dagger \tag{3.1.7}$$

Defined in this way, the operators a_α^+ and a_α obey the commutation (for bosons) or anticommutation (for fermions) relations:

$$[a_\alpha, a_\beta^+]_\pm = \delta_{\alpha\beta}\,, \tag{3.1.8}$$

$$[a_\alpha, a_\beta]_\pm = [a_\alpha^+, a_\beta^+]_\pm = 0\,. \tag{3.1.9}$$

The use of the creation and annihilation operators allows to reduce many of the calculations in the Fock space to algebraic manipulations with the (anti)commutation relations.

Example: In our calculations with electrons, we will use the limit of an infinite system size with the states φ_α being plane waves (parametrized by the wave vector k):

$$\varphi_k(x) = e^{ikx} \tag{3.1.10}$$

Those states are normalized to

$$\int d^3x\, \varphi_k^*(x)\varphi_{k'}(x) = (2\pi)^3\delta(k-k')\,. \tag{3.1.11}$$

Correspondingly, the creation and annihilation operators associated with $\varphi_k(x)$ obey the (anti)commutation relations

$$[a_k, a_{k'}^+]_\pm = (2\pi)^3 \delta(k-k')\,. \tag{3.1.12}$$

By defining the Fourier transforms

$$a^+(x) = \int \frac{d^3k}{(2\pi)^3}\, e^{-ikx} a_k^+\,, \tag{3.1.13}$$

$$a(x) = \int \frac{d^3k}{(2\pi)^3}\, e^{ikx} a_k\,, \tag{3.1.14}$$

$$\tag{3.1.15}$$

the creation/annihilation operators in the coordinate space obey the relations

$$[a(x), a^+(x')]_\pm = \delta(x-x')\,. \tag{3.1.16}$$

3.1.3 One- and two-body operators in the Fock space

For any operator A acting in the single-particle space $\mathcal{H}$, we may construct the corresponding em one-particle operator $A_{(*)}$ in the Fock space $\mathcal{F}_\pm(\mathcal{H})$, whose action is given by the sum of the operators A acting on each particle. One can show that this operator may be written in terms of the creation and annihilation operators as

$$A_{(*)} = \sum_{ij} a_\alpha^+ A_{\alpha\beta} a_\beta\,, \tag{3.1.17}$$

where the sum is over the basis of the single-particle space $\mathcal{H}$ and $A_{\alpha\beta}$ are the matrix elements of A.

Example 1: Particle-number operator. $A = 1$ counts the particles. The total number of particles is given by

$$N = \sum_\alpha a_\alpha^+ a_\alpha\,. \tag{3.1.18}$$

Example 2: Free-particle Hamiltonian. The Hamiltonian of a free particle is diagonal in the momentum space: $E = \varepsilon_k$. Its counterpart in the Fock space can therefore be written as

$$H = \int \frac{d^3k}{(2\pi)^3}\, a_k^+ (\varepsilon_k - \mu) a_k\,, \tag{3.1.19}$$

where ε_k is the energy dispersion [$\varepsilon_k = \hbar^2 k^2/(2m)$ for a particle in an empty space], and μ is the chemical potential (which we usually include in the Hamiltonian in the Fock space). In the case of a quadratic spectrum, we can also rewrite the same operator in the coordinate space:

$$H = \int d^3x\, a^+(x) \left(-\frac{\hbar^2}{2m}\nabla^2 - \mu \right) a(x)\,. \tag{3.1.20}$$

A similar construction is possible for operators involving two and more particles. Consider, for example, the case of a *two-particle operator* V. It acts in the space of two particles $\mathcal{H} \otimes \mathcal{H}$. Let us denote its matrix elements by

$$V_{\alpha\beta,\gamma\delta} = \langle \varphi_\alpha \otimes \varphi_\beta | V | \varphi_\gamma \otimes \varphi_\delta \rangle\,. \tag{3.1.21}$$

Since the particles are indistinguishable, the matrix elements are invariant with respect to the permutation of the two particles:

$$V_{\alpha\beta,\gamma\delta} = V_{\beta\alpha,\delta\gamma}\,. \tag{3.1.22}$$

Then we can define the operator in the Fock space $\mathcal{F}_\pm(\mathcal{H})$, whose action is given by the sum of the operator V acting on *each pair of particles*. One can show that this operator may be written in the second-quantized form as

$$V_{(*)} = \frac{1}{2}\sum_{\alpha,\beta,\gamma,\delta} a^+_\alpha a^+_\beta V_{\alpha\beta,\gamma\delta} a_\delta a_\gamma\,. \tag{3.1.23}$$

Note the factor 1/2 (to avoid the double counting of partice pairs) and the ordering of the creation and annihilation operators (all the creation operators on the left of all the annihilation operators to avoid the self-interaction of particles).

Example: Potential interaction $V(x)$. The second-quantized form of the interaction takes the form

$$U = \frac{1}{2}\int d^3x\, d^3y\, a^+(x)\, a^+(y)\, V(x-y)\, a(y)\, a(x)\,. \tag{3.1.24}$$

3.1.4 Diagonalization of quadratic Hamiltonians

Hamiltonians quadratic with respect to the creation and annihilation operators (both bosonic and fermionic) have very remarkable properties:

1. They can be diagonalized and thus reduced to the case of noninteracting particles;
2. At any temperature, their equilibrium states obey the Wick theorem.

For the sake of generality (with a future application to superconductivity in mind), we consider the general case of a quadratic Hamiltonian

$$H = \begin{pmatrix} a^+ & a \end{pmatrix} \begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix} \begin{pmatrix} a \\ a^+ \end{pmatrix}\,, \tag{3.1.25}$$

where H_{ij} are $N \times N$ blocks (N is the dimension of the single-particle Hilbert space).

Such a Hamiltonian can be diagonalized, i.e., brought to the form

$$H = \sum_{\alpha=1}^{N} \varepsilon_\alpha b^+_\alpha b_\alpha + E_0 \tag{3.1.26}$$

where $\varepsilon_\alpha \geq 0$ (the energies of excitations), the operators b_α are linear combinations of a_α and a^+_α,

$$b_\alpha = u_{\alpha\beta} a_\beta + v_{\alpha\beta} a^+_\beta\,, \tag{3.1.27}$$

$$b^+_\alpha = u^*_{\alpha\beta} a^+_\beta + v^*_{\alpha\beta} a_\beta\,, \tag{3.1.28}$$

$$\tag{3.1.29}$$

obeying the same (anti)commutation relations:

$$[b_\alpha, b^+_\beta]_\pm = \delta_{\alpha\beta}\,, \tag{3.1.30}$$

$$[b_\alpha, b_\beta]_\pm = [b^+_\alpha, b^+_\beta]_\pm = 0\,. \tag{3.1.31}$$

Mathematically, in the fermionic case, such a diagonalization is always possible. In the bosonic case, one needs to require that the quadratic form (3.1.25) is positive-definite (if one treats a^+ and a as complex-conjugate numbers). Physically, any bosonic Hamiltonian must be positive-definite, since otherwise its spectrum would be unbounded from below.

We do not prove here this theorem about diagonalization: you can find a detailed proof and discussion in the book of Blaizot and Ripka [BR].

The practical algorithm for diagonalizing a quadratic Hamiltonian (3.1.25) consists in writing a linear combination (3.1.29) and then solving the eigenvalue problem

$$[H, b^+] = \varepsilon b^+ \,. \tag{3.1.32}$$

Note that if the Hamiltonian conserves the number of particles (i.e., $H_{12} = H_{21} = 0$), then we can put $v = 0$, and the problem reduces to diagonalizing a single-particle Hamiltonian.

3.1.5 Wick theorem

Consider a quadratic Hamiltonian (3.1.25) (bosonic or fermionic). Then, for any set of operators $A_1, \ldots, A_M$ linear in a and a^+, at any temperature, the thermal average of the product

$$\langle A_1 \ldots A_M \rangle_T = \frac{\mathrm{tr}\left(e^{-\beta H} A_1 \ldots A_M\right)}{\mathrm{tr}\left(e^{-\beta H}\right)} \tag{3.1.33}$$

can be expressed in terms of pairwise averages:

$$\langle A_1 \ldots A_M \rangle_T = \sum (\pm 1)^\sigma \langle A_{i_1} A_{i_2} \rangle_T \ldots \langle A_{i_{M-1}} A_{i_M} \rangle_T \,, \tag{3.1.34}$$

where the sum is taken over all partitions (often called *contractions*) of the operators A_i into $M/2$ pairs. The ordering of the operators witin each pair must coincide with the ordering of the operators in the left-hand side (i.e., in the above notation, $i_1 < i_2$, $i_3 < i_4$, etc.). In the fermionic case, the sign $(-1)^\sigma$ is the parity of the permutation $(1, \ldots, M) \mapsto (i_1, \ldots, i_M)$. There are no sign factors in the bosonic case.

For a proof of the Wick theorem, see the book [BR] or M. Gaudin, Nucl. Phys. **15**, 89 (1960) [in French].

Example: Wick theorem for a product of $M = 4$ operators.

$$\langle A_1 A_2 A_3 A_4 \rangle_T = \langle A_1 A_2 \rangle_T \langle A_3 A_4 \rangle_T \pm \langle A_1 A_3 \rangle_T \langle A_2 A_4 \rangle_T + \langle A_1 A_4 \rangle_T \langle A_2 A_3 \rangle_T \,. \tag{3.1.35}$$

Wick theorem can be applied for

1. Calculations of correlation functions in a free-particle system

2. Including interactions perturbatively, which leads to a diagrammatic expansion.

Problem Set 4

Problem 4.1

(a) Verify the following identities for commutators $[A, B] = AB - BA$ and anticommutators $\{A, B\} = AB + BA$:

$$[A, BC] = [A, B]\, C + B\, [A, C] = \{A, B\}\, C - B\, \{A, C\}$$
$$\{A, BC\} = [A, B]\, C + B\, \{A, C\} = \{A, B\}\, C - B\, [A, C]$$

These relations [called the distributive law for commutators] are helpful for commuting products of creation and annihilation operators.

Note: always use commutators for bosonic operators and anticommutators for fermionic operators. Products of an even number of fermionic operators count as bosonic operators.

(b) Verify by an explicit calculation that the free-particle Hamiltonian

$$H = \int \frac{d^3k}{(2\pi)^3}\, a_k^+ (\varepsilon_k - \mu) a_k \,,$$

commutes with the particle-number operator

$$N = \int \frac{d^3k}{(2\pi)^3}\, a_k^+ a_k \,,$$

Hint: the calculation can be simplified by using the relations derived in part (a).

Problem 4.2

Consider one fermionic level. The Fock space consists of two states: empty $|0\rangle$ (0 particles) and occupied $|1\rangle$ (1 particle). The fermionic creation and annihilation operators act as

$$a\,|0\rangle = 0\,, \qquad a\,|1\rangle = |0\rangle\,,$$
$$a^+\,|0\rangle = |1\rangle\,, \qquad a^+\,|1\rangle = 0\,.$$

(a) Verify the anticommutation relations

$$\{a, a^+\} = 1\,, \qquad \{a, a\} = \{a^+, a^+\} = 0\,.$$

(b) Now suppose that the particle has a positive energy, and therefore at zero temperature the system is in the ground state $|0\rangle$. Verify that, in this state, the Wick theorem (3.1.35) holds for the product of four operators aa^+aa^+:

$$\langle aa^+aa^+\rangle_{T=0} = \ldots$$

(c) At a finite temperature, the system will be at a statistical mixture of two states: the state $|0\rangle$ with a probability p and the state $|1\rangle$ with the probability $1 - p$. Verify that the Wick theorem for the expectation value $\langle aa^+aa^+\rangle$ still holds.