5 The formalism of second quantization

Systems consisting of many identical particles form the prevailing part of the physical world. Typical examples are e.g. a solid consisting of electrons in a lattice of ions or a heavy nucleus built out of many nucleons. While the classical treatement of identical particles does not differ from the treatement of nonidentical ones - classical theory relies on the assumption that the motion of each individual particle can always be followed[1] - indistinguishability of identical[2] particles imposes additional requirements on the quantum theory of systems consisting of identical, indistinguishable particles: vectors representing their states in a Hilbert space must have definite symmetry properties with respect to interchanging labels of indistinguishable particles. Imposing this requirement in the ordinary approach based on the multi-particle wave function is rather cumbersome. In this section presented is a convenient formulation - called "second quantization" - of quantum mechanics of systems composed of many identical indistinguishable particles, allowing to automatically take into account these symmetry requirements. Its most characteristic feature is the use of the creation and annihilation operators in terms of which any operator acting in the relevant Hilbert space can be expressed and the action of which on vectors representing system's states is particularly simple. The true essence of this formulation is however the introduction of the "big" Hilbert space $\mathcal{H}$ the vectors of which can represent states of an arbitrary, also infinite, and even of indefinite numbers of particles. (It is this Hilbert space in which the action of the creation and annihilation operators is naturally defined). Quantum mechanics formulated using this formalism, when restricted to a subspace of $\mathcal{H}$ corresponding to a fixed number N of particles (this is possible if the system's Hamiltonian commutes with the particle number operator), can be made fully equivalent to the quantum mechanics based on the N-particle Schrödinger equation supplemented with the appropriate symmetry requirements. However, the second quantization also opens up essentially new possibilities.[3] First of all, by allowing to form in the "big" Hilbert space $\mathcal{H}$ superpositions of vectors representing different (also infinite) numbers of particles, second quantization enables one to consider systems of interacting relativistic particles because, as will be demonstrated in Chapter 7, Poincaré covariance of transition amplitudes characterizing scattering processes (covariance of the S-matrix) necessarily enforces nonconservation of the number of particles by the time evolution (relativistic Hamiltonians cannot commute with particle number operators). Second quantization constitutes therefore a link between the ordinary quantum mechanics of many-particle systems and the relativistic quantum field theory. Moreover, nonseparability of this "big"

[1] Indistinguishability of identical particles must, nevertheless, be taken into account in classical statistical mechanics to avoid the Gibbs paradox, that is nonextensiveness of entropy.

[2] One should distinguish the notions of identity and indistinguishability: N oscillators of the same type are identical but even in the quantum theory are treated as distinguishable.

[3] In view of this the sometimes encountered statement that "second quantization" is simply a misnomer, because it is just another formulation of the ordinary quantum mechanics based on the multi-particle Schrödinger equation (and not a new conceptual step, similar to the transition from classical to quantum mechanics) does not seem fully justified.

Hilbert space $\mathcal{H}$ (the lack of a countable basis) leads to the existence of infinitely many unitarily inequivalent representations by operators acting in it of the basic commutation rules (of the abstract operator algebra) defining the quantum theory. In other words, the "big" Hilbert space $\mathcal{H}$ furnishes a reducible representation of the abstract operator algebra. Any such representation defines in $\mathcal{H}$ a separable subspace called Fock space and it is the dynamics of the considered physical system and the imposed boundary conditions which select the proper Fock space in which states of the system physically accessible in the "thermodynamic limit" (i.e. when the number of degrees of freedom becomes infinite) are represented. This profound property of the big Hilbert space $\mathcal{H}$ is at the heart of the possibility of capturing within this formulation such phenomena as the Bose-Einstein condensation in systems of bosons or spontaneous ("parametrical" or dynamical) breaking of various symmetries in nonrelativistic as well as in relativistic systems.

5.1 Multi-particles Hilbert spaces

Consider first a system of N *distinguishable* particles (for example all having different masses). The Hilbert space of a system of N mutually interacting such particles is the N-fold tensor product $\mathcal{H}^{(N)} = \mathcal{H}_N^{(1)} \otimes \ldots \otimes \mathcal{H}_1^{(1)}$ of one-particle Hilbert spaces of individual particles;[4] it is spanned by the state-vectors having the form of the tensor product

$$|\Psi\rangle = |\psi_N\rangle \otimes \ldots \otimes |\psi_2\rangle \otimes |\psi_1\rangle \,, \tag{5.1}$$

in which each of the individual state-vectors $|\psi_k\rangle$, $k = 1, \ldots, N$, belongs to the separate one-particle Hilbert space $\mathcal{H}_k^{(1)}$ of the k-th particle. The scalar product of two such states of N particles is simply given by the formula

$$\langle\Phi|\Psi\rangle = \langle\phi_N|\psi_N\rangle \cdot \ldots \cdot \langle\phi_1|\psi_1\rangle \,, \tag{5.2}$$

in which each of the factors $\langle\phi_k|\psi_k\rangle$ is the scalar product in the respective one-particle space $\mathcal{H}_k^{(1)}$. If the normalized vectors $|l_k\rangle$, $l_k = 1, 2, \ldots, \infty$ form a countable orthonormal (in the sense of the respective scalar products) basis of the k-th particle Hilbert space $\mathcal{H}_k^{(1)}$, the product state-vectors

$$|l_N, \ldots, l_2, l_1\rangle \equiv |l_N\rangle \otimes \ldots \otimes |l_2\rangle \otimes |l_1\rangle \,, \tag{5.3}$$

form the associated countable basis of $\mathcal{H}^{(N)}$. For example, if all N considered particles are spinless (or their spin degrees of freedom are neglected altogether) and can move in the infinite three-dimensional space, the normalized to unity state-vectors $|(l^x l^y l^z)_k\rangle$ or

[4] All these one-particle Hilbert spaces fall, in the nonrelativistic case, into classes of identical (isomorphic) spaces classified by the spin of the particle they correspond to. One-particle Hilbert spaces $\mathcal{H}^{(1)}$ of particles of spin s are all isomorphic to the (2s+1)-fold Cartesian product of the $L_2(\mathbb{R}^3)$ spaces (treated as vector spaces over $\mathbb{C}$) i.e. to the tensor product of $L_2(\mathbb{R}^3)$ and a $2s+1$ dimensional vector space over $\mathbb{C}$.

$|(l^r l^\theta l^\varphi)_k\rangle$ (l^θ and l^φ stand here, somewhat unconventionally, for the orbital momentum quantum numbers) of the three-dimensional harmonic oscillator (of arbitrary frequencies ω_k which can be different for each of the different one-particle Hilbert spaces $\mathcal{H}_k^{(1)}$ and within each $\mathcal{H}_k^{(1)}$ could even be different for diffent directions) can be taken for $|l_k\rangle$ (l is then a three-index $l^x l^y l^z$ or $l^r l^\theta l^\varphi$), because in the position representation any normalizable wave function $\psi(\mathbf{x})$ can be written as a superposition of the functions $\psi_{(l^x l^y l^z)}(\mathbf{x}) = \langle \mathbf{x}|l^x l^y l^z\rangle = \psi_{l^x}(x)\psi_{l^y}(y)\psi_{l^z}(z)$ or $\psi_{(l^r l^\theta l^\varphi)_k}(r,\theta,\varphi) = \langle r,\theta,\varphi|l^r l^\theta l^\varphi\rangle = \psi_{l^r}(r)Y_{l^\theta l^\varphi}(\theta,\varphi)$, where $Y_{l^\theta l^\varphi}(\theta,\varphi)$ are the spherical harmonics. Similarly, if the system of N particles is enclosed in a box of volume $V = L^3$ (and periodic boundary conditions are imposed on the wave function of each individual particle), the vectors

$$|\mathbf{p}_N,\ldots,\mathbf{p}_2,\mathbf{p}_1\rangle = |\mathbf{p}_N\rangle\otimes\ldots\otimes|\mathbf{p}_2\rangle\otimes|\mathbf{p}_1\rangle\,, \tag{5.4}$$

with $\mathbf{p}_k = (2\pi/L)\mathbf{n}_k$ (in this case $\psi_{\mathbf{p}}(\mathbf{x}) = \langle\mathbf{x}|\mathbf{p}\rangle = (1/\sqrt{V})\exp(i\mathbf{p}\cdot\mathbf{x})$), can be taken for the basis of $\mathcal{H}^{(N)}$. That the vectors (5.3) or (5.4) form a (countable) basis of $\mathcal{H}^{(N)}$ follows from the simple observation that any normalizable wave function $\Psi(\mathbf{x}_1,\ldots,\mathbf{x}_N)$ of N particles can be written as a superposition

$$\Psi(\mathbf{x}_N,\ldots,\mathbf{x}_1) = \sum_{l_N}\ldots\sum_{l_1} c_{l_N\ldots l_1}\,\psi_{l_N}(\mathbf{x}_N)\cdot\ldots\cdot\psi_{l_1}(\mathbf{x}_1)\,,$$

of the products $\psi_{l_N}(\mathbf{x}_N)\cdot\ldots\cdot\psi_{l_1}(\mathbf{x}_1)$ with

$$\sum_{l_N}\ldots\sum_{l_1}|c_{l_N\ldots l_1}|^2 < \infty\,.$$

The completeness relation then reads ($\hat{1}^{(N)}$ is the unit operator in $\mathcal{H}^{(N)}$)

$$\hat{1}^{(N)} = \sum_{l_N}\ldots\sum_{l_1}|l_N,\ldots,l_1\rangle\langle l_1,\ldots,l_N|\,. \tag{5.5}$$

It is also possible, as it is customary in one-particle quantum mechanics, to take for the basis of $\mathcal{H}^{(N)}$ the generalized (non-normalizable) vectors[5]

$$|\mathbf{x}_N,\ldots,\mathbf{x}_2,\mathbf{x}_1\rangle \equiv |\mathbf{x}_N\rangle\otimes\ldots\otimes|\mathbf{x}_2\rangle\otimes|\mathbf{x}_1\rangle\,, \tag{5.6}$$

te scalar product of which is

$$\langle\mathbf{y}_1,\ldots,\mathbf{y}_N|\mathbf{x}_N,\ldots,\mathbf{x}_1\rangle = \delta^{(3)}(\mathbf{y}_N-\mathbf{x}_N)\cdot\ldots\cdot\delta^{(3)}(\mathbf{y}_1-\mathbf{x}_1)\,, \tag{5.7}$$

or the generalized (if the theory is formulated in the infinite space) vectors

$$|\mathbf{p}_N,\ldots,\mathbf{p}_2,\mathbf{p}_1\rangle \equiv |\mathbf{p}_N\rangle\rangle\otimes\ldots\otimes|\mathbf{p}_2\otimes|\mathbf{p}_1\rangle\,, \tag{5.8}$$

[5]More precisely covectors, that is elements of the dual space.

with the scalar product

$$\langle \mathbf{q}_1, \ldots, \mathbf{q}_N | \mathbf{p}_N, \ldots, \mathbf{p}_1 \rangle = (2\pi)^3 \delta^{(3)}(\mathbf{q}_N - \mathbf{p}_N) \cdot \ldots \cdot (2\pi)^3 \delta^{(3)}(\mathbf{q}_1 - \mathbf{p}_1) \,. \tag{5.9}$$

The completeness relations in these cases read

$$\begin{aligned} \hat{1}^{(N)} &= \int d^3\mathbf{x}_N \ldots \int d^3\mathbf{x}_1 \, |\mathbf{x}_N, \ldots, \mathbf{x}_1\rangle\langle \mathbf{x}_1, \ldots, \mathbf{x}_N| \\ &= \int \frac{d^3\mathbf{p}_N}{(2\pi)^3} \ldots \int \frac{d^3\mathbf{p}_1}{(2\pi)^3} \, |\mathbf{p}_N, \ldots, \mathbf{p}_1\rangle\langle \mathbf{p}_1, \ldots, \mathbf{p}_N| \,. \end{aligned} \tag{5.10}$$

Internal degrees of freedom (spin) can be easily incorporated into this formalism by including the spin labels $\sigma_k = -s_k, \ldots, +s_k$ in the labels l_k of states of indistinguishable particles or using the variables $(\mathbf{x}_k, \sigma_k)$ or $(\mathbf{p}_k, \sigma_k)$ instead of $\mathbf{x}_k$ or $\mathbf{p}_k$.

The scalar product[6] of a state-vector of the form (5.1) with the basis vectors (5.6) gives then the N-particle wave function

$$\Psi(\mathbf{x}_N, \ldots, \mathbf{x}_1) = \langle \mathbf{x}_1, \ldots, \mathbf{x}_N | \Psi \rangle = \psi_N(\mathbf{x}_N) \cdot \ldots \cdot \psi_1(\mathbf{x}_1) \,. \tag{5.11}$$

The wave-function (more generally, the state-vector) of a linear superposition of the state-vectors of the form (5.1) or (5.3) cannot in general be written as a product of one-particle wave functions (one-particle state-vectors); states represented by vectors $|\Psi\rangle$ which do not factorize as (5.1) are called *entangled* states and play crucial roles in modern quantum optics and quantum information theory.

Consider now a system consisting of N identical and *indistinguishable* particles of one type,[7] bosons or fermions (continuing to omit in the notation their spin labels). In this case the requirement of the Bose-Einstein or Fermi-Dirac statistics has to be implemented: state-vectors should be symmetric with respect to interchanges of variables of any two identical bosons and antisymmetric with respect to interchanges of variables of any two fermions.[8] This requirement has to be added as an extra rule selecting possible state-vectors in $\mathcal{H}^{(N)}$ spanned by vectors of the form (5.1). In the framework of the nonrelativistic quantum mechanics it cannot be given any sound foundation; the Bose-Einstein (Fermi-Dirac) statistics obeyed by systems of many identical particles having integer (half-integer) spin must simply be regarded as a phenomenological input.[9] Justification of this celebrated *spin-statistics connection* comes only from the relativistic quantum field theory; this will become evident in Chapter 8. This spin-statistics connection is implemented

[6] Or, more precisely, the value of the covector (5.6) on the vector (5.1).

[7] Generalization of the formalism to several types of identical and indistinguishable particles is straightforward.

[8] In two spatial dimensions there are more possibilities.

[9] The Planck sectrum of the black body radiation can be taken for the empirical evidence that photons obey the Bose-Einstein statistics (are bosons); similarly, stability of matter is the best physical indication that electrons (and nucleons) obey the Pauli exclusion principle (are fermions).

by defining the state-vectors $|\psi_1, \psi_2, \dots \psi_N\rangle$ spanning the Hilbert space $\mathcal{H}^{(N)}$ of a system of N identical and indistinguishable particles in terms of the one-particle state-vectors by the formula

$$|\psi_N, \dots, \psi_2, \psi_1\rangle = \frac{1}{\sqrt{N!}} \sum_P \zeta^P |\psi_{P(N)}\rangle \otimes \dots \otimes |\psi_{P(2)}\rangle \otimes |\psi_{P(1)}\rangle \,, \tag{5.12}$$

in which $|\psi_i\rangle$, $i = 1, \dots, N$ are some arbitrary one-particle state-vectors belonging to a one-particle space $\mathcal{H}^{(1)}$ and P denotes permutations of the labels of indistinguishable particles. We have introduced here the symbol ζ

$$\zeta = \begin{cases} +1 & \text{if the particles are bosons} \\ -1 & \text{if the particles are fermions} \end{cases},$$

and by ζ^P understand, if the particle are fermions, the sign of the permutation P. ($\zeta^P = 1$ if particles are bosons). For example, if there are $N = 2$ indistinguishable particles which can be in two one-particle states $|a\rangle$ and $|b\rangle$, the prescription (5.12) yields the following three state-vectors

$$\begin{aligned} |a, b\rangle &= \frac{1}{\sqrt{2!}} \left(|a\rangle \otimes |b\rangle + |b\rangle \otimes |a\rangle \right), \\ |a, a\rangle &= \sqrt{2}\, |a\rangle \otimes |a\rangle \,, \\ |b,\, b\rangle &= \sqrt{2}\, |b\rangle \otimes |b\rangle \,, \end{aligned} \tag{5.13}$$

if these particles are indistinguishable bosons and only one state-vector

$$|a, b\rangle = \frac{1}{\sqrt{2!}} \left(|a\rangle \otimes |b\rangle - |b\rangle \otimes |a\rangle \right),$$

if they are indistinguishable fermions. The scalar product (obtained by extending by linearity the scalar product (5.2)) of state-vectors of the form (5.12) is

$$\begin{aligned} \langle \varphi_1, \dots, \varphi_N | \psi_N, \dots, \psi_1 \rangle &= \frac{1}{N!} \sum_P \sum_Q \zeta^P \zeta^Q \langle \varphi_{Q(N)} | \psi_{P(N)} \rangle \cdot \dots \cdot \langle \varphi_{Q(1)} | \psi_{P(1)} \rangle \\ &= \frac{1}{N!} \sum_R \sum_Q \zeta^R \langle \varphi_N | \psi_{R(N)} \rangle \cdot \dots \cdot \langle \varphi_1 | \psi_{R(1)} \rangle \\ &= \sum_R \zeta^R \langle \varphi_N | \psi_{R(N)} \rangle \cdot \dots \cdot \langle \varphi_1 | \psi_{R(1)} \rangle \,, \end{aligned} \tag{5.14}$$

(in the second step a new permutation $R = PQ^{-1}$ has been defined, its sign is $\zeta^R = \zeta^P \zeta^Q$). If the particles are fermions, (5.14) is just the determinant

$$\langle \varphi_1, \dots, \varphi_N | \psi_N, \dots, \psi_1 \rangle = \begin{vmatrix} \langle \varphi_N | \psi_N \rangle & \dots & \langle \varphi_N | \psi_1 \rangle \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \langle \varphi_1 | \psi_N \rangle & \dots & \langle \varphi_1 | \psi_1 \rangle \end{vmatrix},$$

while if they are bosons, the scalar product differs from the determinant by having all signs in the Laplace expansion positive. Notice that in the example (5.13) of $N = 2$ particles the state-vectors $|a, a\rangle$ and $|b, b\rangle$ of bosons are not properly normalized even if the one-particle state-vectors $|a\rangle$ and $|b\rangle$ are orthonormal: $\langle a, a|a, a\rangle = \langle b, b|b, b\rangle = 2$.

Let us now construct a basis of the (anti)symmetrized N-particle Hilbert space $\mathcal{H}^{(N)}$. Let $|l\rangle = |1\rangle, |2\rangle, \ldots$ be a countable, complete set of normalizable and orthonormal one-particle state-vectors (forming a basis of the proper Hilbert space $\mathcal{H}^{(1)}$ of a single particle) labeled by $l = 1, 2, \ldots, \infty$, that is such that

$$\langle l'|l\rangle = \delta_{l'l}\,, \qquad\qquad \sum_l |l\rangle\langle l| = \hat{1}^{(1)}\,.$$

Again, if the system of spinless particles is enclosed in a box of finite volume L^3, the momentum operator eigenvectors $|\mathbf{k}\rangle$ with wave-vectors $\mathbf{k} = (2\pi/L)\mathbf{n}$ can be taken for $|l\rangle$'s; in the infinite volume one can take for $|l\rangle$ the three-dimensional harmonic oscillator state-vectors $|l^x l^y l^z\rangle$ (or the vectors $|l^r l^\theta l^\varphi\rangle$ in the angular momentum representation). If particles have a nonzero spin s, the appropriate spin label $\sigma = -s, \ldots, +s$ must be included in the label l. As an orthonormal basis of the (proper) Hilbert space $\mathcal{H}^{(N)}$ of N indistinguishable bosons one can then take the vectors[10]

$$\frac{1}{\sqrt{n_1!\,n_2!\ldots}}\,|l_N, \ldots, l_2, l_1\rangle \qquad \text{with} \qquad l_1 \le l_2 \le \ldots \le l_N\,, \tag{5.15}$$

where $|l_1, l_2, \ldots, l_N\rangle$ are the vectors of the form (5.12) and n_1 is the number of l_1 occurrences in the sequence $l_1, l_2, \ldots, l_N$, n_2 is the number of l_2 occurrences, etc. Of course, $n_1 + n_2 + \ldots = N$. As an ortonormal basis of the Hilbert space $\mathcal{H}^{(N)}$ of N indistinguishable fermions one takes instead the vectors (the label l in this case must necessarily include also a spin variable)

$$|l_N, \ldots, l_2, l_1\rangle \qquad \text{with} \qquad l_1 < l_2 < \ldots < l_N\,. \tag{5.16}$$

If in the example (5.13) of $N = 2$ bosons the whole $\mathcal{H}^{(1)}$ is spanned by only two vectors $|a\rangle$ and $|b\rangle$, the basis of $\mathcal{H}^{(2)}$ can be formed by the vectors:

$$\frac{1}{\sqrt{2!}}\,|a, a\rangle\,, \qquad \frac{1}{\sqrt{2!}}\,|b, b\rangle\,, \qquad |a, b\rangle\,.$$

The factors of $1/\sqrt{2!}$ included in the first two basis vectors ensure their proper normalization. More generally, since when particles are bosons (cf. (5.14))

$$\langle l'_1, \ldots l'_N|l_N, \ldots, l_1\rangle = \sum_P \langle l'_N|l_{P(N)}\rangle \cdot \ldots \cdot \langle l'_1|l_{P(1)}\rangle\,, \tag{5.17}$$

[10]It is assumed that the labels l of the basis state-vectors $|l\rangle$ forming a countable set, can be ordered in some natural way.

we see that the scalar product is nonzero only if each l'_i finds its counterpart among the l_i's. If there are n_i occurrences of a particular l'_i in the sequences $l'_1, \ldots l'_N$ and $l_1, \ldots, l_N$ (which is possible only if the considered particles are bosons), then there are $n_i!$ equal and nonzero terms contributing to the sum in (5.17). The factors $1/\sqrt{n_i!}$ in the definition of the basis state-vectorss (5.15) of N indistinguishable bosons cancel then the factors $n_i!$ arising in the scalar product.

The completeness relation in the space of N identical bosons or fermions can be conveniently written in the form

$$\frac{1}{N!}\sum_{l_N}^{\infty}\ldots\sum_{l_1}^{\infty}|l_N,\ldots,l_1\rangle\langle l_1,\ldots l_N| = \hat{1}^{(N)}\,, \tag{5.18}$$

in which the orderings of l_i's appearing in the definitions of the basis vectors (5.15) and (5.16) are *not* respected. Instead, the factor $1/N!$ ensures the cancellation of the multiple counting of the same states. To understand better its working, let us take three indistinguishable bosons, each of which can be in one of the two states $|a\rangle$ or $|b\rangle$ and consider the contribution of the basis vector $(1/\sqrt{2!}\,)|a,a,b\rangle$ to the completeness relation (5.18). In the decomposition of the unit operator only a single term of the form

$$\hat{1}^{(3)} = \ldots + \frac{1}{2!}\,|a,a,b\rangle\langle b,a,a| + \ldots$$

should be present. The prescription (5.18) gives

$$\hat{1}^{(3)} = \ldots + \frac{1}{3!}\Big(|a,a,b\rangle\langle b,a,a| + |a,b,a\rangle\langle a,b,a| + |b,a,a\rangle\langle a,a,b|\Big) + \ldots$$

which is the same taking into account the symmetry of the state-vectors. With this convention it is possible to work also with the bases formed out of generalized (i.e. non-normalizable) symmetrized or antisymmetrized state-vectors like e.g. the (here we make the spin labels explicit) $|\mathbf{p}_1\sigma_1,\ldots,\mathbf{p}_N\sigma_N\rangle$ ones in the infinite volume; the unit operator $\hat{1}^{(N)}$ is then decomposed as:

$$\hat{1}^{(N)} = \frac{1}{N!}\int\frac{d^3\mathbf{p}_N}{(2\pi)^3}\ldots\frac{d^3\mathbf{p}_1}{(2\pi)^3}\sum_{\sigma_N}\ldots\sum_{\sigma_1}|\mathbf{p}_N\sigma_N,\ldots,\mathbf{p}_1\sigma_1\rangle\langle\mathbf{p}_1\sigma_1,\ldots,\mathbf{p}_N\sigma_N|\,. \tag{5.19}$$

If the system is enclosed in a box of volume $V = L^3$ and periodic boundary conditions are imposed, the integrals over $d^3\mathbf{p}_i/(2\pi)^3$ are replaced by discrete sums $\sum_{\mathbf{p}_i}$ - see the footnote below the formula (5.40).

It is important to stress that any two bases like (5.15) (like (5.16)) of the Hilbert space $\mathcal{H}^{(N)}$ of N bosons (N fermions) formed out of two different bases $|l\rangle$ and $|\tilde{l}\rangle$ of the one-particle space $\mathcal{H}^{(1)}$ are unitarily equivalent. This means that any vector of the basis (5.15) (of the basis (5.16)) can be written as a linear combination of the vectors $|\tilde{l}_N,\ldots,\tilde{l}_2,\tilde{l}_1\rangle/\sqrt{\tilde{n}_1!\tilde{n}_2!\ldots}$ (of the vectors $|\tilde{l}_N,\ldots,\tilde{l}_2,\tilde{l}_1\rangle$). In other words, any vector of the

basis (5.15) (of the basis (5.16)) has nonzero scalar products (in $\mathcal{H}^{(N)}$) with at least a finite number of the vectors $|\tilde{l}_N, \ldots, \tilde{l}_2, \tilde{l}_1\rangle/\sqrt{\tilde{n}_1!\tilde{n}_2!\ldots}$ (of the vectors $|\tilde{l}_N, \ldots, \tilde{l}_2, \tilde{l}_1\rangle$).

All this works in the same way with arbitrary $N \geq 1$. It proves convenient to formally include the $N = 0$ case, by adopting the convention that the $\mathcal{H}^{(0)}$ Hilbert space is spanned by a single (normalized to unity) vector $|\text{void}\rangle$ in most texts misleadingly called the "vacuum", or, less misleadingly, the Fock vacuum vector.[11] That is, the zero-particles Hilbert space $\mathcal{H}^{(0)}$ is one-dimensional (all other Hilbert spaces with $N \geq 1$ are all countably infinite dimensional). One then formally introduces the "big" Hilbert space $\mathcal{H}$

$$\mathcal{H} = \oplus_{N=0}^{\infty} \mathcal{H}^{(N)} \,, \tag{5.20}$$

the vectors of which have the form

$$\mathcal{H} \ni |\Psi\rangle = |\Psi^{(0)}\rangle + |\Psi^{(1)}\rangle + |\Psi^{(2)}\rangle + \ldots \tag{5.21}$$

with $|\Psi^{(N)}\rangle$ belonging to $\mathcal{H}^{(N)}$ and $|\Psi^{(0)}\rangle = a|\text{void}\rangle$. This construction is not so unnatural as it might seem at first sight. In a typical accelerator experiment a well defined two-particle state is prepared, say $|e^+e^-\rangle$ in an electron-positon (e^+e^-) collision, and, after the interaction (collision), the state of the system is represented by a vector which in fact is a superposition of vectors belonging to different multi-particle spaces $\mathcal{H}^{(N)}$, corresponding to all possible many-particle states that can be created in this collision (of course selection rules following from e.g the electric charge conservation, impose here some constraints). Therefore the final state is a (in general infinite) superposition of vectors corresponding to different numbers of particles[12]

$$|\Psi\rangle = a\,|e^+e^-\rangle + b\,|e^+e^-\gamma\rangle + c\,|q\bar{q}\rangle + d\,|q\bar{q}g\rangle + e\,|q\bar{q}q\bar{q}\rangle + \ldots$$

where a, b, c, d, e are some complex numbers. Registration of a concrete final state by the detector has the effect of reducing this state-vector of the system. Thus, at least in physics of relativistic particles in which (as will be seen) particle number conservation is impossible, the big Hilbert space (5.20) is the proper arena in which to formulate a theory of physical processes. The possibility of treating systems with variable number

[11] We denote this vector $|\text{void}\rangle$ in order to distinguish this "technical" "no particle" vector from the state-vectors $|\Omega_0\rangle$ and $|\Omega\rangle$, commonly called "vacua", which will be the true ground-state vectors, that is the lowest energy eigenvectors, of the free H_0 and interacting $H = H_0 + V_{\text{int}}$ Hamiltonians of systems of free or interacting particles (or fields), respectively.

[12] This argument is heuristic and may be somewhat misleading. As a matter of facts, the vector $|e^+e^-\rangle$ representing the real initial state is an *in* state (analogous to the ones defined at the end of Section 1.3) while the vectors onto which one projects it to find the probability of registering a particular final state are all *out* vectors also representing definite sets of detectable particles. In general both, the *in* and *out* vectors, are related in a complicated way to the basis states formed as tensor products of one-particle state-vectors (representing states of individual underlying "fundamental" particles which should not, at least in the relativistic theory, be identified whith ones prepared and detected in high-energy physics experiments). Nevertheless, an *in* vector like $|e^+e^-\rangle$, still is a superposition of infinitely many *out* vectors representing definite sets of particles in the final state. This will become more clear in Section 7.3.

of particles is useful also in nonrelativistic physics. Investigating statistical properties of physical systems one usually prefers to work with the Grand Canonical Ensemble, corresponding to the system the number of particles of which is allowed to fluctuate;[13] the big Hilbert space (5.20) is then the proper space in which acts the statistical operator $\hat{\rho}$ of the ensemble. Finally, the possibility of forming superpositions of state-vectors corresponding to different numbers of particles is crucial for theories of various phenomena like e.g. superconductivity in which, if the thermodynamic limit $N \to \infty$, $V \to \infty$ with $\rho = N/V$ kept fixed is to be taken, some symmetries must become spontaneously broken.

In the "big" Hilbert space (5.20) the scalar product is defined as

$$\langle \Phi | \Psi \rangle = \sum_{N=0}^{\infty} \langle \Phi^{(N)} | \Psi^{(N)} \rangle \,, \tag{5.22}$$

that is, vectors belonging entirely to $\mathcal{H}^{(N)}$ and $\mathcal{H}^{(M)}$ are declared to be orthogonal if $N \neq M$. The formal (for reasons which we explain below) completeness relation in $\mathcal{H}$ reads

$$\hat{1} = |\text{void}\rangle\langle\text{void}| + \sum_{N=1}^{\infty} \frac{1}{N!} \sum_{l_N,\ldots,l_1} |l_N,\ldots,l_1\rangle\langle l_1,\ldots,l_N| \,. \tag{5.23}$$

For example, in the position basis it takes the form (we again make the spin labels α - which at least in nonrelativistic mechanics can be given a meaning in terms of a one-particle spin operator - explicit here)

$$\hat{1} = |\text{void}\rangle\langle\text{void}| + \sum_{N=1}^{\infty} \frac{1}{N!} \int d\mathbf{x}_N \ldots \int d\mathbf{x}_1 \sum_{\sigma_N,\ldots,\sigma_1} |\mathbf{x}_N\sigma_N,\ldots,\mathbf{x}_1\sigma_1\rangle\langle\mathbf{x}_1\sigma_1,\ldots,\mathbf{x}_N\sigma_N|, \tag{5.24}$$

and formally the most general form of a state belonging to $\mathcal{H}$ has the form

$$|\Psi\rangle = a|\text{void}\rangle + \sum_{N=1}^{\infty} \frac{1}{N!} \int d\mathbf{x}_N \ldots \int d\mathbf{x}_1 \sum_{\sigma_N,\ldots,\sigma_1} |\mathbf{x}_N\sigma_N,\ldots,\mathbf{x}_1\sigma_1\rangle \Psi^{(N)}_{\sigma_N,\ldots,\sigma_1}(\mathbf{x}_N,\ldots,\mathbf{x}_1) \,,$$

in which $\Psi^{(N)}_{\sigma_N,\ldots,\sigma_1}(\mathbf{x}_N,\ldots,\mathbf{x}_1) \equiv \langle \mathbf{x}_N\sigma_N,\ldots,\mathbf{x}_1\sigma_1|\Psi^{(N)}\rangle$ is the wave function of the N-particle component of the state $|\Psi\rangle$. The function $\Psi^{(N)}_{\sigma_N,\ldots,\sigma_1}(\mathbf{x}_N,\ldots,\mathbf{x}_1)$ of a system of N bosons is totally symmetric while a similar function of a system of N fermions is totally antisymmetric in all groups of its arguments corresponding to individual particles. If $|\Psi^{(N)}\rangle$ is of the form (5.12) then

$$\Psi^{(N)}_{\sigma_N,\ldots,\sigma_1}(\mathbf{x}_N,\ldots,\mathbf{x}_1) = \begin{vmatrix} \langle \mathbf{x}_N\sigma_N|\psi_N\rangle & \ldots & \langle \mathbf{x}_N\sigma_N|\psi_1\rangle \\ \cdot & \ldots & \cdot \\ \cdot & \ldots & \cdot \\ \cdot & \ldots & \cdot \\ \langle \mathbf{x}_1\sigma_1|\psi_N\rangle & \ldots & \langle \mathbf{x}_1\sigma_1|\psi_1\rangle \end{vmatrix}_{\zeta} , \tag{5.25}$$

[13] To be clear: it is the number of particles of the real physical system that can fluctuate due to its contact with the surrounding; the number of particles of each of the systems forming the corresponding Grand Canonical Ensemble is fixed (but it is different in different members of the ensemble).

where the symbol ζ means the determinant in the case of fermions (called the *Slater determinant*) and for bosons the so-called *permanent* of the matrix which is computed similarly as the determinant except for taking everywhere positive signs (the precise definition is given by (5.14) with φ_i replaced by $\mathbf{x}_i, \sigma_i$).

The seemingly innocuous formal step of forming the Hilbert space $\mathcal{H}$ as the direct sum of infinitely many Hilbert spaces $\mathcal{H}^{(N)}$ has a profound mathematical consequence: the constructed space is not separable[14] that is, it has no countable basis - as can be shown, the power of the set of basis vectors (5.15) or (5.16) with arbitrarily large N is equal to the power of the continuum. Infinitely many different separable Hilbert subspaces (which all can be given the structure of the so-called Fock space which will be introduced shortly), with countable bases can be chosen in $\mathcal{H}$ (5.20), all of which, if no cutoff of some sort (effectively reducing the number of degrees of freedom being taken into account) is imposed that is, when the number of degrees of freedom involved becomes infinite, are orthogonal to one another. In view of this, the unit operator $\hat{1}$ defined in (5.23) is in such a case only the unit operator in a particular Fock space singled out by the choice of the one-particle space basis $|l\rangle$ of $\mathcal{H}^{(1)}$.

This can be illustrated most simply on the example of N spins[15] $s = \frac{1}{2}$ (forming e.g. a D-dimensional lattice). The natural basis of states of such a system is represented by the vectors (we assume spins are numbered from 1 to N) $|\sigma_N, \ldots, \sigma_1\rangle = |\sigma_N\rangle \otimes \ldots \otimes |\sigma_1\rangle$ which are tensor products of the state-vectors $|\sigma_i\rangle = |\pm\rangle$ forming a basis of the one-spin space. In the space of a single spin one can, however, equally well take as the basis the vectors $|\sigma_i\rangle^\theta$: $|+\rangle^\theta = \cos(\theta/2)|+\rangle + \sin(\theta/2)|-\rangle$ and $|-\rangle^\theta = -\sin(\theta/2)|+\rangle + \cos(\theta/2)|-\rangle$ with an arbitrary angle θ. If the vectors $|\sigma_N, \ldots, \sigma_1\rangle^\theta = |\sigma_N\rangle^\theta \otimes \ldots \otimes |\sigma_1\rangle^\theta$ are taken as the basis of the N-spin Hilbert space, in the limit $N = \infty$ all vectors of the basis $|\sigma_N, \ldots \sigma_1\rangle^\theta$ will have zero scalar products with all vectors of the basis $|\sigma_N, \ldots, \sigma_1\rangle$. For instance

$$^\theta\langle +, \ldots, +|+, \ldots, +\rangle = \lim_{N\to\infty} (\cos\theta/2)^N = 0\,,$$

etc., if $\theta \neq 0$. Therefore in the limit $N = \infty$ no one vector of the first basis can be expressed as a linear combination of vectors of the second one.

To explain the implications of this, it is instructive to consider a system of N spins (magnetic moments) interacting with one another which at low temperatures exhibits (because of the interactions of spins) spontaneous polarization, i.e. a nonzero mean value $\overline{S^z}$ of the z component $S^z = \sum_{i=1}^N \hat{S}_i^z$ of the total spin, which formally should be obtained

[14]The reader should be warned that mathematicians see this differently: they always work with $\oplus_{N=0}^{N_{\max}} \mathcal{H}^{(N)}$ and only at the end consider the limit $N_{\max} \to \infty$. For this reason they maintain that the Hilbert space constructed in this way is separable. But for forming a mental picture of the working of many physical systems it is better to see things as presented here.

[15]The spins are distinguishable; nevertheless, their Hilbert space in the limit $N \to \infty$ becomes identical with the one of indistinguishable fermions (see the occupation number representation below) and, hence, nonseparable.

as

$$\overline{S^z} = \mathrm{Tr}\Big(\hat{\rho}\,\hat{S}^z\Big)\,, \tag{5.26}$$

with $\hat{\rho} = Z_{\mathrm{stat}}^{-1}\exp(-\hat{H}/k_{\mathrm{B}}T)$ and $\hat{S}^z = \hat{s}_1^z + \ldots + s_N^z$, where $\hat{H}$ is an invariant (by assumption) with respect to simultaneous rotation of all spins Hamiltonian and $Z_{\mathrm{stat}} = \mathrm{Tr}\exp(-\hat{H}/k_{\mathrm{B}}T)$. However, as long as N is finite the value of $\overline{S^z}/N$ given by formula (5.26) is exactly zero because of the assumed rotational invariance. Of course, in Nature N is also finite, but the residual interactions with the surrounding, not accounted (by the very definition of the ensemble - recall my statistical physics lectures) in the Hamiltonian $\hat{H}$ used for statististical physics computations, always break this invariance. Thermal fluctuations, necessarily present, do tend to erase the mean value of the total spin but because the system is large (macroscopic), the probability that they flip simultaneously (almost) all spins (so that the change of the total spin of the system is done at the least energy cost - successive fliping of individual spins would cost a large amount of energy which the system, if not (absolutely) adiathermally isolated in the macroscopic sense, would have to absorb from the environment) from a configuration determined by a first random external perturbation (or rather by the way the real system has been prepared) grows with N; therefore the flip of the total spin is extremely improbable and never happens during the measurement of the magnetization of a real specimen. This is the reason why the magnetization of the real system is nonzero.

To reflect this state of affairs in the statistical approach, one takes the thermodynamic limit selecting first a particular basis $|\sigma_N, \ldots \sigma_1\rangle^\theta$; in the limit $N = \infty$ this has the effect that the formula (5.26) gives a nonzero magnetization precisely owing to the orthogonality of all states $|\sigma_N, \ldots \sigma_1\rangle^{\theta'}$ with $\theta' \neq \theta$. This means that the trace in this formula effectively gets restricted to only one of infinitely many orthogonal Fock spaces which in the limit $N = \infty$ are spanned by the bases $|\sigma_N, \ldots \sigma_1\rangle^\theta$ with different angles θ. The direction of the mean magnetization is in this way selected "by hands", just by taking the thermodynamic limit using one particular out of many possible bases (but since as a result of the underlying symmetry all directions are equivalent this is not a problem). This can be improved by placing the system in a constant magnetic field which singles out a direction in space and therefore makes the energy cost of configurations with the total spin not aligned with the magnetic field very high, infinite in the limit $N = \infty$; this suppresses their contributions to the trace in (5.26). In this way the applied field automatically selects one particular base $|\sigma_N, \ldots \sigma_1\rangle^\theta$. In this approach the magnetization is nonzero even at finite N because the external field explicitly breaks the rotational invariance and the limit of zero external magnetic field is to be taken after the thermodynamic limit $N \to \infty$.

5.2 Creation and annihilation operators

The construction (5.20) of the big Hilbert space $\mathcal{H}$ enables the introduction of the creation and annihilation operators. Let $|\varphi\rangle$ be a one-particle state. With any such state it is

possible to associate the corresponding *creation* operator $a^\dagger(\varphi)$ acting in $\mathcal{H}$ and mapping $\mathcal{H}^{(N)}$ into $\mathcal{H}^{(N+1)}$. On vectors $|\psi_1,\ldots,\psi_N\rangle$ of the form (5.12) its action is defined by the formula

$$a^\dagger(\varphi)|\psi_N,\ldots,\psi_1\rangle = |\varphi,\psi_N,\ldots,\psi_1\rangle\,, \tag{5.27}$$

and is extended to the entire $\mathcal{H}$ by linearity. The *annihilation* operator $a(\varphi)$ is defined as the Hermitian conjugate of $a^\dagger(\varphi)$ through the equality (cf. the definition (4.1))

$$\begin{aligned}\langle\chi_1,\ldots,\chi_{N-1}|a(\varphi)|\psi_N,\ldots,\psi_1\rangle &= \big(\langle\psi_1,\ldots,\psi_N|a^\dagger(\varphi)|\chi_{N-1},\ldots,\chi_1\rangle\big)^* \\ &= \begin{vmatrix} \langle\psi_N|\varphi\rangle & \langle\psi_N|\chi_{N-1}\rangle & \ldots & \langle\psi_N|\chi_1\rangle \\ \cdot & \cdot & \ldots & \cdot \\ \cdot & \cdot & \ldots & \cdot \\ \cdot & \cdot & \ldots & \cdot \\ \langle\psi_1|\varphi\rangle & \langle\psi_1|\chi_{N-1}\rangle & \ldots & \langle\psi_1|\chi_1\rangle \end{vmatrix}^*_\zeta .\end{aligned}$$

The Laplace expansion (valid for determinants and permanents alike) gives

$$\langle\chi_1,\ldots,\chi_{N-1}|a(\varphi)|\psi_N,\ldots,\psi_1\rangle = \sum_{k=1}^{N}\zeta^{k-1}\langle\psi_k|\varphi\rangle^* \begin{vmatrix}\text{without the } k\text{−th row} \\ \text{and the first column}\end{vmatrix}^*_\zeta .$$

From this formula it is easy to read-off the following rule:

$$a(\varphi)|\psi_N,\ldots,\psi_1\rangle = \sum_{k=1}^{N}\zeta^{k-1}\langle\varphi|\psi_k\rangle|\psi_N,\ldots(\text{no }\psi_k)\ldots,\psi_1\rangle\,, \tag{5.28}$$

which shows that $a(\varphi)$ acting on a state -vector $|\Psi^{(N)}\rangle$ of the form (5.12) gives zero if $|\varphi\rangle$ is orthogonal to all one-particle states $|\psi_i\rangle$ building $|\Psi^{(N)}\rangle$. The factor ζ^{k-1} appearing in (5.28) can be understood as a sign factor arising when ψ_k is moved from its k-th position in the ket to the last position, at which $a(\varphi)$ can annihilate it.

Using the definitions (5.27) and (5.28) it is easy to show that

$$\begin{aligned} a^\dagger(\varphi_1)\,a^\dagger(\varphi_2) &= \zeta\,a^\dagger(\varphi_2)\,a^\dagger(\varphi_1)\,, \\ a(\varphi_1)\,a(\varphi_2) &= \zeta\,a(\varphi_2)\,a(\varphi_1)\,, \end{aligned} \tag{5.29}$$

that is, the creation operators associated with one-particle states of bosons commute ($\zeta=+1$) and those associated with fermion states anticommute ($\zeta=-1$) and the same holds true for the annihilation operators. It follows, that the fermionic operators are nilpotent:

$$a^2(\varphi) = (a^\dagger(\varphi))^2 = 0\,. \tag{5.30}$$

It is also easy to prove that

$$\big[a(\varphi_1),\ a^\dagger(\varphi_2)\big]_{-\zeta} = \langle\varphi_1|\varphi_2\rangle\,, \tag{5.31}$$

where the subscript $-\zeta$ denotes the commutator if the particles are bosons and the anti-commutator if they are fermions (the scalar product on the right hand side is that of the one-particle space $\mathcal{H}^{(1)}$).

Creation and annihilation operators can be associated with any complete set of one-particle states $|l\rangle$. If the vectors $|l\rangle$ form a countable orthonormal basis of $\mathcal{H}^{(1)}$, then

$$[a_{l'},\ a_l^\dagger]_{-\zeta} = \delta_{l'l}\,, \qquad [a_{l'},\ a_l]_{-\zeta} = [a_{l'}^\dagger,\ a_l^\dagger]_{-\zeta} = 0\,. \tag{5.32}$$

(If, instead, the $|l\rangle$'s are generalized vectors, then $[a_{l'},\ a_l^\dagger]_{-\zeta} = c_l\,\delta(l'-l)$ with the factor c_l depening on the character of the label l and the adopted convention - cf. Section 2.5). For future use note also that if the particles are fermions, the rule (5.32) is symmetric with respect to the interchange $a_l \leftrightarrow a_l^\dagger$, i.e. the algebraic properties of the fermionic annihilation and creation operators are the same. This property will be exploited in Section 5.4. The action of the fermionic operators $a_{l'}$ and $a_l^\dagger$ on the basis vectors (5.16) is

$$\begin{aligned} a_l\,|l_N,\ldots,l_2,l_1\rangle &= \sum_{k=1}^{N}(-1)^{N-k}\delta_{ll_k}|l_N,\ldots(\text{no } l_k)\ldots,l_1\rangle\,,\\ a_l^\dagger\,|l_N,\ldots,l_2,l_1\rangle &= |l,l_N,\ldots,l_2,l_1\rangle = \pm|l_N,\ldots,l,\ldots,l_1\rangle\,. \end{aligned} \tag{5.33}$$

The sign $\pm$ depends on the number of interchanges needed to move l to the appropriate position (in agreement with the ordering specified in (5.16)); if l is equal to one of the l's in the ket the action of $a_l^\dagger$ gives zero. The action of the bosonic operators is similar (in this case no extra signs are involved). It is useful to note that the state-vectors $|l_1,\ldots,l_N\rangle$ which span $\mathcal{H}^{(N)}$ and are used in (5.15) and (5.16) can be in both cases represented as

$$|l_N,\ldots,l_1\rangle = a_{l_N}^\dagger\ldots a_{l_1}^\dagger|\text{void}\rangle\,. \tag{5.34}$$

The order of the creation operators in this formula (important if the particles are fermions) should of course follow the conventions adopted in (5.15) and (5.16) as follows from the definition (5.27). The formula (5.34) also provides the justification for writing the element of $\mathcal{H}^{(N)*}$ conjugated to $|l_N,\ldots,l_1\rangle$ as $\langle l_1,\ldots,l_N|$. The Hilbert (sub)space spanned by all vectors of the form (5.34) with N arbitrarily large, but finite (as required by mathematicians) is called *the Fock space* built on the vector $|\text{void}\rangle$. In the limit $N\to\infty$ the "location" of this subspace in the "big" Hilbert space $\mathcal{H}$ (5.20) depends of course (as argued) on the choice of the basis $|l\rangle$ of the one-particle space $\mathcal{H}^{(1)}$. It is possible, however, to construct in $\mathcal{H}$ (5.20) also other Fock spaces built on other "void" vectors (specified by some conditions - see e.g. Section 5.5).

To represent the action of the operators $a_{l'}$ and $a_l^\dagger$ on the basis vectors (5.15) in a different way which, in the case of bosons is particularily convenient, one introduces first the so-called *occupation number representation* by changing the notation used for the vectors (5.15) or (5.16) forming countable bases of the Hilbert spaces $\mathcal{H}^{(N)}$ of N bosons

or fermions, respectively. To this ends one defines[16]

$$|n_1, n_2, \ldots\rangle \equiv \frac{1}{\sqrt{n_1!\, n_2! \ldots}} \, |\ldots, 2, \ldots, 2, 1, \ldots, 1\rangle \,, \tag{5.35}$$

In this notation the numbers n_1, n_2, etc. simply indicate how many particles occupy a given (discrete) one-particle state $|l\rangle$ (if the particles are fermions, only $n_l = 0$ or 1 are possible). Of course, vectors belonging to $\mathcal{H}^{(N)}$ are restricted by the condition $n_1 + n_2 + \ldots = N$. Removing this restriction one obtains a set of vectors belonging to the "big" Hilbert space $\mathcal{H}$ defined by (5.20). The set of such vectors is uncountable - its power is equal to the power of the continuum.[17] This shows that the Hilbert space $\mathcal{H}$ constructed as in (5.20) is not separable and the state-vectors $|n_1, n_2, \ldots\rangle$ with $N = n_1 + n_2 + \ldots$ arbitrarily large but finite span in fact only a separable subspace (a Fock space) of the entire big Hilbert space. In the occupation number representation the action of the bosonic creation and annihilation operators looks familiar:

$$\begin{aligned} a_l \, |n_1, n_2, \ldots, n_l, \ldots\rangle &= \sqrt{n_l} \, |n_1, n_2, \ldots, n_l - 1, \ldots\rangle \,, \\ a_l^\dagger |n_1, n_2, \ldots, n_l, \ldots\rangle &= \sqrt{n_l + 1} \, |n_1, n_2, \ldots, n_l + 1, \ldots\rangle \,. \end{aligned} \tag{5.36}$$

For completeness we give also the action of the fermionic operators on the basis vectors (5.16) written in this notation:

$$\begin{aligned} a_l \, |n_1, n_2, \ldots, n_l, \ldots\rangle &= \begin{cases} 0 & \text{if } \; n_l = 0 \\ \eta |n_1, n_2, \ldots, n_l - 1, \ldots\rangle & \text{if } \; n_l = 1 \end{cases} , \\ a_l^\dagger \, |n_1, n_2, \ldots, n_l, \ldots\rangle &= \begin{cases} 0 & \text{if } \; n_l = 1 \\ \eta |n_1, n_2, \ldots, n_l + 1, \ldots\rangle & \text{if } \; n_l = 0 \end{cases} , \end{aligned} \tag{5.37}$$

where $\eta = (-1)^p$, $p = \sum_{l'<l} n_{l'}$. In both cases, the operator $a_l^\dagger a_l$ counts therefore the number of particles occupying the (one-particle) state $|l\rangle$.

In many applications of the developed formalism to systems of many particles, particularily in its applications to statistical physics problems, it is most convenient to associate the creation and annihilation operators with the basis of $\mathcal{H}^{(1)}$ formed by the plane waves $|\mathbf{p}\rangle$ (in the case of spin zero bosons) or $|\mathbf{p}, \sigma\rangle$ in general, with periodic boundary conditions imposed in the finite a box of volume $V = L^3$; the one-particle basis state-vectors are then normalized by the condition

$$\langle \mathbf{p}'\sigma' | \mathbf{p}\sigma \rangle = \delta_{\mathbf{p}'\mathbf{p}} \, \delta_{\sigma'\sigma} \,, \tag{5.38}$$

[16] Since the state-vectors $|n_1, n_2, \ldots\rangle$ usually are not represented as in (5.34), we will not write them as $|\ldots, n_2, n_1\rangle$, which could seem more in line with the notation adopted for the state-vectors $|l_N, \ldots, l_2, l_1\rangle$.

[17] This is particularly easy to demonstrate in the case of fermions: it suffices to notice that any infinite sequence of numbers $n_1 n_2 n_3 \ldots$, in which each $n_l = 0$, or 1, treated as the binary coding of an integer, can be uniquely mapped onto the infinite sequence of integer numbers $p_1 p_2 p_3 \ldots$, $0 \leq p_l < 9$ and the decimal fractions $0.p_1 p_2 p_3 \ldots$ fill the entire segment $[0, 1)$ - a set the power of which is equal to the power of the continuum.

and the corresponding wave functions are[18] $(\psi_{\mathbf{p}\sigma})_\alpha(\mathbf{x}) = (1/\sqrt{V})\,\delta_{\alpha\sigma}\,e^{i\mathbf{p}\cdot\mathbf{x}}$. In the limit $V \to \infty$, i.e. when the individual particles can move in the infinite space, the basis of the momentum states normalized in the box gets replaced by the basis formed by the generalized momentum state-vectors normalized to the delta function[19]

$$\langle \mathbf{p}', \sigma' | \mathbf{p}, \sigma \rangle = (2\pi)^3 \delta^{(3)}(\mathbf{p}' - \mathbf{p}) \delta_{\sigma'\sigma}\,,$$

with the corresponding wave functions $(\psi_{\mathbf{p}\sigma})_\alpha(\mathbf{x}) \equiv \langle \mathbf{x}, \alpha | \mathbf{p}, \sigma \rangle = \delta_{\alpha\sigma} e^{i\mathbf{p}\cdot\mathbf{x}}$. The creation and annihilation operators associated with these bases satisfy the (anti)commutation rules

$$[a_{\mathbf{p}\sigma},\ a^\dagger_{\mathbf{p}'\sigma'}]_{-\zeta} = \delta_{\mathbf{p}'\mathbf{p}}\,\delta_{\sigma'\sigma}\,, \qquad \text{or} \qquad [a_\sigma(\mathbf{p}),\ a^\dagger_{\sigma'}(\mathbf{p}')]_{-\zeta} = (2\pi)^3 \delta^{(3)}(\mathbf{p}' - \mathbf{p})\,\delta_{\sigma'\sigma}\,, \quad (5.39)$$

and the N-particle Hilbert spaces $\mathcal{H}^{(N)}$ are spanned by the (generalized if the particles are not confined to a finite volume) vectors[20]

$$\begin{aligned} |\mathbf{p}_N\sigma_N, \ldots, \mathbf{p}_2\sigma_2, \mathbf{p}_1\sigma_1\rangle &= a^\dagger_{\mathbf{p}_N\sigma_N} \ldots a^\dagger_{\mathbf{p}_2\sigma_2}\, a^\dagger_{\mathbf{p}_1\sigma_1} |\text{void}\rangle\,, \qquad (5.40)\\ \text{or} \qquad &= a^\dagger_{\sigma_N}(\mathbf{p}_N) \ldots a^\dagger_{\sigma_2}(\mathbf{p}_2)\, a^\dagger_{\sigma_1}(\mathbf{p}_1) |\text{void}\rangle\,. \end{aligned}$$

In nonrelativistic physics one also uses as the basis of $\mathcal{H}^{(1)}$ the position generalized vectors $|\mathbf{x}, \alpha\rangle$. The associated creation and annihilation operators satify then the rules

$$[a_\alpha(\mathbf{x}),\ a^\dagger_{\alpha'}(\mathbf{x}')]_{-\zeta} = \delta(\mathbf{x}' - \mathbf{x})\,\delta_{\alpha'\alpha}\,, \qquad (5.41)$$

and the N-particle Hilbert spaces $\mathcal{H}^{(N)}$ are spanned by the vectors

$$|\mathbf{x}_N\alpha_N, \ldots, \mathbf{x}_2\alpha_2, \mathbf{x}_1\alpha_1\rangle = a^\dagger_{\alpha_N}(\mathbf{x}_N) \ldots a^\dagger_{\alpha_2}(\mathbf{x}_2)\, a^\dagger_{\alpha_1}(\mathbf{x}_1) |\text{void}\rangle\,. \qquad (5.42)$$

The operators $a_\alpha(\mathbf{x})$ and $a^\dagger_\alpha(\mathbf{x})$ in this case denoted usually by $\hat\psi_\alpha(\mathbf{x})$ and $\hat\psi^\dagger_\alpha(\mathbf{x})$ (or $\hat\phi(\mathbf{x})$ and $\hat\phi^\dagger(\mathbf{x})$ if the particles are spinless bosons) and are called field operators.

[18] This is a somewhat stupid notation for α, strictly speaking, is also a spin label like σ - simply $(\psi_{\mathbf{p}\sigma})_\alpha(\mathbf{x}) = \langle \mathbf{x}, \alpha | \mathbf{p}, \sigma \rangle$, where $|\mathbf{x}, \alpha\rangle$ represent the particle as $\mathbf{x}$ with the spin projection on the chosen axis equal α - but one commonly treats it as a label of the "floor" of a $2s+1$-component "wave function" of the state $|\mathbf{p}, \sigma\rangle$. The only justification of writing α on ψ instead of σ is perhaps that in the relativistic case the index carried by the field operator will not have the meaning of the spin label.

[19] In the relativistic case it will be convenient to slightly modify this normalization.

[20] Recall that if the particles are bosons, these state-vectors are not properly normalized if two or more momenta and spins coincide; in practical computations this is taken care of by usig the unit operator decomposition in the form

$$\hat{1}^{(N)} = \frac{1}{N!} \sum_{\mathbf{p}_N\sigma_N} \cdots \sum_{\mathbf{p}_1\sigma_1} |\mathbf{p}_N\sigma_N, \ldots, \mathbf{p}_1\sigma_1\rangle\langle \mathbf{p}_1\sigma_1, \ldots, \mathbf{p}_N\sigma_N|,$$

in the case of the normalization in the box or in the form (5.19) in the case of the normalization in the infinite space. Note also that the rule (5.47) and the prescription (5.34) imply that in making the transition from the normalization in the box to the one in the infinite space, the vectors (5.40) normalized in the box should be replaced by those normalized in the infinite space multiplied by the factor $V^{-N/2}$ (the vectors $|\text{void}\rangle$ are normalized in the same way in both cases); together with the rule (5.48) this ensures that the unit operator decomposition given here is consistent with the one given in (5.19).

In order to write down the relations between the creation and annihilation operators associated with different bases of the one-particle Hilbert space, it is sufficient to observe that if a one-particle state-vector $|\psi\rangle$ is a linear superposition of some other vectors, e.g. if

$$|\psi\rangle = c_1\,|\psi_1\rangle + c_2\,|\psi_2\rangle\,, \tag{5.43}$$

then from the definition (5.27) it immediately follows that

$$\begin{aligned} a^\dagger(\psi) &= c_1\,a^\dagger(\psi_1) + c_2\,a^\dagger(\psi_2)\,,\\ a(\psi) \;&= c_1^*\,a(\psi_1) \;+\; c_2^*\,a(\psi_2)\,. \end{aligned} \tag{5.44}$$

Therefore, since

$$|\mathbf{x},\alpha\rangle = \sum_{\mathbf{p},\sigma} |\mathbf{p},\sigma\rangle \left(\frac{1}{\sqrt{V}}\,\delta_{\sigma\alpha}\,e^{i\mathbf{p}\cdot\mathbf{x}}\right)^*, \qquad |\mathbf{p},\sigma\rangle = \int_V d^3\mathbf{x} \sum_\alpha |\mathbf{x},\alpha\rangle \frac{1}{\sqrt{V}}\,\delta_{\sigma\alpha}\,e^{i\mathbf{p}\cdot\mathbf{x}},$$

in the finite volume (with periodic boundary conditions imposed) and

$$|\mathbf{x},\alpha\rangle = \int \frac{d^3\mathbf{p}}{(2\pi)^3} \sum_\sigma |\mathbf{p},\sigma\rangle \left(\delta_{\sigma\alpha}\,e^{i\mathbf{p}\cdot\mathbf{x}}\right)^*, \qquad |\mathbf{p},\sigma\rangle = \int d^3\mathbf{x} \sum_\alpha |\mathbf{x},\alpha\rangle\,\delta_{\sigma\alpha}\,e^{i\mathbf{p}\cdot\mathbf{x}}\,,$$

in the infinite space, the creation and annihilation operators associated with these bases are related by

$$\begin{aligned} \hat\psi^\dagger_\alpha(\mathbf{x}) &= \sum_{\mathbf{p},\sigma} a^\dagger_{\mathbf{p},\sigma}\,\frac{1}{\sqrt{V}}\,\delta_{\sigma\alpha}\,e^{-i\mathbf{p}\cdot\mathbf{x}}\,, \qquad a^\dagger_{\mathbf{p},\sigma} = \int_V d^3\mathbf{x} \sum_\alpha \hat\psi^\dagger_\alpha(\mathbf{x})\,\frac{1}{\sqrt{V}}\,\delta_{\alpha\sigma}\,e^{i\mathbf{p}\cdot\mathbf{x}}\,,\\ \hat\psi_\alpha(\mathbf{x}) &= \sum_{\mathbf{p},\sigma} a_{\mathbf{p},\sigma}\,\frac{1}{\sqrt{V}}\,\delta_{\sigma\alpha}\,e^{i\mathbf{p}\cdot\mathbf{x}}\,, \qquad a_{\mathbf{p},\sigma} = \int_V d^3\mathbf{x} \sum_\alpha \hat\psi_\alpha(\mathbf{x})\,\frac{1}{\sqrt{V}}\,\delta_{\alpha\sigma}\,e^{-i\mathbf{p}\cdot\mathbf{x}}\,, \end{aligned} \tag{5.45}$$

in the finite volume (with periodic boundary conditions) and by

$$\begin{aligned} \hat\psi^\dagger_\alpha(\mathbf{x}) &= \int \frac{d^3\mathbf{p}}{(2\pi)^3} \sum_\sigma a^\dagger_\sigma(\mathbf{p})\,\delta_{\sigma\alpha}\,e^{-i\mathbf{p}\cdot\mathbf{x}}\,, \qquad a^\dagger_\sigma(\mathbf{p}) = \int d^3\mathbf{x} \sum_\alpha \hat\psi^\dagger_\alpha(\mathbf{x})\,\delta_{\alpha\sigma}\,e^{i\mathbf{p}\cdot\mathbf{x}}\,,\\ \hat\psi_\alpha(\mathbf{x}) &= \int \frac{d^3\mathbf{p}}{(2\pi)^3} \sum_\sigma a_\sigma(\mathbf{p})\,\delta_{\sigma\alpha}\,e^{i\mathbf{p}\cdot\mathbf{x}}\,, \qquad a_\sigma(\mathbf{p}) = \int d^3\mathbf{x} \sum_\alpha \hat\psi_\alpha(\mathbf{x})\,\delta_{\alpha\sigma}\,e^{-i\mathbf{p}\cdot\mathbf{x}}\,, \end{aligned} \tag{5.46}$$

in the infinite space. The rules allowing to perform the transition from expressions involving creation and annihilation operators associated with the momentum basis in the discrete and in the continuous normalizations are as follows:

$$a^\dagger_{\mathbf{p},\sigma} \leftrightarrow \frac{1}{\sqrt{V}}\,a^\dagger_\sigma(\mathbf{p})\,, \qquad a_{\mathbf{p},\sigma} \leftrightarrow \frac{1}{\sqrt{V}}\,a_\sigma(\mathbf{p})\,. \tag{5.47}$$

and

$$\sum_{\mathbf{p}} \equiv \sum_{n_x,n_y,n_z} \longleftrightarrow \frac{V}{(2\pi)^3}\int d^3\mathbf{p}\,. \tag{5.48}$$

The second one readily follows from the fact that if periodic boundary conditions are imposed in the box of volume $L\times L\times L$, the factor $(L/2\pi)^3 = V/(2\pi)^3$, as explained in Section 2.5, plays the role of the density of allowed states in the space of wave vectors.[21] With these rules one has

$$\int_V d^3\mathbf{x}\sum_\alpha \hat\psi^\dagger_\alpha(\mathbf{x})\hat\psi_\alpha(\mathbf{x}) = \sum_{\mathbf{p},\sigma} a^\dagger_{\mathbf{p},\sigma}a_{\mathbf{p},\sigma} \leftrightarrow \int\frac{d^3\mathbf{p}}{(2\pi)^3}\sum_\sigma a^\dagger_\sigma(\mathbf{p})a_\sigma(\mathbf{p}) = \int d^3\mathbf{x}\sum_\alpha \hat\psi^\dagger_\alpha(\mathbf{x})\hat\psi_\alpha(\mathbf{x})\,,$$

etc.

More generally, if the functions $(u_{l\sigma})_\alpha(\mathbf{x}) \equiv \langle \mathbf{x},\alpha|l,\sigma\rangle$ form a complete orthonormal set (the spin label σ is here singled out from the general one-particle state label l), such that

$$|\mathbf{x},\alpha\rangle = \sum_{l,\sigma}|l,\sigma\rangle\langle l,\sigma|\mathbf{x},\alpha\rangle = \sum_{l,\sigma}|l,\sigma\rangle\,(u_{l,\sigma})^*_\alpha(\mathbf{x})\,, \tag{5.49}$$

then

$$\hat\psi^\dagger_\alpha(\mathbf{x}) = \sum_{l,\sigma} a^\dagger_{l,\sigma}\,(u_{l\sigma})^*_\alpha(\mathbf{x})\,, \qquad \hat\psi_\alpha(\mathbf{x}) = \sum_{l,\sigma} a_{l,\sigma}\,(u_{l\sigma})_\alpha(\mathbf{x})\,, \tag{5.50}$$

$$a^\dagger_{l,\sigma} = \int d^3\mathbf{x}\sum_\alpha (u_{l\sigma})_\alpha(\mathbf{x})\,\hat\psi^\dagger_\alpha(\mathbf{x})\,, \qquad a_{l,\sigma} = \int d^3\mathbf{x}\sum_\alpha (u^*_{l\sigma})_\alpha(\mathbf{x})\,\hat\psi_\alpha(\mathbf{x})\,. \tag{5.51}$$

The use of the functions $(u_{l\sigma})_\alpha(\mathbf{x})$ in place of the plane waves may be more convenient if particles of the considered system all move in an external spatially inhomogeneous potential. Using the general formulae (5.51) and exploiting the completeness of the set of functions $(u_{l\sigma})_\alpha(\mathbf{x})$ as well as the commutation rules (5.32) one can check that the field operators (bosonic and fermionic alike) always satisfy the (anti)commutation relations

$$\begin{aligned}
&[\hat\psi_\alpha(\mathbf{x}),\,\hat\psi^\dagger_\beta(\mathbf{y})]_{-\zeta} = \delta_{\alpha\beta}\delta^{(3)}(\mathbf{x}-\mathbf{y})\,,\\
&[\hat\psi_\alpha(\mathbf{x}),\,\hat\psi_\beta(\mathbf{y})]_{-\zeta} = [\hat\psi^\dagger_\alpha(\mathbf{x}),\,\hat\psi^\dagger_\beta(\mathbf{y})]_{-\zeta} = 0\,.
\end{aligned} \tag{5.52}$$

5.3 Hamiltonian and other operators

The main advantage of introducing the annihilation and creation operators is that essentially all operators acting in the "big" Hilbert space (5.20) of many indistinguishable

[21] It should be also noted that both $\sum_{\mathbf{p}}$ and $V/(2\pi)^3 d^3\mathbf{p}$ are dimensionless ($\mathbf{p}$ is the wave vector of dimension length^{-1}).

particles can be represented in terms of them in a simple and very convenient for practical computations form. Here we consider in some details only the so-called one-particle operators which like the kinetic energy operator, the total momentum operator, etc. have additive character with respect to individual particles of the system and operators which represent binary interactions (these are additive with respect to pairs of particles). Other operators, e.g. ones representing three-body interactions can be constructed along the same lines.

In general an operator of the form $O = O_N^{(1)} \otimes \ldots \otimes O_2^{(1)} \otimes O_1^{(1)}$ acts on a state-vector $|\Psi\rangle$ of the form (5.1) of a system of N-particles (not necessarily indistinguishable) according to the rule

$$O|\Psi\rangle = O_N^{(1)}|\psi_N\rangle \otimes \ldots \otimes O_2^{(1)}|\psi_2\rangle \otimes O_1^{(1)}|\psi_1\rangle \,. \tag{5.53}$$

The operators $O_i^{(1)}$ act here in separate Hilbert spaces of individual particles and are therefore formally "different". The above rule extends by linearity to (anti)symmetrized vectors (5.12) representing states of identical indistinguishable particles. To preserve the subspaces of completely symmetrized or antisymmetrized state-vectors, admitted can only be the operators $O = O_N^{(1)} \otimes \ldots \otimes O_2^{(1)} \otimes O_1^{(1)}$ which are symmetric with respect to interchanges of $O_l^{(1)} \leftrightarrow O_k^{(1)}$, $1 \leq l, k \leq N$. In this case distinguished is a class of operators of the form

$$O^{(N)} = \sum_{i=1}^{N} \hat{1}^{(1)} \otimes \ldots \otimes O_i^{(1)} \otimes \ldots \otimes \hat{1}^{(1)} \,, \tag{5.54}$$

(the lower index i labels here only the position of the same one-particle operator $O^{(1)}$ in the tensor product) which have additive character with respect to individual particles. An example of the operator of this type is e.g. the N-particle kinetic energy operator

$$\hat{T}^{(N)} = \sum_{i=1}^{N} \hat{1}^{(1)} \otimes \ldots \otimes \frac{\hat{\mathbf{P}}_i^{(1)2}}{2m} \otimes \ldots \otimes \hat{1}^{(1)} \,, \tag{5.55}$$

acting in $\mathcal{H}^{(N)}$ which in many cases plays the role of the free Hamiltonian H_0 of the system of N indistinguishable particles. The state-vectors (5.40), normalized either in the finite-volume or in the infinite space, are its eigenvectors with the eigenvalue $\hbar^2(\mathbf{p}_1^2 + \ldots + \mathbf{p}_N^2)/2m$. Another operator of this class is the particle number operator

$$\hat{N}^{(N)} = N\, \hat{1}^{(1)} \otimes \ldots \otimes \hat{1}^{(1)} \,, \tag{5.56}$$

which is proportional to the unit operator on $\mathcal{H}^{(N)}$.

Operators of this class can be easily expressed in terms of the creation and annihilation operators. This also promotes them to operators defined on the whole big Hilbert space (5.20). In order to represent operators of the form (5.54) in terms of the annihilation and creation operators it is convenient to consider first a particular operator of this sort,

namely $O^{(1)} = |l\rangle\langle l'|$ (the spin label is now included in the general labels l and l'). Its action

$$O|\psi_N, \ldots, \psi_2, \psi_1\rangle = \langle l'|\psi_N\rangle\, |l, \psi_{N-1}, \ldots, \psi_1\rangle + \langle l'|\psi_{N-1}\rangle\, |\psi_N, l, \ldots, \psi_1\rangle + \ldots$$

on a state-vector of the form (5.12) is readily seen to be identical with the action of the operator $a_l^\dagger a_{l'}$ (c.f. the formulae (5.28) and (5.27)). Since any one-particle operator $O^{(1)}$ can be written in the form

$$\hat{O}^{(1)} = \sum_l \sum_{l'} |l\rangle\langle l|O^{(1)}|l'\rangle\langle l'| \equiv \sum_l \sum_{l'} \hat{O}^{(1)}_{ll'}\, |l\rangle\langle l'|\,, \tag{5.57}$$

one concludes that

$$O = \sum_l \sum_{l'} O^{(1)}_{ll'}\, a_l^\dagger\, a_{l'}\,. \tag{5.58}$$

Taking for example $O^{(1)} = \hat{1}^{(1)}$ (the one-particle unit operator), the matrix elements of which are $O^{(1)}_{ll'} = \langle l|\hat{1}^{(1)}|l'\rangle = \delta_{ll'}$, one gets the operator $\hat{N}$ counting the number of particles of the system (for definiteness we consider here the system in the infinite space):

$$\hat{N} = \sum_l a_l^\dagger a_l = \int d^3\mathbf{x} \sum_\alpha \hat{\psi}^\dagger_\alpha(\mathbf{x})\, \hat{\psi}_\alpha(\mathbf{x}) = \int \frac{d^3\mathbf{p}}{(2\pi)^3} \sum_\sigma a^\dagger_\sigma(\mathbf{p})\, a_\sigma(\mathbf{p})\,. \tag{5.59}$$

Similarly, taking for $O^{(1)}$ the one-particle momentum operator $\hat{\mathbf{P}}^{(1)}$ we obtain the operator $\hat{\mathbf{P}}$ of the total momentum of the system:[22]

$$\hat{\mathbf{P}} = \int \frac{d^3\mathbf{p}}{(2\pi)^3} \sum_\sigma \hbar\mathbf{p}\, a^\dagger_\sigma(\mathbf{p}) a_\sigma(\mathbf{p}) = \int d^3\mathbf{x} \sum_\alpha \hat{\psi}^\dagger_\alpha(\mathbf{x})(-i\hbar\nabla_{\mathbf{x}})\hat{\psi}_\alpha(\mathbf{x})\,, \tag{5.60}$$

(recall that $\mathbf{p}$ is the wave vector, not the momentum). In the similar way it is possible to construct also the total angular momentum $\hat{\mathbf{J}}$ and boost $\hat{\mathbf{K}}$ operators of the system of free particles.[23] Each of these operators is originally a one-particle operator of the general

[22]The second form of this operator follows from the matrix element

$$\langle \mathbf{x}|\hat{\mathbf{P}}^{(1)}|\mathbf{y}\rangle = i\hbar\, \frac{\partial}{\partial \mathbf{y}}\, \delta^{(3)}(\mathbf{y} - \mathbf{x})\,,$$

of the one-particle momentum operator $\hat{\mathbf{P}}^{(1)}$ which correctly gives

$$\langle \mathbf{x}|\mathbf{P}^{(1)}|\psi\rangle = \int d^3\mathbf{y}\, \langle \mathbf{x}|\hat{\mathbf{P}}^{(1)}|\mathbf{y}\rangle\, \langle \mathbf{y}|\psi\rangle = -i\hbar\, \frac{\partial}{\partial \mathbf{x}}\, \psi(\mathbf{x})\,.$$

[23]The operators $\hat{\mathbf{P}}$ and $\hat{\mathbf{J}}$ constructed in this way retain their role also in the presence of interactions; the concrete form of the boost operator $\hat{\mathbf{K}}$ may in principle depend on the form of the interaction as a result of the last commutation relation (4.50).

form (5.54). The corresponding exponentialized symmetry operators (see Chapter 4), e.g. the rotation operator $U^{(N)}(\boldsymbol{\theta}) = \exp(-i\boldsymbol{\theta}\cdot\hat{\mathbf{J}}^{(N)})$, are then operators of the form $U^{(N)} = U^{(1)}\otimes\ldots\otimes U^{(1)}$ (i.e. they have the form of tensor products of operators acting on states of individual particles) and act on N-particle state-vectors according to the rule (5.53). This rule becomes automatically implemented (and simultaneously the symmetry operators get promoted to ones acting in the entire Hilbert space (5.20)) when the symmetry generators are written in terms of the creation and annihilation operators and get exponentialized.

If (indistinguishable) particles are not interacting with one another but all move in some external (spin independent) potential $V_{\rm pot}(\mathbf{x})$, their nonrelativistic Hamiltonian is the sum (over particles) of the one-particle operators $H^{(1)} = \hat{T}^{(1)} + \hat{V}^{(1)} = \hat{\mathbf{P}}^{(1)2}/2m + V^{(1)}_{\rm pot}(\hat{\mathbf{x}})$ the matrix elements of which between the position operator eigenstates are

$$\langle\mathbf{x}|H^{(1)}|\mathbf{y}\rangle = -\frac{\hbar^2}{2m}\nabla^2_{\mathbf{y}}\,\delta^{(3)}(\mathbf{y}-\mathbf{x}) + V_{\rm pot}(\mathbf{x})\,\delta^{(3)}(\mathbf{y}-\mathbf{x})\,. \tag{5.61}$$

In the second quantization formalism it takes, therefore, the form

$$H = \int d^3\mathbf{x}\sum_\alpha \hat{\psi}^\dagger_\alpha(\mathbf{x})\left[-\frac{\hbar^2}{2m}\nabla^2_{\mathbf{x}} + V_{\rm pot}(\mathbf{x})\right]\hat{\psi}_\alpha(\mathbf{x})\,. \tag{5.62}$$

To rewrite it in the momentum representation (in the normalization in the infinite space) we use the formulae

$$\langle\mathbf{p},\sigma|T^{(1)}|\mathbf{p}',\sigma'\rangle = \frac{\hbar^2\mathbf{p}^2}{2m}\,(2\pi)^3\delta^{(3)}(\mathbf{p}-\mathbf{p}')\,\delta_{\sigma\sigma'}\,,$$

and

$$\langle\mathbf{p},\sigma|V^{(1)}|\mathbf{p}',\sigma'\rangle = \delta_{\sigma\sigma'}\int d^3\mathbf{x}\int d^3\mathbf{y}\,\langle\mathbf{p}|\mathbf{x}\rangle\langle\mathbf{x}|V_{\rm pot}|\mathbf{y}\rangle\langle\mathbf{y}|\mathbf{p}'\rangle = \tilde{V}_{\rm pot}(\mathbf{p}-\mathbf{p}')\,\delta_{\sigma\sigma'}\,,$$

where $\tilde{V}_{\rm pot}(\mathbf{q})$ is the Fourier transform of the potential $V_{\rm pot}(\mathbf{x})$:

$$\tilde{V}_{\rm pot}(\mathbf{q}) = \int d^3\mathbf{x}\,V_{\rm pot}(\mathbf{x})\,e^{-i\mathbf{q}\cdot\mathbf{x}}\,,\qquad V_{\rm pot}(\mathbf{x}) = \int\frac{d^3\mathbf{q}}{(2\pi)^3}\,\tilde{V}_{\rm pot}(\mathbf{q})\,e^{i\mathbf{q}\cdot\mathbf{x}}\,. \tag{5.63}$$

Thus, in the momentum representation we get

$$\begin{aligned} H &= \int\frac{d^3\mathbf{p}}{(2\pi)^3}\,\frac{\hbar^2\mathbf{p}^2}{2m}\sum_\sigma a^\dagger_\sigma(\mathbf{p})\,a_\sigma(\mathbf{p}) + \int\frac{d^3\mathbf{p}}{(2\pi)^3}\int\frac{d^3\mathbf{p}'}{(2\pi)^3}\sum_\sigma a^\dagger_\sigma(\mathbf{p}')\,\tilde{V}_{\rm pot}(\mathbf{p}'-\mathbf{p})\,a_\sigma(\mathbf{p}) \\ &= \int\frac{d^3\mathbf{p}}{(2\pi)^3}\,\frac{\hbar^2\mathbf{p}^2}{2m}\sum_\sigma a^\dagger_\sigma(\mathbf{p})\,a_\sigma(\mathbf{p}) + \int\frac{d^3\mathbf{q}}{(2\pi)^3}\,\tilde{V}_{\rm pot}(\mathbf{q})\int\frac{d^3\mathbf{p}}{(2\pi)^3}\sum_\sigma a^\dagger_\sigma(\mathbf{p}+\mathbf{q})\,a_\sigma(\mathbf{p})\,. \end{aligned} \tag{5.64}$$

The same Hamiltonian in the momentum representation but with the normalization in the finite volume V (and periodic boundary conditions) is then obtained with the help of

the rules[24] (5.47) and (5.48) and reads:

$$H = \sum_{\mathbf{p},\sigma} \frac{\hbar^2 \mathbf{p}^2}{2m}\, a^\dagger_{\mathbf{p},\sigma} a_{\mathbf{p},\sigma} + \frac{1}{V} \sum_{\mathbf{q}} \tilde{V}_{\rm pot}(\mathbf{q}) \sum_{\mathbf{p},\sigma} a^\dagger_{\mathbf{p}+\mathbf{q},\sigma} a_{\mathbf{p},\sigma}\,. \tag{5.65}$$

Of course, if instead of the one-particle bases formed by the generalized vectors $|\mathbf{x}\rangle$ or $|\mathbf{p}\rangle$ one uses as the complete set the eigenvectors $|l\rangle$ corresponding to the eigenvalues ε_l of the full one-particle Hamiltonian $H^{(1)} = \hat{\mathbf{P}}^2/2m + V_{\rm pot}(\hat{\mathbf{x}})$, the "second-quantized" Hamiltonian H will take the simple form

$$H = \sum_l \varepsilon_l\, a^\dagger_l a_l\,, \tag{5.66}$$

(the range of the label l may in this case consist of a discrete and a continuous part). Note also that the operator

$$\hat{n}(\mathbf{x}) = \sum_\alpha \hat{\psi}^\dagger_\alpha(\mathbf{x}) \hat{\psi}_\alpha(\mathbf{x})\,, \tag{5.67}$$

has the natural interpretation of the operator of the particle number density at the point $\mathbf{x}$ (the number of particles per unit volume). The operator (5.59) counting the number of particles is given by $\hat{N} = \int d^3\mathbf{x}\, \hat{n}(\mathbf{x})$.

Another class of operators which can be straightforwardly expressed through the creation and annihilation operators form the operators of binary interactions acting in the spaces $\mathcal{H}^{(N)}$ with $N \geq 2$. Such operators can be written in the general form

$$\hat{V}_{\rm int} = \frac{1}{2} \sum_{i\neq j}^{N} V_{\rm int}(\hat{1} \otimes \ldots \otimes \hat{O}^{(1)}_i \otimes \ldots \otimes \hat{1},\, \hat{1} \otimes \ldots \otimes \hat{O}^{(1)}_j \otimes \ldots \otimes \hat{1})\,, \tag{5.68}$$

where $V_{\rm int}(x,y)$ is a real-valued symmetric, $V_{\rm int}(x,y) = V_{\rm int}(y,x)$, function of two arguments; correspondingly to the character of the operators $O^{(1)}_i$, the arguments x, y may be of the vector character. To express such operators, promoting them thereby to operators acting in the big Hilbert space (5.20), in terms of the creation and annihilation operators it is necessary[25] to take as the basis of the $\mathcal{H}^{(N)}$ space the state-vectors $a^\dagger_{l_1} \ldots a^\dagger_{l_N}|{\rm void}\rangle$ in which $a^\dagger_l$ are the creation operators associated with the orthonormal basis of $\mathcal{H}^{(1)}$ formed out of eigenvectors $|l\rangle$ of the operator $O^{(1)}$: $\langle l'|O^{(1)}|l\rangle = o_l\, \delta_{l'l}$. It is then easy to check that the matrix elements of (5.68)

$$\langle l'_1, \ldots, l'_N|\hat{V}_{\rm int}|l_N, \ldots, l_1\rangle = \frac{1}{2} \sum_{i\neq j} V_{\rm int}(o_{l_i}, o_{l_j}) \langle l'_1, \ldots, l'_N|l_N, \ldots, l_1\rangle\,,$$

[24] Direct transition from (5.62) to the momentum representation in the finite volume using the expressions (5.45) encounters the problem that the function $V_{\rm pot}(\mathbf{x})$ is usually not periodic in the volume V, so its Fourier transform must be taken in the infiite space.

[25] For the function $V_{\rm int}(x,y)$ may not be expandable in the Taylor series around the point $(0,0)$.

are identical with the corresponding matrix elements of the operator[26]

$$\frac{1}{2}\sum_{l',l} V_{\rm int}(o_{l'}, o_l)\, a_l^\dagger a_{l'}^\dagger a_{l'} a_l\,, \tag{5.69}$$

defined on the entire big Hilbert space (5.20).

The simplest operator of this kind is the potential energy operator of the binary spin-independent interactions which in the ordinary formulation (in terms of the wave functions $\Psi_{\sigma_1,\ldots,\sigma_N}(\mathbf{x}_1,\ldots,\mathbf{x}_N)$ with imposed symmetry requirements) in the N-body quantum mechanics has the form

$$\hat{V}_{\rm int} = \frac{1}{2}\sum_{i\neq j} V_{\rm int}^{(2)}(\hat{1}\otimes\ldots\otimes\hat{\mathbf{x}}_i\otimes\ldots\otimes\hat{1},\, \hat{1}\otimes\ldots\otimes\hat{\mathbf{x}}_j\otimes\ldots\otimes\hat{1})\,. \tag{5.70}$$

Its action in the big Hilbert space (5.20) of indistinguishable particles is represented by the operator

$$\hat{V}_{\rm int} = \frac{1}{2}\int d^3\mathbf{x}\int d^3\mathbf{y}\sum_{\alpha\beta}\hat{\psi}_\alpha^\dagger(\mathbf{x})\,\hat{\psi}_\beta^\dagger(\mathbf{y})\,V(\mathbf{x},\mathbf{y})\,\hat{\psi}_\beta(\mathbf{y})\,\hat{\psi}_\alpha(\mathbf{x})\,, \tag{5.71}$$

One can easily include also spin-dependent binary interactions by writing

$$\hat{V}_{\rm int} = \frac{1}{2}\int d^3\mathbf{x}\int d^3\mathbf{y}\sum_{\alpha'\alpha}\sum_{\beta'\beta}\hat{\psi}_{\alpha'}^\dagger(\mathbf{x})\,\hat{\psi}_{\beta'}^\dagger(\mathbf{y})\,V_{\alpha'\beta',\beta\alpha}(\mathbf{x},\mathbf{y})\,\hat{\psi}_\beta(\mathbf{y})\,\hat{\psi}_\alpha(\mathbf{x})\,. \tag{5.72}$$

In both these formulae the integrals are either over a finite volume V in which the interacting particles are enclosed or over the entire infinite sppace.

The operators (5.71) and (5.72) are said to be *normally ordered* with respect to the vector $|\text{void}\rangle$, because the operators $\hat{\psi}$ which annihilate this vector stand to the right of the operators $\hat{\psi}^\dagger$. In this respect (5.71) differs from the operator

$$\hat{V}'_{\rm int} = \frac{1}{2}\int d^3\mathbf{x}\int d^3\mathbf{y}\,\hat{n}(\mathbf{x})\hat{n}(\mathbf{y})V(\mathbf{x},\mathbf{y})\,,$$

with $\hat{n}(\mathbf{x})$ given by (5.67) by a local term $(1/2)\int d^3\mathbf{x}V(\mathbf{x},\mathbf{x})\hat{n}(\mathbf{x})$ which usually is infinite. Normal ordering is a necessary condition for the equivalence of the second-quantized form of the nonrelativistic many-body theory with its ordinary formulation based on the N-body Schrödinger equation. Since such an equivalence of the relativistic theory is not possible, normal ordering of interaction operators $\hat{V}_{\rm int}$ ceases to be in this case a necessary requirement. It is also to be noted that the interaction operators (5.71) or (5.72) are spatially nonlocal (they involve two integrals over the space) - in this respect they differ from the interaction operators used in relativistic theories which are always assumed

[26]The ordering of the operators $a_{l'}$ and a_l (and of $a_l^\dagger$ and $a_{l'}^\dagger$) is crucial if they are fermionic!

to be local; nonlocality of the operators (5.71) or (5.72) is another consequence of their direct relation to operators used in the traditional formulation of the many-body quantum mechanics in terms of the multi-particle wave functions and ensures that no infinites[27] (of the sort which are typical of relativistic theories) are encountered in computations of quantities characterizing many-body systems.[28]

In their most general forms the interactions (5.71) and (5.72) are neither translationally nor rotationally invariant that is, the total momentum $\hat{\mathbf{P}}$ and the total angular momentum $\hat{\mathbf{J}}$ operators would not commute with the complete Hamiltonian

$$H = -\frac{\hbar^2}{2m}\int d^3\mathbf{x} \sum_\alpha \hat{\psi}^\dagger_\alpha(\mathbf{x})\boldsymbol{\nabla}^2\hat{\psi}_\alpha(\mathbf{x}) + \hat{V}_{\rm int}\,, \tag{5.73}$$

and, therefore, would not generate symmetries of the system. The interaction $\hat{V}_{\rm int}$ of the form (5.71) or (5.72) commutes with the total momentum operator $\hat{\mathbf{P}}$ (in all cases given by (5.60)) only if the function $V(\mathbf{x},\mathbf{y})$, or the function $V_{\alpha'\beta',\beta\alpha}(\mathbf{x},\mathbf{y})$, depends only on the difference $\mathbf{x}-\mathbf{y}$. Rotational invariance of the spin-independent interaction (5.71) is in turn ensured if $V(\mathbf{x}-\mathbf{y})$ depends on $|\mathbf{x}-\mathbf{y}|$: the operators $\hat{\mathbf{J}}$, the precise form of which depends on the spin s of the particles, constructed out of the creation and annihilation operators following the general prescription (5.58) and the formula (4.78) commute then with the Hamiltonian. Spin-dependent interaction operators (5.72), to lead to the rotational invariance, must depend in a specific way (depending on the spin s of the interacting particles) on the spin indices α, β, ... ; for instance, if the interacting particles are spin 1/2 fermions, the binary interaction must be of the form

$$V_{\alpha'\beta',\beta\alpha}(\mathbf{x},\mathbf{y}) = V_{\rm pot1}(|\mathbf{x}-\mathbf{y}|)\,\delta_{\alpha'\alpha}\delta_{\beta'\beta} + V_{\rm pot2}(|\mathbf{x}-\mathbf{y}|)\,\boldsymbol{\sigma}_{\alpha'\alpha}\cdot\boldsymbol{\sigma}_{\beta'\beta}\,.$$

with only two independent functions $V_{\rm pot1}(|\mathbf{x}|)$ and $V_{\rm pot2}(|\mathbf{x}|)$ and the spin indices of the spin dependent term carried by the Pauli matrices $\boldsymbol{\sigma}_{\alpha'\alpha}$. In the case of the theory formulated in the infinite space out of the creation and annihilation operators one can also explicitly construct the boost operators $\hat{\mathbf{K}}$ which together the operators $\hat{\mathbf{P}}$ and $\hat{\mathbf{J}}$ and the Hamiltonian (5.73) satisfy the necessary commutation rules (4.50). The whole Galileo group discussed in Section 4.3 is then the symmetry group of the considered system of interacting particles and is realized by the symmetry operators in the Hilbert space.

Using now the rules (5.46) pertaining to the theory formulated in the infinite space it is straightforward to write the operators (5.71) or (5.72) in terms of the creation and annihilation operators associated with the momentum basis. If the interaction (5.70) is translationally invariant (the theory is formulated in the in the infinite spce), the spin

[27] Except for those - the so called infrared divergences - which are related to the long range character of the assumed potential $V_{\rm pot}(\mathbf{x}-\mathbf{y})$.

[28] Infinities in nonrelativistic theories appear, however, if nonlocal interactions are replaced by effective local ones (see Section 5.5).

dependent interaction (5.72) takes the form

$$\hat{V}_{\rm int} = \frac{1}{2}\int \frac{d^3\mathbf{q}}{(2\pi)^3}\int \frac{d^3\mathbf{p}}{(2\pi)^3}\int \frac{d^3\mathbf{k}}{(2\pi)^3}\sum_{\alpha'\alpha,\beta'\beta} a^\dagger_{\alpha'}(\mathbf{p}+\mathbf{q})\, a^\dagger_{\beta'}(\mathbf{k}-\mathbf{q})\, \tilde{V}_{\alpha'\beta',\beta\alpha}(\mathbf{q})\, a_\beta(\mathbf{k})\, a_\alpha(\mathbf{p})\,, \quad (5.74)$$

in which $\tilde{V}_{\alpha'\beta',\beta\alpha}(\mathbf{q})$ is the Fourier transform of $V_{\alpha'\beta',\beta\alpha}(\mathbf{x}-\mathbf{y})$:

$$V_{\alpha'\beta',\beta\alpha}(\mathbf{x}-\mathbf{y}) = \int \frac{d^3\mathbf{q}}{(2\pi)^3}\, \tilde{V}_{\alpha'\beta',\beta\alpha}(\mathbf{q})\, e^{i\mathbf{q}\cdot(\mathbf{x}-\mathbf{y})}\,. \quad (5.75)$$

Rotational invariance further restricts its dependence on the spin indices and restricts the dependence of the Fourier transforms of the independent functions like $V_{\rm pot1}(|\mathbf{x}|)$ and $V_{\rm pot2}(|\mathbf{x}|)$ in the case of spin 1/2 fermions, on $\mathbf{q}$ to the dependence on $|\mathbf{q}|$.

The momentum space form of the operator (5.72) in the case of particles confined to a box of volume V (with periodic boundary conditions imposed) can be obtained by applying to (5.74) the rules (5.48) and (5.47):

$$\hat{V}_{\rm int} = \frac{1}{2V}\sum_{\mathbf{q}}\sum_{\mathbf{p},\alpha'\alpha}\sum_{\mathbf{k},\beta'\beta} a^\dagger_{\mathbf{p}+\mathbf{q},\alpha'} a^\dagger_{\mathbf{k}-\mathbf{q},\beta'} \tilde{V}_{\alpha'\beta',\beta\alpha}(\mathbf{q})\, a_{\mathbf{k},\beta}\, a_{\mathbf{p},\alpha}\,. \quad (5.76)$$

(Notice the inverse volume factor in front) The action of $\hat{V}_{\rm int}$ in the momentum basis (5.40) of $\mathcal{H}^{(N)}$ in both cases: of the theory formulated in the infinite space and in the finite volume, can be graphically represented as in Figure 5.1.

It is also easy to check that every operator $\hat{V}_{\rm int}$ of the form (5.72), and more generally, of the form (5.69), commutes, as could be expected, with the particle number operator (5.59):

$$[\hat{V}_{\rm int},\ \hat{N}] = 0\,. \quad (5.77)$$

As a result, the complete Hamiltonians of the form (c.f. (5.66))

$$H = \sum_l \varepsilon_l a^\dagger_l a_l + \hat{V}_{\rm int}\,, \quad (5.78)$$

with $\hat{V}_{\rm int}$ of the general form (5.69) have separate vacua - the ground states - $|\Omega\rangle$ (which should be rather denoted $|\Omega^{(N)}\rangle$) in each subspace $\mathcal{H}^{(N)}$ of the bg Hilbert space (5.20).

We have discussed here only two classes of operators which are most typical in applications of the second quantization formalism to many-body problems. More generally, it can be easily shown (essentially by using the mathematical induction) that any operator $\hat{O}$ defined on the entire Hilbert space (5.20) by giving its matrix elements between all possible states $|l_1,\ldots,l_N\rangle$ and $\langle l'_N,\ldots,l'_{N'}|$ of some basis (of a Fock space) with arbitrary

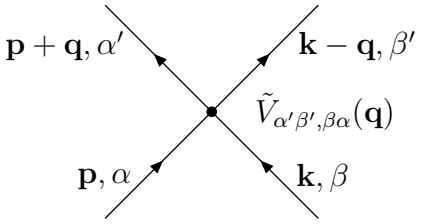

Figure 5.1: Graphical representation of the two-particle interaction (5.74) or (5.76) which conserves the total momentum in the momentum representation.

N and N' (the operator $\hat{O}$ need not commute with the particle number operator (5.59)) can be written in the form (ordered normally with respect to the $|\text{void}\rangle$ vector)

$$\hat{O}=\sum_{N=0}^{\infty}\sum_{N'=0}^{\infty}\sum_{l_N,\ldots,l_1}\sum_{l'_{N'},\ldots,l'_1} c^{N,N'}_{l_N,\ldots,l_1;l'_{N'},\ldots,l'_1}\, a^{\dagger}_{l_N}\ldots a^{\dagger}_{l_1}\, a_{l'_{N'}}\ldots a_{l'_1}\,, \tag{5.79}$$

by appropriately adjusting the coefficients $c^{N,N'}_{l_1,\ldots,l_N;l'_1,\ldots,l'_{N'}}$. In particular, the creation and annihilation operators allow to construct various forms of interactions, also of the nonlocal type, like (omitting the spin labels)

$$\int\frac{d^3\mathbf{p}'_2}{(2\pi)^3}\int\frac{d^3\mathbf{p}_2}{(2\pi)^3}\int\frac{d^3\mathbf{p}'_1}{(2\pi)^3}\int\frac{d^3\mathbf{p}_1}{(2\pi)^3}\,\tilde{V}(\mathbf{p}'_1-\mathbf{p}_1,\mathbf{p}'_2-\mathbf{p}_2)\,a^{\dagger}(\mathbf{p}'_1)\,a^{\dagger}(\mathbf{p}'_2)a(\mathbf{p}_2)\,a(\mathbf{p}_1)\,, \tag{5.80}$$

corresponding to the general form (5.70) of the binary interaction (with $V^{(2)}(\mathbf{x},\mathbf{y})$ being a symmetric function of two independent spatial arguments) and similar ones having more integrals over independent wave vectors and/or more creation and annihilation operators. Such interactions of systems of N nonrelativistic particles are constrained only by the requirement that they commute with the operator $\hat{N}$ (5.59) that is, must involve equal numbers of the creation and annihilation operators. It will be seen (Section 7.8), however, that the requirement that the scattering amplitudes satisfy the cluster decomposition principle (Section 7.8) enforces the presence of one delta function (which effectively reduces the number of independent wave vectors) in the kernel $\tilde{V}(\mathbf{p}_1,\ldots,\mathbf{p}_{2M})$ (in fact the reasons for which the formalism of the creation and annihilation operators is so useful in nonrelativistic quantum mechanics of many particle systems is that is allows to easily satisfy the cluster decomposition principle). We will also see, that the requirement of relativistic covariance of transition amplitudes (S-matrix elements) imposes much more stringent constraints on possible forms of interactions and makes it impossible to maintain the particle number conservation.

It should be clear (this has been already stressed) that as long as the (ordered normally with respect to the $|\text{void}\rangle$ vector) Hamiltonian operator H commutes with the particle number operator $\hat{N}$ (5.59) and the admitted states of the system are superpositions of only state-vectors with the same (finite) number N of particles, the formalism developed here

is equivalent to the one based of the multi-particle Schrödinger equation (again omitting spin labels)

$$i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{x}_1,\ldots,\mathbf{x}_N,t)=H(\mathbf{x}_1,\ldots,\mathbf{x}_N)\Psi(\mathbf{x}_1,\ldots,\mathbf{x}_N,t)\,, \tag{5.81}$$

in which the Hamiltonian is symmetric with respect to permutations of the variables of the N particles and the wave-fuctions $\Psi(\mathbf{x}_1,\ldots,\mathbf{x}_N,t)$ are either totally symmetric or totally antisymmetric. More precisely, the equation

$$i\hbar\frac{d}{dt}|\Psi(t)\rangle=H|\Psi(t)\rangle\,, \tag{5.82}$$

which in the formalism of second quantization determines the time evolution in the big Hilbert space $\mathcal{H}=\oplus_{N=0}^{\infty}\mathcal{H}^{(N)}$ of state-vectors $|\Psi(t)\rangle$ having components belonging to each of the subspaces $\mathcal{H}^{(N)}$

$$a|\text{void}\rangle,\qquad |\Psi^{(1)}\rangle,\qquad |\Psi^{(2)}\rangle\,,\qquad \ldots$$

breaks up into an infinite set of uncoupled, independent Schrödinger equations (5.81) corresponding to $N=1,2,\ldots$ particles. This is easily seen by closing (5.82) with $\langle\mathbf{x}_N,\ldots,\mathbf{x}_1|$, $N=1,2,\ldots$ from the left and using the orthogonality of vectors belonging to different $\mathcal{H}^{(N)}$'s, and the fact that H commutes with $\hat{N}$ (it has vanishing matrix elements between vectors belonging to different $\mathcal{H}^{(N)}$'s). The $N=0$ component of the equation (5.82) is trivial ($0=0$) because for consistency with $\dot{a}=0$ Hamiltonians of systems of nonrelativistic particles should always be constructed so that $H|\text{void}\rangle=0$ that is, with terms involving (equal numbers of) creation and annihilation operators ordered normally with respect to the vector $|\text{void}\rangle$. Normally ordered (with respect to the $|\text{void}\rangle$ vector) form of such Hamiltonians is crucial for the equivalence also because it eliminates certain contributions to amplitudes which are absent in the conventional formulation in terms of the many-body Schrödinger equation. Hamiltonians of interacting relativistic particles cannot commute with the operators of particle numbers and, as a result, in the relativistic case the equation (5.82) would lead to infinitely many coupled equations. It has been already remarked that in this case normal ordering of interaction operators is not a necessary requirement.

The formalism of second quantization is exceptionally flexible and allows also to go far beyond the quantum mechanics based on the N-body Schrödinger equation (5.81). Owing to the fact that the creation and annihilation operators can be associated with quantum states of individual elements of physical systems it allows to easily build (effective) Hamiltonians of emergent phenomena without taking into account the (complicated) underlying dynamics of the more fundamental particles constituting the system. The simplest example are interactions of electrons with phonons which are quantum excitations of lattices consisting of molecules (which themselves are composed of electrons and nuclei): once the states of the lattice are represented as in Section 5.6 in terms of phonons and the associated creation and annihilation operators introduced, it is possible to write

Hamiltonians coupling directly free electrons of a solid with phonons treated as particles (such effective Hamiltonians do not, however, preserve the number of phonons and in this respect resemble Hamiltonians of relativistic particles; phonons are rather quasi-particles than particles). Many other models of similar kind, for instance of particles on lattices capable of hopping from one lattice site to others (generically called Hubbard models) can be costructed using this formalism and find their applications in condensed matter physics in building effective models of a huge variety of phenomena.

The final remark is that the second quantized version of the nonrelativistic quantum theory of many-particle systems as well as all models formulated using this formalism are obviously models of the usual quantum mechanics in which the central role is played by the Hamiltonian operator and its spectrum. The fact that the formalism of second quantization is especially useful in investigating many-body problems, or statistical physics problems in which the statistical operators $\hat{\rho} = Z_{\mathrm{stat}}^{-1} \exp(-\hat{H}/k_{\mathrm{B}}T)$ of the Canonical Ensemble or $\hat{\rho} = Z_{\mathrm{stat}}^{-1} \exp(-(\hat{H} - \mu\hat{N})/k_{\mathrm{B}}T)$ of the Grand Canonical Ensemble play the most important roles, does not preclude applying it also to few-body probems of quantum mechanics, like e.g. the scattering problems (this requires only that the relevant theories be formulated in the infinite space rather than in the finite volume). It is also useful to keep in mind that in the formalism of second quantization all standard rules of quantum mechanics which are formulated in terms of state-vectors and matrix elements of operators, such as e.g. perturbative expansions (stationary and time-dependent ones - see Section 2.1), for computing energy spectra and transition probabilities remain valid and can be used to analyse properties of interacting many particle systems. New is only the method of computing the requisite matrix elements.

5.4 Ground state of a system of fermions. Holes

The formalism of the second quantization applied to systems composed of fermions and to systems composed of bosons is superficially very similar. The only difference seems to be that the creation and annihilation operators associated with bosons satisfy the commutation rules while those associated with fermions - the anticommutation rules. (In addition fermionic operators necessarily carry a spin label). This is indeed so if this formalism is applied to few-body problems, like the mentioned scattering problems. What makes the behaviour of (nonrelativistic) bosonic and fermionic systems really very different is the structure of their respective ground states when the numbers of particles in the system are very large (the systems are macroscopic). Of course, the true system's ground state (ground states in different $\mathcal{H}^{(N)}$ subspaces, in the case of nonrelativistic systems) $|\Omega\rangle$ depends on the precise form of the system's complete Hamiltonian that is, on the particle's interactions, but the essential difference can be seen already in the absence of any interaction (especially if one considers thermodynamic properties of the system).

Consider first a system of N identical indistinguishable fermions the unperturbed

Hamiltonian H_0 of which is obtained by neglecting their mutual interactions (it can therefore correspond to a system of fermions confined in some external potential). It is therefore essentially the sum of the form (5.54) of one-particle operators $H^{(1)}$. Let $|l\rangle$ be the eigenvectors of $H^{(1)}$:

$$H^{(1)}|l\rangle = \varepsilon_l|l\rangle\,, \tag{5.83}$$

where $l = 1, 2, \ldots$ (we assume that the spectrum of $H^{(1)}$ is discrete either because the system is enclosed in a finite volume or because the particles are effectively confined by an external potential). Written in terms of the creation and annihilation operators associated with the states $|l\rangle$ the free Hamiltonian H_0 of the system takes the simple form (5.66) and as a basis of the N-particle Hilbert space $\mathcal{H}^{(N)}$ it is convenient to take the state-vectors

$$|l_N, \ldots, l_2, l_1\rangle = a^\dagger_{l_N} \ldots a^\dagger_{l_2} a^\dagger_{l_1}|\text{void}\rangle\,, \tag{5.84}$$

with $l_1 < l_2 < \ldots < l_N$ corresponding to the ordering $\varepsilon_{l_1} \leq \varepsilon_{l_2} \ldots \leq \varepsilon_{l_N}$ of the energies.

If the complete Hamiltonian of the system (i.e. H_0 plus the interaction term $\hat{V}_{\text{int}}$) commutes with the particle number operator $\hat{N}$ (5.59), one is not interested in the state $|\text{void}\rangle$ but rather in the state $|\Omega_0\rangle$ which is the lowest energy eigenvector of H_0 in the subspace $\mathcal{H}^{(N)}$ of the big Hilbert space $\mathcal{H}$. It is clear that if $N > 2s + 1$ (s is the spin the fermions), the eigenvalue of H_0 on $|\Omega_0\rangle$ cannot be equal to $N\varepsilon_1$ because of the Pauli exclusion principle reflected in the antisymmetry of N-particle states with respect to interchanges of particles: each fermion has to occupy a separate one-particle state. If the energy eigenvalues of the one-particle Hamiltonian $H^{(1)}_0$ are, as has been assumed, ordered so that[29] $\varepsilon_1 \leq \varepsilon_2 \leq \varepsilon_3 \leq \ldots$, the state $|\Omega_0\rangle$ of the lowest possible energy - the (unperturbed) ground state called also the free vacuum state - is

$$|\Omega_0\rangle = |N, \ldots, 3, 2, 1\rangle = a^\dagger_N \ldots a^\dagger_3 a^\dagger_2 a^\dagger_1|\text{void}\rangle\,, \tag{5.85}$$

(i.e. $|\Omega_0\rangle$ corresponds to the basis vector (5.84) with $l_1 = 1, l_2 = 2$, etc.) and

$$E_{\Omega_0} = \varepsilon_1 + \varepsilon_2 + \ldots + \varepsilon_N > N\varepsilon_1\,. \tag{5.86}$$

One says that one-particle states which are occupied in the system's ground-state (in the absence of mutual particle interactions) all lie below the *Fermi energy* $\varepsilon_{\text{F}} \equiv \varepsilon_N$, or below the *Fermi level*, whereas those which are unoccupied are above the Fermi level.[30]

For example, if $H^{(1)} = \hat{\mathbf{P}}^2/2m_f$, the energy E_{Ω_0} of the ground state of N noninteracting spin s (half-integer) fermions of mass m_f enclosed in the volume $V = L^3$ (with

[29] If the particle energy does not depend on the direction of its spin, there are always $2s + 1$ distinct one-particle states with the same energy; the degeneracy of excited energy levels can be even higher if e.g. energy does not depend on the direction of the particle's momentum.

[30] In fact, when the interactions are spin independent and the numbers N_σ (such that $\sum_{\sigma=-s}^{s} N_\sigma = N$) of fermions with the spin projection σ are fixed the relevant ground state $|\Omega_0\rangle$ is characterized by $2s+1$ Fermi energies $\varepsilon_{\text{F}\sigma}$.

periodic boundary conditions imposed), N_σ of which have spin projection σ is given by the expression

$$E_{\Omega_0} = \sum_{\sigma=-s}^{s} \sum_{\mathbf{k}}^{|\mathbf{k}|<p_{\mathrm{F}\sigma}} \frac{\hbar^2 \mathbf{k}^2}{2m_f}\,, \tag{5.87}$$

in which the inner sum runs over wave vectors $\mathbf{k}$ of the form $\mathbf{k} = (2\pi/L)\mathbf{n}$ (here $\mathbf{n}$ are vectors having integer components) and the Fermi wave wectors $p_{\mathrm{F}\sigma}$ are determined by the numbers N_σ:

$$N_\sigma = \sum_{\mathbf{k}}^{|\mathbf{k}|<p_{\mathrm{F}\sigma}} 1\,. \tag{5.88}$$

In the thermodynamic limit, applying the rule (5.48) one gets

$$E_{\Omega_0} = \frac{V}{6\pi^2}\,\frac{3}{5}\,\frac{\hbar^2}{2m_f} \sum_{\sigma=-s}^{s} p_{\mathrm{F}\sigma}^5\,, \qquad N_\sigma = \frac{V}{6\pi^2}\,p_{\mathrm{F}\sigma}^3\,. \tag{5.89}$$

Since $\sum_{\sigma=-s}^{s} N_\sigma = N$, it is convenient to introduce the overall Fermi vector k_{F} defined by $(g_s = 2s+1)$

$$N = g_s V \int \frac{d^3\mathbf{k}}{(2\pi)^3}\,\theta(k_{\mathrm{F}} - |\mathbf{k}|), \tag{5.90}$$

so that $k_{\mathrm{F}} = ((6\pi^2/g_s)(N/V))^{1/3}$ and to define the fractions $x_\sigma \equiv p_{\mathrm{F}\sigma}/k_{\mathrm{F}}$, satisfying the sum rule $x_{-s} + \ldots + x_s = 1$. The ground state energy density takes then the form

$$\frac{E_{\Omega_0}}{V} = \frac{k_{\mathrm{F}}^3}{6\pi^2}\,\frac{3}{5}\,\frac{\hbar^2 k_{\mathrm{F}}^2}{2m_f} \sum_{\sigma=-s}^{s} x_\sigma^5\,. \tag{5.91}$$

If $s = 1/2$ and $P = (N_+ - N_-)/N$ the energy density expressed in terms of the polarization P of the system reads

$$\frac{E_{\Omega_0}}{V} = \frac{k_{\mathrm{F}}^3}{6\pi^2}\,\frac{3}{5}\,\frac{\hbar^2 k_{\mathrm{F}}^2}{2m_f}\left[(1+P)^{5/3} + (1-P)^{5/3}\right]. \tag{5.92}$$

When mutual interactions, represented by $\hat{V}_{\mathrm{int}}$, of the considered fermions are taken into account, the basis vectors (5.84) will not in general be eigenvectors of the complete Hamiltonian $H = H_0 + \hat{V}_{\mathrm{int}}$. Even if the system is initially prepared in the ground state (5.85) of H_0, the probability of finding it later in a state of a higher H_0 energy will be nonzero - the perturbation $\hat{V}_{\mathrm{int}}$ will cause transitions (see Chapter 2 for a discussion when such transitions can be physically relevant) between the eigenstates of H_0. In the perturbative expansion this can be interpreted as successive actions of $\hat{V}_{\mathrm{int}}$ which e.g. in

the case of a binary interaction of the general form (5.69) removes two particles from two filled one-particle states and puts them into two available empty ones. In particular, removing a particle from a one-particle state of energy $\varepsilon_{\tilde{l}}$ below the Fermi level $\varepsilon_{\rm F}$ and putting it into a state of energy ε_l above it can be viewed as creation of a *hole* of energy $-\varepsilon_{\tilde{l}}$ and of a *particle* of energy $\varepsilon_l > \varepsilon_{\tilde{l}}$ (one interprets then the ground state $|\Omega_0\rangle$ as a state with no particles, or better, with no excitations).

This view can be formalized by redefining the creation and annihilation operators corresponding to the H_0 one-particle eigenstates $|\tilde{l}\rangle$ with $1 \leq \tilde{l} \leq N$ and to its eigenstates $|l\rangle$ with $l > N$ as follows (notice that the redefinition depends on the number N of fermions forming the system):

$$\left.\begin{array}{l} a_{\tilde{l}} \equiv d_{\tilde{l}}^\dagger \\ a_{\tilde{l}}^\dagger \equiv d_{\tilde{l}} \end{array}\right\} \quad \text{if} \quad 1 \leq \tilde{l} \leq N\,, \quad \text{and} \quad \left.\begin{array}{l} a_l \equiv b_l \\ a_l^\dagger \equiv b_l^\dagger \end{array}\right\} \quad \text{if} \quad N < l\,. \tag{5.93}$$

It is obvious that now ($l > N$, $\tilde{l} \leq N$)

$$b_l|\Omega_0\rangle = 0\,, \qquad d_{\tilde{l}}|\Omega_0\rangle = 0\,. \tag{5.94}$$

Because the fermionic creation and annihilation operators satisfy the *anticommutation rules* which are symmetric (with respect to interchanging a_l and $a_l^\dagger$), the redefinition (5.93) is perfectly possible: $d_{\tilde{l}}^\dagger$ and $d_{\tilde{l}}$ have all the necessary algebraic properties to be interpreted as fermionic creation and annihilation operators, respectively. Therefore the vectors (5.84) (which can be created by the successive actions of $\hat{V}_{\rm int}$ on the ground state $|\Omega_0\rangle$ of H_0 in the N-fermion sector) forming the basis of the space $\mathcal{H}^{(N)}$ of the system of N fermions can equivalently be written in the form

$$|l_1, \ldots, l_m, \tilde{l}_1, \ldots, \tilde{l}_n\rangle \equiv b_{l_1}^\dagger \ldots b_{l_m}^\dagger d_{\tilde{l}_1}^\dagger \ldots d_{\tilde{l}_n}^\dagger |\Omega_0\rangle\,, \tag{5.95}$$

in which all labels l_i correspond to one-particle states lying above the Fermi level (unoccupied in the ground state) and all labels $\tilde{l}_j$ correspond to one-particle states below the Fermi level (filled in the ground-state). One interprets such states as consisting of m "particles" and n "holes" or $n+m$ "excitations" (of course $n = m \leq N$ because $\hat{V}_{\rm int}$ conserves the number of particles and there are N fermions).

The form of the particle (fermion) number operator $\hat{N}$ (5.59) rewritten accordingly (its last term is a c-number),

$$\hat{N} = \sum_{l>N} b_l^\dagger b_l - \sum_{\tilde{l}\leq N} d_{\tilde{l}}^\dagger d_{\tilde{l}} + N\hat{1}\,, \tag{5.96}$$

suggests that a hole should be ascribed the fermionic number -1 (that is, it can be viewed as -1 particle, or as an "antiparticle"). The free Hamiltonian rewritten in terms of the new operators takes the form

$$H_0 = \sum_{l=1}^{\infty} \varepsilon_l\, a_l^\dagger a_l = \sum_{l>N} \varepsilon_l\, b_l^\dagger b_l + \sum_{\tilde{l}\leq N} \varepsilon_{\tilde{l}}\, d_{\tilde{l}} d_{\tilde{l}}^\dagger$$

$$= \sum_{l>N} \varepsilon_l \, b_l^\dagger b_l + \sum_{\tilde{l}\leq N} (-\varepsilon_{\tilde{l}}) \, d_{\tilde{l}}^\dagger d_{\tilde{l}} + \hat{1} \sum_{\tilde{l}\leq N} \varepsilon_{\tilde{l}} \, . \tag{5.97}$$

The last c-number term is simply the energy E_{Ω_0} of the ground-state $|\Omega_0\rangle$ of H_0 (of the system of N mutually noninteracting fermions). This means that we consider "particles" and "holes" as positive and negative energy excitations, respectively over the ground state of energy E_{Ω_0}. The interpretation of holes as particles carrying negative fermionic number can be made even more suggestive if the one-particle Hamiltonian $H^{(1)}$ is shifted by an appropriate negative constant (equal $-\varepsilon_{\rm F}$), so that in (5.83) all one-particle states $|\tilde{l}\rangle$ with $\tilde{l} = 1, 2, \ldots, N$ have negative energies[31] ($\varepsilon_{\tilde{l}} \to \varepsilon_{\tilde{l}} - \varepsilon_{\rm F} < 0$). The last sum in (5.97), which in some problems (when only differences of energy levels are important) can simply be discarded as physically uninteresting,[32] is then negative while as is clear from penultimate term in (5.97), each created hole increases energy of the system (because its creation corresponds to removing from the system of a particle in the negative energy state). Thus both types of system's excitations (particles and holes-antiparticles) carry now positive energies. Finally, the formulae (5.50) rewritten in terms of the new operators take the forms

$$\begin{aligned} \hat{\psi}_\alpha(\mathbf{x}) &= \sum_{l>N} b_l \, (u_l)_\alpha(\mathbf{x}) + \sum_{\tilde{l}\leq N} d_{\tilde{l}}^\dagger \, (v_{\tilde{l}})_\alpha(\mathbf{x}) \, , \\ \hat{\psi}_\alpha^\dagger(\mathbf{x}) &= \sum_{l>N} b_l^\dagger \, (u_l)_\alpha^*(\mathbf{x}) + \sum_{\tilde{l}\leq N} d_{\tilde{l}} \, (v_{\tilde{l}})_\alpha^*(\mathbf{x}) \, , \end{aligned} \tag{5.98}$$

where we have defined $(v_{\tilde{l}})_\alpha(\mathbf{x}) \equiv (u_{\tilde{l}})_\alpha$ when $\tilde{l} \leq N$. (The operators $\hat{\psi}_\alpha(\mathbf{x})$ and $\hat{\psi}_\alpha^\dagger(\mathbf{x})$ must have as many components as do have the functions $(u_l)_\alpha(\mathbf{x})$ and $(v_{\tilde{l}})_\alpha$). In this form the operators $\hat{\psi}_\alpha(\mathbf{x})$ and $\hat{\psi}_\alpha^\dagger(\mathbf{x})$ bear close resemblance to relativistic field operators (which will be introduced in Chapter 8).

Any interaction operator $\hat{V}_{\rm int}$ of a system of many fermions (if the system of many fermions is enclosed in a box of finite volume the redefinitions (5.93) can be made with respect to the ground state of H_0 consisting of the kinetic energy only and the interaction of particles with an external potential - if present - can be included in $\hat{V}_{\rm int}$) written in terms of the original creation and annihilation operators $a_{\mathbf{p},\sigma}$ and $a_{\mathbf{p},\sigma}^\dagger$ can be expressed in terms of the operators of particles and holes defined in (5.93) and its terms can be interpreted as creating and/or annihilating a number of particles and/or holes. The interaction operator $\hat{V}_{\rm int}$, originally normally ordered with respect to the vector $|\text{void}\rangle$ will then not be normally

[31] In the similar spirit, it is convenient to change the labeling of the now negative energy one-particle eigenstates $|\tilde{l}\rangle$ which are eigenvectors of the one-particle momentum $\hat{\mathbf{P}}^{(1)}$ and the one-particle spin $\hat{S}^{z(1)}$ operators with the eigenvalues $+\mathbf{p}$ and $+\sigma$ so that they are denoted $|-\mathbf{p}, -\sigma\rangle$; an unoccupied negative energy one-particle state denoted now $|\mathbf{p}, \sigma\rangle$ - a hole - contributes then $+\mathbf{p}$ and $+\sigma$ to the total system's momentum and the total system's z-axis spin projection.

[32] There are, however, problems in which this term or, more precisely, differences of such terms specific for systems with the same total number N of fermions but different numbers of fermions with different spin projections, is physically relevant.

ordered with respect to the ground state $|\Omega_0\rangle$ but can be brought to such a form by an appropriate rearrangment (as in (5.96) and (5.97)) of its terms using the anticommutation relations.

The possibility of defining a set of operators which all annihilate the N-particle ground state $|\Omega_0\rangle$ (the operators $d_{\tilde{l}}$ and b_l) and the possibility of splitting the field operators $\hat{\psi}_\alpha(\mathbf{x})$ and $\hat{\psi}^\dagger_\alpha(\mathbf{x})$ as in (5.98) is of great help in applying to Green's functions (which will be introduced and briefly discussed in Section 5.7), or to the formula (1.38) allowing to compute corrections to the ground state energy, the standard Dyson perturbative expansion (presented in Section 5.8): the usefulness of this expansion relies on the possibility of using the Wick theorem (see Section 5.9) which in turn is most efficient if such a set of operators annihilating the ground state $|\Omega_0\rangle$ exists. Fermionic systems are in this respect "easier" than systems consisting mutually interacting bosons because the ground-state of N mutually noninteracting bosons

$$|\Omega_0\rangle = |N, 0, 0, \ldots\rangle\,, \tag{5.99}$$

(written here in the occupation number notation) and $\langle\Omega_0|$ are not annihilated by the operators $a_{l=1}$, $a^\dagger_{l=1}$, respectively ($|l=1\rangle$ is here the lowest energy state of the one-particle Hamiltonian $H^{(1)}$) or $a_{\mathbf{p}=\mathbf{0}}$, $a^\dagger_{\mathbf{p}=\mathbf{0}}$, if the system of bosons is enclosed in a finite volume (with periodic conditions are imposed) and the kinetic energy operator is taken for H_0. A trick enabling using the Wick theorem in perturbative computations of quantities characterizing systems of many bosons is illustrated in the next Section in which a correction to the ground state energy of many bosons is computed using the Bogolyubov transformation.

The interpretation of excitations of a system of fermions in terms of "holes" and particles proves extremely useful in applications to solid state physics and condensed matter physics. Furthermore, the reasoning (the essence of which is the transition from the quantum mechanics of a single particle to the many-particle theory) put forward by Dirac to make sense out of the negative energy solutions of his relativistic wave equation for charged spin $\frac{1}{2}$ particles is in fact application of the same idea. The only difference with the non-relativistic theory of a system of fermions developed in this section is that the energy spectrum of the one-particle Hamiltonian corresponding to the Dirac equation is unbounded from below and therefore the c-number constants (treated as unphysical) in (5.96) and in (5.97) are infinite. While (superficially) successful in solving the problem of negative energy states associated with relativistic wave equations for fermions, this reasoning, for obvious reasons, cannot solve the analogous problem of relativistic wave equations, like the Klein-Gordon one, supposed to apply to bosons. As will be shown, relativistic quantum mechanics of many particles of arbitrary spins (half-integer as well as integer) can, nevertheless, be consistently formulated without any reference to relativistic wave equations. Wave equations are not the basis of the relativistic quantum field theory (although such an impression can be drawn from older textbooks). It might therefore seem that in the modern approach to quantum field theory the interpretation of negative energy states as holes is obsolete and should be regarded purely as a historical

curiosity were it not for the fact that the picture of a filled sea of negative energy states comes back (in a somewhat different disguise) in the path integral approach to quantum field theories involving fermions and seems indispensable to understand highly nontrivial nonperturbative phenomena like nonconservation of the fermion number or the baryon number.

5.5 Energy of the ground state of a system of many bosons

To illustrate the difference in the structure of the ground states of systems of N fermions and bosons we consider here a simple model of the interaction of nonrelativistic bosons. This will also give the opportunity to demonstrate the trick called the Bogolyubov transformation which will be mentioned also in setting the general framework for relativistic particles interactions in Chapter 7.

The Hamiltonian of the system of bosons of mass M and (for simplicity) spin 0 enclosed in the box of volume V will be taken in the form

$$H = H_0 + V_{\rm int} = \sum_{\mathbf{p}} \frac{\hbar^2 \mathbf{p}^2}{2M}\, a^\dagger_{\mathbf{p}} a_{\mathbf{p}} + \frac{g}{2V} \sum_{\mathbf{q}} \sum_{\mathbf{p}_1,\mathbf{p}_2} a^\dagger_{\mathbf{p}_1+\mathbf{q}} a^\dagger_{\mathbf{p}_2-\mathbf{q}} a_{\mathbf{p}_2} a_{\mathbf{p}_1}\,. \tag{5.100}$$

The interaction $V_{\rm int}$ is local here, i.e. the general translationally invariant potential $V_{\rm pot}(\mathbf{x},\mathbf{y}) = V_{\rm pot}(\mathbf{x}-\mathbf{y})$ of (5.71) of the binary interactions is taken in the singular form $g\,\delta^{(3)}(\mathbf{x}-\mathbf{y})$. As potentials of interaction of nonrelativistic particles forming real systems is spatially nonlocal (and nonlocal interactions are naturally used in the formulation of the same problem in the traditional language of the N-body Schrödinger equation), this requires some explanation. Moreover, such a local interaction will, in general, lead to infinities when it is used e.g. to compute corrections to the system's ground-state energy (computing the gas ground-state energy is equivalent to investigating its zero temperature properties) or in the Born series (in the formalism of second quantization most efficiently implemented by using the general formulation of the scattering theory outlined in Chapter 7) to compute the amplitude $f(k,\theta)$ of the elastic scattering of two bosons ($k = |\mathbf{k}|$ is here the center of mass momentum of the colliding particles). A realistic nonlocal interaction of the form (5.72), even if having a hard core character (e.g. infinite for $|\mathbf{x}-\mathbf{y}|$ smaller than some distance), certainly leads to a well defined, finite ground-state energy and a finite scattering amplitude,

If the gas of N bosons is sufficiently diluted, which means that its density N/V is much smaller than the length scale R characterizing the true interaction potential $V_{\rm pot}(\mathbf{x}-\mathbf{y})$, one can expect that its properties are mostly determined by (rare) low energy binary collisions. On the other hand, if energies $\hbar^2\mathbf{k}^2/2M$ of the colliding particles are low, the elastic scattering amplitudes can be reliably approximated by a few first terms of their expansion in powers of kR. It should be therefore possible - and this is in fact one of the cornerstones of the whole quantum field theory successes in accounting for high energy

physics phenomena - to capture the properties of the gas using an *effective theory* with interactions having strictly local character, provided one takes the point of view that it is valid only up to momenta (wave vectors) $|\mathbf{k}|$ smaller than some cutoff scale Λ. Computing within such an effective theory, the Hamiltonian of which should in principle include all possible interaction terms (with arbitrary coupling constants like g - the interaction in (5.100) should be viewed as a first term of an infinite set of interactions) respecting symmetries of the considered system, the ground-state energy or the elastic scattering amplitude one has to cut all integrals over the wave vectors at Λ, thus avoiding infinities caused by the local character of the interaction. All quantities computed within the effective theory depend then, in addition to their dependence on the coupling constants like g, also on the cutoff Λ. Moreover, the couplings themselves should be treated as implicitly dependent on the cutoff. The correct strategy is then to treat e.g. the computation of the s-wave scattering length a_0 (to obtain the first term $-a_0$ of the expansion of $f(k,\theta)$ in powers of k the effective theory interaction explicitly included in the Hamiltonian (5.100) is sufficient) as *determining* the value of the coupling g in (5.100) in terms of the measurable s-wave scattering length a_0 (for a fixed value of the cutoff Λ) and then to express the computed ground-state energy in terms of a_0 (instead of g. The result which we need here (it will be derived in Section 7.4) reads

$$g = \frac{4\pi\hbar^2}{M}\, a_0 \left(1 + \frac{2}{\pi}\, a_0\Lambda + \dots\right). \tag{5.101}$$

Below we will see that infinities (terms growing with the ultraviolet cutoff Λ) present in the computation of the ground state energy of the system of N bosons using the Hamiltonian (5.100) will disappear when the result is expressed in terms of the measurable scattering length a_0, instead of the unknown coupling g. This is in fact the essence of the *renormalization* procedure which is one of the main issues in relativistic field theories (which necessarily have a local character) and will in this context be discussed in Chapter 14.

It is clear, that in the absence of any interactions the energy of the system of N bosons enclosed in the box of volume V is exactly zero, because they all can and will occupy the $\mathbf{k} = \mathbf{0}$ one-particle state. Therefore the occupation number $n_{\mathbf{0}} = N$. This is the well known phenomenon of the Bose-Einstein condensation discussed in all textbooks of statistical physics (from the point of view of statistical mechanics the system is considered here at zero temperature T). It can be expected, that in the presence of interactions (at $T = 0$) $n_{\mathbf{0}}$ will still be large, of order N, and that the energy of the ground state can be reliably computed using the local effective Hamiltonian (5.100). The first assumption gives rise to the so-called Bogolyoubov trick which essentially consists of replacing the operators $a^\dagger_{\mathbf{0}}$ and $a_{\mathbf{0}}$ by the c-number

$$a^\dagger_{\mathbf{0}} \to \sqrt{n_{\mathbf{0}}}\,, \qquad a_{\mathbf{0}} \to \sqrt{n_{\mathbf{0}}}\,. \tag{5.102}$$

This can be rigorously shown to be a correct procedure in the thermodynamic limit $N \to \infty$, $V \to \infty$, at fixed N/V. One can also expect that in the ground state only one-particle

states with small $|\mathbf{k}|$ are significantly populated, in conjuction with the substitutions (5.102) leads to the model interaction Hamiltonian[33]

$$V_{\rm int} = \frac{g}{2V}\left[n_{\mathbf{0}}^2 + 2\,n_{\mathbf{0}}\sum_{\mathbf{p}\neq\mathbf{0}}\left(a_{\mathbf{p}}^\dagger a_{\mathbf{p}} + a_{-\mathbf{p}}^\dagger a_{-\mathbf{p}}\right) + n_{\mathbf{0}}\sum_{\mathbf{p}\neq\mathbf{0}}\left(a_{\mathbf{p}}^\dagger a_{-\mathbf{p}}^\dagger + a_{\mathbf{p}} a_{-\mathbf{p}}\right)\right] + \tilde{V}_{\rm int}\,. \quad (5.103)$$

$\tilde{V}_{\rm int}$ stands here for terms with three and four operators and the terms bilinear in these operators have been written for convenience in the form symmetric w.r.t. the interchange $\mathbf{p}\leftrightarrow-\mathbf{p}$. In turn, the particle number operator becomes

$$\hat{N} = n_{\mathbf{0}} + \frac{1}{2}\sum_{\mathbf{p}\neq\mathbf{0}}\left(a_{\mathbf{p}}^\dagger a_{\mathbf{p}} + a_{-\mathbf{p}}^\dagger a_{-\mathbf{p}}\right). \quad (5.104)$$

Since the number of particles in the system is fixed, the operator $\hat{N}$ can be replaced by the c-number N. Upon using (5.104) to eliminate $n_{\mathbf{0}}$ (moving terms with more than two operators to $\tilde{V}_{\rm int}$ which gets, therefore, modified), the complete effective Hamiltonian (5.100) takes the form[34]

$$\begin{aligned} H &= \frac{gN^2}{2V} + \frac{1}{2}\sum_{\mathbf{p}\neq\mathbf{0}}\left[\left(\frac{\hbar^2\mathbf{p}^2}{2M} + \frac{gN}{V}\right)\left(a_{\mathbf{p}}^\dagger a_{\mathbf{p}} + a_{-\mathbf{p}}^\dagger a_{-\mathbf{p}}\right) + \frac{gN}{V}\left(a_{\mathbf{p}}^\dagger a_{-\mathbf{p}}^\dagger + a_{\mathbf{p}} a_{-\mathbf{p}}\right)\right] + \tilde{V}_{\rm int} \\ &= \tilde{H}_0 + \tilde{V}_{\rm int}\,. \end{aligned} \quad (5.105)$$

In the thermodynamic limit, i.e. when the substitutions (5.102) are exact, this form of the Hamiltonian is fully equivalent to the original one. It should be, however noticed that this Hamiltonian does not commute with the the operator $\hat{N}' = \sum_{\mathbf{p}\neq\mathbf{0}} a_{\mathbf{p}}^\dagger a_{\mathbf{p}}$ counting the number of particles outside the condensate. The energy of the ground state of bosons can be now computed by finding the exact spectrum of $\tilde{H}_0$ and corrections to it induced by the interaction $\tilde{V}_{\rm int}$. The first approximation to the ground state energy of the system of N bosons is therefore given by the ground state energy of $\tilde{H}_0$.

The spectrum of $\tilde{H}_0$ can be found using the Bogolyubov transformation which is analogous to the transformation used in Section 1.3 to find the exact spectrum of the

[33] To obtain its part proportional to $n_{\mathbf{0}}$ it is convenient to write the operators in $V_{\rm int}$ of (5.100) as the sum of two terms

$$\sum_{\mathbf{p}_1,\mathbf{p}_2} a_{\mathbf{p}_1}^\dagger a_{\mathbf{p}_2}^\dagger a_{\mathbf{p}_2} a_{\mathbf{p}_1} + \sum_{\mathbf{q}\neq\mathbf{0}}\sum_{\mathbf{p}_1,\mathbf{p}_2} a_{\mathbf{p}_1+\mathbf{q}}^\dagger a_{\mathbf{p}_2-\mathbf{q}}^\dagger a_{\mathbf{p}_2} a_{\mathbf{p}_1}\,.$$

In the first one (in which $\mathbf{q}=\mathbf{0}$) either $\mathbf{p}_1=\mathbf{0}$, $\mathbf{p}_2\neq\mathbf{0}$, or the other way around ($\mathbf{p}_1=\mathbf{p}_2=\mathbf{0}$ gives the term proportional to $n_{\mathbf{0}}^2$). In the second term (with $\mathbf{q}\neq\mathbf{0}$) either $\mathbf{p}_1=\mathbf{p}_2=\mathbf{0}$, or $\mathbf{p}_1=\mathbf{0}$ and $\mathbf{p}_2=\mathbf{q}$, or $\mathbf{p}_1=-\mathbf{q}$ and $\mathbf{p}_2=\mathbf{0}$, or $\mathbf{p}_1=-\mathbf{q}$ and $\mathbf{p}_2=\mathbf{q}$. It should be noted that no term linear in the operators can arise.

[34] The first its term, $gN^2/2V$, is (in the thermodynamic limit) the same as the order g correction to the ground state energy which would be obtained by applying the ordinary Raileigh - Schrödinger formula $E_\Omega = E_{\Omega_0} + \langle\Omega_0^{(N)}|V_{\rm int}|\Omega_0^{(N)}\rangle + \ldots$ (in which $E_{\Omega_0}=0$) to $V_{\rm int}$ of (5.100) and $|\Omega_0^{(N)}\rangle$ given by (5.99).

Hamiltonian of the perturbed oscillator. In the present case one defines new operators

$$a_{\mathbf{p}} = u_{\mathbf{p}}\, A_{\mathbf{p}} - v_{\mathbf{p}}\, A^{\dagger}_{-\mathbf{p}}\,, \qquad a^{\dagger}_{\mathbf{p}} = u_{\mathbf{p}}\, A^{\dagger}_{\mathbf{p}} - v_{\mathbf{p}}\, A_{-\mathbf{p}}\,. \tag{5.106}$$

Assuming that the coefficients $u_{\mathbf{p}}$ and $v_{\mathbf{p}}$ are real and depend only on $|\mathbf{p}|$, it is easy to see that the requirement that $A_{\mathbf{p}}$ and $A^{\dagger}_{\mathbf{p}}$ satisfy the commutation rules $[A_{\mathbf{p}'},\, A^{\dagger}_{\mathbf{p}}] = \delta_{\mathbf{p}'\mathbf{p}}$, $[A_{\mathbf{p}'},\, A_{\mathbf{p}}] = [A^{\dagger}_{\mathbf{p}'},\, A^{\dagger}_{\mathbf{p}}] = 0$, imposes the conditions

$$u^2_{\mathbf{p}} - v^2_{\mathbf{p}} = 1\,. \tag{5.107}$$

Hence, the coefficients can be represented as $u_{\mathbf{p}} = \cosh\vartheta_{\mathbf{p}}$, $v_{\mathbf{p}} = \sinh\vartheta_{\mathbf{p}}$. The angles $\vartheta_{\mathbf{p}}$ can be now adjusted to bring $\tilde{H}_0$ into the diagonal form, that is to ensure the absence in it of terms with $A^{\dagger}_{\mathbf{p}}A^{\dagger}_{-\mathbf{p}}$ and $A_{\mathbf{p}}A_{-\mathbf{p}}$. A short calculation leads to

$$\tanh 2\vartheta_{\mathbf{p}} = \frac{gN/V}{(gN/V) + (\hbar^2\mathbf{p}^2/2M)}\,. \tag{5.108}$$

The Hamiltonian $\tilde{H}_0$ expressed in terms of the $A^{\dagger}_{\mathbf{p}}$ and $A_{\mathbf{p}}$ operators takes then the form[35]

$$\begin{aligned}\tilde{H}_0 = \frac{gN^2}{2V} - \frac{1}{2}\sum_{\mathbf{p}\neq\mathbf{0}}\left[\left(\frac{\hbar^2\mathbf{p}^2}{2M} + \frac{gN}{V}\right) - \sqrt{\left(\frac{\hbar^2\mathbf{p}^2}{2M} + \frac{gN}{V}\right)^2 - \left(\frac{gN}{V}\right)^2}\right] \\ + \frac{1}{2}\sum_{\mathbf{p}\neq\mathbf{0}}\sqrt{\left(\frac{\hbar^2\mathbf{p}^2}{2M} + \frac{gN}{V}\right)^2 - \left(\frac{gN}{V}\right)^2}\left(A^{\dagger}_{\mathbf{p}}A_{\mathbf{p}} + A^{\dagger}_{-\mathbf{p}}A_{-\mathbf{p}}\right).\end{aligned} \tag{5.109}$$

It is now clear (by the same argument as that used in Section 1.3) that the ground state of $\tilde{H}_0$ is the state $|\tilde{\Omega}_0\rangle$ annihilated by all $A_{\mathbf{p}}$ operators and its energy is given by the first line of the above formula. The sum over $\mathbf{p}$ in this expression is divergent, but in line with the remarks made before it should be cut off at $|\mathbf{p}| = \Lambda$. It is convenient to rewrite this ground state energy in the form

$$\begin{aligned}E_{\tilde{\Omega}_0} = \frac{gN^2}{2V} - \frac{g^2N^2M}{2\hbar^2V^2}\sum_{\mathbf{p}}\frac{1}{\mathbf{p}^2} \\ -\frac{1}{2}\sum_{\mathbf{p}\neq\mathbf{0}}\left[\left(\frac{\hbar^2\mathbf{p}^2}{2M} + \frac{gN}{V}\right) - \sqrt{\left(\frac{\hbar^2\mathbf{p}^2}{2M} + \frac{gN}{V}\right)^2 - \left(\frac{gN}{V}\right)^2} - \frac{g^2N^2M}{\hbar^2V^2\mathbf{p}^2}\right].\end{aligned}$$

In the thermodynamic limit the sums over $\mathbf{p}$ can be replaced by the integrals using the prescription (5.48); the first line then is

$$\frac{gN^2}{2V} - \frac{g^2N^2M}{2\hbar^2V}\,\frac{1}{2\pi^2}\int_0^{\Lambda} d|\mathbf{p}| = \frac{N^2}{V}\left(\frac{1}{2}\,g - \frac{g^2M}{4\pi^2\hbar^2}\,\Lambda\right), \tag{5.110}$$

[35] To arrive at this form of $\tilde{H}_0$ one uses the following relations: if $\tanh 2\vartheta = x$, then $e^{2\vartheta} = \sqrt{(1+x)/(1-x)} = (1+x)/\sqrt{1-x^2}$, $e^{-2\vartheta} = (1-x)/\sqrt{1-x^2}$, $\sinh 2\vartheta = x/\sqrt{1-x^2}$, $\cosh 2\vartheta = 1/\sqrt{1-x^2}$ and $\sinh^2\vartheta = (-1+\cosh 2\vartheta)/2$, $\cosh^2\vartheta = (1+\cosh 2\vartheta)/2$.

while the integral over $|\mathbf{p}|$ obtained in the second line is convergent (the integrand behaves as $1/|\mathbf{p}|^4$) and the cutoff Λ in it can be sent to infinity. The crucial step is now to express the ground state energy through the measurable parameter a_0 using the relation (5.101). The expression (5.110) becomes then independent of Λ up to terms of order a_0^2 and simply reads $(N^2/V)(2\pi\hbar^2/M)a_0$. Making in the second integral the substitution $x = |\mathbf{p}|\sqrt{V\hbar^2/2MgN}$ one obtains the integral which Mathematica does readily[36] and the ground state energy of the system of N interacting bosons can be cast in the form[37]

$$\frac{E_{\tilde{\Omega}_0}}{N} = \frac{N}{V}\,\frac{2\pi\hbar^2}{M}\,a_0\left[1 + \frac{128}{15}\left(\frac{N}{V}\,\frac{a_0^3}{\pi}\right)^{1/2} + \ldots\right]. \tag{5.111}$$

It is finite and is, in the approximation employed here, "universal" in the sense that it does not depend on all details of the two-body interaction potential $V_{\rm pot}(\mathbf{x}-\mathbf{y})$, but only on the scattering length a_0 this interaction gives rise to. The energy spectrum of the system of N interacting bosons is in this approximation also universal (depends only on the s-wave scattering length a_0 and not on the detailed form of the two-body potential $V_{\rm pot}(\mathbf{x}-\mathbf{y})$).

The developed approach allows also to estimate the number of interacting bosons occupying the $\mathbf{p} = \mathbf{0}$ one-particle state. In the same approximation as (5.111) the occupation numbers $n_{\mathbf{p}}$ with $\mathbf{p} \neq \mathbf{0}$ is given by

$$n_{\mathbf{p}} = \langle\tilde{\Omega}_0|a_{\mathbf{p}}^\dagger a_{\mathbf{p}}|\tilde{\Omega}_0\rangle = v_{\mathbf{p}}^2\,\langle\tilde{\Omega}_0|A_{-\mathbf{p}}A_{-\mathbf{p}}^\dagger|\tilde{\Omega}_0\rangle = v_{\mathbf{p}}^2\,,$$

and (in the thermodynamic limit)

$$n_{\mathbf{0}} = N - \sum_{\mathbf{p}\neq\mathbf{0}} v_{\mathbf{p}}^2 = N - V\int\frac{d^3\mathbf{p}}{(2\pi)^3}\,\frac{1}{2}\left(\frac{\frac{\hbar^2\mathbf{p}^2}{2M} + \frac{gN}{V}}{\sqrt{\left(\frac{\hbar^2\mathbf{p}^2}{2M} + \frac{gN}{V}\right)^2 - \left(\frac{gN}{V}\right)^2}} - 1\right)$$

Making again the substitution $x = |\mathbf{p}|\sqrt{V\hbar^2/2MgN}$ one obtains

$$n_{\mathbf{0}} = N - \frac{V}{4\pi^2}\,\frac{2MgN}{\hbar^2V}\left(\frac{2MgN}{\hbar^2V}\right)^{1/2}\int_0^\infty dx\,x^2\left(\frac{x^2+1}{\sqrt{x^4+2x^2}} - 1\right),$$

that is (the integral equals $\sqrt{2}/3$)

$$n_{\mathbf{0}} = N\left[1 - \frac{8}{3}\left(\frac{N}{V}\,\frac{a_0^3}{\pi}\right)^{1/2} + \ldots\right]. \tag{5.112}$$

[36]The integral is

$$\int_0^\infty dx\,x^2\left(x^2 + 1 - \sqrt{x^4+2x^2} - \frac{1}{2x^2}\right) = -\frac{8\sqrt{2}}{15}\,.$$

[37]After the integration the second is proportional to $g^{5/2}$; consistency then requires to replace g in it by $(4\pi\hbar^2/M)a_0$.

Thus even at zero temperature not all interacting bosons occupy the $\mathbf{p} = \mathbf{0}$ one-particle state.

Since in the new formulation all operators $A_{\mathbf{p}}$ annihilate the $\tilde{H}_0$ ground state $|\tilde{\Omega}_0\rangle$, the Dyson expansion employing the Wick theorem can be used to compute further corrections to the energy of the ground state of the system. (Within the effective field theory approach this requires including in the effective Hamiltonian (5.100) further local terms the coefficients of which should be determined by matchig onto the higher partial wave scattering lengths and effective ranges parametrizing the low nergy expansion of the scattering amplitude of two bosons.)

The same effective interaction (5.100) with exactly the same justification as in the bosonic case can be used to determine corrections to the ground state energy of a diluted gas of N fermions (corrections to the result (5.91)). The order g corrections can be computed by applying the standard Rayleigh - Schrödinger perturbative expansion. The resulting order g correction is finite and the result (5.101) (which, as will be seen, applies also to fermions) truncated to the term proportional to a_0 can be used to express the ground state energy density $E_\Omega/V = E_{\Omega_0}/V + \mathcal{O}(g)$ in terms of the s-wave scattering length a_0. Further corrections (of order g^2 and higher) can be also computed (most easily by exploiting the formula (1.38)). They are UV divergent and must be computed using some UV regularization like e.g. the cutoff Λ used here. But similarly as here, the ultraviolet cutoff Λ disappears if the computed energy is systematically expressed using the complete result (5.101) in terms of the measurable scattering length a_0.

5.6 Analogy with coupled harmonic oscillators

In order to provide a link between quantum mechanics of systems of many bosons and quantization of classical fields we now consider quantization of a system of N coupled harmonic oscillators to which in the approximation of small departures from the (classical) equilibrium solution any system of e.g. point masses connected by springs (e.g. playing the role of a model of a crystall lattice) of classical fields (nonrelativistic as well as relativistic) can be reduced. The classical Lagrangian of such a system has in general the form

$$L_0 = \frac{1}{2}\sum_{i,j} T_{ij}\,\dot{q}^i\dot{q}^j - \frac{1}{2}\sum_{i,j} V_{ij}\,q^i q^j\,, \tag{5.113}$$

in which V_{ij} and T_{ij} are (constant, i.e. q-independent) symmetric and positive definite $N \times N$ matrices.[38] The canonical momenta conjugated to the variables q^i are $p_j = T_{ji}\dot{q}^i$ and the corresponding classical Hamiltonian reads

$$H_0 = \frac{1}{2}\sum_{i,j}(T^{-1})^{ij}p_i p_j + \frac{1}{2}\sum_{i,j} V_{ij}q^i q^j\,. \tag{5.114}$$

[38]Here we are more restrictive than one usually is in classical mechanics and assume that both T and V matrices have strictly positive eigenvalues.

Upon quantization $q^i(t)$ and $p_i(t)$ become Schrödinger picture operators satisfying the standard relation $[\hat{q}^i,\ \hat{p}_j] = i\hbar\,\delta^i_j$ but the Hamiltonian (5.114) expressed through the operators a_i and $a_i^\dagger$ related in the standard way (1.40) to $\hat{q}^i$ and $\hat{p}_j$ would not have the form of the sum of the $a_i^\dagger a_i$ terms. To find the spectrum and the Hamiltonian eigenvectors one can solve first the classical problem by introducing the normal mode coordinates $Q^a(t)$ through the formula

$$q^i(t) = A^i_{(a)} Q^a(t)\,, \tag{5.115}$$

where the vectors $A^i_{(a)}$ $a = 1, \ldots, N$ are solutions of the eigenproblem

$$\left(-\omega_a^2 T_{ij} + V_{ij}\right) A^j_{(a)} = 0\,. \tag{5.116}$$

The vectors $A^i_{(a)}$ should be chosen orthonormal in the scalar product set by the matrix T_{ij}: $A^i_{(a)} T_{ij} A^j_{(b)} = \delta_{ab}$. The Lagrangian (5.113) expressed through the normal variables is (working out the potential energy terms one exploits the equation (5.116)) takes the form

$$\begin{aligned} L_0 &= \frac{1}{2} T_{ij} A^i_{(a)} \dot{Q}^a A^j_{(b)} \dot{Q}^b - \frac{1}{2} V_{ij} A^i_{(a)} Q^a A^j_{(b)} Q^b \\ &= \frac{1}{2}\delta_{ab}\dot{Q}^a\dot{Q}^b - \frac{1}{2} A^i_{(a)} Q^a \omega_b^2 T_{ij} A^j_{(b)} Q^b = \frac{1}{2}\delta_{ab}\dot{Q}^a\dot{Q}^b - \frac{1}{2}\omega_b^2\delta_{ab} Q^a Q^b\,. \end{aligned}$$

To the old momenta p_i, the momenta P_a conjugated to the new variables Q^a are related by[39] $P_a = p_i A^i_{(a)}$ and, since $(T^{-1})^{ij} = A^i_{(a)} A^j_{(a)}$, the corresponding Hamiltonian is

$$H_0 = \frac{1}{2} P_a P_a + \frac{1}{2}\,\omega_a^2 Q^a Q^a\,. \tag{5.117}$$

The system can be now quantized by promoting the variables $Q^a(t)$ and $P_a(t)$ to Schrödinger picture (time independent) operators. It can be checked that the commutation relations of the canonical variables remain unchanged: $[\hat{Q}^a,\, \hat{P}_b] = i\hbar\,\delta^a_b$ (because the transformation (5.115) is a canonical transformation which does not change the Poisson brackets). Next, one defines the operators

$$A_a = \sqrt{\frac{\omega_a}{2\hbar}}\left(\hat{Q}^a + \frac{i}{\omega_a}\,\hat{P}_a\right), \qquad A_a^\dagger = \sqrt{\frac{\omega_a}{2\hbar}}\left(\hat{Q}^a - \frac{i}{\omega_a}\,\hat{P}_a\right), \tag{5.118}$$

which satisfy the relation $[A_a,\ A_b^\dagger] = \delta_{ab}$. The Hamiltonian of the system expressed in terms of these operators is already diagonal:

$$H_0 = \sum_{a=1}^{N} \hbar\omega_a \left(A_a^\dagger A_a + \frac{1}{2}\right). \tag{5.119}$$

[39] As usually,

$$P_a = \frac{\partial \tilde{L}(Q,\,\dot{Q})}{\partial \dot{Q}^a} = \frac{\partial L(q(Q),\,\dot{q}(Q,\dot{Q}))}{\partial \dot{q}^i}\,\frac{\partial \dot{q}^i}{\partial \dot{Q}^a} \equiv p_i\,\frac{\partial q^i}{\partial Q^a}\,,$$

because $\partial\dot{q}^i/\partial\dot{Q}^a = \partial q^i/\partial Q^a$.

The eigenvectors of H_0 are therefore of the form

$$|n_1, n_2, \ldots, n_N\rangle = \left(\prod_{a=1}^{N} \frac{\left(A_a^\dagger\right)^{n_a}}{\sqrt{n_a!}} \right) |0, 0, \ldots, 0\rangle \,, \tag{5.120}$$

where $|0, 0, \ldots, 0\rangle$ (with N zeroes) is the system's ground-state annihilated by all A_a's. In this respect it is similar to the vector $|\text{void}\rangle$ spanning the subspace $\mathcal{H}^{(0)}$ of the big Hilbert space (5.20) but in contrast to it, it represents a real physical state (characterized e.g. by nonzero fluctuations of the variables Q_a) of the system of real oscillators. The energy of the state (5.120) is

$$E_{n_1,n_2,\ldots,n_N} = \sum_{\alpha=1}^{N} n_a \hbar\omega_a + \frac{1}{2} \sum_{a=1}^{N} \hbar\omega_a \,. \tag{5.121}$$

The second term - the energy of the ground state can be subtracted if we declare that we are interested only in the differences of energies of the states.

The operator (5.119) can e.g. be the Hamiltonian of quantized vibrations of a crystal lattice.[40] The same structure, with $N = \infty$ and a replaced by $(\mathbf{k}, \lambda)$ was also obtained in Section 3.8 as a result of quantizing the free electromagnetic radiation field enclosed in a box. By analogy with the form of the Hamiltonian

$$H = \sum_{\mathbf{p}} \varepsilon_{\mathbf{p}} \, a_{\mathbf{p}}^\dagger a_{\mathbf{p}} \,,$$

of a system of N noninteracting spinless particles (with periodic boundary conditions in a box of volume $V = L^3$), in the second quantization formalism discussed in the preceding sections, the crystal lattice quantum states $|n_1, n_2, \ldots, n_N\rangle$ (the states $|n_{\mathbf{k}_1\lambda_1}, n_{\mathbf{k}_2\lambda_2}, \ldots\rangle$ of the radiation field quantized in the box) are interpreted as the states consisting of n_1 phonons of type 1 ($n_{\mathbf{k}_1\lambda_1}$ photons with the wave vector $\mathbf{k}_1$ and the polarization λ_1), n_2 phonons of type 2 ($n_{\mathbf{k}_2\lambda_2}$ photons of type two), etc. (there are N types of phonons corresponding to N different lattice vibration modes of frequencies ω_α; the number of the "types" of photons, i.e. photons of different wave vectors $\mathbf{k}$, is not limited). Since the energy (5.121) of such states is additive (the energy contributed by each phonon or photon is independent of the presence of other phonons or photons), phonons or photons which are excitations of the Hamiltonians of the form (5.119) are interpreted as mutually noninteracting.

The action of the operators A_a and $A_a^\dagger$ on the states (5.120) is standard:

$$\begin{aligned} A_a^\dagger |n_1, \ldots, n_a, \ldots, n_N\rangle &= \sqrt{n_a + 1}\, |n_1, \ldots, n_a + 1, \ldots, n_N\rangle \\ A_a |n_1, \ldots, n_a, \ldots, n_N\rangle &= \sqrt{n_a}\, |n_1, \ldots, n_a - 1, \ldots, n_N\rangle \,. \end{aligned} \tag{5.122}$$

[40] In the case of a crystal lattice one usually neglects boundary effects and considers $N = \infty$ coupled oscillators; after a change of the variables, the normal modes are then labeled by a continuous parameter $\mathbf{K}$, $-\pi/a \le K^i \le \pi/a$ (called quasi-momentum) rather than by a discrete index a. The occupation number representation (5.120) has then to be replaced by the representation (5.124).

It corresponds to the action of the bosonic particles creation and annihilation operators in the occupation number representation (5.35). There is however one difference between the second-quantized version of nonrelativistic quantum mechanics of particles and phonons: in the former case the number N of particles is fixed (in nonrelativistic systems it does not change in time, even if the interactions are taken into account), so that in the occupation number representation always $n_1 + n_2 + \ldots = N$. In the latter case, the system can be excited to an arbitrary state $|n_1, \ldots, n_a, \ldots, n_N\rangle$ and the numbers n_a which are eigenvalues of the operators $A_a^\dagger A_a$ (giving the number of phonons of type a) and, therefore, also eigenvalues of the operator of the total number of phonons

$$\hat{N} = \sum_{a=1}^{N} A_a^\dagger A_a \,, \tag{5.123}$$

can be arbitrary integers. In contrast, it is the number N of the phonon types that is finite. The difference disappears however if one allows for arbitrary numbers of particles (e.g. by working in the Grand Canonical Ensemble) in the first case and for an infinite number of vibration modes in the second case.

The basis of states of phonons can be also labeled differently, namely as:

$$|a_1, a_2, \ldots, a_n, \ldots\rangle = A_{a_1}^\dagger A_{a_2}^\dagger \ldots A_{a_n}^\dagger \ldots |\Omega_0\rangle \,, \tag{5.124}$$

where $a_1 \leq a_2 \leq \ldots$ and the state-vector $|\Omega_0\rangle \equiv |0, 0, \ldots, 0\rangle$ (with N zeroes) is the same ground state as in (5.120). The state-vectors $|a_1, a_2, \ldots, a_n, \ldots\rangle$ are related to the basis vectors (5.120) by

$$\begin{aligned} |1, \ldots, 1, 2, \ldots, 2, \ldots, N, \ldots, N\rangle &= \left(A_1^\dagger\right)^{n_1} \left(A_2^\dagger\right)^{n_2} \ldots \left(A_N^\dagger\right)^{n_N} |\Omega_0\rangle \\ &= \sqrt{n_1! n_2! \ldots n_N!}\, |n_1, n_2 \ldots, n_N\rangle \,. \end{aligned} \tag{5.125}$$

For small numbers of phonons this new representation is more convenient. The action of the creation and annihilation operators on the states (5.124) is given by

$$\begin{aligned} A_a^\dagger |a_1, \ldots, a_n, \ldots\rangle &= |a, a_1, \ldots, a_n, \ldots\rangle \,, \\ A_a |a_1, \ldots, a_n, \ldots\rangle &= \sum_{k=1}^{N} \delta_{a_k, a} |a_1, \ldots, (\text{no } a_k), \ldots\rangle \,, \end{aligned} \tag{5.126}$$

and looks the same as the action (5.27) and (5.28) of the creation and annihilation operators corresponding to one-particle states. Thus, barring the difference just explained, quantized harmonic vibrations of a crystal lattice interpreted in terms of phonons are formally equivalent to a system of many free bosons.

Consider finally perturbations of the initial Lagrangian (5.113) by polynomial terms of order higher than second in the variables q_i

$$V_{\text{int}} = \sum_{i,j,k=1}^{N} V_{ijk}\, q^i q^j q^k + \sum_{i,j,k,l=1}^{N} V_{ijkl}\, q^i q^j q^k q^l + \ldots \tag{5.127}$$

When rewritten in terms of the operators A_α, $A_\alpha^\dagger$ they give rise (among others) to terms of the form (B, Cm $D, \ldots$ are in general complex constants)

$$V_{\rm int} \ni B\, A_a^\dagger A_b^\dagger A_c^\dagger + C\, A_a^\dagger A_b^\dagger A_c + D\, A_a^\dagger A_b^\dagger A_c^\dagger A_d^\dagger + \ldots + {\rm H.c.}\,, \tag{5.128}$$

which contain nonequal numbers of the creation and annihilation operators and, hence, do not commute with the operator (5.123) of the total number of phonons. The time evolution will therefore not preserve the number of phonons. In contrast, Hamiltonians of nonrelativistic particle systems always preserve the number of particles. We will see however, that the requirement of relativistic covariance of transition amplitudes enforces nonconservation of the number of particles. Hence, relativistic quantum mechanics of particles naturally acquires features of phonon systems.

5.7 One-particle (two-point) nonrelativistic Green's funtions

Very important objects in the second-quantized formulation of quantum mechanics of many-body systems and of quantum field theory in general are various Green's functions. The causal (also called Feynmanian) ones are defined as true vacuum (the complete Hamiltonian $H = H_0 + V_{\rm int}$, normalized to unity ground state $|\Omega\rangle$) expectation values of chronological products of strings of Heisenberg picture operators $O_a^H(t)$ (the index a may stand here, as in (5.129), also for the space argument $\mathbf{x}$ of the operator) taken at different times

$$iG_{abc\ldots}(t_a, t_b, t_c, \ldots) = \langle\Omega|{\rm T}\, O_a^H(t_a) O_b^H(t_b) O_c^H(t_c) \ldots |\Omega\rangle\,.$$

In the nonrelativistic many-body theory (and also in the relativistic quantum field theory - see Section 13.3) a distinguished role play the so-called one-particle causal Green's functions (from another point of view classified as two-point Green's functions of the elementary field operators of the theory)

$$iG_{\alpha\beta}^{\rm cau}(t, \mathbf{x}; t', \mathbf{x}') = \langle\Omega|{\rm T}\psi_\alpha^H(t, \mathbf{x})\, \psi_\beta^{\dagger H}(t', \mathbf{x}')|\Omega\rangle\,, \tag{5.129}$$

in which the field operators $\psi_\alpha^H(t, \mathbf{x})$, $\psi_\beta^{\dagger H}(t, \mathbf{x})$ are the Heisenberg picture counterparts of the Schrödinger picture operators defined by (5.45), if the system is enclosed in the finite volume V (and periodic boundary conditions are imposed), (5.46) if it is considered in the infinite space, or, if one associates the creation and annihilation operators with a $\mathcal{H}^{(1)}$ basis other than the momentum one, by (5.50). The ground state $|\Omega\rangle$ is in this case the ground state of the complete Hamiltonian in the N-particle subspace $\mathcal{H}^{(N)}$. One should also recall that the chronological product of bosonic operators is defined as in (1.8), and that of fermionic operators is defined with the minus sign in terms in which the fermionic operators stand in an odd order with respect to their order under the symbol T of the chronological product.

In the nonrelativistic many-body theory the distinguished role of the functions (5.129) stems from the fact that many quantities characterizing the system can be extracted from

them. For example, if an single-particle operator $\hat{O}^{(1)}$ is written in the form (5.58) in the position basis

$$\hat{O} = \int d^3\mathbf{x}\, \hat{O}(\mathbf{x}) = \int d^3\mathbf{x} \sum_{\alpha,\beta} \psi^\dagger_\beta(\mathbf{x})\, O_{\beta\alpha}(\mathbf{x})\psi_\alpha(\mathbf{x})\,, \tag{5.130}$$

($O_{\beta\alpha}(\mathbf{x}) \equiv \langle \mathbf{x}, \beta|\hat{O}^{(1)}|\mathbf{x}, \alpha\rangle$ can also be a differential operator as in (5.60) or (5.62)), the ground state expectation value of $\hat{O}(\mathbf{x})$ can be obtained as (the upper sign applies to bosons; the lower one - to fermions)

$$\langle\Omega|\hat{O}(\mathbf{x})|\Omega\rangle = \pm \lim_{\mathbf{x}'\to\mathbf{x}} \sum_{\alpha,\beta} O_{\beta\alpha}(\mathbf{x})\, iG^{\rm cau}_{\alpha\beta}(t, \mathbf{x}; t^+, \mathbf{x}')\,, \tag{5.131}$$

where $t^+ \equiv t + 0$ (i.e. $t' \to t^+$). For instance, the total kinetic energy of all particles constituting the system can be obtained as

$$\langle\Omega|\hat{T}|\Omega\rangle = \pm \int d^3\mathbf{x} \lim_{\mathbf{x}'\to\mathbf{x}} \left(-\frac{\hbar^2}{2m}\,\boldsymbol{\nabla}^2_{\mathbf{x}}\right) iG^{\rm cau}_{\alpha\beta}(t, \mathbf{x}; t^+, \mathbf{x}')\,, \tag{5.132}$$

and the total number N_σ of particles with the spin projection σ in the system (computed as the ground state expectation value of the particle number operator (5.59)) as

$$\langle\Omega|\hat{N}_\sigma|\Omega\rangle = \pm \int d^3\mathbf{x} \lim_{\mathbf{x}'\to\mathbf{x}} iG^{\rm cau}_{\sigma\sigma}(t, \mathbf{x}; t^+, \mathbf{x}')\,. \tag{5.133}$$

In the case of the Hamiltonian $H = H_0 + V_{\rm int} = T + V_{\rm int}$, where $V_{\rm int}$ is a binary interactions of the form (5.72) with $V_{\alpha'\beta',\beta\alpha}(\mathbf{x}, \mathbf{y}) = V_{\beta'\alpha',\alpha\beta}(\mathbf{y}, \mathbf{x})$ it is easy to show that the complete ground state expectation value of the Hamiltonian, that is the system's ground state energy E_Ω, can be extracted from (5.129) in the similar way. To show this one exploits the fact that the Heisenberg picture field operator $\psi^H_\alpha(t, \mathbf{x})$ satisfies the equation (1.15), which here reads (we consider time-independent Hamiltonians H)

$$i\hbar\,\frac{\partial}{\partial t}\,\psi^H_\alpha(t, \mathbf{x}) = [\psi^H_\alpha(t, \mathbf{x}),\, H] = e^{iHt/\hbar}\,[\psi_\alpha(\mathbf{x}),\, H]e^{\,-iHt/\hbar}\,. \tag{5.134}$$

Computing the commutator on the right-had side using, if $\psi_\alpha(\mathbf{x})$ is a bosonic operator, the formula $[A,\, BC] = [A,\, B]C + B\,[A,\, C]$ or $[A,\, BC] = \{A,\, B\}C - B\,\{A,\, C\}$ if it is fermionic, and the rules (5.52), one finds

$$[\psi_\alpha(\mathbf{x}),\, H] = -\frac{\hbar^2}{2m}\,\boldsymbol{\nabla}^2_{\mathbf{x}}\psi_\alpha(\mathbf{x}) + \int d^3\mathbf{y}\, \psi^\dagger_\beta(\mathbf{y})V_{\alpha\beta,\beta'\alpha'}(\mathbf{x}, \mathbf{y})\psi_{\beta'}(\mathbf{y})\psi_{\alpha'}(\mathbf{x})\,,$$

This inserted into (5.134) leads to the relation

$$\left(i\hbar\,\frac{\partial}{\partial t} + \frac{\hbar^2}{2m}\,\boldsymbol{\nabla}^2_{\mathbf{x}}\right)\psi^H_\alpha(t, \mathbf{x}) = \int d^3\mathbf{y}\, \psi^{\dagger H}_\beta(t, \mathbf{y})V_{\alpha\beta,\beta'\alpha'}(\mathbf{x}, \mathbf{y})\psi^H_{\beta'}(t, \mathbf{y})\psi^H_{\alpha'}(t, \mathbf{x})\,,$$

which, when multiplied from the left with $\psi^{\dagger H}_\alpha(t',\mathbf{x})$, summed over α and integrated over $d^3\mathbf{x}$ allows to extract the ground state expectation value of the interaction operator $V_{\rm int}$ from the Green's function (5.129):

$$\langle\Omega|V_{\rm int}|\Omega\rangle = \pm\frac{1}{2}\int d^3\mathbf{x}\lim_{\mathbf{x}'\to\mathbf{x}}\lim_{t'\to t^+}\left(i\hbar\,\frac{\partial}{\partial t}+\frac{\hbar^2}{2m}\,\boldsymbol{\nabla}^2_{\mathbf{x}}\right)iG^{\rm cau}_{\alpha\beta}(t,\mathbf{x};t',\mathbf{x}')\,. \tag{5.135}$$

Combining this with the formula (5.132) one gets[41]

$$E_\Omega = \langle\Omega|H_0+V_{\rm int}|\Omega\rangle = \pm\frac{1}{2}\int d^3\mathbf{x}\lim_{\mathbf{x}'\to\mathbf{x}}\lim_{t'\to t^+}\left(i\hbar\,\frac{\partial}{\partial t}-\frac{\hbar^2}{2m}\,\boldsymbol{\nabla}^2_{\mathbf{x}}\right)iG^{\rm cau}_{\alpha\beta}(t,\mathbf{x};t',\mathbf{x}')\,. \tag{5.136}$$

The formulae (5.132) and (5.133) can be readily checked by applying them to the system of free fermions enclosed in the volume V (with periodic boundary conditions imposed). In this case the total kinetic energy is the total energy of the system and the Heisenberg picture operators coincide with the interaction picture ones. The splitting (5.98) of the interaction picture field operator $\psi^I_\alpha(\mathbf{x})$ in this case reads[42] (we assume for simplicity that $p_{\rm F}$ is independent of the spin projection σ, that is that the system consists of equal numbers $N_\sigma = N/g_s$, $g_s = 2s+1$, of fermions with all possible spin projections $\sigma = -s,\ldots,+s$)

$$\psi^I_\sigma(t,\mathbf{x}) = \frac{1}{\sqrt{V}}\sum_{|\mathbf{p}|>p_{\rm F}} b_{\mathbf{p},\sigma}\,e^{-i\omega_{\mathbf{p}}t+i\mathbf{p}\cdot\mathbf{x}} + \frac{1}{\sqrt{V}}\sum_{|\mathbf{p}|<p_{\rm F}} d^\dagger_{-\mathbf{p},-\sigma}\,e^{-i\omega_{\mathbf{p}}t+i\mathbf{p}\cdot\mathbf{x}}\,.$$

Here $\omega_{\mathbf{p}} = \hbar\mathbf{p}^2/2m \equiv \varepsilon_{\mathbf{p}}/\hbar$. The Hermitian conjugate operator $\psi^{\dagger I}_\alpha(t,\mathbf{x})$ decomposes analogously. Since (cf. the formulae (5.93) and (5.94))

$$b_{\mathbf{p},\sigma}|\Omega_0\rangle = d_{\mathbf{p},\sigma}|\Omega_0\rangle = 0\,, \qquad \langle\Omega_0|b^\dagger_{\mathbf{p},\sigma} = \langle\Omega_0|d^\dagger_{\mathbf{p},\sigma} = 0\,,$$

it is straightforward to evaluate the two vacuum expectation values in the definition of the fermionic Green's function (5.129) and to obtain

$$iG^{(0)\rm cau}_{\alpha\beta}(t,\mathbf{x};t',\mathbf{x}') = \frac{\delta_{\alpha\beta}}{V}\sum_{\mathbf{p}} e^{-i\omega_{\mathbf{p}}(t-t')}\,e^{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{x}')}\,[\theta(t-t')\theta(|\mathbf{p}|-p_{\rm F})-\theta(t'-t)\theta(p_{\rm F}-|\mathbf{p}|)]\,.$$

Using now the integral representations of the Heaviside theta functions

$$\pm\theta(\pm t) = i\int_{-\infty}^{\infty}\frac{d\Omega}{2\pi}\,\frac{e^{-i\Omega t}}{\Omega\pm i0}\,, \tag{5.137}$$

[41] The formula (5.136) is, however, not very practical; much more efficient is the the formula (1.38) which is not restricted to quartic (two-body) interactions and allows to express the difference $E_\Omega - E_{\Omega_0}$ in terms of connected "vacuum" Feynman diagrams.

[42] Although energies of one-particle states are still $\hbar^2\mathbf{p}^2/2m$ ($\varepsilon_{\rm F}$ has not been subtracted), the operators $a_{\mathbf{p},\sigma}$ and $a^\dagger_{\mathbf{p},\sigma}$ with $|\mathbf{p}| < p_{\rm F}$ are denoted here respectively $d^\dagger_{-\mathbf{p},-\sigma}$ and $d_{-\mathbf{p},-\sigma}$, in agreement with the remark made in the second footnote of Section 5.4.

this can be cast in the form

$$iG^{(0)\mathrm{cau}}_{\alpha\beta}(t,\mathbf{x};t',\mathbf{x}') = \sum_{\mathbf{p}} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi}\, e^{-i\omega(t-t')}\, e^{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{x}')}\, i\tilde{G}^{(0)\mathrm{cau}}_{\alpha\beta}(\omega,\mathbf{p})\,,$$

$$i\tilde{G}^{(0)\mathrm{cau}}_{\alpha\beta}(\omega,\mathbf{p}) = i\,\frac{\delta_{\alpha\beta}}{V}\left[\frac{\theta(|\mathbf{p}|-p_{\mathrm{F}})}{\omega-\omega_{\mathbf{p}}+i0} + \frac{\theta(p_{\mathrm{F}}-|\mathbf{p}|)}{\omega-\omega_{\mathbf{p}}-i0}\right]. \tag{5.138}$$

The function $iG^{(0)\mathrm{cau}}_{\alpha\beta}(t,\mathbf{x};t',\mathbf{x}')$ in the limit $V\to\infty$ can be obtained applying now the rule (5.48). Using the result (5.138) the formulae (5.132) and (5.133) can readily be checked.

If $V_{\mathrm{int}} \neq 0$, the exact Green's function cannot be found in the closed form and to apply the formulae (5.133), (5.132) or (5.136) it must be computed e.g. perturbatively using the Dyson expansion presented in Section 5.8 and the Wick theorem (or approximated by another method). The free Green's function obtained here and its Fourier transform $i\tilde{G}^{(0)\mathrm{cau}}_{\alpha\beta}(\omega,\mathbf{p})$ is then the key element of perturbative computation of causal Green's functions of systems of interacting fermions.

However, more important than the possibility of using the Green's function (5.129) in the formulae (5.133), (5.132) or (5.136) is the fact - true also in the relativistic theory - that its Fourier transform $\tilde{G}^{\mathrm{cau}}_{\alpha\beta}$, if the system is closed (its Hamiltonian is time independent), depends on only one frequency variable. This allows to analyze the analytic structure of $\tilde{G}^{\mathrm{cau}}_{\alpha\beta}$ as a function of the complex frequency variable ω in general terms and to demonstrate its relation to the spectrum of excitations of the system. Here we discuss this using the example of a translationally invariant system of fermions of arbitrary (half-integer) spin s enclosed in the finite volume (with periodic boundary conditions imposed) and assuming that the interaction of fermions is spin-independent (and that the numbers N_σ of fermions of different spin projections σ are all equal). Of particular importance will be the analytic structure of $\tilde{G}_{\alpha\beta}$ in the infinite volume limit.

To simplify the notation we will introduce the "four-vectors" $x=(t,\mathbf{x})$ and $\hat{P}=(\hat{H},\hat{\mathbf{P}})$ where $\hat{\mathbf{P}}$ is the momentum operator (5.60) and $\hat{H}$ is the system's complete Hamiltonian. We will also set $\hbar=1$. Assuming that the system is translationally invariant, that is that $[\hat{H},\,\hat{\mathbf{P}}]=0$, allows to simultaneously diagonalize these operators, introducing the in each N-particle subspace $\mathcal{H}^{(N)}$ eigenvectors $|n,N\rangle$ of $\hat{H}$ and $\hat{\mathbf{P}}$ corresponding to the eigenvalues $P_n=(E_n,\mathbf{P}_n)$. If the Heisenberg picture field operators are represented in the form[43]

$$\psi^H_\alpha(t,\mathbf{x}) = e^{i\hat{P}\cdot x}\,\psi_\alpha(\mathbf{0})\,e^{-i\hat{P}\cdot x}\,, \qquad \psi^{H\dagger}_\beta(t',\mathbf{x}') = e^{i\hat{P}\cdot x'}\,\psi^\dagger_\beta(\mathbf{0})\,e^{-i\hat{P}\cdot x'}\,, \tag{5.139}$$

one can, inserting the complete set of vectors $|n,N\pm1\rangle$ between the field operators

[43]The operator $\psi^H_\alpha(t,\mathbf{x})$ (and similarly $\psi^{\dagger H}_\alpha(t,\mathbf{x})$) can always be written as $e^{iHt}e^{-i\hat{\mathbf{P}}\cdot\mathbf{x}}\psi_\alpha(\mathbf{0})\,e^{i\hat{\mathbf{P}}\cdot\mathbf{x}}e^{-iHt}$; the condition $[\hat{\mathbf{P}},\,H]=0$ allows to write this as in (5.139); of course for the possiblity of factorizing the dependence of the Green's function on $\mathbf{x}$ and t crucial is rather the fact that the operators H and $\hat{\mathbf{P}}$ have common eigenvectors.

in each of the two terms[44] of the Green's function (5.129), represent it in the form[45] $iG^{\rm cau}_{\alpha\beta}(t,\mathbf{x};0,\mathbf{0}) \equiv iG^{\rm cau}_{\alpha\beta}(x)$

$$\begin{aligned} iG^{\rm cau}_{\alpha\beta}(x) = \quad & \theta(t)\sum_n e^{-i(P_n-P_\Omega)\cdot x}\langle\Omega|\psi_\alpha(\mathbf{0})|n,N+1\rangle\langle n,N+1|\psi^\dagger_\beta(\mathbf{0})|\Omega\rangle \\ & -\theta(-t)\sum_n e^{i(P_n-P_\Omega)\cdot x}\langle\Omega|\psi^\dagger_\beta(\mathbf{0})|n,N-1\rangle\langle n,N-1|\psi_\alpha(\mathbf{0})|\Omega\rangle\,. \end{aligned}$$

Using again the trick (5.137) to replace the Heaviside theta functions by the integrals and shifting appropriately the integration variables in both terms one obtains

$$\begin{aligned} iG^{\rm cau}_{\alpha\beta}(x) = & \sum_n \int \frac{d\omega}{2\pi}\,\frac{i}{\omega-(E_n-E_\Omega)+i0}\,e^{-i\omega t}\,e^{i\mathbf{P}_n\cdot\mathbf{x}}\,\langle\ldots n,N+1\ldots\rangle \\ & +\sum_n \int \frac{d\omega}{2\pi}\,\frac{i}{\omega+(E_n-E_\Omega)-i0}\,e^{-i\omega t}\,e^{-i\mathbf{P}_n\cdot\mathbf{x}}\,\langle\ldots n,N-1\ldots\rangle\,. \end{aligned}$$

It has been assumed here that $\mathbf{P}_\Omega = \mathbf{0}$. One has also to keep in mind that the energies E_n and total momenta $\mathbf{P}_n$ in the first (second) line are the Hamiltonian and $\hat{\mathbf{P}}$ eigenvalues in the $N+1$-particle ($N-1$-particle) subspace. In contrast, E_Ω is the energy of the H ground state in the N-particle sector.

Computing the (finite volume) Fourier transform

$$i\tilde{G}^{\rm cau}_{\alpha\beta}(\omega,\mathbf{k}) = \int_{-\infty}^{\infty} dt\,\int_V d^3\mathbf{x}\,e^{i\omega t}\,e^{-i\mathbf{k}\cdot\mathbf{x}}\,iG^{\rm cau}_{\alpha\beta}(t,\mathbf{x})\,,$$

using the standard relations

$$\int_{-\infty}^{\infty} dt\,e^{i(\omega-\omega')t} = 2\pi\delta(\omega-\omega')\,, \qquad \int_V d^3\mathbf{x}\,e^{-i(\mathbf{k}-\mathbf{P})\cdot\mathbf{x}} = V\,\delta_{\mathbf{k},\mathbf{P}}\,, \tag{5.140}$$

one obtains

$$\begin{aligned} \tilde{G}^{\rm cau}_{\alpha\beta}(\omega,\mathbf{k}) = & V\sum_n \delta_{\mathbf{k},\mathbf{P}_n}\frac{\langle\Omega|\psi_\alpha(\mathbf{0})|n,N+1\rangle\langle n,N+1|\psi^\dagger_\beta(\mathbf{0})|\Omega\rangle}{\omega-(E_n-E_\Omega)+i0} \\ & +V\sum_n \delta_{\mathbf{k},-\mathbf{P}_n}\frac{\langle\Omega|\psi^\dagger_\beta(\mathbf{0})|n,N-1\rangle\langle n,N-1|\psi_\alpha(\mathbf{0})|\Omega\rangle}{\omega+(E_n-E_\Omega)-i0}\,. \end{aligned}$$

[44] It should be clear that if $[H,\,\hat{N}]=0$, i.e. when the number of particles in the system is conserved, as is in the case of nonrelativistic systems, the action of $\psi^\dagger_\beta$ (ψ_α) on the H ground state $|\Omega\rangle$ in the N-particle subspace produces a state belonging to the $N+1$ ($N-1$) particle subspace; this readily follows from the commutation rules $[\hat{N},\,\psi^\dagger_\alpha(\mathbf{x})] = +\psi^\dagger_\alpha(\mathbf{x})$, $[\hat{N},\,\psi_\alpha(\mathbf{x})] = -\psi_\alpha(\mathbf{x})$ (valid for bosonic and fermionic field operators alike) which imply $\hat{N}\psi^\dagger_\alpha(\mathbf{x})|\Omega\rangle = (N+1)\psi^\dagger_\alpha(\mathbf{x})|\Omega\rangle$, $\hat{N}\psi_\alpha(\mathbf{x})|\Omega\rangle = (N-1)\psi_\alpha(\mathbf{x})|\Omega\rangle$, if $\hat{N}|\Omega\rangle = N|\Omega\rangle$.

[45] This representation makes it clear that in the case of a translationally invariant (homogeneous) system considered here the Green's function depends only on the differences $t-t'$ and $\mathbf{x}-\mathbf{x}'$.

The Kronecker deltas have the effect that the total momenta of the intermediate states $|n, N+1\rangle$ and $|n, N-1\rangle$ must be equal $\mathbf{k}$ and $-\mathbf{k}$, respectively. At this point it is convenient to rearrange the denominators:

$$\omega - [E_n(N+1) - E_\Omega(N)] + i0 = \omega - [E_n(N+1) - E_\Omega(N+1)] - \mu + i0\,,$$
$$\omega + [E_n(N-1) - E_\Omega(N)] - i0 = \omega + [E_n(N-1) - E_\Omega(N-1)] - \mu - i0\,,$$

identifying $E_\Omega(N+1) - E_\Omega(N)$ and $E_\Omega(N) - E_\Omega(N-1)$ (these two differences should coincide in the thermodynamic limit) with the chemical potential μ on account of the thermodynamical relation $\mu = (\partial U/\partial N)_{S,V}$ (here the temperature $T = 0$, so $dU = -p\,dV + \mu\,dN$ and the condition of constancy of S is irrelevant). Thus,

$$\tilde{G}^{\mathrm{cau}}_{\alpha\beta}(\omega, \mathbf{k}) = V \sum_n \delta_{\mathbf{k},\mathbf{P}_n} \frac{\langle\Omega|\psi_\alpha(\mathbf{0})|n, N+1\rangle\langle n, N+1|\psi^\dagger_\beta(\mathbf{0})|\Omega\rangle}{\omega - \mu - (E_n - E_\Omega)_{N+1} + i0}$$
$$+ V \sum_n \delta_{\mathbf{k},-\mathbf{P}_n} \frac{\langle\Omega|\psi^\dagger_\beta(\mathbf{0})|n, N-1\rangle\langle n, N-1|\psi_\alpha(\mathbf{0})|\Omega\rangle}{\omega - \mu + (E_n - E_\Omega)_{N-1} - i0}\,. \tag{5.141}$$

These formulae show that as long as the volume V is finite, and therefore the Hamiltonian spectrum is discrete, the causal Green's function Fourier transform $\tilde{G}^{\mathrm{cau}}_{\alpha\beta}(\omega, \mathbf{k})$, treated as a function of the complex variable ω, is a meromorphic function which (provided the corresponding matrix elements in the numerator are nonvanishing) has simple poles at exact excitation energies of the system with one more particle just below the real ω axis, starting from $\omega = \mu$ and at exact excitation energies of the system with one particle less just above the real ω axis for $\omega < \mu$.

Before investigating the analytic structure of $\tilde{G}^{\mathrm{cau}}_{\alpha\beta}(\omega, \mathbf{k})$ in the infinite volume limit, it is convenient to introduce the retarded and advanced Green's functions throught the formulae[46]

$$iG^{\mathrm{ret}}_{\alpha\beta}(t, \mathbf{x}; t', \mathbf{x}') = \quad \theta(t - t')\langle\Omega|\{\psi^H_\alpha(t, \mathbf{x}),\, \psi^{H\dagger}_\beta(t', \mathbf{x}')\}|\Omega\rangle\,,$$
$$iG^{\mathrm{adv}}_{\alpha\beta}(t, \mathbf{x}; t', \mathbf{x}') = -\theta(t' - t)\langle\Omega|\{\psi^H_\alpha(t, \mathbf{x}),\, \psi^{H\dagger}_\beta(t', \mathbf{x}')\}|\Omega\rangle\,, \tag{5.142}$$

Proceeding analogously as with the causal funcion, one obtains the following Fourier transforms of these functions

$$\tilde{G}^{\mathrm{ret/adv}}_{\alpha\beta}(\omega, \mathbf{k}) = V \sum_n \delta_{\mathbf{k},\mathbf{P}_n} \frac{\langle\Omega|\psi_\alpha(\mathbf{0})|n, N+1\rangle\langle n, N+1|\psi^\dagger_\beta(\mathbf{0})|\Omega\rangle}{\omega - \mu - (E_n - E_\Omega)_{N+1} \pm i0}$$
$$+ V \sum_n \delta_{\mathbf{k},-\mathbf{P}_n} \frac{\langle\Omega|\psi^\dagger_\beta(\mathbf{0})|n, N-1\rangle\langle n, N-1|\psi_\alpha(\mathbf{0})|\Omega\rangle}{\omega - \mu + (E_n - E_\Omega)_{N-1} \pm i0}\,. \tag{5.143}$$

[46] If the operators ψ_α and $\psi^\dagger_\beta$ are bosonic, the anticommutators are replaced by the commutators and the minus sign in the formula for $iG^{\mathrm{adv}}_{\alpha\beta}$ is absent.

They are also meromorphic functions of the complex variable ω but $\tilde{G}^{\rm ret}_{\alpha\beta}(\omega,\mathbf{k})$ is analytic in the upper half plane (all its simple poles are below the real axis) while $\tilde{G}^{\rm adv}_{\alpha\beta}(\omega,\mathbf{k})$ is analytic in the lower half plane (all its simple poles are above the real axis). It is also clear that for real ω they are related to one another by the relation[47]

$$[\tilde{G}^{\rm ret}_{\alpha\beta}(\omega,\mathbf{k})]^* = \tilde{G}^{\rm adv}_{\beta\alpha}(\omega,\mathbf{k})\,. \tag{5.144}$$

To simplify the discussion it will be convenient to assume now that the interaction of the considered fermions are spin independent and therefore $\tilde{G}^{\rm x}_{\alpha\beta}(\omega,\mathbf{k}) = \delta_{\alpha\beta}\tilde{G}^{\rm x}(\omega,\mathbf{k})$ where x = cau, ret, adv. Therefore

$$\tilde{G}^{\rm x}(\omega,\mathbf{k}) = \frac{1}{g_s}\sum_{\alpha}\tilde{G}^{\rm x}_{\alpha\alpha}(\omega,\mathbf{k})\,.$$

One can now take the limit of infinite volume. It is natural to expect that in this limit the spectrum of the complete Hamiltonian becomes extremely dense and, because the uncertainty principle constrains the possible energy resolution which can be achieved in a finite measurement time, individual energy levels can no longer be resolved (from the practical point of view the system's spectrum becomes quasicontinuous); the sums over n in the formulae (5.141) and (5.143) should be therefore replaced by integrals over the (quasi)continuous spectra of H eigenvalues. We define therefore the two spectral functions $A(E,\mathbf{k})$ and $B(E,\mathbf{k})$ by the relations

$$\begin{aligned} dE'\,A(E',\mathbf{k}) &= \frac{V}{g_s}\sum_{n}\sum_{\alpha}\ \delta_{\mathbf{k},\mathbf{P}_n}\langle\Omega|\psi_\alpha(\mathbf{0})|n,N+1\rangle\langle n,N+1|\psi^\dagger_\alpha(\mathbf{0})|\Omega\rangle\,,\\ dE'\,B(E',\mathbf{k}) &= \frac{V}{g_s}\sum_{n}\sum_{\alpha}\delta_{-\mathbf{k},\mathbf{P}_n}\langle\Omega|\psi^\dagger_\alpha(\mathbf{0})|n,N-1\rangle\langle n,N-1|\psi_\alpha(\mathbf{0})|\Omega\rangle\,, \end{aligned} \tag{5.145}$$

in which the summations (the first over the H spectrum in the $\mathcal{H}^{(N+1)}$ subspace and the second one in $\mathcal{H}^{(N-1)}$) extend to such n's that $E' \le E_n - E_\Omega \le E' + dE'$. The Fourier transform of the causal Green's function $\tilde{G}^{\rm cau}(\omega,\mathbf{k})$ in the infinite volume limit can be then represented by the integral

$$\tilde{G}^{\rm cau}(\omega,\mathbf{k}) = \int_0^\infty dE\left(\frac{A(E,\mathbf{k})}{\omega-\mu-E+i0} + \frac{B(E,\mathbf{k})}{\omega-\mu+E-i0}\right), \tag{5.146}$$

and the retarded and advanced ones by similar integrals but the retarded one with $+i0$ in both denominators and the advanced one with $-i0$'s.

The functions $A(E,\mathbf{k})$ and $B(E,\mathbf{k})$ satisfy the sum rule which follows from the anticommutation relation (5.52). Indeed, inserting the complete set of the Hamltonian

[47] Indeed, the numerator of $[\tilde{G}^{\rm ret}_{\alpha\beta}(\omega,\mathbf{k})]^*$ written in the mathematical notation as $(\Omega|\psi_\alpha n)^*(n|\psi^\dagger_\beta\Omega)^* = (\psi_\alpha n|\Omega)(\psi^\dagger_\beta\Omega|n)$ can be, with the help of the rule (4.1), written in the form $(n|\psi^\dagger_\alpha\Omega)(\Omega|\psi_\beta n) = (\Omega|\psi_\beta n)(n|\psi^\dagger_\alpha\Omega)$ which is just the numerator of $\tilde{G}^{\rm adv}_{\beta\alpha}(\omega,\mathbf{k})$.

eigenvectors into the relation $\langle\Omega|\{\psi_\alpha(\mathbf{x}),\ \psi^\dagger_\alpha(\mathbf{0})\}|\Omega\rangle = \delta^{(3)}(\mathbf{x})$, summing over the spin label α, multiplying both sides by $e^{-i\mathbf{k}\cdot\mathbf{x}}$ and integrating over the volume V using the relation (5.140) one arrives at

$$\frac{V}{g_s}\sum_n\sum_\alpha \delta_{\mathbf{k},\mathbf{P}_n}\langle\ldots n, N+1\ldots\rangle + \frac{V}{g_s}\sum_n\sum_\alpha \delta_{-\mathbf{k},\mathbf{P}_n}\langle\ldots n, N-1\ldots\rangle = 1\,.$$

Recalling now the definitions of the spectral functions $A(E,\mathbf{k})$ and $B(E,\mathbf{k})$ one concludes that

$$\int_0^\infty dE\,[A(E,\mathbf{k}) + B(E,\mathbf{k})] = 1\,. \tag{5.147}$$

It follows then from (5.146) that in the limit $|\omega| \to \infty$, when the factors $\mu \pm E$ in the denominators in (5.146) can be neglected, all the three Green's functions $\tilde{G}^{\rm x}(\omega,\mathbf{k})$ (x = cau, ret, adv) vanish as $1/\omega$.

The well-known Sochocki formula (C.2) allows now to obtain the real and imaginary parts of $\tilde{G}^{\rm cau}(\omega,\mathbf{k})$, $\tilde{G}^{\rm ret}(\omega,\mathbf{k})$ and $\tilde{G}^{\rm adv}(\omega,\mathbf{k})$ treated as functions of the *real* variable ω:

$$\begin{aligned}\mathrm{Re}\,\tilde{G}^{\rm cau}(\omega,\mathbf{k}) &= \mathrm{Re}\,\tilde{G}^{\rm ret}(\omega,\mathbf{k})\\ &= \mathrm{Re}\,\tilde{G}^{\rm adv}(\omega,\mathbf{k}) = \mathrm{P}\int_0^\infty dE\left(\frac{A(E,\mathbf{k})}{\omega-\mu-E} + \frac{B(E,\mathbf{k})}{\omega-\mu+E}\right),\end{aligned} \tag{5.148}$$

(P stands for the principal value) and

$$\mathrm{Im}\,\tilde{G}^{\rm cau}(\omega,\mathbf{k}) = \begin{cases} -\pi A(\omega-\mu,\mathbf{k})\,, & \omega > \mu,\\ \pi B(\mu-\omega,\mathbf{k})\,, & \omega < \mu,\end{cases} \tag{5.149}$$

$$\mathrm{Im}\,\tilde{G}^{\rm ret/adv}(\omega,\mathbf{k}) = \begin{cases} \mp\pi A(\omega-\mu,\mathbf{k})\,, & \omega > \mu,\\ \mp\pi B(\mu-\omega,\mathbf{k})\,, & \omega < \mu,\end{cases}\,. \tag{5.150}$$

The comparison of these formulae leads to the conclusion that for real ω

$$\begin{aligned}\tilde{G}^{\rm cau}(\omega,\mathbf{k}) &= \tilde{G}^{\rm adv}(\omega,\mathbf{k})\,, \qquad \text{for } \omega < \mu\,,\\ \tilde{G}^{\rm cau}(\omega,\mathbf{k}) &= \tilde{G}^{\rm ret}(\omega,\mathbf{k})\,, \qquad \text{for } \omega > \mu\,,\end{aligned} \tag{5.151}$$

(the same is also true before taking the infinite volume limit).

Making now in the expression (5.148) for $\mathrm{Re}\,\tilde{G}^{\rm ret}(\omega,\mathbf{k})$ the changes of the variables: $\omega' = E+\mu$ in the A-term and $\omega' = -E+\mu$ in the B-term, one obtains

$$\mathrm{Re}\,\tilde{G}^{\rm ret}(\omega,\mathbf{k}) = \mathrm{P}\int_\mu^\infty d\omega'\,\frac{A(\omega'-\mu,\mathbf{k})}{\omega-\omega'} + \mathrm{P}\int_{-\infty}^\mu d\omega'\,\frac{B(\mu-\omega',\mathbf{k})}{\omega-\omega'}\,,$$

and then using the relations (5.150) one arrives at

$$\mathrm{Re}\,\tilde{G}^{\rm ret}(\omega,\mathbf{k}) = -\frac{\mathrm{P}}{\pi}\int_{-\infty}^\infty d\omega'\,\frac{\mathrm{Im}\,\tilde{G}^{\rm ret}(\omega',\mathbf{k})}{\omega-\omega'}\,. \tag{5.152}$$

This relation between the real and imaginary parts of $\tilde{G}^{\rm ret}(\omega,\mathbf{k})$ holding for the real variable ω means - c.f. Appendix C - that $\tilde{G}^{\rm ret}(\omega,\mathbf{k})$ can be analytically continued from the real axis into complex values of ω and the resulting function will be analytic in the upper half-plane of the complex variable ω. Analogous reasoning shows that the real and imaginary parts of $\tilde{G}^{\rm adv}(\omega,\mathbf{k})$, treated as functions of real ω, satisfy the relation which guarantees that $\tilde{G}^{\rm adv}(\omega,\mathbf{k})$ continued into the complex ω plane will be analytic in the lower half-plane. These results are consistent with the observation that because $G^{\rm ret}(t,\mathbf{x})$ is in (5.142) defined to be zero for $t<0$, in the integral

$$\tilde{G}^{\rm ret}(\omega,\mathbf{k})=\int_{-\infty}^{\infty}dt\,e^{i\omega t}\int d^3\mathbf{x}\,e^{-i\mathbf{k}\cdot\mathbf{x}}\,G^{\rm ret}(t,\mathbf{x})=\int_{0}^{\infty}dt\,e^{i\omega t}\int d^3\mathbf{x}\,e^{-i\mathbf{k}\cdot\mathbf{x}}\,G^{\rm ret}(t,\mathbf{x})\,,$$

defining its Fourier transform, the analytic continuation of ω into the upper half-plane: $\omega\to x+iy$ with $y>0$, produces the damping factor e^{-ty} which, if $G^{\rm ret}(t,\mathbf{x})$ does not itself grow exponentially as $t\to\infty$, certainly makes the integrand convergent and, therefore, finite. The integral defining the Fourier transform of $G^{\rm adv}(t,\mathbf{x})$ acquires a similar damping factor when ω is continued into the lower half-plane.

As a matter of facts, the functions $\tilde{G}^{\rm ret}(\omega,\mathbf{k})$ and $\tilde{G}^{\rm adv}(\omega,\mathbf{k})$ can be obtained from the single function $\tilde{G}(z,\mathbf{k})$ of the complex variable z defined as

$$\tilde{G}(z,\mathbf{k})=\int_{0}^{\infty}dE\left(\frac{A(E,\mathbf{k})}{z-\mu-E}+\frac{B(E,\mathbf{k})}{z-\mu+E}\right).\tag{5.153}$$

$\tilde{G}^{\rm ret}(\omega,\mathbf{k})$ is the limiting value of $\tilde{G}(z,\mathbf{k})$ for $z=\omega+i0$ and $\tilde{G}^{\rm adv}(\omega,\mathbf{k})$ for $z=\omega-i0$. The function $\tilde{G}(z,\mathbf{k})$ defined by the integral (5.153) has a branch cut with a finite discontinuity along the entire real axis but is otherwise analytic both in the lower and upper half-planes of complex z. However, $\tilde{G}(z,\mathbf{k})$ given in the upper half-plane (lower half-plane) of the z variable by the integral (5.153) can be continued across the branch cut: the continuation gives in the lower (upper) half-plane another branch of $\tilde{G}(z,\mathbf{k})$ which is not analytic: it can have there poles.[48]

[48] This can be illustrated by a simple example (the real constant a is assumed to be positive; the integral can be easily evaluated by the residue method)

$$g(z)=\int_{-\infty}^{\infty}dy\,\frac{1}{z-y}\,\frac{a}{y^2+a^2}=\begin{cases}\pi/(z+ia) & {\rm Im}z>0\\ \pi/(z-ia) & {\rm Im}z<0\end{cases}.$$

The function $g(z)$ is thus analytic in the upper and lower half-planes of complex z and along the real axis $z=x$ it has the discontinuity $g(x+i0)-g(x-i0)=-2i\pi a/(x^2+a^2)$ which can be also computed using the formula (C.2)

$$g(x\pm i0)=\int_{-\infty}^{\infty}dy\,\frac{a}{y^2+a^2}\left\{P\,\frac{1}{x-y}\mp i\pi\delta(x-y)\right\}.$$

It is also clear that the function $\pi/(z+ia)$ ($g(z)$ in the upper half-plane) can be continued across the cut but the continuation has in the lower half plane a simple pole at $z=-ia$.

Thus the analytic structure of the functions $\tilde{G}^{\rm cau}(\omega,\mathbf{k})$ and $\tilde{G}^{\rm ret/adv}(\omega,\mathbf{k})$ changes dramatically with taking the limit of infinite volume: simple poles which at the finite volume are located just above and just below the real axis after taking the limit coalesce into the branch cut covering the whole real axis[49] while new poles may emerge on the branches of $\tilde{G}^{\rm ret/adv}(\omega,\mathbf{k})$ obtained by continuing these functions across the branch cut from the half-planes at which they are analytic.

Since for $\omega > \mu$ ($\omega < \mu$) $\tilde{G}^{\rm cau}(\omega,\mathbf{k})$ coincides with $\tilde{G}^{\rm ret}(\omega,\mathbf{k})$ (coincides with $\tilde{G}^{\rm adv}(\omega,\mathbf{k})$) it too can be continued from the upper (lower) half-plane, where it is analytic, across the branch cut into the lower (upper) half-plane, where it can have poles.

The physical interpretation of the possible poles of the Fourier transform of the causal Green's function can be clarified by the following reasoning. Let the system of N interacting fermions be at time t' in its ground state. Its Schrödinger picture state vector $|\Omega(t')\rangle$ at t' is therefore given by $U(t',0)|\Omega(0)\rangle = U(t',0)|\Omega\rangle$, where $|\Omega\rangle$ is the system's ground state vector in the Heisenberg Picture (see Section 1.1). Adding to the system a particle (with the spin projection β) at the point $\mathbf{x}'$ at t' is represented by the action on $|\Omega(t')\rangle$ of the Schrödinger picture operator $\psi^\dagger_\beta(\mathbf{x}')$. The state of the system with the added particle at a later instant $t > t'$ is then represented by the state-vector $U(t,t')\psi^\dagger_\beta(\mathbf{x}')|\Omega(t')\rangle$. One can then ask, what is the overlap of this state with the state of the system obtained by adding to the ground state a particle (with the spin projection α) at $\mathbf{x}$ at the moment t, that is, the overlap with the state represented by $\psi^\dagger_\alpha(\mathbf{x})|\Omega(t)\rangle$? The scalar product of these two states is easily seen - c.f. the formulae (1.4) and (1.12) - to be given by

$$\theta(t-t')\langle\Omega(t)|\psi_\alpha(\mathbf{x})U(t,t')\psi^\dagger_\beta(\mathbf{x}')|\Omega(t')\rangle = \theta(t-t')\langle\Omega|\psi^H_\alpha(t,\mathbf{x})\psi^{\dagger H}_\beta(t',\mathbf{x}')|\Omega\rangle\,.$$

Analogously, removing a particle (in the spin state α) at the point $\mathbf{x}$ from the system which is in its (N-particle) ground state $|\Omega(t)\rangle$ at the moment t and finding the overlap at a later moment t' of the state of the system perturbed in this way with its state obtained by removing a particle at $\mathbf{x}'$ (and the spin state β) from the ground state at $t' > t$ is represented by

$$\theta(t'-t)\langle\Omega(t')|\psi^\dagger_\beta(\mathbf{x}')U(t',t)\psi_\alpha(\mathbf{x})|\Omega(t)\rangle = \theta(t'-t)\langle\Omega|\psi^{\dagger H}_\beta(t',\mathbf{x}')\psi^H_\alpha(t,\mathbf{x})|\Omega\rangle\,.$$

Thus the answers to both questions are directly given by the causal Green's function (5.129). It should also be clear that the answers to the analogous questions but when to or from the system true ground state a particle not at a definite space points but in a one-particle state with a definite momentum $\mathbf{k}$ (we have here in mind a translationally invariant system) is added or removed is given by the spatial Fourier transform

$$G^{\rm cau}_{\alpha\beta}(t-t',\mathbf{k}) = \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\,e^{-i\omega(t-t')}\,\tilde{G}^{\rm cau}_{\alpha\beta}(\omega,\mathbf{k})\,. \tag{5.154}$$

[49] Due to a different dispersion relation - the dependence on the momentum $\mathbf{p}$ of energies of one-particle states - of "fundamental" constituents of relativistic systems, the branch cuts of Green's functions of some operators in relativistic theories are expected to extend to $\mp\infty$ only from some threshold values $\mp\omega_{\rm thr}$; and to have in the "gap" (at real values of the frequency variable) poles corresponding to states of a stable "physical" particles.

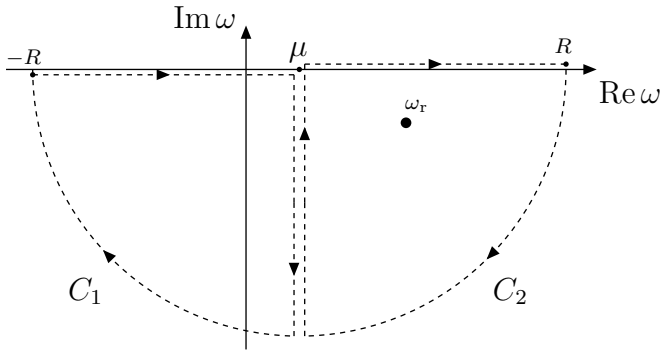

Figure 5.2: Integration contours used to compute $G^{\rm cau}_{\alpha\beta}(t,\mathbf{k})$.

To see what consequences for the answers have possible poles of the Fourier transform $\tilde{G}^{\rm cau}_{\alpha\beta}(\omega,\mathbf{k})$, let us assume that it has a simple pole at $\omega=(E_{\rm r}-i\Gamma_{\rm r})/\hbar$ with $E_{\rm r}>\mu$, $\Gamma_{\rm r}>0$ and the residue $\mathcal{Z}_{\rm r}$ (which for simplicity will be assumed here to be real) and consider (5.154) for $t-t'\equiv t>0$. We will assume that the interactions are spin independent and, therefore, $\tilde{G}^{\rm x}_{\alpha\beta}(\omega,\mathbf{k})=\delta_{\alpha\beta}\tilde{G}^{\rm x}(\omega,\mathbf{k})$. To evaluate the integral over all real values of ω in (5.154) one can split it into two domains: $(-\infty,\mu)$ and (μ,∞). In the first domain - c.f. (5.151) - $\tilde{G}^{\rm cau}(\omega,\mathbf{k})=\tilde{G}^{\rm adv}(\omega,\mathbf{k})$ and since the latter function has no poles in the lower half-plane, the integral over the closed contour C_1 shown in Figure 5.2 is zero. In the second domain $\tilde{G}^{\rm cau}(\omega,\mathbf{k})=\tilde{G}^{\rm ret}(\omega,\mathbf{k})$ and the result of the integration over the closed contour C_2 (which lies on the continuation of $\tilde{G}^{\rm ret}(\omega,\mathbf{k})$ into the lower half-plane) in Figure 5.2 is determined by the assumed single simple pole at $\omega_{\rm r}=(E_{\rm r}-i\Gamma_{\rm r})/\hbar$. Since we consider the case $t>0$, the integrals over the two arcs of C_1 and C_2 are likely to vanish (and we assume they do) in the limit of the arcs radii R tending to infinity, owing to the Jordan lemma. One can therefore write

$$G^{\rm cau}_{\alpha\beta}(t,\mathbf{k})=\delta_{\alpha\beta}\int_{-i\infty+\mu/\hbar}^{\mu/\hbar}\frac{d\omega}{2\pi}\,e^{-i\omega t}\left[G^{\rm adv}(\omega,\mathbf{k})-G^{\rm ret}(\omega,\mathbf{k})\right]-i\mathcal{Z}_{\rm r}\,e^{-(iE_{\rm r}+\Gamma_{\rm r})t/\hbar}\,.$$

If $E_{\rm r}-\mu\gg\Gamma_{\rm r}$ and the time t is such that $t(E_{\rm r}-\mu)\gg\hbar$ but $t\Gamma_{\rm r}\lesssim\hbar$, the integral in the above formula can be neglected: indeed, the contribution to the integral arising from the parts of the integration path far removed from the point $\omega=\mu$ are strongly suppressed by the exponential factor; the contribution of the part of the path close to the real axis can be estimated by approximating there the $\tilde{G}^{\rm ret}(\omega,\mathbf{k})$ by its behaviour $\approx\mathcal{Z}_{\rm r}/(\omega-(E_{\rm r}-i\Gamma_{\rm r})/\hbar)$ near the pole; owing to the relation (5.144)

$$\tilde{G}^{\rm adv}(\omega,\mathbf{k})-\tilde{G}^{\rm ret}(\omega,\mathbf{k})\approx\frac{2i\mathcal{Z}_{\rm r}\Gamma_{\rm r}/\hbar}{(\omega-E_{\rm r}/\hbar)^2+\Gamma_{\rm r}^2/\hbar^2}\,,$$

and after substituting $u=i(\omega-\mu/\hbar)$ the integral becomes

$$-\frac{2\mathcal{Z}_{\rm r}\Gamma_{\rm r}}{\hbar}\int_0^\infty\frac{du}{2\pi}\,\frac{e^{-i\mu t/\hbar}\,e^{-ut}}{(\mu/\hbar-E_{\rm r}/\hbar-iu)^2+\Gamma_{\rm r}^2/\hbar^2}\,,$$

and can be estimated to be[50] approximately equal $-(\mathcal{Z}_{\rm r}/\pi)[\Gamma_{\rm r}/(E_{\rm r}-\mu)][\hbar/t(E_{\rm r}-\mu)]e^{-i\mu t/\hbar}$, that is, it is suppressed by both factors in the last two brackets.

Thus, the overlap of the two states corresponding to adding to the system an extra particle (creating in it a particle-like exitation) at two different times is given by $G^{\rm cau}(t,\mathbf{k}) \approx -i\mathcal{Z}_{\rm r}\exp(-(iE_{\rm r}+\Gamma_{\rm r})t/\hbar)$ and vanishes exponentially with the time separation t. $\Gamma_{\rm r}$ can be then interpreted as the width (inverse lifetime) of the created particle excitation.

If $t<0$ (i.e. $t'>t$) analogous role play possible poles of the function $\tilde{G}^{\rm adv}(\omega,\mathbf{k})$ (of $\tilde{G}^{\rm ret}(\omega,\mathbf{k})$) in the upper half-plane at $\omega_{\rm r}=E_{\rm r}+i\Gamma_{\rm r}$ with $E_{\rm r}-\mu<0$, $\Gamma_{\rm r}>0$ which correspond to dissipating hole-type (quasi-hole) excitations.

5.8 Dyson perturbative expansions

Ground state expectation values of chronological products of Heisenberg picture operators contain a lot of interesting information about physical systems. In view of this it is important to have a systematic method of their computation using an expansion in the interaction term $V_{\rm int}$ of the system's Hamiltonian $H=H_0+V_{\rm int}$. Such an expansion, called Dyson expansion, can be formulated and relies on the Gell-Mann - Low construction of the ground state vector of H presented in Section 1.2. It is fairly general and applies to ordinary quantum mechanics, quantum theory of many-particle systems as well as to relativistic quantum field theories.

Let $O_1^H(t)$, $O_2^H(t)$, etc. be some Heisenberg picture operators obtained[51] in the standard way (Section 1.1) from their Schrödinger picture counterparts. In order to compute the Green's function

$$iG(t_1,t_2,\ldots)=\langle\Omega|{\rm T}[O_1^H(t_1)O_2^H(t_2)\ldots]|\Omega\rangle=\frac{\langle\Omega|T[O_1^H(t_1)O_2^H(t_2)\ldots]|\Omega\rangle}{\langle\Omega|\Omega\rangle}\,, \quad (5.155)$$

one represents the normalized to unity ground state vectors $|\Omega\rangle$ and $\langle\Omega|$ of the system ($\langle\Omega|\Omega\rangle=1$) using the result of Section 1.2 in the forms[52]

$$\langle\Omega|=\frac{\langle\Omega_0|U_I(\infty,0)}{\langle\Omega_0|U_I(\infty,0)|\Omega_0\rangle}\,\frac{1}{C}\,,\qquad |\Omega\rangle=\frac{1}{C}\,\frac{U_I(0,-\infty)|\Omega_0\rangle}{\langle\Omega_0|U_I(0,-\infty)|\Omega_0\rangle}\,. \quad (5.156)$$

In the formula (5.155) the factors C and $\langle\Omega_0|U_I^\varepsilon(0,-\infty)|\Omega_0\rangle$, which are left undetermined

[50] The integral receives the main contribution from the domain $0\le u\lesssim 1/t$ in which $e^{-ut}\approx 1$; since it is assumed that $E_{\rm r}-\mu\gg\hbar/t\gtrsim\hbar u$, and $E_{\rm r}-\mu\gg\Gamma_{\rm r}$, the denominator of the integrand can be approximated by $(E_{\rm r}-\mu)^2/\hbar^2$.

[51] In applications to many-body problems and to quantum field theory the operators O depend usually also on position variables $\mathbf{x}$. This dependence will be not displayed, as it plays no role here.

[52] The interaction picture evolution operators $U_I(\infty,0)$ and $U_I(0,-\infty)$ should be understood as the $\varepsilon\to 0^+$ limits of the operators $U_I^{-\varepsilon}(\infty,0)$ and $U_I^\varepsilon(0,-\infty)$, respectively.

by the Gell-Mann - Low construction, cancel out and one obtains

$$G(t_1, t_2, \ldots) = \frac{\langle \Omega_0 | U_I(\infty, 0) \mathrm{T}[O_1^H(t_1) O_2^H(t_2) \ldots] U_I(0, -\infty) | \Omega_0 \rangle}{\langle \Omega_0 | U_I(\infty, 0) U_I(0, -\infty) | \Omega_0 \rangle} \,. \tag{5.157}$$

The denominator (in the limit $\varepsilon \to 0^+$) is simply $\langle \Omega_0 | U_I(\infty, -\infty) | \Omega_0 \rangle$. To bring the numerator to a more manageable form one writes (cf. the formulae (1.12) and (1.24))

$$\begin{aligned} O^H(t) &= U^\dagger(t,0) O^S U(t,0) = U^\dagger(t,0) e^{-iH_0 t} O^I(t) e^{iH_0 t} U(t,0) \\ &= U_I^\dagger(t,0) O^I(t) U_I(t,0) = U_I(0,t) O^I(t) U_I(t,0) \,, \end{aligned}$$

which allows, using the composition rules satisfied by the evolution operators, to write the string of operators in the numerator in the form

$$U_I(\infty, 0) \mathrm{T}[U_I(0, t_1) O_1^I(t_1) U_I(t_1, t_2) O_2^I(t_2) \ldots O_n^I(t_n) U_I(t_n, 0)] U_I(0, -\infty) \,.$$

The last step is to show that this can be written as

$$\mathrm{T}\left(O_1^I(t_1) O_2^I(t_2) \cdots \exp\left\{ -i \int_{-\infty}^{\infty} dt \, V_{\mathrm{int}}^I(t) \right\} \right) . \tag{5.158}$$

To see this one expands the expression (5.158) into the power series in the interaction V_{int}^I:

$$\sum_{N=0}^{\infty} \frac{(-i)^N}{N!} \int_{-\infty}^{\infty} d\tau_1 \ldots \int_{-\infty}^{\infty} d\tau_N \, \mathrm{T}[O_1^I(t_1) O_2^I(t_2) \cdots V_{\mathrm{int}}^I(\tau_1) \cdots V_{\mathrm{int}}^I(\tau_N)] \,, \tag{5.159}$$

and for each fixed ordering of times $t_1 > \ldots > t_n$ splits the N-dimensional integration domain into subdomains in which the times are ordered as follows:

$$\tau_{01}, \ldots, \tau_{0N_0} > t_1 > \tau_{11}, \ldots, \tau_{1N_1} > t_2 \ldots > t_n > \tau_{nN_1}, \ldots, \tau_{nN_n} \,,$$

summing over all different possible assignements of N integration times τ_i into groups of N_0, N_1, ... elements (times) subjected to the condition $N_0 + N_1 + \ldots + N_n = N$. Since all interaction terms $V_{\mathrm{int}}^I(\tau)$ are identical, the assignement of the times τ_i into groups specified by the above inequality can be done in $N!/N_0!N_1! \ldots N_n!$ equivalent ways giving each the same contribution. One then sees that the original expression (5.159) written as

$$\begin{aligned} &\sum_{N=0}^{\infty} \frac{(-i)^N}{N!} \sum_{N_0, \ldots, N_n} \frac{N!}{N_0! \ldots N_n!} \, \delta_{N, N_0 + \ldots + N_n} \\ &\qquad \int_{t_1}^{\infty} d\tau_{01} \ldots d\tau_{0N_0} \int_{t_2}^{t_1} d\tau_{11} \ldots d\tau_{1N_1} \ldots \int_{-\infty}^{t_n} d\tau_{n1} \ldots d\tau_{nN_n} \, \mathrm{T}[\ldots] \,, \end{aligned}$$

breaks up into n independent sums giving the evolution operators $U_I(\infty, t_1)$, $U_I(t_1, t_2)$, etc. sandwitched between the operators $O_1^I(t_1)$, $O_1^I(t_2)$ etc. because it is now clear that

for a fixed ordering of times $t_1 > t_2 > \ldots > t_n$ the chronological product in (5.159) can be written as

$$\mathrm{T}[V^I_{\rm int}(\tau_{01})\cdots V^I_{\rm int}(\tau_{0N_0})]\, O^I(t_1)\, \mathrm{T}[V^I_{\rm int}(\tau_{11})\cdots V^I_{\rm int}(\tau_{1N_1})]\, O^I(t_2)\ldots \mathrm{T}[V^I_{\rm int}(\tau_{n1})\cdots V^I_{\rm int}(\tau_{nN_n})]\,.$$

In this way the Green's function (5.155) gets represented as the ratio of the free ground states $|\Omega_0\rangle$ expectation values of two operator expressions: (5.158) and

$$U_I(\infty,-\infty) = \mathrm{T}\exp\biggl\{-i\int_{-\infty}^{\infty} dt\, V^I_{\rm int}(t)\biggr\}\,,$$

involving only interaction picture operators. Each term of the expansion of the numerator and of the denominator can be, therefore, worked out using the Wick theorem formulated in Section 5.9 which allows to write chronologically ordered strings of the interaction picture operators O^I and $V^I_{\rm int}$ (each of which is built out of some elementary operators of the theory) as products of the free ground state $|\Omega_0\rangle$ expectation values of all possible pairings (to be defined in Section 5.9) of elementary operators. This leads to Feynman diagrams which represent different contributions to the successive terms of the Dyson expansion and allow to easily, by appealing to the so-called Feynman rules, write down the corresponding analytical expressions. This will be discussed in due course (and in more detail in the relativistic case when theories of interacting relativistic particles will have been formulated).

It should finally be stressed that the validity of the Dyson expansion requires, in agreement with the remarks made at the end of Section 1.2, that the state-vector $|\Omega_0\rangle$ be adiabatically connected to the true ground state $|\Omega\rangle$ of the complete Hamiltonian. If it is not, one has to reformulate the theory so that the vector $|\tilde{\Omega}_0\rangle$ of a new free Hamiltonian $\tilde{H}_0$ satisfies this requirement.

It is instructive to consider at this point the analogous perturbative expansions of quantities of interest in statistical physics. Working in the Grand Canonical Ensemble one is interested in the statistical sum $\Xi_{\rm stat}(T,V,\mu)$ and

$$\Xi_{\rm stat}(T,V,\mu) = \mathrm{Tr}_{\mathcal{H}}\Bigl(e^{-\hat{K}/k_{\rm B}T}\Bigr)\,, \tag{5.160}$$

in which[53]

$$\hat{K} = \hat{H} - \mu\hat{N} = \hat{H}_0 + \hat{V}_{\rm int} - \mu\hat{N} \equiv \hat{K}_0 + \hat{V}_{\rm int}\,, \tag{5.161}$$

and various thermal Greens functions defined as

$$-G(\tau_a,\tau_b,\ldots) = \mathrm{Tr}_{\mathcal{H}}\bigl(\hat{\rho}\,\mathrm{T}_\tau[O^K_1(\tau_a)O^K_2(\tau_b)\ldots]\bigr)\,, \tag{5.162}$$

[53] If the interaction $\hat{V}_{\rm int}$ preserves spin of individual particles it is appropriate to associate separate chemical potentials μ_σ with fermions having different spin projections σ, that is to replace $\mu\hat{N}$ by $\sum_\sigma \mu_\sigma \hat{N}_\sigma$.

where T_τ is the chronological ordering with respect to the (imaginary) "time" τ, $\hat{\rho} = \Xi_{\mathrm{stat}}^{-1} e^{-\beta \hat{K}}$ is the statistical operator of the Grand Canonical Ensemble and the operators $O^K(\tau)$ in the so called K-picture are defined as

$$O^K(\tau) = e^{\tau K}\, O\, e^{-\tau K}\,. \tag{5.163}$$

In particular the two-point (single-particle) thermal Green's function reads

$$-G_{\alpha\beta}(\tau, \mathbf{x}, \tau', \mathbf{x}') \equiv \mathrm{Tr}_{\mathcal{H}}\Big(\hat{\rho}\, \mathrm{T}_\tau[\hat{\psi}_\alpha^K(\tau, \mathbf{x}) \hat{\psi}_\beta^{\dagger K}(\tau,' \mathbf{x}')]\Big)\,. \tag{5.164}$$

Notice that (except at $\tau = 0$) $\hat{\psi}_\beta^{\dagger K}(\tau, \mathbf{x}) \neq [\hat{\psi}_\beta^K(\tau, \mathbf{x})]^\dagger$.

As in the zero-temperature formalism, by which term one means computing expectation values of operators in the system's ground state $|\Omega\rangle$, instead of averages over the statistical ensemble, one is interested in converting the problem of computing the Green's functions (5.162) into a problem of computing the chronological averages of I-picture operators defined by $O^I(\tau) = e^{\tau \hat{K}_0} O\, e^{-\tau \hat{K}_0}$ and related to the K-picture ones by

$$O^K(\tau) = U_I(0, \tau)\, O^I(\tau)\, U_I(\tau, 0)\,, \tag{5.165}$$

where the thermal I-picture "imaginary time" evolution operator $U_I(\tau, \tau')$ is given by

$$U_I(\tau, \tau') = e^{\tau \hat{K}_0}\, e^{-(\tau - \tau')\hat{K}}\, e^{-\tau' \hat{K}_0}\,, \tag{5.166}$$

and satisfies the equation

$$\frac{d}{d\tau}\, U_I(\tau, \tau') = -V_{\mathrm{int}}^I(\tau)\, U_I(\tau, \tau')\,, \tag{5.167}$$

in which $V_{\mathrm{int}}^I(\tau) = e^{\tau \hat{K}_0} V_{\mathrm{int}} e^{-\tau \hat{K}_0}$, with the initial condition $U_I(\tau, \tau) = \hat{1}$. Although not unitary, it too satisfies the composition rule

$$U_I(\tau, \tau')\, U_I(\tau', \tau'') = U_I(\tau, \tau'')\,. \tag{5.168}$$

Similarly as the analogous equation discussed in Section 1.1, the equation (5.167) can be converted into an integral equation and solved iteratively; the result is the formula

$$U_I(\tau, \tau') = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \int_{\tau'}^{\tau} d\tau_1 \,\ldots \int_{\tau'}^{\tau} d\tau_n\, \mathrm{T}_\tau[V_{\mathrm{int}}^I(\tau_1) \ldots V_{\mathrm{int}}^I(\tau_n)]\,. \tag{5.169}$$

Since the definition (5.166) can be rewritten as $e^{-\tau \hat{K}} = e^{-\tau \hat{K}_0}\, U_I(\tau, 0)$, the formula (5.169) evaluated at $\tau = \beta = 1/k_{\mathrm{B}}T$ immediately gives the expansion of the statistical sum of the interacting system (whose Hamiltonian is $H = H_0 + V_{\mathrm{int}}$) in terms of the correlation functions of the noninteracting system

$$\begin{aligned} \Xi_{\mathrm{stat}} &= \mathrm{Tr}\Big(e^{-\beta \hat{K}}\Big) = \mathrm{Tr}\Big(e^{-\beta \hat{K}_0}\, U_I(\beta, 0)\Big) \\ &= \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \int_0^{\beta} d\tau_1 \,\ldots \int_0^{\beta} d\tau_n\, \mathrm{Tr}\,\Big(e^{-\beta \hat{K}_0}\, \mathrm{T}_\tau[V_{\mathrm{int}}^I(\tau_1) \ldots V_{\mathrm{int}}^I(\tau_n)]\Big)\,. \end{aligned} \tag{5.170}$$

The thermal Green's functions (5.162) can be expressed similarly. Let $\tau_1 > \tau_2 > \ldots$ Then

$$-G(\tau_a, \tau_b, \ldots) = \frac{\mathrm{Tr}\Big(e^{-\beta \hat{K}_0}\, U_I(\beta, 0)\, U_I(0, \tau_a) O_1^I(\tau_a) U_I(\tau_a, \tau_b) O_1^I(\tau_b) \ldots U_I(\tau_d, 0)]\Big)}{\mathrm{Tr}\Big(e^{-\beta \hat{K}_0}\, U_I(\beta, 0)\Big)}\,.$$

Similar expressions can be also written for other orderings of the imaginary times τ_1, τ_2, ... It follows that one can write the following perturbative expansion of the numerator

$$\sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \int_0^\beta d\tau_1 \ldots \int_0^\beta d\tau_n \,\mathrm{Tr}\,\Big(e^{-\beta \hat{K}_0}\, \mathrm{T}_\tau [V_{\mathrm{int}}^I(\tau_1) \ldots V_{\mathrm{int}}^I(\tau_n) O^I(\tau_a) \ldots O^I(\tau_d)]\Big)\,. \quad (5.171)$$

Together with the expansion (5.170) this gives the perturbative expansion of the thermal Green's functions. Successive terms of these expansions can be, with the help of the thermal analog of the Wick theorem, represented by Feynman diagrams and evaluated using the appropriate modification of the usual Feynman rules.

It is striking to realize that the expansion obtained here, relying essentially on algebraic relations between operators, seems to be valid independently of whether the ground state $|\Omega\rangle$ of the interacting system can be reached adiabatically starting from the ground state $|\Omega_0\rangle$, as requires the expansion of the zero temeprature Green's functions. Thus it superficially seems not to be subjected to the restrictions imposed by the validity of the Gell-Mann - Low construction which exclude in particular interesting cases of symmetry breaking as discussed at the end od Section 1.2. As a matter of facts, however, all complications with the use of the Gell-Mann - Low construction are in the present case hidden in the symbol Tr of the trace: in view of the discussed nonseparability of the big Hilbert space (5.20) one has to decide over which of its separable subspaces the trace is to be taken and this, in the cases of symmetry breaking (phase transitions), is precisely equivalent to the problem with the use of the Gell-Mann - Low construction in the zero temperature case.

5.9 Wick theorem

An efficient tool for computing matrix elements of strings of operators arising in problems of many-body quantum mechanics as well as of relativistic quantum field theory (and sometimes even in ordinary quantum mechanics e.g. of the harmonic oscillator(s)) is the Wick theorem. It will be formulated here in the most general form[54] in order to allow an easy adaptation to the case of current interest. We assume therefore that there is a set of operators A_i with the label i belonging to a (finite or countably or even uncountably infinite) set of indices which are decomposable (according to some rule which depends on

[54] L.G. Molinari, ArXiv:1710.09248 [math-phys].

the situation - see below for illustrating examples) into two parts

$$A_i = A_i^{(+)} + A_i^{(-)}\,, \tag{5.172}$$

so that[55]

$$[A_i^{(+)},\, A_j^{(+)}]_\mp = [A_i^{(-)},\, A_j^{(-)}]_\mp = 0\,, \qquad [A_i^{(+)},\, A_j^{(-)}]_\mp = \hat{1}\cdot a_{ij}\,, \tag{5.173}$$

where the factors a_{ij} are c-numbers. This is the crucial assumption on which the theorem rests: if the last commutator is not a c-number, the Wick theorem is invalid. It is important to stress that $(A_i^{(\pm)})^\dagger$ is not necessarily equal to $A_i^{(\mp)}$ (although in some specific cases this may be so): if $(A_i^{(\pm)})^\dagger \neq A_i^{(\mp)}$ (i.e. when $A^\dagger \neq A$) then A_i and $A_i^\dagger$ are both included in the set of the A_i operators and are simply distinguished by different values of the index i. In some cases one of the two parts, either $A_i^{(+)}$ or $A_i^{(-)}$, of an operator A_i may vanish (be a zero operator). Finally, although the main results of the Wick theorem can be stated in the operator form (independent of the structure of the Hilbert space in which the operators act), it is most useful if there is a state-vector $|\mathrm{vac}\rangle$ such that for all values of the index[56] i

$$A_i^{(+)}|\mathrm{vac}\rangle = 0\,, \qquad \langle\mathrm{vac}|A_i^{(-)} = 0\,. \tag{5.174}$$

A product (a string) of n operators $A_i^{(+)}$ and $A_j^{(-)}$ is *normally ordered* (with respect to the state $|\mathrm{vac}\rangle$, if such a state-vector exists) if it has the form

$$A_1^{(-)}\cdots A_k^{(-)} A_{k+1}^{(+)}\cdots A_n^{(+)}\,. \tag{5.175}$$

Usefullness of the Wick theorem follows from the fact that the $|\mathrm{vac}\rangle$ state expectation values of normally ordered products of operators vanish (unless the product is the unit operator). By decomposing individual operators A_i as in (5.172) and performing a series of appropriate algebraic operations (involving commuting/anticommuting the operators $A_i^{(\pm)}$) every product $A_1\cdots A_n$ (and every time ordered product $\mathrm{T}(A_1\cdots A_n)$ - see below) of n operators A_i can be brough (in the case of time ordered product only if the time dependence of operators is of a particular form) into the form of a sum of (in general 2^n) strings of normally ordered operators. This is automatized by the Wick theorem.

Define first the operation, denoted $:\ :$, of normal ordering which amounts to replacing the product of n operators $A_i^{(\pm)}$ by its normal form

$$:A_1^{(\pm)}\cdots A_n^{(\pm)}:\ \equiv (-1)^P A_{i_1}^{(-)}\cdots A_{i_k}^{(-)} A_{i_{k+1}}^{(+)}\cdots A_{i_n}^{(+)}\,, \tag{5.176}$$

[55]The symbol $[\cdot\,,\,\cdot]_\mp$ means the anticommutator, if both operators are fermionic and the commutator in other cases.

[56]It might seem more logical to call $A_i^{(-)}$ that part of the operator A_i that annihilates $|\mathrm{vac}\rangle$; yet this is not the convention adopted is standard textbooks on relativistic quantum field theory (another example of a lasting stupid tradition).

where P is the number of transpositions of fermionic operators in the overall permutation needed to convert the original string of operators (in which some of the opertators may be fermionic and others bosonic) into the ordering on the right hand side. The action of the normal ordering operation is extended to the complete operators A_i by linearity. For instance

$$\begin{aligned} :A_1A_2: &= :(A_1^{(+)} + A_1^{(-)})(A_2^{(+)} + A_2^{(-)}): \\ &= :A_1^{(+)}A_2^{(+)} + A_1^{(-)}A_2^{(-)} + A_1^{(-)}A_2^{(+)} + A_1^{(+)}A_2^{(-)}: \\ &= A_1^{(+)}A_2^{(+)} + A_1^{(-)}A_2^{(-)} + A_1^{(-)}A_2^{(+)} \pm A_2^{(-)}A_1^{(+)} \,. \end{aligned} \tag{5.177}$$

(The sign of the last term in the last line is negative only if both operators, A_1 and A_2, are fermionic). From the rule (5.176) and the extension of the normal ordering by linearity it follows that

$$:A_1 \cdots A_n: = (-1)^P :A_{i_1} \cdots A_{i_n}: \,, \tag{5.178}$$

where again P is the number of interchanges of fermionic operators.

A product $A_1 \cdots A_n$ of n operators A_i having the structure (5.172) can always be written as a sum of normally ordered products. If $n = 2$ this is trivial

$$A_1A_2 = :A_1A_2: + [A_1^{(+)}, A_2^{(-)}]_\mp \,, \tag{5.179}$$

as can be straightforwardly seen from (5.177). Here by virtue of the basic assumption underlying the Wick theorem the second term is a c-number. To write the statement in the general case one defines the *contraction* (or the *pairing*) of two operators A_1 and A_2 by

$$[A_1A_2] \equiv \overbrace{A_1A_2} \equiv A_1A_2 - :A_1A_2: \,. \tag{5.180}$$

From (5.177) or from (5.179) one then gets that

$$\overbrace{A_1A_2} = [A_1^{(+)}, A_2^{(-)}]_\mp = \langle \mathrm{vac}|A_1A_2|\mathrm{vac}\rangle \,, \tag{5.181}$$

where the last form of the contraction requires that there be a state-vector $|\mathrm{vac}\rangle$ annihilated by all $A_i^{(+)}$ (which in application usually is the case). With the help of the rule (5.178) the contraction operation of two operators A and A' is now extended to the case of a product of an arbitrary number of operators:

$$\overbrace{A(A_1 \ldots A_n)A'} \equiv (\zeta_{A'})^P \overbrace{AA'} \, (A_1 \ldots A_n) \,. \tag{5.182}$$

Here $\zeta_{A'} = -1$ if A' is fermionic and $+1$ otherwise; P is the number of fermionic operators in the string $A_1 \ldots A_n$. The formula (5.182) defines operationally the meaning of the

symbol on the left hand side. The *Wick theorem* (applied to ordinary products of operators A_i) can be now written in the form

$$\begin{aligned} A_1 \dots A_n = & :A_1 \dots A_n: \\ & + \sum_{(i,j)} :A_1 \dots \overbrace{A_i \dots A_j} \dots A_n: \\ & + \sum_{(i,j),(k,l)} :A_1 \dots \overbrace{A_i \dots \overbrace{A_k \cdots A_j} \cdots A_l} \dots A_n: \\ & + \dots \end{aligned} \tag{5.183}$$

If the contraction of a pair of operators is defined by the first equality[57] (5.181), it is an operator relation and does not rely on whether there is the state-vector $|\mathrm{vac}\rangle$ annihilated by all A_i^-. If, however, such a vector exists, (5.183) implies that $\rangle\mathrm{vac}|A_1 \dots A_n|\mathrm{vac}\rangle$ vanishes, if the number n of operators is odd, while if it is even, it is given by the sum over all possible pairings of all n operators in the string. The purely algebraic proof (based on mathematical induction) is not very exciting, so the reader is referred to the cited paper of L.G. Molinari.

The simplest (somewhat trivial) example of the operators A_i is provided by the position and momentum operators $A_{2i-1} = \hat{x}_i \propto a_i + a_i^\dagger$, and $A_{2i} = \hat{p}_i \propto i(a_i - a_i^\dagger)$, where $i = 1, \dots, N$, of a system of N (identical or not identical, uncoupled or coupled) harmonic oscillators. In this case case $(A_i^{(\pm)})^\dagger = A_i^{(\mp)}$ and the role of the state-vector $|\mathrm{vac}\rangle$ is played by the ground state-vector $|0, 0 \dots\rangle$ of the system of mutually uncoupled oscillators. Most naturally the operators A_i appear in the second quantization formalism. Their set is then formed by the field operators $\psi_\alpha(\mathbf{x})$ and $\psi_\alpha^\dagger(\mathbf{x})$ of identical bosons or fermions given either by (5.45), (5.46) or, in general, by (5.50). Each of the operators A_i has in this case only one part $A_i^{(+)}$ or $A_i^{(-)}$ (the second part of each operator A_i vanishes) and the vector $|\mathrm{vac}\rangle$ is just the vector $|\mathrm{void}\rangle$. However if the system consists of N fermions, the field operators $\hat{\psi}_\alpha(\mathbf{x})$ and $\hat{\psi}_\alpha^\dagger(\mathbf{x})$ playing the roles of the operators A_i can (and in applications this is more convenient) be decomposed as in (5.98). In this case each operator A_i has both parts, $A_i^{(+)}$ and $A_i^{(-)}$, nonvanishing and $(A_i^{(+)})^\dagger \neq A_i^{(-)}$. The role of the state $|\mathrm{vac}\rangle$ is then played by the state $|\Omega_0\rangle$ in the chosen N-fermion sector of the Hilbert space (one is interested in normal ordering with respect to the vector $|\Omega_0\rangle$). As already remarked, the nonrelativistic field operators decomposed as in (5.98) have the structure very similar to relativistic field operators which will be constructed in Chapter 8. Relativistic field opertors provide, therefore, another example of the operators A_i decomposable into $A_i^{(+)}$ and $A_i^{(-)}$ the role of which play, respectively, the parts of these operators involving the annihilation and creation operators of the particle (if the particle with which a given field operator is associated is neutral - in this case $(A_i^{(\pm)})^\dagger = A_i^{(\mp)}$, $A_i^\dagger = A_i$) or involving the annihilation operators of the particle and creation operators of its atiparticle (if the particle with which the field operator is associated is not neutral - in this case $(A_i^{(\pm)})^\dagger \neq A_i^{(\mp)}$ and

[57] Recall again that the commutator in it must be a c-number!

$A_i^\dagger \neq A_i$). The role of the state $|\text{vac}\rangle$ is then played by the ground state vector $|\Omega_0\rangle$ of the Hamiltonian H_0 of noninteracting particles which (in virtually all cases) is identical with the vector $|\text{void}\rangle$ of the big Hilbert space (5.20). Finally, if the system consists of N nonrelativistic bosons it is impossible to decompose the field operators $\hat{\phi}_\alpha(\mathbf{x})$ and $\hat{\phi}_\alpha^\dagger(\mathbf{x})$ in such a way that their parts $A_i^{(+)}$ annihilate the the H_0 ground state $|\Omega_0\rangle = |N, 0, 0, \ldots\rangle$ that is, normal ordering with respect to $|\Omega_0\rangle$ cannot be defined.[58] This becomes possible only after the momentum space operators $a_{\mathbf{p}=\mathbf{0}}$ and $a_{\mathbf{p}=\mathbf{0}}^\dagger$ are replaced by c-numbers - as suggested by Bogolyubov and an appropriate transformation analogous to the one considered in Section 5.5 is effected.

The Wick theorem applies also to chronological products of time-dependent operators $A_i(t_i)$ provided the time dependence of the operators $a_a(t)$ and $a_a^\dagger(t)$ out of which $A_i^{(+)}$ and $A_i^{(-)}$, respectively, are constructed as their linear combinations, is of the form of c-number phase factors (as is the case when $a_a(t) = \exp(-i\omega_a t)a_a$ and $a_a^\dagger = \exp(i\omega_a t)a_a^\dagger$; the Wick theorem does not apply to Heisenbeg picture operators!). In the case of two operators it takes the form (although the meaning of the contraction is different here, we continue to use the same symbol)

$$\mathrm{T}[A_1(t_1)A_1(t_2)] = :A_1(t_1)A_1(t_2): + \overbrace{A(t_1)A}(t_2)\,. \tag{5.184}$$

The contraction is defined here by

$$\overbrace{A_1(t_1)A_2}(t_2) \equiv \mathrm{T}[A_1(t_1)A_2(t_2)] - :A_1(t_1)A_2(t_2):\ . \tag{5.185}$$

Assuming that the state $|\text{vac}\rangle$ annihilated by all $A_i^{(+)}$ exists, it can be evaluated as

$$\overbrace{A(t_1)A}(t_2) = \langle\text{vac}|\mathrm{T}[A_1(t_1)A_1(t_2)]|\text{vac}\rangle\,. \tag{5.186}$$

The right hand side of the generalization of the above result to chronological product of n operators $T[A_1(t_1)\ldots A_n(t_n)]$ takes exactly the form as in (5.183) with the contractions on the right hand side now given by (5.185). In applications of this version of the Wick theorem it happens, as when it is applied to work out successive terms (5.159) of the Dyson expansion, especially in nonrelativistic many-body problems, that under the symbol of the chronological ordering stand groups of operators depending on the same time variable and ordered normally within the groups (they come from the same interaction operator $V_{\text{int}}^I(t)$); in such cases in (5.183) one should omit the contractions of operators belonging to one and the same such group.

5.10 Summary

We have constructed the second quantized version of quantum mechanics of nonrelativistic many-particle systems starting from its standard version based on the multiparticle Schrödinger equation and multiparticle wave functions $\Psi(\mathbf{x}_1\sigma_1, \ldots, \mathbf{x}_N\sigma_N)$.

[58] But of course with respect to the $|\text{void}\rangle$ vector this is possible as discussed above.

An alternative approach would be to start from symmetry principles and to assume that the Galileo group is realized (projectively) in some Hilbert space (playing the role of the "big" Hilbert space $\mathcal{H}$) by unitary operators. One could then classify possible eigenvectors $|\mathbf{p}, \sigma\rangle$ of the commuting Galileo group generators $H, \mathbf{P}$ and identify them with particles. Operators $a_\sigma(\mathbf{p})$ and $a^\dagger_\sigma(\mathbf{p})$ could be then associated with these states. Finally interactions V_{int} could be constructed from the operators $a_\sigma(\mathbf{p})$ and $a^\dagger_\sigma(\mathbf{p})$ respecting the assumed symmetry principles.

We will follow such an approach in the next chapters to construct the Hilbert space of relativistic quantum theory of particles.

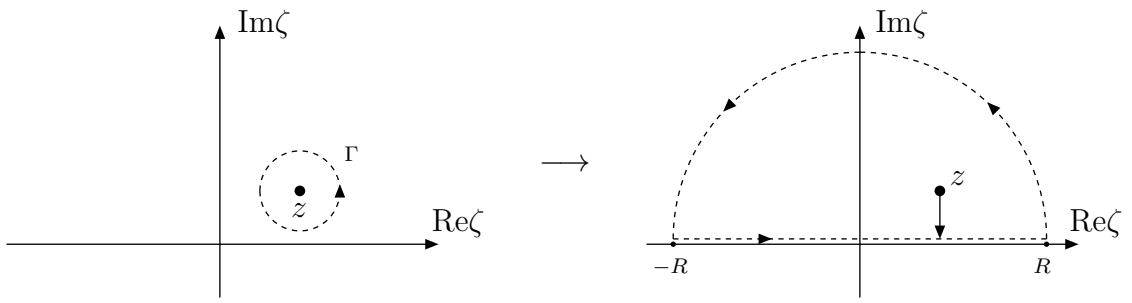

Figure C.1: Deformation of the integration contour Γ leading to the dispersion relations (C.3) satisfied by $f(\zeta)$ analytic in the upper half-plane of the complex variable ζ.

C Dispersion relations

Let $f(z)$ be a function analytic in the upper half-plane of its complex variable z. Then if the integration contour Γ encircling the point z lies entirely in the upper half plane - see the left Figure C.1 - the function $f(z)$ satusfies the well-known Cauchy relation

$$f(z) = \frac{1}{2\pi i}\oint_\Gamma d\zeta\, \frac{f(\zeta)}{\zeta - z}\,. \tag{C.1}$$

As the integrand $f(\zeta)/(\zeta - z)$ has in the upper plane no other poles than the one at $\zeta = z$, the integration contour Γ can be deformed as in the right Figure C.1. Assuming that the integral over the large semicircle vanishes in the limit of the semicircle radius R going to infinity, setting $z = x + i\varepsilon_1$ and $\zeta = y + i\varepsilon_2$ with $0 < \varepsilon_2 < \varepsilon_1$ (to keep the pole above the path of the integration, as is clear from the right Figure C.1) one gets

$$f(x + i0) = \frac{1}{2\pi i}\int_{-\infty}^{\infty} dy\, \frac{f(y)}{y - x - i0}\,,$$

where the integral is taken over y lying at the upper side of the real axis in the complex ζ plane. Splitting now $f(x)$ and $f(y)$ into their real and imaginary parts: $f(x) = \mathrm{Re}f(x) + i\mathrm{Im}f(x)$, etc., and employing the Sochocki formula

$$\frac{1}{x \pm i0} = \mathrm{P}\frac{1}{x} \mp i\pi\,\delta(x)\,, \tag{C.2}$$

one obtains

$$\mathrm{Re}f(x) + i\mathrm{Im}f(x) = \frac{1}{2\pi i}\int_{-\infty}^{\infty} dy\,(\mathrm{Re}f(y) + i\mathrm{Im}f(y))\left\{\mathrm{P}\frac{1}{y - x} + i\pi\,\delta(y - x)\right\}.$$

Finally, equating the real and imaginary parts of both sides, one arrives at the dispersion relations

$$\begin{aligned}\mathrm{Re}\, f(x) &= \mathrm{P}\int_{-\infty}^{\infty}\frac{dy}{\pi}\,\frac{\mathrm{Im}\, f(y)}{y - x}\,,\\ \mathrm{Im}\, f(x) &= -\mathrm{P}\int_{-\infty}^{\infty}\frac{dy}{\pi}\,\frac{\mathrm{Re}\, f(y)}{y - x}\,.\end{aligned} \tag{C.3}$$

If the function $f(z)$ is analytic in the lower half-plane of the complex variable z, a reasoning analogous to the one presented here leads to the relations

$$\begin{aligned} \mathrm{Re}\, f(x) &= -\mathrm{P}\int_{-\infty}^{\infty} \frac{dy}{\pi}\, \frac{\mathrm{Im}\, f(y)}{y-x}\,, \\ \mathrm{Im}\, f(x) &= \mathrm{P}\int_{-\infty}^{\infty} \frac{dy}{\pi}\, \frac{\mathrm{Re}\, f(y)}{y-x}\,, \end{aligned} \tag{C.4}$$

in which the integrals are taken over the lower side of the real axis.