5 The formalism of second quantization

Systems consisting of many identical particles form the prevailing part of the physical world. A typical example are electrons in a lattice of ions in a solid or nucleons in a heavy nucleus. 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 imposes additional requirements on the quantum theory of identical particles: vectors representing states must have definite symmetry properties with respect to interchanging labels of identical particles. Imposing this requirement in the ordinary approach based on the multiparticle-wave function is rather cumbersome. In this section a convenient formulation - called "second quantization" - of quantum mechanics of systems composed of many identical particles, allowing to automatically take into account these symmetry requirements, is presented. Its most characteristic feature is the use of the creation and annihilation operators in terms of which any operator can be expressed and whose action on the system's states is particularly simple. The true essence of this formulation is however the introduction of the "big" Hilbert space $\mathcal{H}$ whose vectors can represent states of an arbitrary, also infinite, and even 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), is 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.[2] 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 section 7, Poincaré covariance of transition amplitudes (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

[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] 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) is not entirely true.

relativistic quantum field theory. Moreover, nonseparability of the "big" 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, $\mathcal{H}$ furnishes a reducible representation of the abstract operator algebra. Any such representation selects in $\mathcal{H}$ a separable subspace called Fock space and it is the dynamics of the considered physical system which selects the Fock space in which the physically accessible states of the system are represented. This profound property of the big Hilbert space $\mathcal{H}$ is at the heart of the possibility of describing in 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 Many-particle 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 $\mathcal{H}^{(N)} = \mathcal{H}_1^{(1)} \otimes \ldots \otimes \mathcal{H}_N^{(1)}$ of one-particle Hilbert spaces of individual particles;[3] it is spanned by the state-vectors having the form of the tensor product

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

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

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

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

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

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

[3] 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 of particles of spin s are all isomorphic to the (2s+1)-fold Cartesian product of $L_2(\mathbb{R}^3)$.

altogether) and can move in the infinite three-dimensional space, the three-dimensional isotropic harmonic oscillator normalized to unity state-vectors $|\psi_{(l^x l^y l^z)_k}(\omega_k)\rangle$ or $|\psi_{(l^r l^\theta l^\varphi)_k}(\omega_k)\rangle$ (l^θ stands here, somewhat unconventionally, for the orbital momentum quantum number) can be taken for $|l_k\rangle$ (l_k is then a three-index $l^x l^y l^z$ or $l^r l^\theta l^\varphi$), because in the position (or the momentum) representation any normalizable wave function $\psi(\mathbf{x})$ (or $\psi(\mathbf{p})$) can be written as a superposition of the functions $\psi_{(l^x l^y l^z)}(\mathbf{x}) = \psi_{l^x}(x)\psi_{l^y}(y)\psi_{l^z}(z)$ or $|\psi_{(l^r l^\theta l^\varphi)_k}(\mathbf{x}) = \psi_{l^r}(r)Y_{l^\theta l^\varphi}(\theta,\varphi)$ (or, in the momentum representation, of $\psi_{(l^x l^y l^z)}(\mathbf{p}) = \psi_{l^x}(p^x)\psi_{l^y}(p^y)\psi_{l^z}(p^z)$) with some arbitrary $\omega_k^2 > 0$ (the frequencies ω can be different for diffent particles and in $\psi_{(l^x l^y l^z)}$ could even be different for diffent directions). Similarly, if the system of N particles is enclosed in a box of volume $V = L^3$ (and the periodic boundary conditions are imposed on the wave functions of individual particles), the vectors

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

with $\mathbf{p}_k = (2\pi/L)\mathbf{n}_k$, 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 $\Psi(\mathbf{x}_1, \dots, \mathbf{x}_N)$ of N particles can be written as a superposition

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

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

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

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

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

In the infinite space 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[4]

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

whose scalar products is

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

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

or the generalized vectors

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

with the scalar product

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

The completeness relation in these cases read

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

Internal degrees of freedom (spin) can be easily incorporated into this formalism by including the spin labels $\sigma_k = -s_k, \dots, +s_k$ into l_k's 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[5] of a state of the form (5.1) with the basis vectors (5.6) gives then the N-particle wave function

$$\Psi(\mathbf{x}_1, \dots, \mathbf{x}_N) = \langle \mathbf{x}_N, \dots, \mathbf{x}_1|\Psi\rangle = \psi^{(1)}(\mathbf{x}_1) \cdot \dots \cdot \psi^{(N)}(\mathbf{x}_N)\,. \tag{5.11}$$

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 states); states $|\Psi\rangle$ which do not factorize as (5.1) are called *entangled* states and play crucial role in modern quantum optics and quantum information theory.

Consider now a system consisting of N *indistinguishable* particles of one type,[6] 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.[7] This requirement has to be added as an extra rule selecting possible states. 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

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

[6]Generalization of the formalism to several types of identical particles is straightforward.

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

simply be regarded as a phenomenological input.[8] As will be argued in Section 8, justification of this celebrated *spin-statistics connection* comes only from the relativistic quantum field theory. It is implemented by defining the state-vectors spanning the Hilbert space $\mathcal{H}^{(N)}$ of a system of N identical particles in terms of the one-particle state-vectors by the formula

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

in which $|\psi_i\rangle$ are N arbitrary one-particle states and P denotes their permutations. We have introduced here the symbol ζ

$$\zeta = \begin{cases} +1 & \text{for} \quad \text{bosons} \\ -1 & \text{for} \quad \text{fermions} \end{cases},$$

and by ζ^P understand for fermions the sign of the permutation P. For bosons of course $\zeta^P = 1$. For example, in the case of $N = 2$ particles and two one-particle states $|a\rangle$ or $|b\rangle$ one can construct the following three states

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

if the particles are identical bosons and only one state

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

if they are identical fermions. The scalar product of such states is

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

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

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

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

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 states $|a,a\rangle$ and $|b,b\rangle$ of bosons are not properly normalized even if the one-particle states $|a\rangle$ and $|b\rangle$ are orthonormal: $\langle a,a|a,a\rangle = \langle b,b|b,b\rangle = 2$.

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

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

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 $\mathbf{k} = (2\pi/L)\mathbf{n}$ 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 $\sigma = -s, \dots, +s$ must be included in the label l. As an orthonormal a basis of the Hilbert space $\mathcal{H}^{(N)}$ of N identical bosons one can then take the vectors[9]

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

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

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

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

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, recalling that

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

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 $l'_1,\dots l'_N$ and $l_1,\dots,l_N$ (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 identical 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 therefore conveniently written in the form

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

Note that here 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 consider three 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. In the decomposition of the unit operator only a single term of the form

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

should be present. (5.18) gives

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

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

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

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 $\mathcal{H}^{(1)}$ 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 $|\tilde{l}_1, \tilde{l}_2, \ldots, \tilde{l}_N\rangle/\sqrt{\tilde{n}_1!\tilde{n}_2!\ldots}$ (of the vectors $|\tilde{l}_1, \tilde{l}_2, \ldots, \tilde{l}_N\rangle$). 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 vectors $|\tilde{l}_1, \tilde{l}_2, \ldots, \tilde{l}_N\rangle/\sqrt{\tilde{n}_1!\tilde{n}_2!\ldots}$ (of vectors $|\tilde{l}_1, \tilde{l}_2, \ldots, \tilde{l}_N\rangle$).

All this works in the same way for 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 vector $|\text{void}\rangle$ in most texts misleadingly called the "vacuum", or, less misleadinly, the Fock vacuum vector.[10] That is, the zero-particles Hilbert space $\mathcal{H}^{(0)}$ is one-dimensional (all other Hilbert spaces for $N \geq 1$ are all countably infinite dimensional). One then formally introduces the "big" Hilbert space $\mathcal{H}$

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

whose vectors are of 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,[11] say $|e^+e^-\rangle$ in an 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 some constraints). Therefore the final state is a (in general infinite) superposition of vectors corresponding to different numbers of particles

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

where a, b, c, d, e are some complex number. Measurement of a concrete final state by the detector has the effect of reducing this state-vector of the system.

[10] We denote this vector $|\text{void}\rangle$ in order to distinguish this "technical" "no particle" vector from the state-vectors $|\Omega_0\rangle$ and $|\Omega\rangle$ 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.

[11] The precise way the states like $|e^+e^-\rangle$, representing a well defined number of physically detectable particles, are related to the basis states formed as tensor products of one-particle states will be elucidated in Section 7.2.

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 right arena in which to describe physical processes. The possibility of treating systems with variable number of particles is useful also in nonrelativistic physics. Investigating statistical properties of physical systems one usually prefers to work in the framework of the Grand Canonical Ensemble, in which the number of paricles is allowed to fluctuate. Also one is usually interested in systems having fixed density which requires considering the system of N particles in a finite box of volume V and taking the limits $N \to \infty$, $V \to \infty$ with $\rho = N/V$ kept fixed. Finally, the possibility of forming superpositions of state-vectors corresponding to different number of particles is crucial for description of phenomena as superconductivity in which some symmetries are spontaneously broken.

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, that is it has no countable basis - as will be shown in the next section, 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 (called in this context Fock spaces), with countable bases can be chosen in $\mathcal{H}$ (5.20), all of which are, if the volume of the space is taken to be infnite and/or no UV cutoff (effectively discretizing the space) is imposed, are ortghonal to one another.

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 completeness relation in $\mathcal{H}$ reads

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

For example, in the position basis it takes the form (spin labels can be included here as in (5.19))

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

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

$$|\Psi\rangle = a|\text{void}\rangle + \sum_{N=1}^{\infty} \frac{1}{N!} \int d\mathbf{x}_1 \dots \int d\mathbf{x}_N \, |\mathbf{x}_1,\dots,\mathbf{x}_N\rangle\langle\mathbf{x}_N,\dots,\mathbf{x}_1|\Psi\rangle$$

$$= a|\mathrm{void}\rangle + \sum_{N=1}^{\infty} \frac{1}{N!} \int d\mathbf{x}_1 \dots \int d\mathbf{x}_N \, |\mathbf{x}_1, \dots, \mathbf{x}_N\rangle \Psi_{(N)}(\mathbf{x}_1, \dots, \mathbf{x}_N) \, ,$$

where $\Psi_{(N)}(\mathbf{x}_1, \dots, \mathbf{x}_N) \equiv \langle \mathbf{x}_1, \dots, \mathbf{x}_N | \Psi^{(N)}\rangle$ is the wave function of the N-particle component of the state $|\Psi\rangle$. The function $\Psi_{(N)}(\mathbf{x}_1, \dots, \mathbf{x}_N)$ of a system of bosons is totally symmetric while a similar function of a system of 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 (we again make the spin labels α - which must, and in nonrelativistic mechanics can, be given a meaning in terms of some one-particle spin operator - explicit here)

$$\Psi^{(N)}_{\alpha_1,\dots,\alpha_N}(\mathbf{x}_1, \dots, \mathbf{x}_N) = \left| \begin{array}{ccc} \langle \mathbf{x}_1 \alpha_1 | \psi_1 \rangle & \dots & \langle \mathbf{x}_1 \alpha_1 | \psi_N \rangle \\ \cdot & \dots & \cdot \\ \cdot & \dots & \cdot \\ \cdot & \dots & \cdot \\ \langle \mathbf{x}_N \alpha_N | \psi_1 \rangle & \dots & \langle \mathbf{x}_N \alpha_N | \psi_N \rangle \end{array} \right|_{\zeta} , \quad (5.25)$$

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 calculated as the determinant except for taking everywhere positive signs (the precise definition is given by (5.14) with φ_i replaced by $\mathbf{x}_i$).

5.2 Creation and annihilation operators

Construction 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 of the form (5.12) it is defined by the formula

$$a^\dagger(\varphi)|\psi_1, \dots, \psi_N\rangle = |\varphi, \psi_1, \dots, \psi_N\rangle \, , \quad (5.26)$$

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

$$\langle \chi_{N-1}, \dots, \chi_1 | a(\varphi) | \psi_1, \dots, \psi_N \rangle = \left(\langle \psi_N, \dots, \psi_1 | a^\dagger(\varphi) | \chi_1, \dots, \chi_{N-1} \rangle \right)^*$$
$$= \left| \begin{array}{cccc} \langle \psi_1 | \varphi \rangle & \langle \psi_1 | \chi_1 \rangle & \dots & \langle \psi_1 | \chi_{N-1} \rangle \\ \cdot & \cdot & \dots & \cdot \\ \cdot & \cdot & \dots & \cdot \\ \cdot & \cdot & \dots & \cdot \\ \langle \psi_N | \varphi \rangle & \langle \psi_N | \chi_1 \rangle & \dots & \langle \psi_N | \chi_{N-1} \rangle \end{array} \right|^*_{\zeta} .$$

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

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

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

$$a(\varphi)|\psi_1, \ldots, \psi_N\rangle = \sum_{k=1}^{N} \zeta^{k-1} \langle \varphi | \psi_k \rangle |\psi_1, \ldots (\text{no } \psi_k) \ldots, \psi_N\rangle \,, \qquad (5.27)$$

which shows that $a(\varphi)$ acting on a state $|\Psi^{(N)}\rangle$ 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 (5.27) can be understood as a sign factor arising when ψ_k is moved from its k-th position in the ket to the first position, where $a(\varphi)$ annihilates it.

From the definitions (5.26) and (5.27) it is easy to show that

$$\begin{aligned} a^\dagger(\varphi_1)\, a^\dagger(\varphi_2) &= \zeta\, a^\dagger(\varphi_2)\, a^\dagger(\varphi_1) \,, \\ a(\varphi_1)\, a(\varphi_2) &= \zeta\, a(\varphi_2)\, a(\varphi_1) \,, \end{aligned} \qquad (5.28)$$

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:

$$a^2(\varphi) = (a^\dagger(\varphi))^2 = 0 \,. \qquad (5.29)$$

It is also easy to prove that

$$\big[a(\varphi_1),\ a^\dagger(\varphi_2)\big]_{-\zeta} = \langle \varphi_1 | \varphi_2 \rangle \,, \qquad (5.30)$$

where the subscript $-\zeta$ denotes the commutator for bosons and the anticommutator for fermions.

The 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 basis of $\mathcal{H}^{(1)}$, then

$$[a_{l'},\ a_l^\dagger]_{-\zeta} = \delta_{l'l} \,. \qquad (5.31)$$

(If, instead, the $|l\rangle$'s are generalized vectors, then $[a_{l'},\ a_l^\dagger]_{-\zeta} = \delta(l' - l)$). This means that the annihilation and creation operators of bosons (fermions) commute (anticommute) to 1 (or, in the case of a continuous normalization of the one-particle states, to the appropriate delta function). For future use note also, that for fermions the rule (5.31) 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

$$
\begin{aligned}
a_l\,|l_1, l_2, \dots, l_N\rangle &= \sum_{k=1}^{N} (-1)^{k-1} \delta_{l l_k} |l_1, \dots (\text{no } l_k) \dots, l_N\rangle\,, \\
a_l^\dagger\,|l_1, l_2, \dots, l_N\rangle &= |l, l_1, l_2, \dots, l_N\rangle = \pm |l_1, \dots, l, \dots, l_N\rangle\,, \qquad (5.32)
\end{aligned}
$$

where the sign depends on the number of interchanges needed to put l on the appropriate position (in agreement with the ordering specified in (5.16)).

To represent the action of the bosonic operators $a_{l'}$ and$a_l^\dagger$ on the basis vectors (5.15) it is convenient to introduce 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, by defining

$$
|n_1, n_2, \dots\rangle \equiv \frac{1}{\sqrt{n_1!\, n_2! \dots}}\,|1, \dots, 1, 2, \dots, 2, \dots\rangle\,, \qquad (5.33)
$$

In this notation the numbers n_1, n_2 etc. simply indicate how many particles occupies 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 $n_1 + n_2 + \dots = N$. 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.[12] As a result, the Hilbert space $\mathcal{H}$ constructed as in (5.20) is not separable and the state-vectors $|n_1, n_2, \dots\rangle$ span in fact only a subspace of the big Hilbert space: there are vectors in $\mathcal{H}$ which have zero scalar products with all vectors the $|n_1, n_2, \dots\rangle$.

In the occupation number representation the action of bosonic creation and annihilation operators looks more familiar:

$$
\begin{aligned}
a_l\,|n_1, n_2, \dots, n_l, \dots\rangle &= \sqrt{n_l}\,|n_1, n_2, \dots, n_l - 1, \dots\rangle\,, \\
a_l^\dagger|n_1, n_2, \dots, n_l, \dots\rangle &= \sqrt{n_l + 1}\,|n_1, n_2, \dots, n_l + 1, \dots\rangle\,. \qquad (5.34)
\end{aligned}
$$

[12]This is particularly easy to demonstrate in the case of fermions: it suffices to notice that the infinite sequence of numbers $n_1 n_2 n_3 \dots$, 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 $p_1 p_2 p_3 \dots$, $0 \le p_l < 9$ and the fractions $0.p_1 p_2 p_3 \dots$ fill the entire segment $[0, 1)$ whose power is equal to the power of the continuum.

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

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

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 $|l\rangle$.

The creation and annihiolation operators can be also associated with non-normalizable bases of $\mathcal{H}^{(1)}$, for example with the basis of plane waves $|\mathbf{p}\rangle$ (in the case of spin zero bosons) or $|\mathbf{p}\sigma\rangle$ in general normalized to the delta function in the infinite space[13]

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

for which $\langle \mathbf{x}, \alpha|\mathbf{p}, \sigma\rangle = (\psi_{\mathbf{p}\sigma})_\alpha(\mathbf{x}) = \delta_{\alpha\sigma}e^{i\mathbf{p}\cdot\mathbf{x}}$, or normalized in a box of volume $V = L^3$ with periodic boundary conditions:

$$\langle \mathbf{p}'\sigma'|\mathbf{p}\sigma\rangle = \delta_{\mathbf{p}',\mathbf{p}}\,\delta_{\sigma'\sigma}\,, \tag{5.35}$$

and $(\psi_{\mathbf{p}\sigma})_\alpha(\mathbf{x}) = L^{-3/2}\delta_{\alpha\sigma}e^{i\mathbf{p}\cdot\mathbf{x}}$. The rule (which is frequently used) for transition from the discrete normalization to the continuous one is

$$\sum_{\mathbf{p}} \equiv \sum_{n_x, n_y, n_z} \leftrightarrow \frac{V}{(2\pi)^3}\int d^3\mathbf{p}\,. \tag{5.36}$$

In this basis

$$[a_\sigma(\mathbf{p}),\ a^\dagger_{\sigma'}(\mathbf{p}')]_{-\zeta} = (2\pi)^3\delta^{(3)}(\mathbf{p}' - \mathbf{p})\delta_{\sigma'\sigma} \qquad \text{or} \qquad \delta_{\mathbf{p}',\mathbf{p}}\delta_{\sigma'\sigma}\,, \tag{5.37}$$

and the Hilbert space $\mathcal{H}^{(N)}$ is spanned by the vectors

$$|\mathbf{p}_1\sigma_1, \mathbf{p}_2\sigma_2, \dots, \mathbf{p}_N\sigma_N\rangle = a^\dagger_{\sigma_1}(\mathbf{p}_1)\,a^\dagger_{\sigma_2}(\mathbf{p}_2)\dots a^\dagger_{\sigma_N}(\mathbf{p}_N)|\text{void}\rangle\,. \tag{5.38}$$

One can also use the position basis in which

$$[a_\alpha(\mathbf{x}),\ a^\dagger_{\alpha'}(\mathbf{x}')]_{-\zeta} = \delta(\mathbf{x}' - \mathbf{x})\delta_{\alpha'\alpha}\,, \tag{5.39}$$

and the Hilbert space $\mathcal{H}^{(N)}$ is spanned by the vectors

$$|\mathbf{x}_1\alpha_1, \mathbf{x}_2\alpha_2, \dots, \mathbf{x}_N\alpha_N\rangle = a^\dagger_{\alpha_1}(\mathbf{x}_1)\,a^\dagger_{\alpha_2}(\mathbf{x}_2)\dots a^\dagger_{\alpha_N}(\mathbf{x}_N)|\text{void}\rangle\,. \tag{5.40}$$

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

The operators $a(\mathbf{x})$ and $a^\dagger(\mathbf{x})$ are sometimes denoted by $\hat{\psi}(\mathbf{x})$ and $\hat{\psi}^\dagger(\mathbf{x})$ and called the field operators.

In general, if a one-particle state-vector $|\chi\rangle$ is a linear superposition of some other vectors, e.g. if

$$|\chi\rangle = A\,|\psi\rangle + B\,|\phi\rangle\,, \tag{5.41}$$

then from the definition (5.26) it is clear that

$$\begin{aligned} a^\dagger(\chi) &= A\,a^\dagger(\psi) + B\,a^\dagger(\phi)\,,\\ a(\chi) &= A^* a(\psi) + B^* a(\phi)\,. \end{aligned} \tag{5.42}$$

Since

$$|\mathbf{x},\alpha\rangle = \int \frac{d^3\mathbf{p}}{(2\pi)^3} \sum_\sigma |\mathbf{p},\sigma\rangle\langle\mathbf{p},\sigma|\mathbf{x},\alpha\rangle = \int \frac{d^3\mathbf{p}}{(2\pi)^3} \sum_\sigma |\mathbf{p},\sigma\rangle\,\delta_{\sigma\alpha} e^{-i\mathbf{p}\cdot\mathbf{x}}\,, \tag{5.43}$$

we have

$$a^\dagger_\alpha(\mathbf{x}) = \int \frac{d^3\mathbf{p}}{(2\pi)^3}\, a^\dagger_\alpha(\mathbf{p})\, e^{-i\mathbf{p}\cdot\mathbf{x}}\,, \qquad a_\alpha(\mathbf{x}) = \int \frac{d^3\mathbf{p}}{(2\pi)^3}\, a_\alpha(\mathbf{p})\, e^{+i\mathbf{p}\cdot\mathbf{x}}\,. \tag{5.44}$$

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

$$|\mathbf{x},\alpha\rangle = \sum_{l,\sigma} |l,\sigma\rangle\langle l,\sigma|\mathbf{x},\alpha\rangle = \sum_{l,\sigma} |l,\sigma\rangle\,(u_{l,\sigma})^*_\alpha(\mathbf{x})\,, \tag{5.45}$$

then

$$a^\dagger_\alpha(\mathbf{x}) = \sum_{l,\sigma} a^\dagger_{l,\sigma}\,(u_{l\sigma})^*_\alpha(\mathbf{x})\,, \qquad a_\alpha(\mathbf{x}) = \sum_{l,\sigma} a_{l,\sigma}\,(u_{l\sigma})_\alpha(\mathbf{x})\,, \tag{5.46}$$

$$a^\dagger_{l,\sigma} = \int d^3\mathbf{x} \sum_\alpha (u_{l\sigma})_\alpha(\mathbf{x})\, a^\dagger_\alpha(\mathbf{x})\,, \qquad a_{l,\sigma} = \int d^3\mathbf{x} \sum_\alpha (u^*_{l\sigma})_\alpha(\mathbf{x})\, a_\alpha(\mathbf{x})\,. \tag{5.47}$$

5.3 Hamiltonian and other operators

The annihilation and creation operators allow to represent various operators in a simple form. Let us begin with one-particle operators of the general form

$$O = \sum_{i=1}^N O_i^{(1)}\,, \tag{5.48}$$

where $O_i^{(1)}$ denotes a one-particle operator $O^{(1)}$ acting only on the variables of the i-th particle:

$$O|\psi_1, \psi_2, \ldots, \psi_N\rangle = |\psi'_1, \psi_2, \ldots, \psi_N\rangle + \ldots + |\psi_1, \psi_2, \ldots, \psi'_N\rangle\,. \qquad (5.49)$$

The state-vectors $|\psi_1, \psi_2, \ldots, \psi_N\rangle$ are defined in (5.12) and $|\psi'_i\rangle = O^{(1)}|\psi_i\rangle$. Obviously, if $|\psi_i\rangle$ are all eigenstates of the respective $O_i^{(1)}$'s with the eigenvalues o_{ψ_i}, one gets

$$O|\psi_1, \psi_2, \ldots, \psi_N\rangle = (o_{\psi_1} + o_{\psi_2} + \ldots + o_{\psi_N})|\psi_1, \psi_2, \ldots, \psi_N\rangle\,. \qquad (5.50)$$

An example of the operator of this type is e.g. the kinetic energy operator $T = \sum_{i=1}^{N} \hat{\mathbf{P}}_i^{(1)2}/2m$ which in many cases plays the role of the free Hamiltonian H_0 of the system of particles. Acting on the (generalized) state-vectors (5.38) gives the eigenvalue $(\mathbf{p}_1^2 + \ldots + \mathbf{p}_N^2)/2m$.

To find the representation of a general O of the form (5.48) in terms of the annihilation and creation operators let us consider first a particular operator $O^{(1)} = |l\rangle\langle l'|$ (the spin label is now included in the general label l). The action of the corresponding O of the form (5.48) on a state-vector $|\psi_1, \psi_2, \ldots, \psi_N\rangle$ is

$$O|\psi_1, \psi_2, \ldots, \psi_N\rangle = \langle l'|\psi_1\rangle\, |l, \psi_2, \ldots, \psi_N\rangle + \langle l'|\psi_2\rangle\, |\psi_1, l, \ldots, \psi_N\rangle + \ldots$$

It is easy to see that this action of O is identical with the action of $a_l^\dagger a_{l'}$. Since any one-particle operator can be written in the form

$$O^{(1)} = \sum_l \sum_{l'} |l\rangle\langle l|O^{(1)}|l'\rangle\langle l'| \equiv \sum_l \sum_{l'} O_{ll'}^{(1)}\, |l\rangle\langle l'|\,, \qquad (5.51)$$

one concludes that

$$O = \sum_l \sum_{l'} O_{ll'}^{(1)}\, a_l^\dagger\, a_{l'}\,. \qquad (5.52)$$

Taking for example $O^{(1)} = \hat{1}^{(1)}$ (the one-particle unit operator), whose matrix elements are $O_{ll'}^{(1)} = \langle l|\hat{1}^{(1)}|l'\rangle = \delta_{ll'}$, one gets the operator $\hat{N}$ counting the number of particles of the system:

$$\hat{N} = \sum_l a_l^\dagger a_l = \int d^3\mathbf{x} \sum_\alpha a_\alpha^\dagger(\mathbf{x})\, a_\alpha(\mathbf{x}) = \int \frac{d^3\mathbf{p}}{(2\pi)^3} \sum_\sigma a_\sigma^\dagger(\mathbf{p})\, a_\sigma(\mathbf{p})\,. \qquad (5.53)$$

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:[14]

$$\hat{\mathbf{P}} = \int \frac{d^3\mathbf{p}}{(2\pi)^3} \sum_\sigma \hbar\mathbf{p}\, a_\sigma^\dagger(\mathbf{p}) a_\sigma(\mathbf{p}) = \int d^3\mathbf{x} \sum_\alpha a_\alpha^\dagger(\mathbf{x})(-i\hbar\nabla_\mathbf{x}) a_\alpha(\mathbf{x})\,, \qquad (5.54)$$

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

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

(recall that $\mathbf{p}$ is the wave vector, not the momentum). In the similar way, out of the corresponding one-particle operators, it is possible to construct also the total angular momentum $\mathbf{J}$ and boost $\mathbf{K}$ operators of the system of free particles.

If (identical) particles are not interacting with each other but all move in some external potential $V(\mathbf{x})$, their nonrelativistic Hamiltonian is the sum (over particles) of one-particle operators $H^{(1)} = T^{(1)} + V^{(1)} = \hat{\mathbf{P}}^{(1)2}/2m + V^{(1)}(\hat{\mathbf{x}})$ whose matrix elements are

$$\langle\mathbf{x}|H^{(1)}|\mathbf{y}\rangle = -\frac{\hbar^2}{2m}\nabla^2_{\mathbf{y}}\,\delta^{(3)}(\mathbf{y}-\mathbf{x}) + V(\mathbf{x})\,\delta^{(3)}(\mathbf{y}-\mathbf{x})\,, \tag{5.55}$$

and takes the form

$$H = \int d^3\mathbf{x}\,a^\dagger(\mathbf{x})\left[-\frac{\hbar^2}{2m}\nabla^2_{\mathbf{x}} + V(\mathbf{x})\right]a(\mathbf{x})\,. \tag{5.56}$$

To rewrite it in the momentum representation we use the formulae

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

and

$$\langle\mathbf{p}|V^{(1)}|\mathbf{p}'\rangle = \int d^3\mathbf{x}\int d^3\mathbf{y}\;\langle\mathbf{p}|\mathbf{x}\rangle\langle\mathbf{x}|V^{(1)}|\mathbf{y}\rangle\langle\mathbf{y}|\mathbf{p}'\rangle = \tilde{V}(\mathbf{p}-\mathbf{p}')\,,$$

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

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

Thus, in the momentum representation we get

$$\begin{aligned} H &= \int\frac{d^3\mathbf{p}}{(2\pi)^3}\,\frac{\hbar^2\mathbf{p}^2}{2m}\;a^\dagger(\mathbf{p})\,a(\mathbf{p}) + \int\frac{d^3\mathbf{p}}{(2\pi)^3}\int\frac{d^3\mathbf{p}'}{(2\pi)^3}\,a^\dagger(\mathbf{p}')\,\tilde{V}(\mathbf{p}'-\mathbf{p})\,a(\mathbf{p}) \\ &= \int\frac{d^3\mathbf{p}}{(2\pi)^3}\,\frac{\hbar^2\mathbf{p}^2}{2m}\,a^\dagger(\mathbf{p})\,a(\mathbf{p}) + \int\frac{d^3\mathbf{p}}{(2\pi)^3}\int\frac{d^3\mathbf{q}}{(2\pi)^3}\,a^\dagger(\mathbf{p}+\mathbf{q})\,\tilde{V}(\mathbf{q})\,a(\mathbf{p})\,. \end{aligned} \tag{5.57}$$

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 $|l\rangle$ of the full

---

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

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

one-particle Hamiltonian $H^{(1)} = \hat{\mathbf{P}}^2/2m + V^{(1)}(\hat{\mathbf{x}})$, the "second-quantized" Hamiltonian H will take the simple form

$$H = \sum_l E_l a_l^\dagger a_l \,, \tag{5.58}$$

(the range of the label l may consist of a discrete and a continuous parts). Note also that the operator

$$\rho(\mathbf{x}) = a^\dagger(\mathbf{x}) a(\mathbf{x}) \,, \tag{5.59}$$

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 (5.53) counting the number of particles is given by $\hat{N} = \int d^3\mathbf{x}\, \rho(\mathbf{x})$.

Even more useful is the formalism of the creation and annihilation operators for the 2-particle operators which act on variables of two particles. The most frequently encountered operator of this kind is the potential energy operator of the binary interactions

$$V_{\rm int} = \sum_{i<j} V^{(2)}(\mathbf{x}_i, \mathbf{x}_j) = \frac{1}{2}\sum_{i\neq j} V^{(2)}(\mathbf{x}_i, \mathbf{x}_j) \,, \tag{5.60}$$

where if the particles are identical the function $V^{(2)}$ must be symmetric: $V^{(2)}(\mathbf{x}_i, \mathbf{x}_j) = V^{(2)}(\mathbf{x}_j, \mathbf{x}_i)$. Furthermore, if the system is translationally invariant the function $V^{(2)}$ can depend only on the difference of the positions: $V^{(2)}(\mathbf{x}_i, \mathbf{x}_j) = V^{(2)}(\mathbf{x}_i - \mathbf{x}_j)$. It is easy to see that in the formalism of second quantization on the generalized vectors $|\mathbf{x}_1, \dots, \mathbf{x}_N\rangle$ of the position basis the operator $V_{\rm int}$ must act in the following way

$$V_{\rm int}|\mathbf{x}_1, \dots, \mathbf{x}_N\rangle = \sum_{i<j} V^{(2)}(\mathbf{x}_i, \mathbf{x}_j)|\mathbf{x}_1, \dots, \mathbf{x}_N\rangle \,. \tag{5.61}$$

Indeed, if $V_{\rm int}$ acts as above, using the orthogonality relation

$$\langle \mathbf{x}_N, \dots, \mathbf{x}_1|\mathbf{y}_1, \dots, \mathbf{y}_N\rangle = \sum_P \zeta^P \delta^{(3)}(\mathbf{y}_1 - \mathbf{x}_{P(1)}) \dots \delta^{(3)}(\mathbf{y}_N - \mathbf{x}_{P(N)}) \,,$$

one can write

$$\begin{aligned}
&\frac{1}{N!}\int d^3\mathbf{y}_1 \dots \int d^3\mathbf{y}_N \langle \mathbf{x}_N, \dots, \mathbf{x}_1|V_{\rm int}|\mathbf{y}_1, \dots, \mathbf{y}_N\rangle\langle \mathbf{y}_N, \dots, \mathbf{y}_1|\Psi\rangle \\
&= \frac{1}{N!}\int d^3\mathbf{y}_1 \dots \int d^3\mathbf{y}_N \sum_{i<j} V^{(2)}(\mathbf{y}_i, \mathbf{y}_j)\langle \mathbf{x}_N, \dots, \mathbf{x}_1|\mathbf{y}_1, \dots, \mathbf{y}_N\rangle\langle \mathbf{y}_N, \dots, \mathbf{y}_1|\Psi\rangle \\
&= \sum_{i<j} V^{(2)}(\mathbf{x}_i, \mathbf{x}_j)\langle \mathbf{x}_N, \dots, \mathbf{x}_1|\Psi\rangle = \sum_{i<j} V^{(2)}(\mathbf{x}_i, \mathbf{x}_j)\Psi(\mathbf{x}_1, \dots, \mathbf{x}_N) \,.
\end{aligned}$$

This shows that the action of $V_{\rm int}$ on the N-particle wave function in the position representation is correctly reproduced. In $\mathcal{H}^{(2)}$ the rule (5.61) is satisfied by

$$V_{\rm int}^{(2)} = \frac{1}{2}\int d^3\mathbf{x}\int d^3\mathbf{y}\,|\mathbf{x},\mathbf{y}\rangle\,V(\mathbf{x},\mathbf{y})\,\langle\mathbf{y},\mathbf{x}|\,,$$

and it is not too difficult to guess that in $\mathcal{H}$ the operator $V_{\rm int}$ is given by

$$V_{\rm int} = \frac{1}{2}\int d^3\mathbf{x}\int d^3\mathbf{y}\,a^\dagger(\mathbf{x})\,a^\dagger(\mathbf{y})\,V(\mathbf{x},\mathbf{y})\,a(\mathbf{y})\,a(\mathbf{x})\,, \tag{5.62}$$

(note the reversed order - important if the particles are fermions - of a's compared to $a^\dagger$'s!). Notice also that the operator

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

with $\rho(\mathbf{x})$ given by (5.59) differs from (5.62) by a local term $(1/2)\int d^3\mathbf{x}\,V(\mathbf{x},\mathbf{x})$ which usually is infinite. We have seen that in the quantum theory of radiation (outlined in section 3.8) such infinite terms had to be - due to the improper formulation of that theory - subtracted by hand (using the so-called normal ordering of operators).

If the interaction $V_{\rm int}$ is translationally invariant, using the rules (5.44), in the momentum space representation we get

$$V_{\rm int} = \frac{1}{2}\int\frac{d^3\mathbf{p}}{(2\pi)^3}\int\frac{d^3\mathbf{p}'}{(2\pi)^3}\int\frac{d^3\mathbf{q}}{(2\pi)^3}\,a^\dagger(\mathbf{p}+\mathbf{q})\,a^\dagger(\mathbf{p}'-\mathbf{q})\,\tilde{V}(\mathbf{q})\,a(\mathbf{p}')\,a(\mathbf{p})\,, \tag{5.63}$$

where $\tilde{V}(\mathbf{q})$ is the Fourier transform of $V(\mathbf{x}-\mathbf{y})$:

$$V(\mathbf{x}-\mathbf{y}) = \int\frac{d^3\mathbf{q}}{(2\pi)^3}\,\tilde{V}(\mathbf{q})\,e^{i\mathbf{q}\cdot(\mathbf{x}-\mathbf{y})}\,. \tag{5.64}$$

Thus, the action of $V_{\rm int}$ can be graphically represented as in figure 5.1. It is also easy to check that

$$[V_{\rm int},\ \hat{N}] = 0\,, \tag{5.65}$$

where $\hat{N}$ is the particle number operator (5.53) (the same is true also for the interaction term in (5.57)). If in addition the interaction depends only on differences of coordinates, i.e. if $V^{(2)}(\mathbf{x},\mathbf{y}) = V^{(2)}(\mathbf{x}-\mathbf{y})$, then also

$$[V_{\rm int},\ \hat{\mathbf{P}}] = 0\,, \tag{5.66}$$

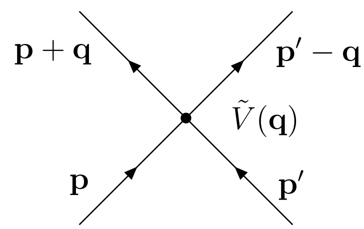

Figure 5.1: Graphical representation of the two-particle interaction (5.67) which conserves the total momentum in the momentum representation.

where $\hat{\mathbf{P}}$ is the total momentum operator (5.54). Thus, the time independent Hamiltonian of the form

$$\begin{aligned} H = & \int \frac{d^3\mathbf{p}}{(2\pi)^3} \frac{\hbar^2 \mathbf{p}^2}{2m} a^\dagger(\mathbf{p})\, a(\mathbf{p}) \\ & + \frac{1}{2} \int \frac{d^3\mathbf{p}}{(2\pi)^3} \int \frac{d^3\mathbf{p}'}{(2\pi)^3} \int \frac{d^3\mathbf{q}}{(2\pi)^3}\, a^\dagger(\mathbf{p}+\mathbf{q})\, a^\dagger(\mathbf{p}'-\mathbf{q})\, \tilde{V}(\mathbf{q})\, a(\mathbf{p}')\, a(\mathbf{p}) \,, \end{aligned} \tag{5.67}$$

commutes with the total momentum operator (5.54). Translations in space and in time are then symmetries of the system. In this case one can also construct the boost operator $\mathbf{K}$ satisfying the necessary commutation rules (4.46). Finally, if $V^{(2)}(\mathbf{x}-\mathbf{y})$ depends only on $|\mathbf{x}-\mathbf{y}|$, the generators $\mathbf{J}$ of the rotations can also be constructed and commute with H. The whole Galileo group discussed in section 4.3 is then the symmetry group of the system and its generators satisfying the commutation rules (4.46) can be explicitly constructed out of the available creation and annihilation operators.

The creation and annihilation operators allow to construct various forms of interactions, also of the nonlocal type, like

$$\int \frac{d^3\mathbf{p}}{(2\pi)^3} \int \frac{d^3\mathbf{p}'}{(2\pi)^3} \int \frac{d^3\mathbf{q}}{(2\pi)^3} \int \frac{d^3\mathbf{q}'}{(2\pi)^3}\, \tilde{V}(\mathbf{p}', \mathbf{p}, \mathbf{q}', \mathbf{q})\, a^\dagger(\mathbf{p}')\, a^\dagger(\mathbf{p}) a(\mathbf{q}')\, a(\mathbf{q}) \,, \tag{5.68}$$

and similar ones having more integrals over independent wave vectors and more creation and annihilation operators. Such interactions of real systems of N nonrelativistic particles are constrained only by the requirement that they commute with the operator $\hat{N}$ (5.53), which means that they must be built of equal numbers of the creation and annihilation operators. We will see that the requirement that the amplitudes satisfy the cluster decomposition principle (section 7.6) enforces the presence of one delta function (which effectively reduces the number of independent wave vectors) in the kernel $\tilde{V}(\mathbf{p}_1, \dots, \mathbf{p}_{2M})$ (in fact the main reason 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 imposes much more stringent constraints on possible forms of interactions and makes it impossible to preserve the particle number conservation.

The second quantized version of quantum theory of many-particle systems is obviously the usual quantum mechanics in which the central role is played by the Hamiltonian operator and its spectrum. 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 - see section 2.1), for computing energy spectra and transition probabilities remain valid. New is only the method of calculating the requisite matrix elements. In particular, it should be clear that as long as the Hamiltonian operator H commutes with the particle number operator $\hat{N}$ (5.53), the formalism developed here is equivalent with the one based of the multi-particle Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{x}_1,\dots,\mathbf{x}_N,t) = H(\mathbf{x}_1,\dots,\mathbf{x}_N)\Psi(\mathbf{x}_1,\dots,\mathbf{x}_N,t)\,. \tag{5.69}$$

More precisely, the equation which determines the time evolution of state-vectors in the big Hilbert space $\mathcal{H} = \oplus_{N=0}^{\infty}\mathcal{H}^{(N)}$,

$$i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle = H|\Psi(t)\rangle\,, \tag{5.70}$$

where $|\Psi(t)\rangle$ has components in each $\mathcal{H}^{(N)}$

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

is equivalent to an infinite set of independent Schrödinger equations (5.69) for $N = 1, 2, \dots$ (for $N = 0$ the equation is trivial because for consistency H should always be constructed so that $H|\mathrm{void}\rangle = 0$). This is easily seen by closing (5.70) with $\langle\mathbf{x}_N,\dots,\mathbf{x}_1|$ 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). Relativistic Hamiltonians do not possess this property and, as a result, in the relativistic case the equation (5.70) leads to infinitely many coupled equations.

5.4 Ground state of a system of fermions. Holes

Consider a system of identical fermions whose unperturbed Hamiltonian H_0 obtained by neglecting their mutual interactions is the sum of one-particle operators $H_0 = \sum_{i=1}^{N} H_i^{(1)}$. Suppose $|l\rangle$ are eigenvectors of the one-particle Hamiltonian $H^{(1)}$

$$H^{(1)}|l\rangle = E_l|l\rangle\,, \tag{5.71}$$

where $l = 1, 2, \ldots$ (we assume that the spectrum of $H^{(1)}$ is discretized e.g. by enclosing the system in a box of volume $V = L^3$; alternatively the considered particles can be confined by an external harmonic oscillator-like potential). As a basis of the N-particle Hilbert space $\mathcal{H}^{(N)}$ one takes then the state-vectors

$$|l_1, l_2, \ldots, l_N\rangle = a^\dagger_{l_1} a^\dagger_{l_2} \ldots a^\dagger_{l_N}|\text{void}\rangle\,, \tag{5.72}$$

with $l_1 < l_2 < \ldots < l_N$. In this basis the free Hamiltonian H_0 of the system takes the simple form

$$H_0 = \sum_l E_l\, a^\dagger_l\, a_l\,. \tag{5.73}$$

If the complete Hamiltonian of the system (i.e. H_0 plus the interaction term V_{int}) commutes with the particle number operator $\hat{N}$ (5.53), 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 for $N > 2$ the energy of this state cannot be $N \times E_1$ 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 $H_0^{(1)}$ are ordered so that[15] $E_1 \leq E_2 \leq E_3 \leq \ldots$, the state of lowest possible energy - called the (unperturbed) ground state - is

$$|\Omega_0\rangle = |1, 2, 3, \ldots, N\rangle = a^\dagger_1 a^\dagger_2 \ldots a^\dagger_N|\text{void}\rangle\,, \tag{5.74}$$

and

$$E_{\Omega_0} = E_1 + E_2 + E_3 + \ldots + E_N > N \times E_1\,. \tag{5.75}$$

One says that all one-particle states which are occupied in the ground state are below the *Fermi level*, whereas those which are unoccupied are above the Fermi level.

When mutual interactions V_{int} of the considered fermions are taken into account the basis vectors (5.72) will not in general be eigenvectors of the

[15]If the particle energy does not depend on the direction of its spin, there are always $2s + 1$ (s is the particle's spin) 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.

total Hamiltonian $H = H_0 + V_{\rm int}$: the perturbation $V_{\rm int}$ will cause transitions between these states. Even if the system is initially in the ground state (5.74) of H_0, the probability of finding it later in state of a higher H_0 energy is nonzero. This can be interpreted as the action of $V_{\rm int}$ which removes a particle from a one-particle state which is filled in the ground state (that is from a state below the Fermi level) and puts it in a higher energy one-particle state above the Fermi level. Such an action, which reduces to moving a particle from a one-particle state $|\tilde{l}\rangle$ below the Fermi level to a state $|l\rangle$ above the Fermi level, can be viewed as creation of a *hole* of energy $-E_{\tilde{l}}$ and of a *particle* of energy $E_l > E_{\tilde{l}}$.

This intuitive picture can be formalized as follows. Let us redefine the creation and annihilation operators corresponding to the (H_0 one-particle eigen)states $|\tilde{l}\rangle$ for $1 \leq \tilde{\leq} N$ and $|l\rangle$ for $N < l$:

$$\left.\begin{array}{l} d_{\tilde{l}} \equiv a^\dagger_{\tilde{l}} \\ d^\dagger_{\tilde{l}} \equiv a_{\tilde{l}} \end{array}\right\} \quad \text{if} \quad 1 \leq \tilde{l} \leq N\,, \qquad \text{and} \qquad \left.\begin{array}{l} b_l \equiv a_l \\ b^\dagger_l \equiv a^\dagger_l \end{array}\right\} \quad \text{if} \quad N < l\,. \tag{5.76}$$

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

$$b_l|\Omega_0\rangle = 0\,, \qquad d_{\tilde{l}}|\Omega_0\rangle = 0\,. \tag{5.77}$$

Because the fermionic creation and annihilation operators satisfy *anticommutation rules* which are symmetric (with respect to interchanging a_l and $a^\dagger_l$), the redefinition (5.76) is perfectly possible: $d^\dagger_{\tilde{l}}$ and $d_{\tilde{l}}$ have all the necessary properties to be interpreted as fermionic creation and annihilation operators, respectively. Therefore one can consider states (created by the actions of $V_{\rm int}$ on the ground state) of the form

$$|l_1, \ldots, l_m, \tilde{l}_1, \ldots, \tilde{l}_n\rangle \equiv b^\dagger_{l_1} \ldots b^\dagger_{l_m} d^\dagger_{\tilde{l}_1} \ldots d^\dagger_{\tilde{l}_n} |\Omega_0\rangle\,, \tag{5.78}$$

where all l_i correspond to one-particle states above the Fermi level (unoccupied in the ground state) and all $\tilde{l}_j$ 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" (of course $n = m$, if H conserves the number of particles).

The particle number operator $\hat{N}$ (5.53) rewritten accordingly (its last term is a c-number),

$$\hat{N} = \sum_{l>N} b^\dagger_\alpha b_\alpha - \sum_{\tilde{l}\leq N} d^\dagger_{\tilde{l}} d_{\tilde{l}} + N\,, \tag{5.79}$$

should be then interpreted as the fermion number operator and its form (5.79) 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

$$
\begin{aligned}
H_0 = \sum_{l=1}^{\infty} E_l\, a_l^\dagger a_l = \sum_{l>N} E_l\, b_l^\dagger b_l + \sum_{\tilde{l}\leq N} E_{\tilde{l}}\, d_{\tilde{l}} d_{\tilde{l}}^\dagger \\
= \sum_{l>N} E_l\, b_l^\dagger b_l + \sum_{\tilde{l}\leq N} (-E_{\tilde{l}})\, d_{\tilde{l}}^\dagger d_{\tilde{l}} + \sum_{\tilde{l}\leq N} E_{\tilde{l}}\,. \qquad (5.80)
\end{aligned}
$$

The last c-number term is simply the energy E_{Ω_0} of the unperturbed ground state $|\Omega_0\rangle$ of H_0. 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 it the one-particle Hamiltonian $H^{(1)}$ is shifted by an appropriate negative constant, so that in (5.71) all one-particle states $|\tilde{l}\rangle$ with $\tilde{l} = 1, 2, \dots, N$ have negative energies. The last sum in (5.80), which can simply be discarded as physically uninteresting (only differences of energy levels are important), is then negative while each created hole (the penultimate term in (5.80)) 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 (5.46) rewritten in terms of the new operators take the forms

$$
\begin{aligned}
\psi(\mathbf{x}) = \sum_{l>N} b_l\, u_l(\mathbf{x}) + \sum_{\tilde{l}\leq N} d_{\tilde{l}}^\dagger\, v_{\tilde{l}}(\mathbf{x})\,, \\
\psi^\dagger(\mathbf{x}) = \sum_{l>N} b_l^\dagger\, u_l^*(\mathbf{x}) + \sum_{\tilde{l}\leq N} d_{\tilde{l}}\, v_{\tilde{l}}^*(\mathbf{x})\,, \qquad (5.81)
\end{aligned}
$$

where we have defined $v_{\tilde{l}}(\mathbf{x}) \equiv u_{\tilde{l}}$ for $\tilde{l} \leq N$. (The operators $\psi(\mathbf{x})$ and $\psi^\dagger(\mathbf{x})$ must have as many components as do have the functions $u_l(\mathbf{x})$ and $v\tilde{l}$). In this form the operators $\psi(\mathbf{x})$ and $\psi^\dagger(\mathbf{x})$ bear close resemblance to relativistic field operators.

Any interaction $V_{\rm int}$ of fermions with an external potential can be decomposed similarly

$$
\begin{aligned}
V_{\rm int} = \sum_{l,l'} V_{ll'} a_l^\dagger a_{l'} = \sum_{ll'>N} V_{ll'} b_l^\dagger b_{b'} + \sum_{l>N,\tilde{l}\leq N} V_{l\tilde{l}} b_l^\dagger d_{\tilde{l}}^\dagger \\
+ \sum_{\tilde{l}\leq N,l>N} V_{\tilde{l}l} d_{\tilde{l}} b_l - \sum_{\tilde{l},\tilde{l}'\leq N} V_{\tilde{l},\tilde{l}'} d_{\tilde{l}}^\dagger d_{\tilde{l}'} + \sum_{\tilde{l}N} V_{\tilde{l}\tilde{l}}\,, \qquad (5.82)
\end{aligned}
$$

into terms having different effects: the first term modifies energy of a "particle" (moving it from one one-particle state above the Fermi level to another such state), the second term creates a “particle-hole” pair, the third term annihilates such a pair; finally, the last term modifies energy of a “hole” (moving it from one one-particle state below the Fermi level to another such state). Similar decomposition can be applied to other multi-particle interactions describing binary and higher interactions between fermions forming the system.

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 (whose essence 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 many-body non-relativistic theory 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 (5.79) and in (5.80) are infinite. While successful in solving the problem of negative energy states associated with relativistic wave equations for fermions, this reasoning, for obvious reason, cannot solve the analogous problem of relativistic wave equations supposed to apply to bosons, like the Klein-Gordon equation. As will be shown, relativistic quantum mechanics of many particles of arbitrary spins can however 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 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 baryon number.

5.5 Analogy with coupled harmonic oscillators

In order to provide a link between quantum mechanics of many particle systems and quantization of classical fields we now consider quantization of a system of N coupled harmonic oscillators to which, in the simple approximation of small departures from the (classical) equilibrium solution any system of e.g. point masses connected by springs can be reduced. The classical

Lagrangian of such a system has in general the form

$$L_0 = \frac{1}{2}\sum_{i,j} T_{ij}\,\dot{q}^i\dot{q}^j - \frac{1}{2}\sum_{i,j} V_{ij}\,q^iq^j\,, \tag{5.83}$$

in which V_{ij} and T_{ij} are symmetric positive definite (constant) $N\times N$ matrices.[16] The canonical momenta conjugated to the variables q^i are $p_j = T_{ji}\dot{q}^i$ and the corresponding classical Hamiltonian reads

$$H_0 = \frac{1}{2}\sum_{i,j}(T^{-1})^{ij}p_ip_j + \frac{1}{2}\sum_{i,j} V_{ij}q^iq^j\,. \tag{5.84}$$

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 (5.84) expressed through the operators a_i and $a^\dagger_i$ related in the standard way to $\hat{q}^i$ and $\hat{p}_j$ would not have the form of the sum of the $a^\dagger_i a_i$ terms. To find the spectrum and the Hamiltonian eigenstates one can solve first the classical problem by introducing normal the mode coordinates $Q^\alpha(t)$ by the formula

$$q^i(t) = A^i_{(\alpha)}Q^\alpha(t)\,, \tag{5.85}$$

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

$$\left(-\omega^2_\alpha T_{ij} + V_{ij}\right)A^j_{(\alpha)} = 0\,. \tag{5.86}$$

The vectors $A^i_{(\alpha)}$ should be chosen orthonormal in the scalar product set by the matrix T_{ij}: $A^i_{(\alpha)}T_{ij}A^j_{(\beta)} = \delta_{\alpha\beta}$. The Lagrangian expressed through the normal variables is (working out the potential energy terms one uses (5.86))

$$\begin{aligned} L_0 &= \frac{1}{2}T_{ij}A^i_{(\alpha)}\dot{Q}^\alpha A^j_{(\beta)}\dot{Q}^\beta - \frac{1}{2}V_{ij}A^i_{(\alpha)}Q^\alpha A^j_{(\beta)}Q^\beta \\ &= \frac{1}{2}\delta_{\alpha\beta}\dot{Q}^\alpha\dot{Q}^\beta - \frac{1}{2}A^i_{(\alpha)}Q^\alpha\omega^2_\beta T_{ij}A^j_{(\beta)}Q^\beta = \frac{1}{2}\delta_{\alpha\beta}\dot{Q}^\alpha\dot{Q}^\beta - \frac{1}{2}\omega^2_\beta\delta_{\alpha\beta}Q^\alpha Q^\beta\,, \end{aligned}$$

To the momenta p_i, the momenta P_α conjugated to the new variables Q^α are related by[17] $P_\alpha = p_iA^i_{(\alpha)}$ and, since $(T^{-1})^{ij} = A^i_{(a)}A^j_{(a)}$, the corresponding Hamiltonian is

$$H_0 = \frac{1}{2}P_\alpha P_\alpha + \frac{1}{2}\,\omega^2_\alpha Q^\alpha Q^\alpha\,. \tag{5.87}$$

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

[17]As usually,

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

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

The system can be now quantized by promoting the variables $Q^\alpha(t)$ and $P_\alpha(t)$ to Schrödinger picture operators. It can be checked that the commutation relations of the canonical variables remain unchanged: $[\hat{Q}^\alpha,\ \hat{P}_\beta] = i\hbar\delta^\alpha_\beta$. Next, we define the operators

$$A_\alpha = \sqrt{\frac{\omega_\alpha}{2\hbar}}\left(\hat{Q}^\alpha + \frac{i}{\omega_\alpha}\,\hat{P}_\alpha\right), \qquad A^\dagger_\alpha = \sqrt{\frac{\omega_\alpha}{2\hbar}}\left(\hat{Q}^\alpha - \frac{i}{\omega_\alpha}\,\hat{P}_\alpha\right), \tag{5.88}$$

which satisfy the relation $[A_\alpha,\ A^\dagger_\beta] = \delta_{\alpha\beta}$. Expressed in terms of these operators the Hamiltonian is diagonal:

$$H_0 = \sum_{\alpha=1}^{N} \hbar\omega_\alpha\left(A^\dagger_\alpha A_\alpha + \frac{1}{2}\right). \tag{5.89}$$

The eigenvectors of H_0 are therefore of the form

$$|n_1, n_2, \dots, n_N\rangle = \left(\prod_{\alpha=1}^{N} \frac{\left(A^\dagger_\alpha\right)^{n_\alpha}}{\sqrt{n_\alpha!}}\right)|0, 0, \dots, 0\rangle\,, \tag{5.90}$$

where $|0, 0, \dots, 0\rangle$ (with N zeroes) is the ground state annihilated by all a_α's. The energy of the state (5.90) is

$$E_{n_1,n_2,\dots,n_N} = \sum_{\alpha=1}^{N} n_\alpha\hbar\omega_\alpha + \frac{1}{2}\sum_{\alpha=1}^{N}\hbar\omega_\alpha\,. \tag{5.91}$$

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 Hamiltonian of this type can describe e.g. quantized vibrations of a crystal lattice.[18] The same structure, with $N = \infty$ and α 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

$$H = \sum_{\mathbf{p}} E(\mathbf{p})\,a^\dagger(\mathbf{p})a(\mathbf{p})\,,$$

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 subsections, the crystal lattice quantum states

[18] In the case of a crystal lattice one usually neglects boundary effects and considers $N = \infty$ coupled oscillators; after the change of variables, the normal modes are then labeled by a continuous parameter $\mathbf{K}$ (called quasi-momentum) rather than by a discrete index α. The occupation number representation (5.90) has then to be replaced by the representation (5.94).

$|n_1, n_2, \ldots, n_N\rangle$ (the states $|n_{\mathbf{k}_1\lambda_1}, n_{\mathbf{k}_2\lambda_2}, \ldots\rangle$ of the radiation field) 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 ($n_{\mathbf{k}_1\lambda_1}$ photons of type two), etc. (there and N possible types of phonons corresponding to N different lattice vibration modes of frequencies ω_α; the number of types of photons is not limited). Since the energy of such a state has the form (5.91), that is, it is additive (the energy contributed by each phonon or photon is independent of the presence of other phonons or photons), the phonons and photon described by the Hamiltonian (5.89) are noninteracting.

The action of the operators A_α and $A^\dagger_\alpha$ on the states (5.90) is standard:

$$\begin{aligned} A^\dagger_\alpha |n_1, \ldots, n_\alpha, \ldots, n_N\rangle &= \sqrt{n_\alpha + 1}\, |n_1, \ldots, n_\alpha + 1, \ldots, n_N\rangle \\ A_\alpha |n_1, \ldots, n_\alpha, \ldots, n_N\rangle &= \sqrt{n_\alpha}\, |n_1, \ldots, n_\alpha - 1, \ldots, n_N\rangle\,. \end{aligned} \tag{5.92}$$

It corresponds to the action of the bosonic particles creation and annihilation operators in the occupation number representation (5.33). 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, the system can be excited to an arbitrary state $|n_1, \ldots, n_\alpha, \ldots, n_N\rangle$ for which the eigenvalues of the operator $A^\dagger_\alpha A_\alpha$ (giving the number of phonons of type α), as well as of the operator of total number of phonons

$$\hat{N} = \sum_{\alpha=1}^{N} A^\dagger_\alpha A_\alpha\,, \tag{5.93}$$

can be arbitrary (in contrast, it is the number 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:

$$|\alpha_1, \alpha_2, \ldots, \alpha_n, \ldots\rangle = A^\dagger_{\alpha_1} A^\dagger_{\alpha_2} \ldots A^\dagger_{\alpha_m} \ldots |\Omega_0\rangle\,, \tag{5.94}$$

where $\alpha_1 \leq \alpha_2 \leq \ldots$ and the state $|\Omega_0\rangle \equiv |0, 0, \ldots, 0\rangle$ (with N zeroes), the ground state of (5.90), is annihilated by all A_α's. The states $|\alpha_1, \alpha_2, \ldots, \alpha_n, \ldots\rangle$ are related to the basis by

$$\begin{aligned} |1, \ldots, 1, 2, \ldots, 2, \ldots, N, \ldots, N\rangle &= \left(A^\dagger_1\right)^{n_1} \left(A^\dagger_2\right)^{n_2} \ldots \left(A^\dagger_N\right)^{n_N} |\Omega_0\rangle \\ &= \sqrt{n_1! n_2! \ldots n_N!}\, |n_1, n_2 \ldots, n_N\rangle\,. \end{aligned} \tag{5.95}$$

For small numbers of phonons this new representation is more convenient. The action of the creation and annihilation operators on the states (5.94) is given by

$$
\begin{aligned}
A^{\dagger}_{\alpha}|\alpha_1,\dots,\alpha_n,\dots\rangle &= |\alpha,\alpha_1,\dots,\alpha_n,\dots\rangle\,,\\
A_{\alpha}|\alpha_1,\dots,\alpha_n,\dots\rangle &= \sum_{k=1}^{N}\delta_{\alpha_k,\alpha}|\alpha_1,\dots,(\text{no }\alpha_k),\dots\rangle\,,
\end{aligned}
\tag{5.96}
$$

and looks the same as the action (5.26) and (5.27) of the creation and annihilation operators corresponding to one-particle states. Thus, barring the difference just explained, the description of quantized crystal lattice vibrations in terms of phonons is formally the same as of many particle systems.

Consider finally perturbations of the initial Lagrangian (5.83) by polynomial terms of order higher than second in the variables q_i

$$
V_{\text{int}} = \sum_{i,j,k=1}^{N} V_{ijk}\,q^i q^j q^k + \sum_{i,j,k,l=1}^{N} V_{ijkl}\,q^i q^j q^k q^l + \dots \tag{5.97}
$$

When rewritten in terms of the operators a_α, $a^{\dagger}_{\alpha}$ they give rise (among others) to terms of the form

$$
V_{\text{int}} \ni B\,A^{\dagger}_{\alpha}A^{\dagger}_{\beta}A^{\dagger}_{\gamma} + C\,A^{\dagger}_{\alpha}A^{\dagger}_{\beta}A_{\gamma} + D\,A^{\dagger}_{\alpha}A^{\dagger}_{\beta}A^{\dagger}_{\gamma}A^{\dagger}_{\kappa} + F\,A_{\alpha}A_{\beta}A_{\gamma}A_{\kappa}\,, \tag{5.98}
$$

which contain nonequal numbers of the creation and annihilation operators and, hence, do not commute with the total number of phonons operator (5.93). 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.

5.6 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 $\Psi(\mathbf{x}_1,\dots,\mathbf{x}_N)$.

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 eigenstates $|\mathbf{p}\rangle$ of commuting Galileo group generators H, $\mathbf{P}$ and identify them with particles. Operators $a(\mathbf{p})$ and $a^\dagger(\mathbf{p})$ could be then associated with these states. Finally interactions V_{int} could be constructed from the operators $a(\mathbf{p})$ and $a^\dagger(\mathbf{p})$ respecting assumed symmetry principles.

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