2

Field Formulation of Many-Body Quantum Physics

A piece of matter composed of a large number of microscopic particles is called a *many-body system*. The microscopic particles may either be all identical or of different species. Examples are crystal lattices, liquids, and gases, all of these being aggregates of molecules and atoms. Molecules are composed of atoms which, in turn, consist of an atomic nucleus and electrons, held together by electromagnetic forces, or more precisely their quanta, the photons. The mass of an atom is mostly due to the nucleus, only a small fraction being due to the electrons and an even smaller fraction due to the electromagnetic binding energy. Atomic nuclei are themselves bound states of nucleons, held together by mesonic forces, or more precisely their quanta, the mesons. The nucleons and mesons, finally, consist of the presently most fundamental objects of nuclear material, called quarks, held together by gluonic forces. Quarks and gluons are apparently as fundamental as electrons and photons. It is a wonderful miracle of nature that this deep hierarchy of increasingly fundamental particles allows a common description with the help of a single theoretical structure called quantum field theory.

As a first step towards developing this powerful theory we shall start from the well-founded Schrödinger theory of nonrelativistic spinless particles. We show that there exists a completely equivalent formulation of this theory in terms of quantum fields. This formulation will serve as a basis for setting up various quantum field theoretical models which can eventually explain the physics of the entire particle hierarchy described above.

2.1 Mechanics and Quantum Mechanics for n Distinguishable Nonrelativistic Particles

For a many-body system with only one type of nonrelativistic spinless particles of mass M, which may be spherical atoms or molecules, the classical Lagrangian has the form

$$L(\mathbf{x}_\nu, \dot{\mathbf{x}}_\nu; t) = \sum_{\nu=1}^{n} \frac{M}{2} \dot{\mathbf{x}}_\nu^2 - V(\mathbf{x}_1, \ldots, \mathbf{x}_n; t), \qquad (2.1)$$

where the arguments $\mathbf{x}_\nu, \dot{\mathbf{x}}_\nu$ in $L(\mathbf{x}_\nu, \dot{\mathbf{x}}_\nu; t)$ stand, pars pro toto, for all positions $\mathbf{x}_\nu$ and velocities $\dot{\mathbf{x}}_\nu$, $\nu = 1, \ldots, n$. The general n-body potential $V(\mathbf{x}_1, \ldots, \mathbf{x}_n; t)$ can usually be assumed to consist of a sum of an *external potential* $V_1(\mathbf{x}_\nu; t)$ and a *pair potential* $V_2(\mathbf{x}_\nu - \mathbf{x}_\mu; t)$, also called *one-* and *two-body-potentials*, respectively:

$$V(\mathbf{x}_1, \ldots, \mathbf{x}_n; t) = \sum_\nu V_1(\mathbf{x}_\nu; t) + \frac{1}{2} \sum_{\nu,\mu} V_2(\mathbf{x}_\nu - \mathbf{x}_\mu; t). \tag{2.2}$$

The second sum is symmetric in μ and ν, so that $V_2(\mathbf{x}_\nu - \mathbf{x}_\mu; t)$ may be taken as a symmetric function of the two spatial arguments — any asymmetric part would not contribute. The symmetry ensures the validity of *Newton's third law* "actio est reactio". The two-body potential is initially defined only for $\mu \neq \nu$, and the sum is restricted accordingly, but for the development to come it will be useful to include also the $\mu = \nu$ -terms into the second sum (2.2), and compensate this by an appropriate modification of the one-body potential $V_1(\mathbf{x}_\nu; t)$, so that the total potential remains the same. Such a rearrangement excludes pair potentials $V_2(\mathbf{x}_\nu - \mathbf{x}_\mu; t)$ which are singular at the origin, such as the Coulomb potential between point charges $V_2(\mathbf{x}_\nu - \mathbf{x}_\mu; t) = e^2/4\pi|\mathbf{x}_\nu - \mathbf{x}_\mu|$. Physically, this is not a serious obstacle since all charges in nature really have a finite charge radius. Even the light fundamental particles electrons and muons possess a finite charge radius, as will be seen in Chapter 12.

At first we shall consider all particles to be distinguishable. This assumption is often unphysical and will be removed later. For the particle at $\mathbf{x}_\nu$, the Euler-Lagrange equation of motion that extremizes the above Lagrangian (2.1) reads [recall Eq. (1.8)]

$$M\ddot{\mathbf{x}}_\nu = -\frac{\partial V_1(\mathbf{x}_\nu; t)}{\partial \mathbf{x}_\nu} - \sum_\mu \frac{\partial}{\partial \mathbf{x}_\nu} V_2(\mathbf{x}_\nu - \mathbf{x}_\mu; t). \tag{2.3}$$

The transition to the Hamiltonian formalism proceeds by introducing the canonical momenta [see (1.10)]

$$\mathbf{p}_\nu = \frac{\partial L}{\partial \dot{\mathbf{x}}_\nu} = M\dot{\mathbf{x}}_\nu, \tag{2.4}$$

and forming the Legendre transform [see (1.9)]

$$\begin{aligned} H(\mathbf{p}_\nu, \mathbf{x}_\nu; t) &= \left[\sum_\nu \mathbf{p}_\nu \dot{\mathbf{x}}_\nu - L(\mathbf{x}_\nu, \dot{\mathbf{x}}_\nu; t) \right]_{\dot{\mathbf{x}}_\nu = \mathbf{p}_\nu/M} \\ &= \sum_\nu \frac{\mathbf{p}_\nu^2}{2M} + \sum_\nu V_1(\mathbf{x}_\nu; t) + \frac{1}{2} \sum_{\nu,\mu} V_2(\mathbf{x}_\nu - \mathbf{x}_\mu; t). \end{aligned} \tag{2.5}$$

From this, the Hamilton equations of motions are derived as [see (1.17)]

$$\dot{\mathbf{p}}_\nu = \{H, \mathbf{p}_\nu\} = -\frac{\partial V_1(\mathbf{x}_\nu; t)}{\partial \mathbf{x}_\nu} - \sum_\mu \frac{\partial}{\partial \mathbf{x}_\nu} V_2(\mathbf{x}_\nu - \mathbf{x}_\mu; t), \tag{2.6}$$

$$\dot{\mathbf{x}}_\nu = \{H, \mathbf{x}_\nu\} = \frac{\partial H}{\partial \mathbf{p}_\nu} = \frac{\mathbf{p}_\nu}{M}, \tag{2.7}$$

with $\{A, B\}$ denoting the Poisson brackets defined in Eq. (1.20):

$$\{A, B\} = \sum_{\nu=1}^{n} \left(\frac{\partial A}{\partial \mathbf{p}_\nu} \frac{\partial B}{\partial \mathbf{x}_\nu} - \frac{\partial B}{\partial \mathbf{p}_\nu} \frac{\partial A}{\partial \mathbf{x}_\nu} \right). \tag{2.8}$$

An arbitrary observable $F(\mathbf{p}_\nu, \mathbf{x}_\nu; t)$ changes as a function of time according to the equation of motion (1.19):

$$\frac{dF}{dt} = \{H, F\} + \frac{\partial F}{\partial t}. \tag{2.9}$$

It is now straightforward to write down the laws of quantum mechanics for the system. We follow the rules in Eqs. (1.236)–(1.238), and take the local basis

$$|\mathbf{x}_1, \ldots, \mathbf{x}_n\rangle \tag{2.10}$$

as eigenstates of the position operators $\hat{\mathbf{x}}_\nu$:

$$\hat{\mathbf{x}}_\nu |\mathbf{x}_1, \ldots, \mathbf{x}_n\rangle = \mathbf{x}_\nu |\mathbf{x}_1, \ldots, \mathbf{x}_n\rangle, \quad \nu = 1, \ldots, n. \tag{2.11}$$

They are orthonormal to each other:

$$\langle \mathbf{x}_1, \ldots, \mathbf{x}_n | \mathbf{x}'_1, \ldots, \mathbf{x}'_n \rangle = \delta^{(3)}(\mathbf{x}_1 - \mathbf{x}'_1) \cdots \delta^{(3)}(\mathbf{x}_n - \mathbf{x}'_n), \tag{2.12}$$

and form a complete basis in the space of localized n-particle states:

$$\int d^3x_1 \cdots d^3x_n \, |\mathbf{x}_1, \ldots, \mathbf{x}_n\rangle\langle\mathbf{x}_1, \ldots, \mathbf{x}_n| = 1. \tag{2.13}$$

An arbitrary state is denoted by a ket vector and can be expanded in this basis by multiplying the state formally with the unit operator (2.13), yielding the expansion

$$|\psi(t)\rangle \equiv 1 \times |\psi(t)\rangle = \int d^3x_1 \cdots d^3x_n \, |\mathbf{x}_1, \ldots, \mathbf{x}_n\rangle\langle\mathbf{x}_1, \ldots, \mathbf{x}_n|\psi(t)\rangle. \tag{2.14}$$

The scalar products

$$\langle \mathbf{x}_1, \ldots, \mathbf{x}_n|\psi(t)\rangle \equiv \psi(\mathbf{x}_1, \ldots, \mathbf{x}_n; t) \tag{2.15}$$

are the wave functions of the n-body system. They are the probability amplitudes for the particle 1 to be found at $\mathbf{x}_1$, particle 2 at $\mathbf{x}_2$, etc..

The Schrödinger equation reads, in operator form,

$$\hat{H}|\psi(t)\rangle = H(\hat{\mathbf{p}}_\nu, \hat{\mathbf{x}}_\nu; t)|\psi(t)\rangle = i\hbar\partial_t|\psi(t)\rangle, \tag{2.16}$$

where $\hat{\mathbf{p}}_\nu$ are Schrödinger's momentum operators, whose action upon the wave functions is specified by the rule

$$\langle \mathbf{x}_1, \ldots, \mathbf{x}_n|\hat{\mathbf{p}}_\nu = -i\hbar\partial_{\mathbf{x}_\nu}\langle\mathbf{x}_1, \ldots, \mathbf{x}_n|. \tag{2.17}$$

Multiplication of (2.16) from the left with the bra vectors $\langle \mathbf{x}_1, \ldots, \mathbf{x}_n |$ yields via (2.17) the Schrödinger differential equation for the wave functions:

$$
\begin{aligned}
H(-i\hbar\partial_{\mathbf{x}_\nu}, \mathbf{x}_\nu; t)\psi(\mathbf{x}_1, \ldots, \mathbf{x}_n; t) & \\
= & \left[-\sum_\nu \frac{\hbar^2}{2M}\partial_{\mathbf{x}_\nu}^2 + \sum_\nu V_1(\mathbf{x}_\nu; t) + \frac{1}{2}\sum_{\nu,\mu} V_2(\mathbf{x}_\nu - \mathbf{x}_\mu; t) \right] \psi(\mathbf{x}_1, \ldots, \mathbf{x}_n; t) \\
= & \ i\hbar\partial_t \psi(\mathbf{x}_1, \ldots, \mathbf{x}_n; t).
\end{aligned} \tag{2.18}
$$

In many physical systems, the potentials $V_1(\mathbf{x}_\nu; t)$ and $V_2(\mathbf{x}_\nu - \mathbf{x}_\mu; t)$ are independent of time. Then we can factor out the time dependence of the wave functions with fixed energy as

$$
\psi(\mathbf{x}_1, \ldots, \mathbf{x}_n; t) = e^{-iEt/\hbar}\psi_E(\mathbf{x}_1, \ldots, \mathbf{x}_n), \tag{2.19}
$$

and find for $\psi_E(\mathbf{x}_1, \ldots, \mathbf{x}_n)$ the time-independent Schrödinger equation

$$
H(-i\hbar\partial_{\mathbf{x}_\nu}, \mathbf{x}_\nu; t)\psi_E(\mathbf{x}_1, \ldots, \mathbf{x}_n) = E\psi_E(\mathbf{x}_1, \ldots, \mathbf{x}_n). \tag{2.20}
$$

2.2 Identical Particles: Bosons and Fermions

The quantum mechanical rules in the last section were written down in the previous section under the assumption that all particles are distinguishable. For most realistic n-body systems, however, this is an unphysical assumption. For example, there is no way of distinguishing the electrons in an atom. Thus not all of the solutions $\psi(\mathbf{x}_1, \ldots, \mathbf{x}_n; t)$ of the Schrödinger equation (2.18) can be physically permissible. Consider the case where the system contains only one species of identical particles, for example electrons. The Hamilton operator in Eq. (2.18) is invariant under all permutations of the particle labels ν. In addition, all probability amplitudes $\langle \psi_1 | \psi_2 \rangle$ must reflect this invariance. They must form a representation space of all permutations. Let T_{ij} be an operator which interchanges the variables $\mathbf{x}_i$ and $\mathbf{x}_j$.

$$
T_{ij}\psi(\mathbf{x}_1, \ldots, \mathbf{x}_i, \ldots, \mathbf{x}_j, \ldots, \mathbf{x}_n; t) \equiv \psi(\mathbf{x}_1, \ldots, \mathbf{x}_j, \ldots, \mathbf{x}_i, \ldots, \mathbf{x}_n; t). \tag{2.21}
$$

It is called a *transposition*. The invariance may then be expressed as $\langle T_{ij}\psi_1 | T_{ij}\psi_2 \rangle = \langle \psi_1 | \psi_2 \rangle$, implying that the wave functions $|\psi_1\rangle$ and $|\psi_2\rangle$ can change at most by a phase:

$$
T_{ij}\psi(\mathbf{x}_1, \ldots, \mathbf{x}_n; t) = e^{i\alpha_{ij}}\psi(\mathbf{x}_1, \ldots, \mathbf{x}_n; t). \tag{2.22}
$$

But from the definition (2.21) we see that T_{ij} satisfies

$$
T_{ij}^2 = 1. \tag{2.23}
$$

Thus $e^{i\alpha_{ij}}$ can only have the values $+1$ or -1. Moreover, due to the identity of all particles, the sign must be the same for any pair ij.

The set of all multiparticle wave functions can be decomposed into wave functions transforming in specific ways under arbitrary permutations P of the coordinates.

It will be shown in Appendix 2A that each permutation P can be decomposed into products of transpositions. Of special importance are wave functions which are completely symmetric, i.e., which are obtained by applying, to an arbitrary n-particle wave function, the operation

$$S = \frac{1}{n!} \sum_P P. \tag{2.24}$$

The sum runs over all $n!$ permutations of the particle indices. Another important type of wave function is obtained by applying the antisymmetrizing operator

$$A = \frac{1}{n!} \sum_P \epsilon_P P \tag{2.25}$$

to the arbitrary n-particle wave function. The symbol ϵ_P is unity for even permutations and -1 for odd permutations. It is called the *parity* of the permutation.

By applying S or A to an arbitrary n-particle wave function one obtains completely symmetric or completely antisymmetric n-particle wave functions. In nature, both signs can occur. Particles with symmetric wave functions are called *bosons*, the others *fermions*. Examples for bosons are photons, mesons, α-particles, or any nuclei with an even atomic number. Examples for fermions are electrons, neutrinos, muons, protons, neutrons, or any nuclei with an odd atomic number.

In two-dimensional multi-electron systems in very strong magnetic fields, an interesting new situation has been discovered. These systems have wave functions which look like those of free quasiparticles on which transpositions T_{ij} yield a phase factor $e^{i\alpha_{ij}}$ which is not equal to ± 1: These quasiparticles are neither bosons nor fermions. They have therefore been called *anyons*. Their existence in two dimensions is made possible by imagining each particle to introduce a singularity in the plane, which makes the plane multisheeted. A second particle moving by 360^0 around this singularity does not arrive at the initial point but at a point lying in a second sheet below the initial point. For this reason, the equation (2.23) needs no longer to be fulfilled.

Distinguishing the symmetry properties of the wave functions provides us with an important tool to classify the various solutions of the Schrödinger equation (2.18). Let us illustrate this by looking at the simplest nontrivial case in which the particles have only a common time-independent external potential $V_1(\mathbf{x}_\nu)$ but are otherwise noninteracting, i.e., their time-independent Schrödinger equation (2.20) reads

$$\sum_\nu \left[-\frac{\hbar^2}{2M} \partial^2_{\mathbf{x}_\nu} + V_1(\mathbf{x}_\nu) \right] \psi_E(\mathbf{x}_1, \ldots, \mathbf{x}_n) = E\psi_E(\mathbf{x}_1, \ldots, \mathbf{x}_n). \tag{2.26}$$

It can be solved by the factorizing ansatz in terms of single-particle states $\psi_{E_{\alpha_\nu}}$ of energy E_{α_ν},

$$\psi_E(\mathbf{x}_1, \ldots, \mathbf{x}_n) = \prod_{\nu=1}^n \psi_{E_{\alpha_\nu}}(\mathbf{x}_\nu), \tag{2.27}$$

with the total energy being the sum of the individual energies:

$$E = \sum_{\nu=1}^{n} E_{\alpha_\nu}. \tag{2.28}$$

The single-particle states $\psi_{E_{\alpha_\nu}}(\mathbf{x}_\nu)$ are the solutions of the one-particle Schrödinger equation

$$\left[-\frac{\hbar^2}{2M}\partial_{\mathbf{x}}^2 + V_1(\mathbf{x}) \right] \psi_{E_\alpha}(\mathbf{x}) = E_\alpha \psi_{E_\alpha}(\mathbf{x}). \tag{2.29}$$

If the wave functions $\psi_{E_\alpha}(\mathbf{x})$ form a complete set of states, they satisfy the one-particle completeness relation

$$\sum_\alpha \psi_{E_\alpha}(\mathbf{x})\psi_{E_\alpha}^*(\mathbf{x}') = \delta^{(3)}(\mathbf{x} - \mathbf{x}'). \tag{2.30}$$

The sum over the labels α may, of course, involve an integral over a continuous part of the spectrum. It is trivial to verify that the set of all products (2.27) is complete in the space of n-particle wave functions:

$$\sum_{\alpha_1,...,\alpha_n} \psi_{E_{\alpha_1}}(\mathbf{x}_1) \cdots \psi_{E_{\alpha_n}}(\mathbf{x}_n)\, \psi_{E_{\alpha_n}}^*(\mathbf{x}_n') \cdots \psi_{E_{\alpha_1}}^*(\mathbf{x}_1')$$

$$= \delta^{(3)}(\mathbf{x}_1 - \mathbf{x}_1') \cdots \delta^{(3)}(\mathbf{x}_n - \mathbf{x}_n'). \tag{2.31}$$

For identical particles, this Hilbert space is greatly reduced. In the case of bosons, only the fully symmetrized products correspond to physical energy eigenstates. We apply the symmetrizing operation S of Eq. (2.24) to the product of single-particle wave functions $\prod_{\nu=1}^{n} \psi_{E_{\alpha_{p(\nu)}}}(\mathbf{x}_\nu)$ and normalize the result to find

$$\psi_{\{E_\alpha\}}^S(\mathbf{x}_1, \ldots, \mathbf{x}_n) = \mathcal{N}_{\{E_\alpha\}}^S S \prod_{\nu=1}^{n} \psi_{E_{\alpha_{p(\nu)}}}(\mathbf{x}_\nu) = \mathcal{N}_{\{E_\alpha\}}^S \frac{1}{n!} \sum_P \prod_{\nu=1}^{n} \psi_{E_{\alpha_{p(\nu)}}}(\mathbf{x}_\nu). \tag{2.32}$$

The sum runs over $n!$ permutations of the indices $\nu = 1, \ldots, n$, the permuted indices being denoted by $p(\nu)$.

Note that $\psi_{\{E_\alpha\}}^S(\mathbf{x}_1, \ldots, \mathbf{x}_n)$ no longer depends on the order of labels of the energies $E_{\alpha_1}, \ldots, E_{\alpha_n}$. This is a manifestation of the indistinguishability of the particles in the corresponding one-particle states indicated by the curly-bracket notation $\psi_{\{E_\alpha\}}^S$. Also the normalization factor is independent of the order and has been denoted by $\mathcal{N}_{\{E_\alpha\}}^S$.

For fermions, the wave functions are

$$\psi_{\{E_\alpha\}}^A(\mathbf{x}_1, \ldots, \mathbf{x}_n) = \mathcal{N}_{\{E_\alpha\}}^A A \prod_{\nu=1}^{n} \psi_{E_{\alpha_{p(\nu)}}}(\mathbf{x}_\nu) = \mathcal{N}_{\{E_\alpha\}}^A \frac{1}{n!} \sum_P \epsilon_P \prod_{\nu=1}^{n} \psi_{E_{\alpha_{p(\nu)}}}(\mathbf{x}_\nu), \tag{2.33}$$

where ϵ_P has the values $\epsilon_P = \pm 1$ for even or odd permutations, respectively.

Instead of the indices on the labels α_ν of the energies, we may just as well symmetrize or antisymmetrize the labels of the position variables:

$$\psi_{\{E_\alpha\}}^{S,A}(\mathbf{x}_1, \ldots, \mathbf{x}_n) = \mathcal{N}_{\{E_\alpha\}}^{S,A} \frac{1}{n!} \sum_P \left\{ \begin{matrix} 1 \\ \epsilon_P \end{matrix} \right\} \prod_{\nu=1}^n \psi_{E_{\alpha_\nu}}(\mathbf{x}_{p(\nu)}). \tag{2.34}$$

See Appendix 2A for more details.

The completely antisymmetrized products (2.33) can also be written in the form of a determinant first introduced by Slater:

$$\psi_{\{E_\alpha\}}^A(\mathbf{x}_1, \ldots, \mathbf{x}_n) = \mathcal{N}_{\{E_\alpha\}}^A \frac{1}{n!} \begin{vmatrix} \psi_{E_{\alpha_1}}(\mathbf{x}_1) & \psi_{E_{\alpha_1}}(\mathbf{x}_2) & \ldots & \psi_{E_{\alpha_1}}(\mathbf{x}_n) \\ \vdots & \vdots & & \vdots \\ \psi_{E_{\alpha_n}}(\mathbf{x}_1) & \psi_{E_{\alpha_n}}(\mathbf{x}_2) & \ldots & \psi_{E_{\alpha_n}}(\mathbf{x}_n) \end{vmatrix}. \tag{2.35}$$

To determine the normalization factors in (2.32)–(2.35), we calculate the integral

$$\int d^3x_1 \cdots d^3x_n \, \psi_{\{E_\alpha\}}^{S\,*}(\mathbf{x}_1, \ldots, \mathbf{x}_n)\psi_{\{E_\alpha\}}^S(\mathbf{x}_1, \ldots, \mathbf{x}_n)$$
$$= \mathcal{N}_{\{E_\alpha\}}^{S\,2} \frac{1}{n!^2} \sum_{P,Q} \prod_{\nu=1}^n \int d^3x_\nu \psi_{E_{\alpha_{p(\nu)}}}^*(\mathbf{x}_\nu)\psi_{E_{\alpha_{q(\nu)}}}(\mathbf{x}_\nu). \tag{2.36}$$

Due to the group property of permutations, the double-sum contains $n!$ identical terms with $P = Q$ and can be rewritten as

$$\int d^3x_1 \cdots d^3x_n \, \psi_{\{E_\alpha\}}^{S\,*}(\mathbf{x}_1, \ldots, \mathbf{x}_n)\psi_{\{E_\alpha\}}^S(\mathbf{x}_1, \ldots, \mathbf{x}_n)$$
$$= \mathcal{N}_{\{E_\alpha\}}^{S\,2} \frac{1}{n!} \sum_P \prod_{\nu=1}^n \int d^3x_\nu \psi_{E_{\alpha_\nu}}^*(\mathbf{x}_\nu)\psi_{E_{\alpha_{p(\nu)}}}(\mathbf{x}_\nu). \tag{2.37}$$

If all single-particle states $\psi_{E_{\alpha_\nu}}(\mathbf{x}_\nu)$ are different from each other, then only the identity permutation $P = 1$ with $p(\nu) = \nu$ survives, and the normalization integral (2.37) fixes

$$\mathcal{N}_{\{E_\alpha\}}^{S\,2} = n!. \tag{2.38}$$

Suppose now that two of the single-particle wave functions $\psi_{E_{\alpha_\nu}}$, say $\psi_{E_{\alpha_1}}$ and $\psi_{E_{\alpha_2}}$, coincide, while all others are different from these and each other. Then only two permutations survive in (2.37): those with $p(\nu) = \nu$, and those in which P is a transposition T_{ij} of two elements (see Appendix 2A). The right-hand side of (2.38) is then reduced by a factor of 2:

$$\mathcal{N}_{\{E_\alpha\}}^{S\,2} = \frac{n!}{2}. \tag{2.39}$$

Extending this consideration to n_1 identical states $\psi_{E_{\alpha_1}}, \ldots, \psi_{E_{\alpha_{n_1}}}$, all $n_1!$ permutations among these give equal contributions to the normalization integral (2.37) and lead to

$$\mathcal{N}_{\{E_\alpha\}}^{S\,2} = \frac{n!}{n_1!} = 1. \tag{2.40}$$

Finally it is easy to see that, if there are groups of $n_1, n_2, \ldots, n_k$ identical states, the normalization factor is

$$\mathcal{N}_{\{E_\alpha\}}^{S}{}^{2} = \frac{n!}{n_1! n_2! \cdots n_k!}. \tag{2.41}$$

For the antisymmetric states of fermion systems, the situation is much simpler. Here, no two states can be identical as is obvious from the Slater determinant (2.35). Similar considerations as in (2.36), (2.37) for the wave functions (2.33) lead to

$$\mathcal{N}_{\{E_\alpha\}}^{A}{}^{2} = n!. \tag{2.42}$$

The projection into the symmetric and antisymmetric subspaces has the following effect upon the completeness relation (2.31): Multiplying it by the symmetrization or antisymmetrization operators

$$\hat{P}^{S,A} = \frac{1}{n!} \sum_P \left\{ \begin{array}{c} 1 \\ \epsilon_P \end{array} \right\}, \tag{2.43}$$

which may be applied upon the particle positions $\mathbf{x}_1, \ldots, \mathbf{x}_n$ as in (2.34), we calculate

$$\sum_{\alpha_1, \ldots, \alpha_n} \left[\mathcal{N}_{\{E_\alpha\}}^{S,A} \right]^2 \psi_{\{E_\alpha\}}^{S,A}(\mathbf{x}_1, \ldots, \mathbf{x}_n) \psi_{\{E_\alpha\}}^{S,A}{}^{*}(\mathbf{x}_1', \ldots, \mathbf{x}_n') = \delta^{(3)S,A}(\mathbf{x}_1, \ldots, \mathbf{x}_n; \mathbf{x}_1', \ldots, \mathbf{x}_n'), \tag{2.44}$$

where the symmetrized or antisymmetrized δ-function is defined by

$$\delta^{(3)S,A}(\mathbf{x}_1, \ldots, \mathbf{x}_n; \mathbf{x}_1', \ldots, \mathbf{x}_n') \equiv \frac{1}{n!} \sum_P \left\{ \begin{array}{c} 1 \\ \epsilon_P \end{array} \right\} \delta^{(3)}(\mathbf{x}_1 - \mathbf{x}_{p(1)}') \cdots \delta^{(3)}(\mathbf{x}_n - \mathbf{x}_{p(n)}'). \tag{2.45}$$

Since the left-hand side of (2.44) is independent of the order of $E_{\alpha_1}, \ldots, E_{\alpha_n}$, we may sum only over a certain order among the labels

$$\sum_{\alpha_1, \ldots, \alpha_n} \longrightarrow n! \sum_{\alpha_1 > \ldots > \alpha_n}. \tag{2.46}$$

If there are degeneracy labels in addition to the energy, these have to be ordered in the same way.

For antisymmetric states, the labels $\alpha_1, \ldots, \alpha_n$ are necessarily different from each other. Inserting (2.42) and (2.46) into (2.45), this gives directly

$$\sum_{\alpha_1 > \ldots > \alpha_n} \psi_{\{E_\alpha\}}^{A}(\mathbf{x}_1, \ldots, \mathbf{x}_n) \psi_{\{E_\alpha\}}^{A}{}^{*}(\mathbf{x}_1', \ldots, \mathbf{x}_n') = \delta^{(3)A}(\mathbf{x}_1, \ldots, \mathbf{x}_n; \mathbf{x}_1', \ldots, \mathbf{x}_n'). \tag{2.47}$$

For the symmetric case we can order the different groups of identical states and denote their common labels by $\alpha_{n_1}, \alpha_{n_2}, \ldots, \alpha_{n_k}$, with the numbers n_ν indicating how often the corresponding label α is present. Obviously, there are $n!/n_1! n_2! \cdots n_k!$ permutations in the completeness sum (2.44) for each set of labels $\alpha_{n_1} > \alpha_{n_2} >$

$\ldots > \alpha_{n_k}$, the divisions by $n_\nu!$ coming from the permutations *within* each group of $n_1, \ldots, n_k$ identical states. This combinatorial factor cancels precisely the normalization factor (2.41), so that the completeness relation for symmetric n-particle states reads

$$\sum_{n_1,\ldots,n_k} \sum_{\alpha_{n_1} > \ldots > \alpha_{n_k}} \psi^S_{\{E_\alpha\}}(\mathbf{x}_1, \ldots, \mathbf{x}_n) \psi^{S\,*}_{\{E_\alpha\}}(\mathbf{x}'_1, \ldots, \mathbf{x}'_n)$$
$$= \delta^{(3)S}(\mathbf{x}_1, \ldots, \mathbf{x}_n; \mathbf{x}'_1, \ldots, \mathbf{x}'_n). \tag{2.48}$$

The first sum runs over the different breakups of the total number n of states into identical groups so that $n = n_1 + \ldots + n_k$.

It is useful to describe the symmetrization or antisymmetrization procedure directly in terms of Dirac's bra and ket formalism. The n-particle states are direct products of single-particle states multiplied by the operator $\hat{P}^{S,A}$, and can be written as

$$|\psi^{S,A}\rangle = \hat{P}^{S,A}|E_{\alpha_1}\rangle \cdots |E_{\alpha_n}\rangle = \mathcal{N}^{S,A} \frac{1}{n!} \sum_P \left\{ \begin{matrix} 1 \\ \epsilon_P \end{matrix} \right\} |E_{\alpha_{p(1)}}\rangle \cdots |E_{\alpha_{p(n)}}\rangle. \tag{2.49}$$

The wave functions (2.32) and (2.33) consist of scalar products of these states with the localized boson states $|\mathbf{x}_1, \ldots, \mathbf{x}_n\rangle$, which may be written as direct products

$$|\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n\rangle = |\mathbf{x}_1\rangle \otimes |\mathbf{x}_2\rangle \otimes \ldots \otimes |\mathbf{x}_n\rangle. \tag{2.50}$$

In this state, the particle with number 1 sits at $\mathbf{x}_1$, the particle with number 2 at $\mathbf{x}_2$, $\ldots$, etc. The symmetrization process wipes out the distinction between the particles $1, 2, \ldots, n$.

Let us adapt the symbolic completeness relation to the symmetry of the wave functions. The general relation

$$\int d^3x_1 \cdots d^3x_n \, |\mathbf{x}_1\rangle\langle \mathbf{x}_1| \otimes \ldots \otimes |\mathbf{x}_n\rangle\langle \mathbf{x}_n| = 1 \tag{2.51}$$

covers *all* square integrable wave functions in the product space. As far as the physical Hilbert space is concerned, it can be restricted as follows:

$$\int d^3x_1 \cdots d^3x_n \, |\mathbf{x}_1, \ldots, \mathbf{x}_n\rangle^{S,A} \; {}^{S,A}\langle \mathbf{x}_1, \ldots, \mathbf{x}_n| = \hat{P}^{S,A}, \tag{2.52}$$

where

$$|\mathbf{x}_1, \ldots, \mathbf{x}_n\rangle^{S,A} = \frac{1}{n!} \sum_P \left\{ \begin{matrix} 1 \\ \epsilon_P \end{matrix} \right\} |\mathbf{x}_{p(1)}, \ldots, \mathbf{x}_{p(n)}\rangle. \tag{2.53}$$

The states are orthonormal in the sense

$${}^{S,A}\langle \mathbf{x}_1, \ldots, \mathbf{x}_n | \mathbf{x}'_1, \ldots, \mathbf{x}'_n\rangle^{S,A} = \delta^{(3)S,A}(\mathbf{x}_1, \ldots, \mathbf{x}_n; \mathbf{x}'_1, \ldots, \mathbf{x}'_n). \tag{2.54}$$

This basis will play an essential role for the introduction of quantum fields.

While the formalism presented so far is applicable to any number of particles, practical calculations usually present a tremendous task. The number of particles is often so large, of the order 10^{23}, that no existing computer could even list the wave functions. On the other hand, macroscopic many-body systems containing such a large number of microscopic particles make up our normal environment, and our experience teaches us that many global phenomena can be predicted quite reliably. They should therefore also be calculable in simple terms. For example, for most purposes a crystal follows the laws of a rigid body, and nothing in theses laws records the immense number of degrees of freedom inherent in a microscopic description. If the solid is excited, there are sound waves in which all the many atoms in the lattice vibrate around their equilibrium positions. Their description requires only a few bulk parameters such as elastic constants and mass density. Phenomena of this type are called *collective phenomena*.

To describe such phenomena, an economic way had to be found which does not require the solution of the Schrödinger differential equation with $3n \sim 10^{23}$ coordinates. We shall later see that field theory provides us with an elegant and efficient access to such phenomena. After a suitable choice of field variables, simple mean-field approximations will often give a rough explanation of many collective phenomena. In the subsequent sections we shall demonstrate how the Schrödinger theory of any number of particles can be transformed into the quantum field theory of a single field.

There is further motivation at a more fundamental level for introducing fields. They offer a natural way of accounting for the symmetry properties of the wave functions, as we shall now see.

2.3   Creation and Annihilation Operators for Bosons

When dealing with n-particle Schrödinger equations, the imposition of symmetry upon the Schrödinger wave functions $\psi(\mathbf{x}_1, \dots, \mathbf{x}_n; t)$ seems to be a rather artificial procedure. There exists an alternative formulation of the quantum mechanics of n particles in which the Hilbert space *automatically* carries the correct symmetry. This formulation may therefore be viewed as a more "natural" description of such quantum systems. The basic mathematical structure which will serve this purpose was first encountered in a particular quantum mechanical description of harmonic oscillators which we now recall. It is well-known that the Hamilton operator of an oscillator of unit mass

$$\hat{H} = \frac{1}{2}\hat{p}^2 + \frac{\omega^2}{2}\hat{q}^2 \tag{2.55}$$

can be rewritten in the form

$$\hat{H} = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right), \tag{2.56}$$

where

$$\hat{a}^\dagger = \frac{\sqrt{\omega}\hat{q} - i\hat{p}/\sqrt{\omega}}{\sqrt{2\hbar}}, \qquad \hat{a} = \frac{\sqrt{\omega}\hat{q} + i\hat{p}/\sqrt{\omega}}{\sqrt{2\hbar}} \tag{2.57}$$

are the so-called *raising* and *lowering* operators. The canonical quantization rules

$$
\begin{aligned}
[\hat{p}, \hat{p}] &= [\hat{x}, \hat{x}] = 0, \\
[\hat{p}, \hat{x}] &= -i\hbar
\end{aligned}
\tag{2.58}
$$

imply that $\hat{a}, \hat{a}^\dagger$ satisfy

$$
\begin{aligned}
[\hat{a}, \hat{a}] &= [\hat{a}^\dagger, \hat{a}^\dagger] = 0, \\
[\hat{a}, \hat{a}^\dagger] &= 1.
\end{aligned}
\tag{2.59}
$$

The energy spectrum of the oscillator follows directly from these commutation rules. We introduce the *number operator*

$$
\hat{N} = \hat{a}^\dagger \hat{a},
\tag{2.60}
$$

which satisfies the equations

$$
[\hat{N}, \hat{a}^\dagger] = \hat{a}^\dagger,
\tag{2.61}
$$

$$
[\hat{N}, \hat{a}] = -\hat{a}.
\tag{2.62}
$$

These imply that $\hat{a}^\dagger$ and $\hat{a}$ raise and lower the eigenvalues of the number operator $\hat{N}$ by one unit, respectively. Indeed, if $|\nu\rangle$ is an eigenstate with eigenvalue ν,

$$
\hat{N}|\nu\rangle = \nu|\nu\rangle,
\tag{2.63}
$$

we see that

$$
\hat{N}\hat{a}^\dagger|\nu\rangle = (\hat{a}^\dagger\hat{N} + \hat{a}^\dagger)|\nu\rangle = (\nu+1)\hat{a}^\dagger|\nu\rangle,
\tag{2.64}
$$

$$
\hat{N}\hat{a}|\nu\rangle = (\hat{a}\hat{N} - \hat{a})|\nu\rangle = (\nu-1)\hat{a}|\nu\rangle.
\tag{2.65}
$$

Moreover, the eigenvalues ν must all be integer numbers n which are larger or equal to zero. To see this, we observe that $\hat{a}^\dagger\hat{a}$ is a positive operator. It satisfies for every state $|\psi\rangle$ in Hilbert space the inequality

$$
\langle\psi|\hat{a}^\dagger\hat{a}|\psi\rangle = \|\hat{a}^\dagger|\psi\rangle\|^2 \geq 0.
\tag{2.66}
$$

Hence there exists a state, usually denoted by $|0\rangle$, whose energy cannot be lowered by one more application of $\hat{a}$. This state will satisfy

$$
\hat{a}|0\rangle = 0.
\tag{2.67}
$$

As a consequence, the operator $\hat{N}$ applied to $|0\rangle$ must be zero. Applying the raising operator $\hat{a}^\dagger$ any number of times, the eigenvalues ν of $\hat{N}$ will cover all integer numbers $\nu = n$ with $n = 0, 1, 2, 3, \ldots$. The corresponding states are denoted by $|n\rangle$:

$$
\hat{N}|n\rangle = n|n\rangle, \quad n = 0, 1, 2, 3, \ldots .
\tag{2.68}
$$

Explicitly, these states are given by

$$
|n\rangle = \mathcal{N}_n(\hat{a}^\dagger)^n|0\rangle,
\tag{2.69}
$$

with some normalization factor $\mathcal{N}_n$, that can be calculated using the commutation rules (2.59) to be

$$\mathcal{N}_n = \frac{1}{\sqrt{n!}}. \tag{2.70}$$

By considering the commutation rules (2.59) between different states $|n\rangle$ and inserting intermediate states, we derive the matrix elements of the operators $\hat{a}, \hat{a}^\dagger$:

$$\langle n'|\hat{a}|n\rangle = \sqrt{n}\,\delta_{n',n-1}, \tag{2.71}$$

$$\langle n'|\hat{a}^\dagger|n\rangle = \sqrt{n+1}\,\delta_{n',n+1}. \tag{2.72}$$

In this way, all properties of the harmonic oscillator are recovered by purely algebraic manipulations, using (2.59) with the condition (2.67) to define the ground state.

This mathematical structure can be used to describe the complete set of symmetric localized states (2.32). All we need to do is reinterpret the eigenvalue n of the operator $\hat{N}$. In the case of the oscillator, n is the principal quantum number of the single-particle state that counts the number of zeros in the Schrödinger wave function. In quantum field theory, the operator changes its role and its eigenvalues n count the number of particles contained in the many-body wave function. The operators $\hat{a}^\dagger$ and $\hat{a}$ which raise and lower n are renamed *creation* and *annihilation operators*, which add or take away a single particle in the state $|n\rangle$. The ground state $|0\rangle$ contains no particle. It constitutes the vacuum state of the n-body system. In the states (2.32), there are n particles at places $\mathbf{x}_1, \ldots, \mathbf{x}_n$. We therefore introduce the spatial degree of freedom by giving $\hat{a}^\dagger, \hat{a}$ a spatial label and defining the operators

$$\hat{a}^\dagger_{\mathbf{x}}, \hat{a}_{\mathbf{x}},$$

which permit the creation and annihilation of a particle localized at the position $\mathbf{x}$.[1]

The operators at different locations are taken to be independent, i.e., they commute as

$$[\hat{a}_{\mathbf{x}}, \hat{a}_{\mathbf{x}'}] = [\hat{a}^\dagger_{\mathbf{x}}, \hat{a}^\dagger_{\mathbf{x}'}] = 0, \tag{2.73}$$

$$[\hat{a}_{\mathbf{x}}, \hat{a}^\dagger_{\mathbf{x}'}] = 0, \quad \mathbf{x} \neq \mathbf{x}'. \tag{2.74}$$

The commutation rule between $\hat{a}^\dagger_{\mathbf{x}}$ and $\hat{a}_{\mathbf{x}'}$ for coinciding space variables $\mathbf{x}$ and $\mathbf{x}'$ is specified with the help of a Dirac δ-function as follows:

$$[\hat{a}_{\mathbf{x}}, \hat{a}^\dagger_{\mathbf{x}'}] = \delta^{(3)}(\mathbf{x} - \mathbf{x}'). \tag{2.75}$$

We shall refer to these $\mathbf{x}$-dependent commutation rules as the *local oscillator algebra*.

The δ-function singularity in (2.75) is dictated by the fact that we want to preserve the raising and lowering commutation rules (2.61) and (2.62) for the particle number at each point $\mathbf{x}$, i.e., we want that

$$[\hat{N}, \hat{a}^\dagger_{\mathbf{x}}] = \hat{a}^\dagger_{\mathbf{x}}, \tag{2.76}$$

---

[1]The label $\mathbf{x}$ in configuration space of the particles bears no relation to the operator $\hat{q}$ in the Hamiltonian (2.55), which here denotes an operator in field space, as we shall better understand in Section 2.8.

$$[\hat{N}, \hat{a}_{\mathbf{x}}] = -\hat{a}_{\mathbf{x}}. \tag{2.77}$$

The total particle number operator is then given by the integral

$$\hat{N} = \int d^3 x \, \hat{a}_{\mathbf{x}}^\dagger \hat{a}_{\mathbf{x}}. \tag{2.78}$$

Due to (2.74), all parts in the integral (2.78) with $\mathbf{x}'$ different from the $\mathbf{x}$ in (2.76) and (2.77) do not contribute. If the integral is supposed to give the right-hand sides in (2.76) and (2.77), the commutator between $\hat{a}_{\mathbf{x}}$ and $\hat{a}_{\mathbf{x}}^\dagger$ has to be equal to a δ-function.

The use of the δ-function is of course completely analogous to that in Subsection 1.4. [recall the limiting process in Eq. (1.160)]. In fact, we could have introduced local creation and annihilation operators with ordinary unit commutation rules at each point by discretizing the space into a fine-grained point-lattice of a tiny lattice spacing ϵ, with discrete lattice points at

$$\mathbf{x_n} = (n_1, n_2, n_3)\epsilon, \qquad n_\nu = 0, \pm 1, \pm 2, \dots \; . \tag{2.79}$$

And for the creation or annihilation of a particle in the small cubic box around $\mathbf{x_n}$ we could have introduced the operators $\hat{a}_{\mathbf{n}}^\dagger$ or $\hat{a}_{\mathbf{n}}$, which satisfy the discrete commutation rules

$$[\hat{a}_{\mathbf{n}}, \hat{a}_{\mathbf{n}'}] = [\hat{a}_{\mathbf{n}}^\dagger, \hat{a}_{\mathbf{n}'}^\dagger] = 0, \tag{2.80}$$

$$[\hat{a}_{\mathbf{n}}, \hat{a}_{\mathbf{n}'}^\dagger] = \delta_{\mathbf{nn}'}^{(3)}. \tag{2.81}$$

For these the total particle number operator is

$$\hat{N} = \sum_{\mathbf{n}} \hat{a}_{\mathbf{n}}^\dagger \hat{a}_{\mathbf{n}}. \tag{2.82}$$

This would amount to identifying $\hat{a}_{\mathbf{n}}$ with a discrete subset of the continuous set of operators $\hat{a}_{\mathbf{x}}$ as follows:

$$\hat{a}_{\mathbf{n}} = \left. \sqrt{\epsilon^3} \, \hat{a}_{\mathbf{x}} \right|_{\mathbf{x} \equiv \mathbf{x_n}}. \tag{2.83}$$

Then the discrete and continuous formulations of the particle number operator would be related by

$$\hat{N} = \sum_{\mathbf{n}} \hat{a}_{\mathbf{n}}^\dagger \hat{a}_{\mathbf{n}} \equiv \epsilon^3 \sum_{\mathbf{x_n}} \hat{a}_{\mathbf{x_n}}^\dagger \hat{a}_{\mathbf{x_n}} \xrightarrow[\epsilon \to 0]{} \int d^3 x \, \hat{a}_{\mathbf{x}}^\dagger \hat{a}_{\mathbf{x}}. \tag{2.84}$$

In the same limit, the commutator

$$\frac{1}{\epsilon^3} [\hat{a}_{\mathbf{n}}, \hat{a}_{\mathbf{n}'}^\dagger] \equiv [\hat{a}_{\mathbf{x_n}}, \hat{a}_{\mathbf{x_{n'}}}^\dagger] = \frac{1}{\epsilon^3} \delta_{\mathbf{nn}'}^{(3)} \tag{2.85}$$

would tend to $\delta^{(3)}(\mathbf{x} - \mathbf{x}')$, which can be seen in the same way as in Eq. (1.160).

We are now ready to define the vacuum state of the many-particle system. It is given by the unique state $|0\rangle$ of the local oscillator algebra (2.73) and (2.74), which contains no particle at *all* places $\mathbf{x}$, thus satisfying

$$\hat{a}_{\mathbf{x}} |0\rangle \equiv 0, \qquad \langle 0| \hat{a}_{\mathbf{x}}^\dagger \equiv 0. \tag{2.86}$$

It will always be normalized to unity:

$$\langle 0|0\rangle = 1. \tag{2.87}$$

We can now convince ourselves that the fully symmetrized Hilbert space of all localized states of n particles may be identified with the states created by repeated application of the local creation operators $\hat{a}_{\mathbf{x}}^{\dagger}$:

$$|\mathbf{x}_1, \ldots, \mathbf{x}_n\rangle^S \equiv \frac{1}{\sqrt{n!}} \hat{a}_{\mathbf{x}_1}^{\dagger} \cdots \hat{a}_{\mathbf{x}_n}^{\dagger} |0\rangle. \tag{2.88}$$

The such-generated Hilbert space will be referred to as the *second-quantized Hilbert space* for reasons to be seen below. It decomposes into a direct sum of n-particle sectors. The symmetry of these states in the position variables is obvious, due to the commutativity (2.73) of all $\hat{a}_{\mathbf{x}_\nu}^{\dagger}, \hat{a}_{\mathbf{x}_\mu}^{\dagger}$ among each other.

Let us verify that the generalized orthonormality relation is indeed fulfilled by the single-particle states. Using the local commutation rules (2.73), (2.74), and the definition of the vacuum state (2.86), we calculate for a single particle

$$
\begin{aligned}
{}^S\langle\mathbf{x}|\mathbf{x}'\rangle^S &= \langle 0|\hat{a}_{\mathbf{x}}\hat{a}_{\mathbf{x}'}^{\dagger}|0\rangle \\
&= \langle 0|\delta^{(3)}(\mathbf{x}-\mathbf{x}') + \hat{a}_{\mathbf{x}'}^{\dagger}\hat{a}_{\mathbf{x}}|0\rangle \\
&= \delta^{(3)}(\mathbf{x}-\mathbf{x}').
\end{aligned}
\tag{2.89}
$$

For two particles we find

$$
\begin{aligned}
{}^S\langle\mathbf{x}_1,\mathbf{x}_2|\mathbf{x}_1',\mathbf{x}_2'\rangle^S &= \frac{1}{2!}\langle 0|\hat{a}_{\mathbf{x}_2}\hat{a}_{\mathbf{x}_1}\hat{a}_{\mathbf{x}_1'}^{\dagger}\hat{a}_{\mathbf{x}_2'}^{\dagger}|0\rangle \\
&= \frac{1}{2!}\left[\delta^{(3)}(\mathbf{x}_1-\mathbf{x}_1')\langle 0|\hat{a}_{\mathbf{x}_2}\hat{a}_{\mathbf{x}_2'}^{\dagger}|0\rangle + \langle 0|\hat{a}_{\mathbf{x}_2}\hat{a}_{\mathbf{x}_1'}^{\dagger}\hat{a}_{\mathbf{x}_1}\hat{a}_{\mathbf{x}_2'}^{\dagger}|0\rangle\right] \\
&= \frac{1}{2!}\left[\delta^{(3)}(\mathbf{x}_1-\mathbf{x}_1')\delta^{(3)}(\mathbf{x}_2-\mathbf{x}_2') + \delta^{(3)}(\mathbf{x}_2-\mathbf{x}_1')\delta^{(3)}(\mathbf{x}_1-\mathbf{x}_2')\right] \\
&= \delta^{(3)S}(\mathbf{x}_1,\mathbf{x}_2;\mathbf{x}_1',\mathbf{x}_2').
\end{aligned}
\tag{2.90}
$$

The generalization to n particles is straightforward, although somewhat tedious. It is left to the reader as an exercise. Later in Section 7.17.1, rules will be derived in a different context by a procedure due to Wick, which greatly simplifies calculations of this type.

2.4 Schrödinger Equation for Noninteracting Bosons in Terms of Creation and Annihilation Operators

Expressing the localized states in terms of the local creation and annihilation operators $\hat{a}_{\mathbf{x}}^{\dagger}, \hat{a}_{\mathbf{x}}$ does not only lead to an automatic symmetrization of the states. It also brings about an extremely simple unified form of the Schrödinger equation, which does not require the initial specification of the particle number n, as in Eq. (2.18).

This will now be shown for the case of identical particles with no two-body interactions $V_2(\mathbf{x}_\nu - \mathbf{x}_\mu; t)$.

In order to exhibit the unified Schrödinger equation for any number of particles, let us first neglect interactions and consider only the motion of the particles in an external potential with the Schrödinger equation:

$$\left\{ \sum_\nu \left[-\frac{\hbar^2}{2M} \partial_{\mathbf{x}_\nu}^2 + V_1(\mathbf{x}_\nu; t) \right] \right\} \psi(\mathbf{x}_1, \ldots, \mathbf{x}_n; t) = i\hbar \partial_t \psi(\mathbf{x}_1, \ldots, \mathbf{x}_n; t). \qquad (2.91)$$

We shall now demonstrate that the $\hat{a}^\dagger, \hat{a}$ -form of this equation, which is valid for any particle number n, reads

$$\hat{H}(t)|\psi(t)\rangle = i\hbar \partial_t |\psi(t)\rangle, \qquad (2.92)$$

where $\hat{H}(t)$ is simply the one-particle Hamiltonian sandwiched between creation and annihilation operators $\hat{a}_\mathbf{x}^\dagger$ and $\hat{a}_\mathbf{x}$ and integrated over $\mathbf{x}$, i.e.,

$$\hat{H}(t) = \int d^3x\, \hat{a}_\mathbf{x}^\dagger \left[-\frac{\hbar^2}{2M} \partial_\mathbf{x}^2 + V_1(\mathbf{x}; t) \right] \hat{a}_\mathbf{x}. \qquad (2.93)$$

The operator (2.93) is called the *second-quantized Hamiltonian*, equation (2.92) the *second-quantized Schrödinger equation*, and the state $|\psi(t)\rangle$ is an arbitrary n-particle state in the second-quantized Hilbert space, generated by multiple application of $\hat{a}_\mathbf{x}^\dagger$ upon the vacuum state $|0\rangle$, as described in the last section. The operator nature of $\hat{a}_\mathbf{x}, \hat{a}_\mathbf{x}^\dagger$ accounts automatically for the many-body content of Eq. (2.92).

This statement is proved by multiplying Eq. (2.92) from the left with

$$^S\langle \mathbf{x}_1, \ldots, \mathbf{x}_n| = \frac{1}{\sqrt{n!}} \langle 0|\hat{a}_{\mathbf{x}_n} \cdots \hat{a}_{\mathbf{x}_1},$$

which leads to

$$\frac{1}{\sqrt{n!}} \langle 0|\hat{a}_{\mathbf{x}_n} \cdots \hat{a}_{\mathbf{x}_1} \hat{H}(t)|\psi(t)\rangle = i\hbar \partial_t \frac{1}{\sqrt{n!}} \langle 0|\hat{a}_{\mathbf{x}_n} \cdots \hat{a}_{\mathbf{x}_1}|\psi(t)\rangle. \qquad (2.94)$$

Here we make use of the property (2.86) of the vacuum state to satisfy $\langle 0|\hat{a}_\mathbf{x}^\dagger = 0$. As a consequence, we may rewrite the left-hand side of (2.94) with the help of a commutator as

$$\frac{1}{\sqrt{n!}} \langle 0|[\hat{a}_{\mathbf{x}_n} \cdots \hat{a}_{\mathbf{x}_1}, \hat{H}]|\psi(t)\rangle.$$

This commutator is easily calculated using the *operator chain rules*

$$[\hat{A}, \hat{B}\hat{C}] = \hat{B}[\hat{A}, \hat{C}] + [\hat{A}, \hat{B}]\hat{C}, \qquad [\hat{A}\hat{B}, \hat{C}] = \hat{A}[\hat{B}, \hat{C}] + [\hat{A}, \hat{C}]\hat{B}. \qquad (2.95)$$

These rules can easily be memorized, noting that their structure is exactly the same as in the Leibnitz rule for derivatives. In the first rule we may imagine A to be a differential operator applied to the product BC, which is evaluated by first

differentiating B, leaving C untouched, and then C, leaving B untouched. In the second rule we imagine C to be a differential operator acting similarly to the left upon the product AB. Generalizing this rule to products of more than two operators we derive

$$
\begin{aligned}
[\hat{a}_{\mathbf{x}_n} \cdots \hat{a}_{\mathbf{x}_1}, \hat{a}_{\mathbf{y}}^\dagger \hat{a}_{\mathbf{z}}] &= [\hat{a}_{\mathbf{x}_n} \cdots \hat{a}_{\mathbf{x}_1}, \hat{a}_{\mathbf{y}}^\dagger]\hat{a}_{\mathbf{z}} + \hat{a}_{\mathbf{y}}^\dagger [\hat{a}_{\mathbf{x}_n} \cdots \hat{a}_{\mathbf{x}_1}, \hat{a}_{\mathbf{z}}] \\
&= \hat{a}_{\mathbf{x}_n} \cdots \hat{a}_{\mathbf{x}_3}\hat{a}_{\mathbf{x}_2}[\hat{a}_{\mathbf{x}_1}, \hat{a}_{\mathbf{y}}^\dagger]\hat{a}_{\mathbf{z}} + [\hat{a}_{\mathbf{x}_n} \cdots \hat{a}_{\mathbf{x}_3}\hat{a}_{\mathbf{x}_2}, \hat{a}_{\mathbf{y}}^\dagger]\hat{a}_{\mathbf{x}_1}\hat{a}_{\mathbf{z}} + \ldots \\
&= \sum_\nu \delta^{(3)}(\mathbf{x}_\nu - \mathbf{y})\hat{a}_{\mathbf{x}_n} \cdots \hat{a}_{\mathbf{x}_{\nu+1}}\hat{a}_{\mathbf{z}}\hat{a}_{\mathbf{x}_{\nu-1}} \cdots \hat{a}_{\mathbf{x}_1}.
\end{aligned}
$$

Multiplying both sides by

$$
\delta^{(3)}(\mathbf{y} - \mathbf{z}) \left[-\hbar^2 \partial_{\mathbf{z}}{}^2 / 2M + V_1(\mathbf{z}; t) \right],
$$

and integrating over $d^3y \, d^3z$ using (2.93) and (2.75) we find

$$
[\hat{a}_{\mathbf{x}_n} \cdots \hat{a}_{\mathbf{x}_1}, \hat{H}(t)] = \sum_\nu \left[-\frac{\hbar^2}{2M}\partial_{\mathbf{x}_\nu}^2 + V_1(\mathbf{x}_\nu; t) \right] \hat{a}_{\mathbf{x}_n} \cdots \hat{a}_{\mathbf{x}_{\nu+1}}\hat{a}_{\mathbf{x}_\nu}\hat{a}_{\mathbf{x}_{\nu-1}} \cdots \hat{a}_{\mathbf{x}_1}, \quad (2.96)
$$

so that (2.94) becomes

$$
\sum_\nu \left[-\frac{\hbar^2}{2M}\partial_{\mathbf{x}_\nu}^2 + V_1(\mathbf{x}_\nu; t) \right]\frac{1}{\sqrt{n!}}\langle 0|\hat{a}_{\mathbf{x}_n} \cdots \hat{a}_{\mathbf{x}_1}|\psi(t)\rangle = i\hbar\partial_t \frac{1}{\sqrt{n!}}\langle 0|\hat{a}_{\mathbf{x}_n} \cdots \hat{a}_{\mathbf{x}_1}|\psi(t)\rangle,
$$
$$(2.97)$$

which is precisely the n-body Schrödinger equation (2.91) for the wave function

$$
\psi(\mathbf{x}_1, \ldots, \mathbf{x}_n; t) \equiv \frac{1}{\sqrt{n!}}\langle 0|\hat{a}_{\mathbf{x}_n} \cdots \hat{a}_{\mathbf{x}_1}|\psi(t)\rangle. \quad (2.98)
$$

2.5 Second Quantization and Symmetrized Product Representation

It is worth pointing out that the mathematical structure exploited in the process of second quantization is of a very general nature.

Consider a set of matrices M_i with indices α', α

$$
(M_i)_{\alpha'\alpha}
$$

which satisfy some matrix commutation rules, say

$$
[M_i, M_j] = i f_{ijk} M_k. \quad (2.99)
$$

Let us sandwich these matrices between creation and annihilation operators which satisfy

$$
\begin{aligned}
[\hat{a}_\alpha, \hat{a}_{\alpha'}] &= [\hat{a}_\alpha^\dagger, \hat{a}_{\alpha'}^\dagger] = 0, \\
[\hat{a}_\alpha, \hat{a}_{\alpha'}^\dagger] &= \delta_{\alpha\alpha'}, \quad (2.100)
\end{aligned}
$$

and form the analogs of "second-quantized operators" (2.93) by defining

$$\hat{M}_i \equiv \hat{a}^\dagger_{\alpha'}(M_i)_{\alpha'\alpha}\hat{a}_\alpha = \hat{a}^\dagger M_i \hat{a}. \tag{2.101}$$

In expressions of this type, repeated indices α, α' imply a summation over all α, α'. This is commonly referred to as *Einstein's summation convention*. On the right-hand side of (2.101) we have suppressed the indices α, α' completely, for brevity. It is now easy to verify, using the operator chain rules (2.95), that the operators $\hat{M}_i$ satisfy the same commutation rules as the matrices M_i:

$$
\begin{aligned}
\left[\hat{M}_i, \hat{M}_j\right] &= \left[\hat{a}^\dagger M_i \hat{a}, \hat{a}^\dagger M_j \hat{a}\right] \\
&= \left[\hat{a}^\dagger M_i \hat{a}, \hat{a}^\dagger\right] M_j \hat{a} + \hat{a}^\dagger M_j \left[\hat{a}^\dagger M_i \hat{a}, \hat{a}\right] \\
&= \hat{a}^\dagger M_i M_j \hat{a} - \hat{a}^\dagger M_j M_i \hat{a} \\
&= \hat{a}^\dagger \left[M_i, M_j\right] \hat{a} = i f_{ijk} \hat{a}^\dagger M_k \hat{a} = i f_{ijk} \hat{M}_k.
\end{aligned}
\tag{2.102}
$$

Thus the "second-quantized" operators $\hat{M}_i$ generate an *operator representation* of the matrices M_i. They can be sandwiched between states in the "second-quantized" Hilbert space generated by applying products of creation operators $\hat{a}^\dagger_n$ upon the vacuum state $|0\rangle$. Thereby they are mapped into an infinite-dimensional matrix representation. On each subspace spanned by the products of a fixed number of creation operators, they generate the symmetrized part of the direct product representation.

The action of the "second-quantized" operators $\hat{M}_i$ upon the large Hilbert space is very simple to calculate. The only commutation rules required are

$$
\begin{aligned}
\left[\hat{M}_i, \hat{a}^\dagger_\alpha\right] &= \hat{a}^\dagger_{\alpha'}(M_i)_{\alpha'\alpha}, \\
\left[\hat{a}_{\alpha'}, \hat{M}_i\right] &= (M_i)_{\alpha'\alpha}\hat{a}_\alpha.
\end{aligned}
\tag{2.103}
$$

From this property we calculate directly the action upon "single-particle states":

$$
\begin{aligned}
\hat{M}_i \hat{a}^\dagger_\alpha |0\rangle &= \left[\hat{M}_i, \hat{a}^\dagger_\alpha\right]|0\rangle = \hat{a}^\dagger_{\alpha'}|0\rangle(M_i)_{\alpha'\alpha}, \\
\langle 0|\hat{a}_{\alpha'}\hat{M}_i &= \langle 0|\left[\hat{a}_{\alpha'}, \hat{M}_i\right] = (M_i)_{\alpha'\alpha}\langle 0|\hat{a}_\alpha.
\end{aligned}
\tag{2.104}
$$

Thus the states $\hat{a}^\dagger_\alpha|0\rangle$ span an invariant subspace and are transformed into each other via the matrix $(M_i)_{\alpha'\alpha}$.

Consider now a state with two particles:

$$\hat{a}^\dagger_{\alpha_1}\hat{a}^\dagger_{\alpha_2}|0\rangle. \tag{2.105}$$

Applying $\hat{M}_i$ to this state yields

$$
\begin{aligned}
\left[\hat{M}_i, \hat{a}^\dagger_{\alpha_1}\hat{a}^\dagger_{\alpha_2}\right] &= \left[\hat{M}_i, \hat{a}^\dagger_{\alpha_1}\right]\hat{a}^\dagger_{\alpha_2} + \hat{a}^\dagger_{\alpha_1}\left[\hat{M}_i, \hat{a}^\dagger_{\alpha_2}\right] \\
&= \hat{a}^\dagger_{\alpha'_1}\hat{a}^\dagger_{\alpha'_2}\left[(M_i)_{\alpha'_1\alpha_1}\delta_{\alpha'_2\alpha_2} + \delta_{\alpha'_1\alpha_1}(M_i)_{\alpha'_2\alpha_2}\right].
\end{aligned}
\tag{2.106}
$$

Multiplying Eq. (2.106) by $|0\rangle$ from the right, we find the transformation law for the two-particle states $\hat{a}_{\alpha_1}^\dagger \hat{a}_{\alpha_2}^\dagger |0\rangle$. They are transformed via the representation matrices

$$(M_i)_{\alpha_1' \alpha_2', \alpha_1 \alpha_2} = (M_i)_{\alpha_1' \alpha_1} \delta_{\alpha_2' \alpha_2} + \delta_{\alpha_1' \alpha_1} (M_i)_{\alpha_2' \alpha_2}. \tag{2.107}$$

Omitting the indices, we may also write the matrices as

$$M_i^{(2)} = M_i \times 1 + 1 \times M_i, \tag{2.108}$$

which is the well-known way of forming representations of a matrix algebra in a direct product space.

Since $a_{\alpha_1}^\dagger$ and $a_{\alpha_2}^\dagger$ commute with each other, the invariant space constructed in this way contains only symmetric tensors, and only the symmetrized part of the matrices $(M_i)_{\alpha_1' \alpha_2', \alpha_1 \alpha_2}$ contribute.

The alert reader will have realized that the same operator structure can be obtained for the *antisymmetrized* parts of the matrices $(M_i)_{\alpha_1' \alpha_2', \alpha_1 \alpha_2}$ by using creation and annihilation operators $a_{\alpha_1}^\dagger$ and a_{α_2} which satisfy the fermionic version of the algebraic rules (2.100):

$$\begin{aligned}
\{\hat{a}_\alpha, \hat{a}_{\alpha'}\} &= \{\hat{a}_\alpha^\dagger, \hat{a}_{\alpha'}^\dagger\} = 0, \\
\{\hat{a}_\alpha, \hat{a}_{\alpha'}^\dagger\} &= \delta_{\alpha\alpha'}.
\end{aligned} \tag{2.109}$$

In these, curly brackets are used to abbreviate *anticommutators*

$$\{A, B\} \equiv AB + BA. \tag{2.110}$$

The first two lines in (2.102) are unchanged since the operator chain rules (2.95) hold for both Bose and Fermi operators. To derive the third line we must use the additional rules

$$\begin{aligned}
[\hat{A}, \hat{B}\hat{C}] &= \{\hat{A}, \hat{B}\}\hat{C} - \hat{B}\{\hat{A}, \hat{C}\}, \\
[\hat{A}\hat{B}, \hat{C}] &= \hat{A}\{\hat{B}, \hat{C}\} - \{\hat{A}, \hat{C}\}\hat{B}.
\end{aligned} \tag{2.111}$$

This fermionic version of the commutation relation (2.102) will form, in Section 2.10, the basis for constructing a second-quantized representation for the n-particle wave functions and Schrödinger operators of fermions.

If M_i are chosen to be representation matrices L_i of the generators of the rotation group (to be discussed in detail in Section 4.1), the law (2.108) represents the quantum mechanical law of addition of two angular momenta:

$$L_i^{(2)} = L_i \times 1 + 1 \times L_i.$$

The generalization to any number of angular momenta is obvious.

Incidentally, any operator which satisfies the same commutation rules with $\hat{M}_i$, as $\hat{a}_\alpha$ in (2.103), i.e., satisfies the commutation rules

$$\begin{aligned}
\left[\hat{M}_i, \hat{O}_\alpha^\dagger\right] &= \hat{O}_{\alpha'}^\dagger (M_i)_{\alpha'\alpha}, \\
\left[\hat{O}_{\alpha'}, \hat{M}_i\right] &= (M_i)_{\alpha'\alpha} \hat{O}_\alpha,
\end{aligned} \tag{2.112}$$

will be referred to as a *spinor operator*. Generalizing this definition, an operator $\hat{O}_{\alpha_1\alpha_2...\alpha_n}$ which commutes with $\hat{M}_i$ like a product $\hat{O}_{\alpha_1}\hat{O}_{\alpha_2}\cdots\hat{O}_{\alpha_n}$, generalizing Eq. (2.106), is called a *multispinor operator* of rank n.

Another type of operators which frequently occurs in quantum mechanics and quantum field theory is a *vector operator*. This is any operator $\hat{O}_j$ which commutes with $\hat{M}_i$ in the same way as $\hat{M}_j$ does in (2.102), i.e.,

$$\left[\hat{M}_i, \hat{O}_j\right] = if_{ijk}\hat{O}_k. \tag{2.113}$$

Its generalization $\hat{O}_{j_1j_2...j_n}$, which commutes with $\hat{M}_i$ as the product of operators $\hat{M}_{j_1}\hat{M}_{j_2}\ldots\hat{M}_{j_n}$, is called a *tensor operator* of rank n.

The many-particle version of the Schrödinger theory is obtained if we view the one-particle Schrödinger equation

$$H(-i\hbar\partial_{\mathbf{x}}, \mathbf{x})\psi(\mathbf{x}, t) = i\hbar\partial_t\psi(\mathbf{x}, t) \tag{2.114}$$

as a matrix equation in the discretized $\mathbf{x}$-space with the lattice positions $\mathbf{x} = (n_1, n_2, n_3)\epsilon$, so that the wave functions $\psi(\mathbf{x}, t)$ correspond to vectors $\psi_{\mathbf{n}}(t)$. Then the differential operator $\partial_i\psi(\mathbf{x})$ becomes simply $\nabla_i\psi(\mathbf{x}) = [\psi(\mathbf{x} + \mathbf{i}\epsilon) - \psi(\mathbf{x})]/\epsilon = [\psi_{\mathbf{n+i}} - \psi_{\mathbf{n}}]/\epsilon$ where $\mathbf{i}$ is the unit vector in the ith direction, and ϵ the lattice spacing. The Laplacian may be viewed as the continuum limit of the matrix

$$\begin{aligned}
\bar{\nabla}_i\nabla_i\psi(\mathbf{x}) &= \frac{1}{\epsilon^2}\sum_{i=1}^3\left[\psi(\mathbf{x} + \mathbf{i}\epsilon) - 2\psi(\mathbf{x}) + \psi(\mathbf{x} - \mathbf{i}\epsilon)\right] \\
&= \frac{1}{\epsilon^2}\sum_{i=1}^3\left[\psi_{\mathbf{n+i}} - 2\psi_{\mathbf{n}} + \psi_{\mathbf{n-i}}\right].
\end{aligned} \tag{2.115}$$

The Schrödinger equation (2.114) is then the $\epsilon \to 0$ -limit of the matrix equation

$$H_{\mathbf{nn'}}\psi_{\mathbf{n'}}(t) = i\hbar\partial_t\psi_{\mathbf{n}}(t). \tag{2.116}$$

The many-particle Schrödinger equation in second quantization form reads

$$\hat{H}|\psi(t)\rangle = i\hbar\partial_t|\psi(t)\rangle, \tag{2.117}$$

with the Hamiltonian operator

$$\hat{H} = \hat{a}_{\mathbf{n'}}^\dagger H_{\mathbf{n'n}}\hat{a}_{\mathbf{n}}. \tag{2.118}$$

It can be used to find the eigenstates in the symmetrized multispinor representation space spanned by

$$\hat{a}_{\mathbf{n}_1}^\dagger\ldots\hat{a}_{\mathbf{n}_N}^\dagger|0\rangle. \tag{2.119}$$

Applying $\hat{H}$ to it we see that this state is multiplied from the right by a direct-product matrix

$$H \times 1 \times \ldots \times 1 + 1 \times H \times \ldots \times 1 + \ldots 1 \times 1 \times \ldots \times H. \tag{2.120}$$

Due to this very general relation, the Schrödinger energy of a many-body system without two- or higher-body interactions is the sum of the one-particle energies.

2.6 Bosons with Two-Body Interactions

We now include two-body interactions. For simplicity, we neglect the one-body potential $V_1(\mathbf{x};t)$ which can be added at the end and search for the second-quantized form of the Schrödinger equation

$$\left[-\sum_\nu \frac{\hbar^2}{2M}\partial^2_{\mathbf{x}_\nu} + \frac{1}{2}\sum_{\mu,\nu} V_2(\mathbf{x}_\nu - \mathbf{x}_\mu;t)\right]\psi(\mathbf{x}_1,\ldots,\mathbf{x}_n;t) = i\hbar\partial_t\psi(\mathbf{x}_1,\ldots,\mathbf{x}_n;t). \quad (2.121)$$

It is easy to see that such a two-body potential can be introduced into the second-quantized Schrödinger equation (2.92) by adding to the Hamilton operator in (2.93) the interaction term

$$\hat{H}_{\text{int}}(t) = \frac{1}{2}\int d^3x\, d^3x' \hat{a}^\dagger_{\mathbf{x}}\hat{a}^\dagger_{\mathbf{x}'}V_2(\mathbf{x}-\mathbf{x}';t)\hat{a}_{\mathbf{x}'}\hat{a}_{\mathbf{x}}. \quad (2.122)$$

To prove this we work out the expectation value

$$\frac{1}{\sqrt{n!}}\langle 0|\hat{a}_{\mathbf{x}_n}\ldots\hat{a}_{\mathbf{x}_1}\hat{H}_{\text{int}}(t)|\psi(t)\rangle = \frac{1}{\sqrt{n!}}\langle 0|[\hat{a}_{\mathbf{x}_n}\ldots\hat{a}_{\mathbf{x}_1},\hat{H}_{\text{int}}(t)]|\psi(t)\rangle. \quad (2.123)$$

We do this by using the local commutation rules (2.73), (2.75), and the vacuum property (2.86). First we generalize Eq. (2.96) to

$$\begin{aligned}
&[\hat{a}_{\mathbf{x}_n}\cdots\hat{a}_{\mathbf{x}_1}, \hat{a}^\dagger_{\mathbf{y}_2}\hat{a}^\dagger_{\mathbf{y}_1}\hat{a}_{\mathbf{z}_1}\hat{a}_{\mathbf{z}_2}]\\
&= [\hat{a}_{\mathbf{x}_n}\cdots\hat{a}_{\mathbf{x}_1}, \hat{a}^\dagger_{\mathbf{y}_2}\hat{a}^\dagger_{\mathbf{y}_1}]\hat{a}_{\mathbf{z}_1}\hat{a}_{\mathbf{z}_2} + \hat{a}^\dagger_{\mathbf{y}_2}\hat{a}^\dagger_{\mathbf{y}_1}[\hat{a}_{\mathbf{x}_n}\cdots\hat{a}_{\mathbf{x}_1}, \hat{a}_{\mathbf{z}_1}\hat{a}_{\mathbf{z}_2}]\\
&= [\hat{a}_{\mathbf{x}_n}\cdots\hat{a}_{\mathbf{x}_1}, \hat{a}^\dagger_{\mathbf{y}_2}]\hat{a}^\dagger_{\mathbf{y}_1}\hat{a}_{\mathbf{z}_1}\hat{a}_{\mathbf{z}_2} + \hat{a}^\dagger_{\mathbf{y}_2}[\hat{a}_{\mathbf{x}_n}\cdots\hat{a}_{\mathbf{x}_1}, \hat{a}^\dagger_{\mathbf{y}_1}]\hat{a}_{\mathbf{z}_1}\hat{a}_{\mathbf{z}_2}\\
&= \sum_\nu \delta^{(3)}(\mathbf{x}_\nu - \mathbf{y}_2)\hat{a}_{\mathbf{x}_n}\cdots\hat{a}_{\mathbf{x}_{\nu+1}}\hat{a}_{\mathbf{x}_{\nu-1}}\cdots\hat{a}_{\mathbf{x}_1}\hat{a}^\dagger_{\mathbf{y}_1}\hat{a}_{\mathbf{z}_1}\hat{a}_{\mathbf{z}_2}\\
&\quad + \hat{a}^\dagger_{\mathbf{y}_2}\sum_\nu \delta^{(3)}(\mathbf{x}_\nu - \mathbf{y}_1)\hat{a}_{\mathbf{x}_n}\cdots\hat{a}_{\mathbf{x}_{\nu+1}}\hat{a}_{\mathbf{x}_{\nu-1}}\cdots\hat{a}_{\mathbf{x}_1}\hat{a}_{\mathbf{z}_1}\hat{a}_{\mathbf{z}_2}. \quad (2.124)
\end{aligned}$$

The second piece does not contribute to Eq. (2.123) since $\hat{a}^\dagger_{\mathbf{y}_2}$ annihilates the vacuum on the left. For the same reason, the first piece can be written as

$$\sum_\nu \delta^{(3)}(\mathbf{x}_\nu - \mathbf{y}_2)[\hat{a}_{\mathbf{x}_n}\cdots\hat{a}_{\mathbf{x}_{\nu+1}}\hat{a}_{\mathbf{x}_{\nu-1}}\cdots\hat{a}_{\mathbf{x}_1}, \hat{a}^\dagger_{\mathbf{y}_1}]\hat{a}_{\mathbf{z}_1}\hat{a}_{\mathbf{z}_2}, \quad (2.125)$$

as long as it stands to the right of the vacuum. Using the commutation rule (2.96), this leads to

$$\begin{aligned}
\langle 0|\hat{a}_{\mathbf{x}_n}\cdots\hat{a}_{\mathbf{x}_1}\hat{a}^\dagger_{\mathbf{y}_2}\hat{a}^\dagger_{\mathbf{y}_1}\hat{a}_{\mathbf{z}_1}\hat{a}_{\mathbf{z}_2}|\psi(t)\rangle &= \sum_{\mu,\nu}\delta^{(3)}(\mathbf{x}_\mu - \mathbf{y}_1)\delta^{(3)}(\mathbf{x}_\nu - \mathbf{y}_2)\\
&\times\langle 0|\hat{a}_{\mathbf{x}_n}\cdots\hat{a}_{\mathbf{x}_{\nu+1}}\hat{a}_{\mathbf{x}_{\nu-1}}\cdots\hat{a}_{\mathbf{x}_{\mu+1}}\hat{a}_{\mathbf{x}_{\mu-1}}\ldots\hat{a}_{\mathbf{x}_1}\hat{a}_{\mathbf{z}_1}\hat{a}_{\mathbf{z}_2}|\psi(t)\rangle. \quad (2.126)
\end{aligned}$$

After multiplying this relation by $V_2(\mathbf{y}_2 - \mathbf{y}_1;t)\delta^{(3)}(\mathbf{y}_1 - \mathbf{z}_1)\delta^{(3)}(\mathbf{y}_2 - \mathbf{z}_2)/2$, and integrating over $d^3y_1\, d^3y_2\, d^3z_1\, d^3z_2$, we find

$$\langle 0|\hat{a}_{\mathbf{x}_n}\cdots\hat{a}_{\mathbf{x}_1}\hat{H}_{\text{int}}|\psi(t)\rangle = \frac{1}{2}\sum_{\mu,\nu}V_2(\mathbf{x}_\nu - \mathbf{x}_\mu;t)\langle 0|\hat{a}_{\mathbf{x}_n}\cdots\hat{a}_{\mathbf{x}_1}|\psi(t)\rangle, \quad (2.127)$$

which is precisely the two-body interaction in the Schrödinger equation (2.121).

Adding now the one-body interactions, we see that an n-body Schrödinger equation with arbitrary one- and two-body potentials can be written in the form of a single operator Schrödinger equation

$$\hat{H}(t)|\psi(t)\rangle = i\hbar\partial_t|\psi(t)\rangle, \tag{2.128}$$

with the second-quantized Hamilton operator

$$\hat{H}(t) = \int d^3x\, \hat{a}_{\mathbf{x}}^\dagger \left[-\frac{\hbar^2}{2M}\partial_{\mathbf{x}}^{\,2} + V_1(\mathbf{x};t) \right] \hat{a}_{\mathbf{x}} + \frac{1}{2}\int d^3x\, d^3x'\, \hat{a}_{\mathbf{x}}^\dagger \hat{a}_{\mathbf{x}'}^\dagger V_2(\mathbf{x} - \mathbf{x}';t)\hat{a}_{\mathbf{x}'}\hat{a}_{\mathbf{x}}. \tag{2.129}$$

The second-quantized Hilbert space of the states $|\psi(t)\rangle$ is constructed by repeated multiplication of the vacuum vector $|0\rangle$ with particle creation operators $\hat{a}_{\mathbf{x}}^\dagger$. The order of the creation and annihilation operators in this Hamiltonian is such that the vacuum, as a zero-particle state, has zero energy:

$$\hat{H}(t)|0\rangle = 0, \qquad \langle 0|\hat{H}(t) = 0, \tag{2.130}$$

as in the original Schrödinger equation.

A Hamiltonian which is a spatial integral over a *Hamiltonian density* $\mathcal{H}(\mathbf{x})$ as

$$H = \int d^3x\, \mathcal{H}(\mathbf{x}), \tag{2.131}$$

is called a *local Hamiltonian*. In (2.129), the free part is local, but the interacting part is not. It consists of an integral over two spatial variables, thus forming a *bilocal* operator.

2.7 Quantum Field Formulation of Many-Body Schrödinger Equations for Bosons

The annihilation operator $\hat{a}_{\mathbf{x}}$ can now be used to define a time-dependent quantum field $\hat{\psi}(\mathbf{x}, t)$ as being the Heisenberg picture of the operator $\hat{a}_{\mathbf{x}}$ (which itself is also referred to as the Schrödinger picture of the annihilation operator). According to Eq. (1.285), the Heisenberg operator associated with $\hat{a}_{\mathbf{x}}$ is

$$a_{\mathbf{x}\mathrm{H}}(t) \equiv [\hat{U}(t, t_a)]^{-1}\hat{a}_{\mathbf{x}}\hat{U}(t, t_a). \tag{2.132}$$

Thus we define

$$\hat{\psi}(\mathbf{x}, t) \equiv a_{\mathbf{x}\mathrm{H}}(t). \tag{2.133}$$

Choosing the time variable $t_a = 0$, the quantum field $\hat{\psi}(\mathbf{x}, t)$ coincides with $\hat{a}_{\mathbf{x}}$ at $t = 0$:

$$\hat{\psi}(\mathbf{x}, 0) \equiv \hat{a}_{\mathbf{x}}. \tag{2.134}$$

The time dependence of $\hat{\psi}(\mathbf{x}, t)$ is ruled by Heisenberg's equation of motion (1.280):

$$\partial_t \hat{\psi}(\mathbf{x}, t) = \frac{i}{\hbar}[\hat{H}_H(t), \hat{\psi}(\mathbf{x}, t)]. \tag{2.135}$$

For simplicity, we shall at first assume the potentials to have no explicit time dependence, an assumption to be removed later. Then Eq. (2.135) is solved by

$$\hat{\psi}(\mathbf{x}, t) = e^{i\hat{H}t/\hbar}\hat{\psi}(\mathbf{x}, 0)e^{-i\hat{H}t/\hbar} = e^{i\hat{H}t/\hbar}\hat{a}_{\mathbf{x}}e^{-i\hat{H}t/\hbar}. \tag{2.136}$$

The Hermitian conjugate of this determines the time dependence of the Heisenberg picture of the creation operator:

$$\hat{\psi}^\dagger(\mathbf{x}, t) = e^{i\hat{H}t/\hbar}\hat{\psi}^\dagger(\mathbf{x}, 0)e^{-i\hat{H}t/\hbar} = e^{i\hat{H}t/\hbar}\hat{a}_{\mathbf{x}}^\dagger e^{-i\hat{H}t/\hbar}. \tag{2.137}$$

At each given time t, the field $\hat{\psi}(\mathbf{x}, t)$ fulfills the same commutation rules (2.73) and (2.74) as $\hat{a}_{\mathbf{x}}$:

$$\begin{aligned}
[\hat{\psi}(\mathbf{x}, t), \hat{\psi}(\mathbf{x}', t)] &= 0, \\
[\hat{\psi}^\dagger(\mathbf{x}, t), \hat{\psi}^\dagger(\mathbf{x}', t)] &= 0, \\
[\hat{\psi}(\mathbf{x}, t), \hat{\psi}^\dagger(\mathbf{x}', t)] &= \delta^{(3)}(\mathbf{x} - \mathbf{x}').
\end{aligned} \tag{2.138}$$

Consider now the Hamiltonian operator (2.129) in the Heisenberg representation. Under the assumption of no explicit time dependence in the potentials we may simply multiply it by $e^{i\hat{H}t/\hbar}$ and $e^{-i\hat{H}t/\hbar}$ from the left and right, respectively, and see that

$$\begin{aligned}
\hat{H}_H(t) = & \int d^3x\, \hat{\psi}^\dagger(\mathbf{x}, t)\left[-\frac{\hbar^2}{2M}\partial_{\mathbf{x}}^2 + V_1(\mathbf{x})\right]\hat{\psi}(\mathbf{x}, t) \\
& + \frac{1}{2}\int d^3x d^3x'\, \hat{\psi}^\dagger(\mathbf{x}, t)\hat{\psi}^\dagger(\mathbf{x}', t)V_2(\mathbf{x} - \mathbf{x}')\hat{\psi}(\mathbf{x}', t)\hat{\psi}(\mathbf{x}, t).
\end{aligned} \tag{2.139}$$

Since $\hat{H}$ commutes with itself, the operator $\hat{H}_H(t)$ is time independent, so that

$$\hat{H}_H(t) \equiv \hat{H}. \tag{2.140}$$

The important point about the expression (2.139) for $\hat{H}$ is now that by containing the time-dependent fields $\hat{\psi}(\mathbf{x}, t)$, it can be viewed as the Hamilton operator of a canonically quantized Heisenberg field. This is completely analogous to the Hamiltonian operator $\hat{H} \equiv H(\hat{p}_H(t), \hat{x}_H(t), t)$ in (1.278). Instead of $p_H(t)$ and $q_H(t)$, we are dealing here with generalized coordinates and their canonically conjugate momenta of the field system. They consist of the Hermitian and anti-Hermitian parts of the field, $\hat{\psi}_R(\mathbf{x}, t)$ and $\hat{\psi}_I(\mathbf{x}, t)$, defined by

$$\hat{\psi}_R \equiv \frac{(\hat{\psi} + \hat{\psi}^\dagger)}{\sqrt{2}}, \qquad \hat{\psi}_I \equiv \frac{(\hat{\psi} - \hat{\psi}^\dagger)}{\sqrt{2}i}. \tag{2.141}$$

They commute like

$$
\begin{aligned}
{[\hat{\psi}_I(\mathbf{x}, t), \hat{\psi}_R(\mathbf{x}', t)]} &= -i\delta^{(3)}(\mathbf{x} - \mathbf{x}'), \\
{[\hat{\psi}_I(\mathbf{x}, t), \hat{\psi}_I(\mathbf{x}', t)]} &= 0, \\
{[\hat{\psi}_R(\mathbf{x}, t), \hat{\psi}_R(\mathbf{x}', t)]} &= 0.
\end{aligned}
\tag{2.142}
$$

These commutation rules are structurally identical to those between the quasi-Cartesian generalized canonical coordinates $\hat{q}_{iH}(t)$ and $\hat{p}_{iH}(t)$ in Eq. (1.97).

In fact, the formalism developed there can be generalized to an infinite set of canonical variables labeled by the space points $\mathbf{x}$ rather than i, i.e., to canonical variables $p_{\mathbf{x}}(t)$ and $q_{\mathbf{x}}(t)$. Then the quantization rules (1.97) take the form

$$
\begin{aligned}
{[\hat{p}_{\mathbf{x}}(t), \hat{q}_{\mathbf{x}'}(t)]} &= -i\hbar\delta^{(3)}(\mathbf{x} - \mathbf{x}'), \\
{[\hat{p}_{\mathbf{x}}(t), \hat{p}_{\mathbf{x}'}(t)]} &= 0, \\
{[\hat{q}_{\mathbf{x}}(t), \hat{q}_{\mathbf{x}'}(t)]} &= 0,
\end{aligned}
\tag{2.143}
$$

which is a local version of the algebra (2.58). The replacement $i \to \mathbf{x}$ can of course be done on a lattice with a subsequent continuum limit as in Eqs. (2.79)–(2.85). When going from the index i to the continuous spatial variable $\mathbf{x}$, the Kronecker δ_{ij} turns into Dirac's $\delta^{(3)}(\mathbf{x} - \mathbf{x}')$, and sums become integrals.

By identifying

$$
\hat{p}_{\mathbf{x}}(t) \equiv \hbar\hat{\psi}_I(\mathbf{x}, t), \qquad \hat{q}_{\mathbf{x}}(t) \equiv \hat{\psi}_R(\mathbf{x}, t),
\tag{2.144}
$$

we now obtain the commutation relations (2.142). In quantum field theory it is customary to denote the canonical momentum variable $p_{\mathbf{x}}(t)$ by the symbol $\pi_{\mathbf{x}}(t)$, and write

$$
\hat{p}_{\mathbf{x}}(t) = \hbar\hat{\psi}_I(\mathbf{x}, t) \equiv \hat{\pi}(\mathbf{x}, t).
\tag{2.145}
$$

Thus the many-body nature of the system may be considered as a consequence of *quantizing the fields* $q_{\mathbf{x}}(t) = \hat{\psi}_R(\mathbf{x}, t)$ and $\hat{p}_{\mathbf{x}}(t) = \hbar\hat{\psi}_I(\mathbf{x}, t)$ canonically via Eq. (2.143).

2.8 Canonical Formalism in Quantum Field Theory

So far, the commutation rules have been imposed upon the fields $\hat{\psi}(\mathbf{x}, t)$ and $\hat{\psi}^\dagger(\mathbf{x}', t)$ by the particle nature of the n-body Schrödinger theory. It is, however, possible to *derive* these rules by applying the standard canonical formalism to the fields $\psi_R(\mathbf{x}, t)$ and $\psi_I(\mathbf{x}, t)$, treating them as generalized Lagrange coordinates. To see this, let us recall once more the general procedure for finding the quantization rules and the Schrödinger equation for a general Lagrangian system with an action

$$
\mathcal{A} = \int dt\, L(q(t), \dot{q}(t)),
\tag{2.146}
$$

where the Lagrangian L is some function of the independent variables $q(t) = (q_1(t), \ldots, q_N(t))$ and their velocities $\dot{q}(t) = (\dot{q}_1(t), \ldots, \dot{q}_N(t))$. The conjugate momenta are defined, as usual, by the derivatives

$$p_i(t) = \frac{\partial L}{\partial \dot{q}_i(t)}. \tag{2.147}$$

The Hamiltonian is given by the Legendre transformation

$$H(p(t), q(t)) = \sum_i p_i(t) q_i(t) - L(q(t), \dot{q}(t)). \tag{2.148}$$

If $q(t)$ are Cartesian or quasi-Cartesian coordinates, quantum physics is imposed in the Heisenberg picture by letting $p_i(t)$, $q_i(t)$ become operators $\hat{p}_{iH}(t)$, $\hat{q}_{iH}(t)$ which satisfy the canonical equal time commutation rules

$$\begin{aligned}
[\hat{p}_{iH}(t), \hat{q}_{jH}(t)] &= -iH\hbar\delta_{ij}, \\
[\hat{p}_{iH}(t), \hat{p}_{jH}(t)] &= [\hat{q}_{iH}(t), \hat{q}_{jH}(t)] = 0,
\end{aligned} \tag{2.149}$$

and postulating the Heisenberg equation of motion

$$\frac{d}{dt}\hat{O}_H = \frac{i}{\hbar}[\hat{H}_H, \hat{O}_H] + \frac{\partial}{\partial t}\hat{O}_H \tag{2.150}$$

for any observable

$$\hat{O}_H(t) \equiv O(\hat{p}_H(t), \hat{q}_H(t), t). \tag{2.151}$$

This formalism holds for any number of Cartesian or quasi-Cartesian variables. It can therefore be generalized to functions of space variables $\mathbf{x_n}$ lying on a lattice with a tiny width ϵ [see (2.79)]. Suppressing the subscripts of $\mathbf{x_n}$, the canonical momenta (2.147) read

$$p_{\mathbf{x}}(t) = \frac{\partial L}{\partial \dot{q}_{\mathbf{x}}(t)}, \tag{2.152}$$

and the Hamiltonian becomes

$$H = \sum_{\mathbf{x}} p_{\mathbf{x}}(t)\dot{q}_{\mathbf{x}}(t) - L(q_{\mathbf{x}}, \dot{q}_{\mathbf{x}}). \tag{2.153}$$

The canonical commutation rules (2.149) become the commutation rules (2.143) of second quantization.

In quantum field theory, the formalism must be generalized to continuous space variables $\mathbf{x}$. For a Hamiltonian (2.153), the action (2.146) is

$$\mathcal{A} = \int dt\, L(t) = \int dt \int d^3x\, \psi_I(\mathbf{x}, t)\hbar\partial_t\psi_R(\mathbf{x}, t) - \int dt\, H[\psi_I, \psi_R], \tag{2.154}$$

where $H[\psi_I, \psi_R]$ denotes the classical Hamiltonian associated with the operator $H_H(t)$ in Eq. (2.139). The derivative term can be written as an integral over a kinetic Lagrangian $L^{\text{kin}}(t)$ as

$$\mathcal{A}^{\text{kin}} = \int dt\, L^{\text{kin}}(t) = \int dt \int d^3x\, \mathcal{L}^{\text{kin}}(\mathbf{x}, t) \equiv \int dt \int d^3x\, \psi_I(\mathbf{x}, t)\hbar\partial_t\psi_R(\mathbf{x}, t). \tag{2.155}$$

Then the lattice rule (2.152) for finding the canonical momentum has the following functional generalization to find the canonical field momentum:

$$p_\mathbf{x}(t) = \frac{\partial L}{\partial \dot{q}_\mathbf{x}(t)} \quad \rightarrow \quad \pi(\mathbf{x},t) \equiv \frac{\partial \mathcal{L}^{\mathrm{kin}}}{\partial \partial_t \psi_R(\mathbf{x},t)} = \hbar \psi_I(\mathbf{x},t), \tag{2.156}$$

in agreement with the identification (2.152) and the action (2.155). The canonical quantization rules

$$\begin{aligned}
[\pi(\mathbf{x},t), \hat{\psi}_R(\mathbf{x}',t)] &= -i\delta^{(3)}(\mathbf{x}-\mathbf{x}'), \\
[\pi(\mathbf{x},t), \pi(\mathbf{x}',t)] &= 0, \\
[\hat{\psi}_R(\mathbf{x},t), \hat{\psi}_R(\mathbf{x}',t)] &= 0
\end{aligned} \tag{2.157}$$

coincide with the commutation rules (2.142) of second quantization. Obviously, the Legendre transformation (2.153) turns L into the correct Hamiltonian H.

More conveniently, one expresses the classical action in terms of complex fields

$$\mathcal{A} = \int dt\, L(t) = \int dt \int d^3x\, \psi^*(\mathbf{x},t)\, i\hbar\partial_t \psi(\mathbf{x},t) - \int dt\, H[\psi,\psi^*], \tag{2.158}$$

and defines the canonical field momentum as

$$\pi(\mathbf{x},t) \equiv \frac{\partial \mathcal{L}^{\mathrm{kin}}}{\partial \partial_t \psi(\mathbf{x},t)} = \hbar \psi^*(\mathbf{x},t). \tag{2.159}$$

Then the canonical quantization rules become

$$\begin{aligned}
[\psi(\mathbf{x},t), \psi^\dagger(\mathbf{x}',t)] &= -i\delta^{(3)}(\mathbf{x}-\mathbf{x}'), \\
[\psi(\mathbf{x},t), \psi(\mathbf{x}',t)] &= 0, \\
[\psi^\dagger(\mathbf{x},t), \psi^\dagger(\mathbf{x}',t)] &= 0.
\end{aligned} \tag{2.160}$$

We have emphasized before that the canonical quantization rules are applicable only if the field space is quasi-Cartesian (see the remark on page 15). For this, the dynamical metric (1.94) has to be q-independent. This condition is violated by the interaction in the Hamiltonian (2.139). There are ambiguities in ordering the field operators in this interaction. These are, however, removed by the requirement that, after quantizing the field system, one wants to reproduce the n-body Schrödinger equation, which requires that the zero-body state has zero energy and thus satisfies Eq. (2.130).

The equivalence of the n-body Schrödinger theory with the above-derived canonically quantized field theory requires specification of the ordering of the field operators after having imposed the canonical commutation rules upon the fields.

By analogy with the definition of a local Hamiltonian we call an action $\mathcal{A}$ *local* if it can be written as a spacetime integral over a *Lagrangian density* $\mathcal{L}(\mathbf{x},t)$:

$$\mathcal{A} = \int dt \int d^3x\, \mathcal{L}(\mathbf{x},t), \tag{2.161}$$

where $\mathcal{L}(\mathbf{x}, t)$ depends only on the fields $\psi(\mathbf{x}, t)$ and their first derivatives. The kinetic part in (2.158) is obviously local, the interacting part is bilocal [recall (2.139)].

For a local theory, the canonical field momentum (2.162) becomes

$$\pi(\mathbf{x}, t) \equiv \frac{\partial \mathcal{L}}{\partial \partial_t \psi(\mathbf{x}, t)} = \hbar \psi^*(\mathbf{x}, t). \tag{2.162}$$

The formal application of the rules (2.143) leads again directly to the commutation rules (2.138) without prior splitting into kinetic part and remainder.

In the complex-field formulation, only $\psi(\mathbf{x}, t)$ has a canonical momentum, not $\psi^*(\mathbf{x}, t)$. This, however, is an artifact of the use of complex field variables. Later, in Section 7.5.1 we shall encounter a more severe problem, where the canonical momentum of a component of the real electromagnetic vector field vanishes as a consequence of gauge invariance, requiring an essential modification of the quantization procedure.

Let us calculate the classical equations of motion for the continuous field theory. They are obtained by extremizing the action with respect to $\psi(x)$ and $\psi^*(x)$. To do this we need the rules of functional differentiation. These rules are derived as follows: we take the obvious differentiation rules stating the independence of generalized Lagrange variables $q_i(t)$, which read

$$\frac{\partial q_i(t)}{\partial q_j(t)} = \delta_{ij}, \tag{2.163}$$

and generalize them to lattice variables

$$\frac{\partial q_{\mathbf{x}}(t)}{\partial q_{\mathbf{x}'}(t)} = \delta_{\mathbf{x}\mathbf{x}'}. \tag{2.164}$$

For continuous field variables, these become

$$\frac{\partial \psi(\mathbf{x}, t)}{\partial \psi(\mathbf{x}', t)} = \delta(\mathbf{x} - \mathbf{x}'). \tag{2.165}$$

The entire formalism can be generalized, thus considering the action as a local functional of fields living in continuous four-dimensional *spacetime*. Then the derivative rules must be generalized further to functional derivatives whose variations satisfy the basic rules

$$\frac{\delta \psi(\mathbf{x}, t)}{\delta \psi(\mathbf{x}', t')} = \delta^{(3)}(\mathbf{x} - \mathbf{x}') \delta(t - t') = \delta^{(4)}(x - x'). \tag{2.166}$$

The functional derivatives of actions which depend on spacetime-dependent fields $\psi(\mathbf{x}, t)$ are obtained by using the chain rule of differentiation together with (2.166). The formalism of functional differentiation and integration will be treated in detail in Chapter 14.

For a local theory, where the action has the form (2.161), and the fields and their canonical momenta (2.162) are time-dependent Lagrange coordinates with differentiation rules (2.165), the extremality conditions lead to the Euler-Lagrange equations

$$\frac{\partial \mathcal{A}}{\partial \psi(\mathbf{x}, t)} = \frac{\partial \mathcal{L}}{\partial \psi(\mathbf{x}, t)} - \partial_t \frac{\delta \mathcal{L}}{\partial \, \partial_t \psi(\mathbf{x}, t)} = 0, \tag{2.167}$$

$$\frac{\partial \mathcal{A}}{\partial \psi^*(\mathbf{x}, t)} = \frac{\partial \mathcal{L}}{\partial \psi^*(\mathbf{x}, t)} - \partial_t \frac{\delta \mathcal{L}}{\partial \, \partial_t^* \psi(\mathbf{x}, t)} = 0. \tag{2.168}$$

The second equation is simply the complex-conjugate of the first.

Note that these equations are insensitive to surface terms. This is why, in spite of the asymmetric appearance of ψ and ψ^* in the action (2.158), the two equations (2.167) and (2.168) are complex conjugate to each other. Indeed, the latter reads explicitly

$$\left[i\hbar\partial_t + \frac{\hbar^2}{2M}\partial_{\mathbf{x}}^2 - V_1(\mathbf{x}) \right] \psi(\mathbf{x}, t) = \int d\mathbf{x}' \, \psi^*(\mathbf{x}', t) V_2(\mathbf{x} - \mathbf{x}'; t) \psi(\mathbf{x}', t) \, \psi(\mathbf{x}, t), \tag{2.169}$$

and it is easy to verify that (2.167) produces the complex conjugate of this.

After field quantization, the above Euler-Lagrange equation becomes an equation for the field operator $\psi(\mathbf{x}', t)$ and its conjugate $\psi^*(\mathbf{x}', t)$ must be replaced by the Hermitian conjugate field operator $\psi^{\dagger *}(\mathbf{x}', t)$.

Let us also remark that the equation of motion (2.168) can be used directly to derive the n-body Schrödinger equation (2.91) once more in another way, by working with time-dependent field operators. As a function of time, an arbitrary state vector evolves as follows:

$$|\psi(t)\rangle = e^{-i\hat{H}t/\hbar}|\psi(0)\rangle. \tag{2.170}$$

Multiplying this by the basis bra-vectors

$$\frac{1}{\sqrt{n!}}\langle 0|\hat{a}_{\mathbf{x}_n} \cdots \hat{a}_{\mathbf{x}_1}, \tag{2.171}$$

we obtain the time-dependent Schrödinger wave function

$$\psi(\mathbf{x}_1, \ldots, \mathbf{x}_n; t). \tag{2.172}$$

Inserting between each pair of $\hat{a}_{\mathbf{x}_\nu}$-operators in (2.171) the trivial unit factors $\mathbf{1} = e^{-i\hat{H}t/\hbar}e^{i\hat{H}t/\hbar}$, each of these operators is transformed into the time-dependent field operators $\hat{\psi}(\mathbf{x}_\nu, t)$, and one has

$$\psi(\mathbf{x}_1, \ldots, \mathbf{x}_n; t) = \frac{1}{\sqrt{n!}}\langle 0|e^{-i\hat{H}t/\hbar}\hat{\psi}(\mathbf{x}_n, t) \cdots \hat{\psi}(\mathbf{x}_1, t)|\psi(0)\rangle. \tag{2.173}$$

Using the zero-energy property (2.130) of the vacuum state, this becomes

$$\psi(\mathbf{x}_1, \ldots, \mathbf{x}_n; t) = \langle \mathbf{x}_1, \ldots, \mathbf{x}_n; t|\psi(0)\rangle. \tag{2.174}$$

The bra-states arising from the application of the time-dependent field operators $\hat{\psi}(\mathbf{x}_i, t)$ to the vacuum state on the left

$$\frac{1}{\sqrt{n!}} \langle 0 | \hat{\psi}(\mathbf{x}_n, t) \cdots \hat{\psi}(\mathbf{x}_1, t), \tag{2.175}$$

define a new time-dependent basis

$$\langle \mathbf{x}_1, \ldots, \mathbf{x}_n; t |, \tag{2.176}$$

with the property

$$\langle \mathbf{x}_1, \ldots, \mathbf{x}_n; t | \psi(0) \rangle \equiv \langle \mathbf{x}_1, \ldots, \mathbf{x}_n | \psi(t) \rangle. \tag{2.177}$$

If we apply to the states (2.175) the differential operator (2.169) and use the canonical equal-time commutation rules (2.138), we may derive once more that $\psi(\mathbf{x}_1, \ldots, \mathbf{x}_n; t)$ obeys the Schrödinger equation (2.18).

The difference between the earlier way (2.98) of defining the wave function and the formula (2.174) is, of course, the second-quantized version of the difference between the Schrödinger and the Heisenberg picture for the ordinary quantum mechanical wave functions. In Eq. (2.98), the states $|\psi(t)\rangle$ are *time-dependent* but the basis ket vectors $\langle \mathbf{x}_1, .., \mathbf{x}_n |$ are not, and with them also the field operators $\hat{\psi}(\mathbf{x}, 0) = \hat{a}_{\mathbf{x}}$ generating them. In Eq. (2.174), on the contrary, the states $\langle \psi(0) |$ are *time-independent* (and may be called Heisenberg states), but the local basis bra states $\langle \mathbf{x}_1, \ldots, \mathbf{x}_n; t |$ are not, and with them the field operators $\hat{\psi}(\mathbf{x}, t)$ generating them. Whatever representation we use, the n-body wave function $\psi(\mathbf{x}_1, \ldots, \mathbf{x}_n, t)$ remains the same and obeys the Schrödinger equation (2.18). The change of picture is relevant only for the operator properties of the many-particle description.

Certainly, there is also the possibility of changing the picture in the Schrödinger wave function $\psi(\mathbf{x}_1, \ldots, \mathbf{x}_n; t)$. But the associated unitary transformation would take place in another Hilbert space, namely in the space of square integrable functions of n arguments, where $\hat{p}$ and $\hat{x}$ are the differential operators $-i\hbar\partial_{\mathbf{x}}$ and $\mathbf{x}$.

When going through the proof that (2.174) satisfies the n-body Schrödinger equation (2.18), we realize that at no place do we need the assumption of time-independent potentials. Thus we can conclude that the canonical quantization scheme for the action (2.158) is valid for an arbitrary explicit time dependence of the potentials in the Hamiltonian operator $\hat{H}$ [see (2.5)]. It is always equivalent to the Schrödinger description for an arbitrary number of particles.

2.9 More General Creation and Annihilation Operators

In many applications it is possible to solve exactly the Schrödinger equation with only the one-body potential $V_1(\mathbf{x}; t)$. In these cases it is useful to employ, instead of the creation and annihilation operators of particles at a point, another equivalent set of such operators which refers, right away, to the corresponding eigenstates. We

do this by expanding the field operator into the complete set of solutions of the one-particle Schrödinger equation

$$\hat{\psi}(\mathbf{x}, t) = \sum_{\alpha} \psi_{E_\alpha}(\mathbf{x}, t) \hat{a}_\alpha. \tag{2.178}$$

If the one-body potential is time-independent and there is no two-body potential, the states have the time dependence

$$\psi_{E_\alpha}(\mathbf{x}, t) = \psi_{E_\alpha}(\mathbf{x}) \, e^{-iE_\alpha t/\hbar}. \tag{2.179}$$

The expansion (2.178) is inverted to give

$$\hat{a}_\alpha = \int d^3x \, \psi_{E_\alpha}^*(\mathbf{x}, t) \hat{\psi}(\mathbf{x}, t), \tag{2.180}$$

which we shall write shorter in a scalar-product notation as

$$\hat{a}_\alpha = (\psi_{E_\alpha}(t), \hat{\psi}(t)). \tag{2.181}$$

As opposed to the Dirac bracket notation to denote basis-independent scalar products, the parentheses indicate more specifically a scalar product between spatial wave functions.

From the commutation rules (2.138) we find that the new operators $\hat{a}_\alpha, \hat{a}_\alpha^\dagger$ satisfy the commutation rules

$$\begin{aligned} [\hat{a}_\alpha, \hat{a}_{\alpha'}] &= [\hat{a}_\alpha^\dagger, \hat{a}_{\alpha'}^\dagger] = 0, \\ [\hat{a}_\alpha, \hat{a}_{\alpha'}^\dagger] &= \delta_{\alpha,\alpha'}. \end{aligned} \tag{2.182}$$

Inserting (2.178) into (2.139) with $V_2 = 0$, we may use the orthonormality relation among the one-particle states $\psi_{E_\alpha}(\mathbf{x})$ to find the field operator representation for the Hamilton operator

$$\hat{H} = \sum_{\alpha} E_\alpha \hat{a}_\alpha^\dagger \hat{a}_\alpha. \tag{2.183}$$

The eigenstates of the time-independent Schrödinger equation

$$\hat{H}|\psi(t)\rangle = E|\psi(t)\rangle \tag{2.184}$$

are now

$$|n_1, \ldots, n_n\rangle = \frac{1}{\sqrt{n_1! \cdots n_n!}} (\hat{a}_{\alpha_1}^\dagger)^{n_1} \cdots (\hat{a}_{\alpha_k}^\dagger)^{n_k} |0\rangle, \tag{2.185}$$

where the prefactor ensures the proper normalization. The energy is

$$E = \sum_{i=1}^{k} E_{\alpha_i} n_i. \tag{2.186}$$

Finally, by forming the scalar products

$$\frac{1}{\sqrt{n!}} \langle 0 | \hat{a}_{\mathbf{x}_n} \cdots \hat{a}_{\mathbf{x}_1} (\hat{a}_{\alpha_1}^\dagger)^{n_1} \cdots (\hat{a}_{\alpha_k}^\dagger)^{n_k} |0\rangle \frac{1}{\sqrt{n_1! \cdots n_k!}}, \tag{2.187}$$

we recover precisely the symmetrized wave functions (2.32) with the normalization factors (2.41).

Similar considerations are, of course, possible in the Heisenberg picture of the operators $\hat{a}_\alpha^\dagger, \hat{a}_\alpha$ which can be obtained from

$$\hat{a}_\alpha(t) = \int d^3x \psi_{E_\alpha}^*(\mathbf{x}) \hat{\psi}(\mathbf{x}, t). \tag{2.188}$$

In the field operator description of many-body systems, the Schrödinger wave function $\psi(\mathbf{x}, t)$ has become a canonically quantized field object. Observe that the field $\psi(\mathbf{x}, t)$ by itself contains all relevant quantum mechanical information of the system via the derivative terms of the action (2.158),

$$\hat{\psi}^\dagger(\mathbf{x}, t) i\hbar \partial_t \hat{\psi}(\mathbf{x}, t) + \frac{\hbar^2}{2M} \hat{\psi}^\dagger(\mathbf{x}, t) \partial_\mathbf{x}^2 \hat{\psi}(\mathbf{x}, t). \tag{2.189}$$

This fixes the relation between wavelength and momentum, and between frequency and energy. The field quantization which introduces the additional processes of particle creation and annihilation is distinguished from this and often referred to as *second quantization.*

It should be kept in mind that, for a given n-body system, second quantization is completely equivalent and does not go beyond the usual n-body Schrödinger theory. It merely introduces the technical advantage of collecting the wave equations for any particle number n in a single operator representation. This advantage is, nevertheless, of great use in treating systems with many identical particles. In the limit of large particle densities, it gives rise to approximations which would be very difficult to formulate in the Schrödinger formulation. In particular, collective excitations of many-particle systems find their easiest explanation in terms of a quantum field formulation.

The full power of quantum fields, however, will unfold itself when trying to explain the physics of relativistic particles, where the number of particles is no longer conserved. Since the second-quantized Hilbert space contains any number of particles, the second-quantized formulation allows naturally for the description of the emission and absorption of fundamental particles, processes which the Schrödinger equation is unable to deal with.

2.10 Quantum Field Formulation of Many-Fermion Schrödinger Equations

The question arises whether an equally simple formalism can be found which automatically leads to the correct antisymmetric many-particle states

$$|\mathbf{x}_1, \ldots, \mathbf{x}_n\rangle^A = \frac{1}{\sqrt{n!}} \sum_P \epsilon_P |\mathbf{x}_{p(1)}\rangle \otimes \ldots \otimes |\mathbf{x}_{p(n)}\rangle. \tag{2.190}$$

This is indeed possible. Let us remember that the symmetry of the wave functions was a consequence of the commutativity of the operators $\hat{\psi}(\mathbf{x}, t)$ for different position

values $\mathbf{x}$. Obviously, we can achieve an antisymmetry in the coordinates by forming product states

$$|\mathbf{x}_1, \ldots, \mathbf{x}_n\rangle^A = \frac{1}{\sqrt{n!}} \hat{a}^\dagger_{\mathbf{x}_1} \cdots \hat{a}^\dagger_{\mathbf{x}_n} |0\rangle \tag{2.191}$$

and requiring anticommutativity of the particle creation and annihilation operators:

$$\{\hat{a}^\dagger_{\mathbf{x}}, \hat{a}^\dagger_{\mathbf{x}'}\} = 0, \qquad \{\hat{a}_{\mathbf{x}}, \hat{a}_{\mathbf{x}'}\} = 0. \tag{2.192}$$

The curly brackets denote the anticommutator defined in Eq. (2.110). To define a closed algebra, we require in addition, by analogy with the third commutation rule (2.75) for bosons, the anticommutation rule

$$\{\hat{a}_{\mathbf{x}}, \hat{a}^\dagger_{\mathbf{x}'}\} = \delta^{(3)}(\mathbf{x} - \mathbf{x}'). \tag{2.193}$$

As in the bosonic case we introduce a vacuum state $|0\rangle$ which is normalized as in (2.87) and contains no particle [cf. (2.86)]:

$$\hat{a}_{\mathbf{x}}|0\rangle = 0 \ , \ \ \langle 0|\hat{a}^\dagger_{\mathbf{x}} = 0. \tag{2.194}$$

The anticommutation rules (2.192) have the consequence that each point can at most be occupied by a single particle. Indeed, applying the creation operator twice to the vacuum state yields zero:

$$\hat{a}^\dagger_{\mathbf{x}} \hat{a}^\dagger_{\mathbf{x}}|0\rangle = \{\hat{a}^\dagger_{\mathbf{x}}, \hat{a}^\dagger_{\mathbf{x}}\}|0\rangle - \hat{a}^\dagger_{\mathbf{x}} \hat{a}^\dagger_{\mathbf{x}}|0\rangle = 0. \tag{2.195}$$

This guarantees the validity of the *Pauli exclusion principle*.

The properties (2.192), (2.193), and (2.194) are sufficient to derive the many-body Schrödinger equations with two-body interactions for an arbitrary number of fermionic particles. It is easy to verify that the second-quantized Hamiltonian has the same form as in Eq. (2.129). The proof proceeds along the same line as in the symmetric case, Eqs. (2.94)–(2.129). A crucial tool is the operator chain rule (2.111) derived for anticommutators. The minus sign, by which anticommutators differ from commutators, cancels out in all relevant equations.

As for bosons we define a time-dependent quantum field for fermions in the Heisenberg picture as

$$\begin{aligned} \hat{\psi}(\mathbf{x}, t) &= e^{i\hat{H}t/\hbar} \hat{\psi}(\mathbf{x}, 0) e^{-i\hat{H}t/\hbar} \\ &= e^{i\hat{H}t/\hbar} \hat{a}_{\mathbf{x}} e^{-i\hat{H}t/\hbar}, \end{aligned} \tag{2.196}$$

and find equal-time anticommutation rules of the same type as the commutation relations (2.138):

$$\begin{aligned} \{\hat{\psi}(\mathbf{x}, t), \hat{\psi}(\mathbf{x}', t)\} &= 0, \\ \{\hat{\psi}^\dagger(\mathbf{x}, t), \hat{\psi}^\dagger(\mathbf{x}', t)\} &= 0, \\ \{\hat{\psi}(\mathbf{x}, t), \hat{\psi}^\dagger(\mathbf{x}', t)\} &= \delta^{(3)}(\mathbf{x} - \mathbf{x}'). \end{aligned} \tag{2.197}$$

The Hamiltonian has again the form Eq. (2.139).

There is only one place where the fermionic case is not completely analogous to the bosonic one: The second-quantized formulation cannot be derived from a standard canonical formalism of an infinite number of generalized coordinates. The standard formalism of quantum mechanics applies only to true physical canonical coordinates $p(t)$ and $q(t)$, and these can never account for anticommuting properties of field variables.[2] Thus an identification analogous to (2.144),

$$\hat{p}_{\mathbf{x}}(t) \equiv \hat{\psi}_I(\mathbf{x}, t), \qquad \hat{q}_{\mathbf{x}}(t) \equiv \hat{\psi}_R(\mathbf{x}, t), \tag{2.198}$$

is at first impossible.

The canonical formalism may nevertheless be generalized appropriately. We may start out with exactly the same classical Lagrangian as in the boson case, Eq. (2.158), but treat the fields formally as anticommuting objects, i.e.,

$$\psi(\mathbf{x}, t)\psi(\mathbf{x}', t') = -\psi(\mathbf{x}', t')\psi(\mathbf{x}, t). \tag{2.199}$$

In mathematics, such objects are called *Grassmann variables*. Using these, we define again classical canonical momenta

$$p_{\mathbf{x}}(t) \equiv \frac{\delta L}{\delta \dot{\psi}(\mathbf{x}, t)} = -i\hbar \psi^\dagger(\mathbf{x}, t) \equiv \pi(\mathbf{x}, t). \tag{2.200}$$

Together with the field variable $q_{\mathbf{x}}(t) = \psi^\dagger(\mathbf{x}, t)$, this is postulated to satisfy the canonical anticommutation rule

$$\{p_{\mathbf{x}}(t), q_{\mathbf{x}'}(t)\} = -i\hbar \delta^{(3)}(\mathbf{x} - \mathbf{x}'). \tag{2.201}$$

2.11 Free Nonrelativistic Particles and Fields

An important way to approach interacting theories is based on perturbative methods. Usually, these begin with the free theory and prescribe how to calculate successive corrections due to the interaction energies. A detailed discussion of how and when this works will be given later. It seems intuitively obvious, however, that at least for weak interactions, the free theory may be a good starting point for an approximation scheme. It is therefore worthwhile to study a few properties of the free theory in detail.

The free-field action is, according to Eqs. (2.158) and (2.139) for $V_1(\mathbf{x}) = 0$ and $V_2(\mathbf{x} - \mathbf{x}') = 0$:

$$\mathcal{A} = \int dt\, d^3x\, \psi^*(\mathbf{x}, t) \left[i\hbar \partial_t + \frac{\hbar^2}{2M} \partial_{\mathbf{x}}^2 \right] \psi(\mathbf{x}, t). \tag{2.202}$$

---

[2]For a detailed discussion of classical mechanics with supersymmetric Lagrange coordinates see A. Kapka, *Supersymmetrie*, Teubner, 1997.

The quantum field $\hat{\psi}(\mathbf{x}, t)$ satisfies the field operator equation

$$\left(i\hbar \partial_t + \frac{\hbar^2}{2M} \partial_{\mathbf{x}}^2 \right) \hat{\psi}(\mathbf{x}, t) = 0, \tag{2.203}$$

with the conjugate field satisfying

$$\hat{\psi}^\dagger(x, t) \left(-i\hbar \overset{\leftarrow}{\partial}_t + \frac{\hbar^2}{2M} \overset{\leftarrow}{\partial}_{\mathbf{x}}^2 \right) = 0. \tag{2.204}$$

The equal-time commutation rules for bosons and fermions are

$$
\begin{aligned}
[\hat{\psi}(\mathbf{x}, t), \hat{\psi}(\mathbf{x}', t)]_{\mp} &= 0, \\
[\hat{\psi}^\dagger(\mathbf{x}, t), \hat{\psi}^\dagger(\mathbf{x}', t)]_{\mp} &= 0, \\
[\hat{\psi}(\mathbf{x}, t), \hat{\psi}^\dagger(\mathbf{x}', t)]_{\mp} &= \delta^{(3)}(\mathbf{x} - \mathbf{x}'),
\end{aligned}
\tag{2.205}
$$

where we have denoted commutator and anticommutator collectively by $[\dots, \dots]_{\mp}$, respectively.

In a finite volume V, the solutions of the free one-particle Schrödinger equation are given by the time-dependent version of the plane wave functions (1.185) [compare (2.179)]:

$$\psi_{\mathbf{p^m}}(\mathbf{x}, t) = \langle \mathbf{x}, t | \mathbf{p^m} \rangle = \langle \mathbf{x}, t | \hat{a}_{\mathbf{p^m}}^\dagger \rangle = \frac{1}{\sqrt{V}} \exp\left\{ \frac{i}{\hbar} \left(\mathbf{p^m} \mathbf{x} - \frac{\mathbf{p}^{\mathbf{m}2}}{2M} t \right) \right\}. \tag{2.206}$$

These are orthonormal in the sense

$$\int d^3x \, \psi_{\mathbf{p^m}}^*(\mathbf{x}, t) \psi_{\mathbf{p^{m'}}}(\mathbf{x}, t) = \delta_{\mathbf{p^m}, \mathbf{p^{m'}}}, \tag{2.207}$$

and complete, implying that

$$\sum_{\mathbf{p^m}} \psi_{\mathbf{p^m}}(\mathbf{x}, t) \psi_{\mathbf{p^m}}^*(\mathbf{x}', t) = \delta^{(3)}(\mathbf{x} - \mathbf{x}'). \tag{2.208}$$

As in Eq. (2.178), we now expand the field operator in terms of these solutions as

$$\hat{\psi}(\mathbf{x}, t) = \sum_{\mathbf{p^m}} \psi_{\mathbf{p^m}}(\mathbf{x}, t) \hat{a}_{\mathbf{p^m}}. \tag{2.209}$$

This expansion is inverted with the help of the scalar product (2.181) as

$$\hat{a}_{\mathbf{p^m}} = (\psi_{\mathbf{p^m}}(t), \hat{\psi}(t)) = \int d^3x \, \psi_{\mathbf{p^m}}^*(\mathbf{x}, t) \hat{\psi}(\mathbf{x}, t). \tag{2.210}$$

In the sequel we shall usually omit the superscript of the momenta $\mathbf{p^m}$ if their discrete nature is evident from the context. The operators $\hat{a}_{\mathbf{p}}$ and $\hat{a}_{\mathbf{p}}^\dagger$, obey the canonical commutation rules corresponding to Eq. (2.182):

$$
\begin{aligned}
[\hat{a}_{\mathbf{p}}, \hat{a}_{\mathbf{p}'}]_{\mp} &= 0, \\
[\hat{a}_{\mathbf{p}}^\dagger, \hat{a}_{\mathbf{p}'}^\dagger]_{\mp} &= 0, \\
[\hat{a}_{\mathbf{p}}, \hat{a}_{\mathbf{p}'}^\dagger]_{\mp} &= \delta_{\mathbf{pp}'},
\end{aligned}
\tag{2.211}
$$

where we have used the modified δ-functions introduced in Eq. (1.196).

In an infinite volume, we use the time-dependent version of the continuous wave functions (1.195)

$$\psi_{\mathbf{p}}(\mathbf{x}, t) = \langle \mathbf{x}, t | \mathbf{p} \rangle = \langle \mathbf{x}, t | \hat{a}_{\mathbf{p}}^\dagger \rangle = \frac{1}{\sqrt{V}} \exp \left\{ \frac{i}{\hbar} \left(\mathbf{p}^{\mathbf{m}} \mathbf{x} - \frac{\mathbf{p}^{\mathbf{m}2}}{2M} t \right) \right\}, \qquad (2.212)$$

which are orthonormal in the sense

$$\begin{aligned}
\int d^3x \, \psi_{\mathbf{p}}^*(\mathbf{x}, t) \psi_{\mathbf{p}'}(\mathbf{x}, t) &= (2\pi\hbar)^3 \delta^{(3)}(\mathbf{p} - \mathbf{p}') \\
&\equiv \delta^{(3)}(\mathbf{p} - \mathbf{p}'),
\end{aligned} \qquad (2.213)$$

and complete, as expressed by

$$\int \frac{d^3p}{(2\pi\hbar)^3} \, \psi_{\mathbf{p}}(\mathbf{x}, t) \psi_{\mathbf{p}}^*(\mathbf{x}', t) \equiv \int \tilde{d}^3p \, \psi_{\mathbf{p}}(\mathbf{x}, t) \psi_{\mathbf{p}}^*(\mathbf{x}', t) = \delta^{(3)}(\mathbf{x} - \mathbf{x}'). \qquad (2.214)$$

In terms of these continuum wave functions, we expand the field operator as

$$\hat{\psi}(\mathbf{x}, t) = \int \tilde{d}^3p \, \psi_{\mathbf{p}}(\mathbf{x}, t) \hat{a}(\mathbf{p}), \qquad (2.215)$$

and have the inverse

$$\hat{a}(\mathbf{p}) = (\psi_{\mathbf{p}}(t), \hat{\psi}(t)) = \int d^3x \, \psi_{\mathbf{p}}^*(\mathbf{x}, t) \hat{\psi}(\mathbf{x}, t). \qquad (2.216)$$

The discrete-momentum operators $\hat{a}_{\mathbf{p}}$, and $\hat{a}_{\mathbf{p}}^\dagger$ and the continuous ones $\hat{a}(\mathbf{p})$ and $\hat{a}^\dagger(\mathbf{p})$, are related by [recall Eq. (1.190)]

$$\hat{a}(\mathbf{p}) = \sqrt{V} \hat{a}_{\mathbf{p}}, \qquad \hat{a}^\dagger(\mathbf{p}) = \sqrt{V} \hat{a}_{\mathbf{p}}^\dagger. \qquad (2.217)$$

For the continuous-momentum operators $\hat{a}(\mathbf{p})$ and $\hat{a}(\mathbf{p})^\dagger$, the canonical commutation rules in Eq. (2.182) take the form

$$\begin{aligned}
[\hat{a}(\mathbf{p}), \hat{a}(\mathbf{p}')]_{\mp} &= [\hat{a}^\dagger(\mathbf{p}), \hat{a}^\dagger(\mathbf{p}')]_{\mp} = 0, \\
[\hat{a}(\mathbf{p}), \hat{a}^\dagger(\mathbf{p}')]_{\mp} &= \delta^{(3)}(\mathbf{p} - \mathbf{p}').
\end{aligned} \qquad (2.218)$$

The time-independent many-particle states are obtained, as in (2.185), by repeatedly applying any number of creation operators $\hat{a}_{\mathbf{p}}^\dagger$ [or $\hat{a}^\dagger(\mathbf{p})$] to the vacuum state $|0\rangle$, thus creating states

$$|n_{\mathbf{p}_1}, n_{\mathbf{p}_2}, \ldots, n_{\mathbf{p}_k}\rangle = \mathcal{N}^{S,A}(\hat{a}_{\mathbf{p}_1}^\dagger)^{n_{\mathbf{p}_1}} \cdots (\hat{a}_{\mathbf{p}_k}^\dagger)^{n_{\mathbf{p}_k}} |0\rangle, \qquad (2.219)$$

where the normalization factor is determined as in Eq. (2.185). For bosons with $n_{\mathbf{p}_1}$ identical states of momentum $\mathbf{p}_1$, with $n_{\mathbf{p}_2}$ identical states of momentum $\mathbf{p}_2$, etc., the normalization factor is

$$\mathcal{N}^S = \frac{1}{\sqrt{n_{\mathbf{p}_1}! \cdots n_{\mathbf{p}_k}!}}. \qquad (2.220)$$

The same formula can be used for fermions, only that then the values of $n_{\mathbf{p}_i}$ are restricted to 0 or 1, and the normalization constant $\mathcal{N}^A$ is equal to 1. The time-independent wave functions are obtained as

$$\langle \mathbf{x}_1, \ldots, \mathbf{x}_n | n_{\mathbf{p}_1}, n_{\mathbf{p}_2}, \ldots, n_{\mathbf{p}_k} \rangle^{S,A} = \frac{\mathcal{N}^{S,A}}{\sqrt{n!}} \tag{2.221}$$
$$\times \langle 0 | \hat{\psi}(\mathbf{x}_n, 0) \cdots \hat{\psi}(\mathbf{x}_1, 0) (\hat{a}_{\mathbf{p}_1}^\dagger)^{n_{\mathbf{p}_1}} \cdots (\hat{a}_{\mathbf{p}_k}^\dagger)^{n_{\mathbf{p}_k}} | 0 \rangle,$$

and the time-dependent ones as

$$\begin{aligned}
\langle \mathbf{x}_1, \ldots, \mathbf{x}_n | n_{\mathbf{p}_1}, n_{\mathbf{p}_2}, \ldots, n_{\mathbf{p}_k}; t \rangle^{S,A} &= \langle \mathbf{x}_1, \ldots, \mathbf{x}_n | n_{\mathbf{p}_1}, n_{\mathbf{p}_2}, \ldots, n_{\mathbf{p}_k} \rangle^{S,A} e^{-iEt/\hbar} \\
&= \frac{\mathcal{N}^{S,A}}{\sqrt{n!}} \langle 0 | \hat{\psi}(\mathbf{x}_n, 0) \cdots \hat{\psi}(\mathbf{x}_1, 0) e^{-i\hat{H}t/\hbar} (\hat{a}_{\mathbf{p}_1}^\dagger)^{n_{\mathbf{p}_1}} \ldots (\hat{a}_{\mathbf{p}_k}^\dagger)^{n_{\mathbf{p}_k}} | 0 \rangle \\
&= \frac{\mathcal{N}^{S,A}}{\sqrt{n!}} \langle 0 | \hat{\psi}(\mathbf{x}_n, 0) \cdots \hat{\psi}(\mathbf{x}_1, 0) [\hat{a}_{\mathbf{p}_1}^\dagger(t)]^{n_{\mathbf{p}_1}} \cdots [\hat{a}_{\mathbf{p}_k}^\dagger(t)]^{n_{\mathbf{p}_k}} | 0 \rangle,
\end{aligned}$$

with the time-dependent creation operators being defined by

$$\hat{a}_{\mathbf{p}}^\dagger(t) \equiv e^{i\hat{H}t/\hbar} \hat{a}_{\mathbf{p}}^\dagger e^{-i\hat{H}t/\hbar}. \tag{2.222}$$

The energy of these states is

$$E = \sum_{i=1}^{k} n_i \varepsilon_{\mathbf{p}_i}, \tag{2.223}$$

where $\varepsilon_{\mathbf{p}} \equiv \mathbf{p}^2/2M$ are the energies of the single-particle wave functions (2.212). The many-body states (2.219) form the so-called *occupation number basis* of the Hilbert space. For fermions, n_i can only be 0 or 1, due to the anticommutativity of the operators $\hat{a}_{\mathbf{p}}$ and $\hat{a}_{\mathbf{p}}^\dagger$ among themselves. The basis states are properly normalized:

$$\langle n_{\mathbf{p}_1} n_{\mathbf{p}_2} n_{\mathbf{p}_3} \ldots n_{\mathbf{p}_k} | n'_{\mathbf{p}_1} n'_{\mathbf{p}_2} n'_{\mathbf{p}_3} \ldots n'_{\mathbf{p}_k} \rangle = \delta_{n_{\mathbf{p}_1} n'_{\mathbf{p}_1}} \delta_{n_{\mathbf{p}_2} n'_{\mathbf{p}_2}} \delta_{n_{\mathbf{p}_3} n'_{\mathbf{p}_3}} \ldots \delta_{n_{\mathbf{p}_k} n'_{\mathbf{p}_k}}. \tag{2.224}$$

They satisfy the completeness relation:

$$\sum_{\mathbf{p}_1 \mathbf{p}_2 \mathbf{p}_3 \cdots} \sum_{n_{\mathbf{p}_1} n_{\mathbf{p}_2} n_{\mathbf{p}_3} \ldots n_{\mathbf{p}_k}} | n_{\mathbf{p}_1} n_{\mathbf{p}_2} n_{\mathbf{p}_3} \ldots n_{\mathbf{p}_k} \rangle \langle n_{\mathbf{p}_1} n_{\mathbf{p}_2} n_{\mathbf{p}_3} \ldots n_{\mathbf{p}_k} | = 1^{S,A}, \tag{2.225}$$

where the unit operator on the right-hand side covers only the physical Hilbert space of symmetric or antisymmetric n-body wave functions.

2.12 Second-Quantized Current Conservation Law

In Subsection 1.3.4 of Chapter 1 we have observed an essential property for the probability interpretation of the Schrödinger wave functions: The probability current density (1.107) and the probability density (1.108) are related by the *local conservation law* (1.109):

$$\partial_t \rho(\mathbf{x}, t) = -\boldsymbol{\nabla} \cdot \mathbf{j}(\mathbf{x}, t). \tag{2.226}$$

This followed directly from the Schrödinger equation (2.169). Since the same equation holds for the field operators, i.e., with $\psi^*(\mathbf{x}', t)$ replaced by $\hat{\psi}^\dagger(\mathbf{x}', t)$, the field operators of charge and current density,

$$
\begin{aligned}
\hat{\rho}(\mathbf{x}, t) &= \hat{\psi}^\dagger(\mathbf{x}, t)\hat{\psi}(\mathbf{x}, t), \\
\hat{\mathbf{j}}(\mathbf{x}, t) &= -i\frac{\hbar}{2M}\hat{\psi}^\dagger(\mathbf{x}, t) \overset{\leftrightarrow}{\boldsymbol{\nabla}} \hat{\psi}(\mathbf{x}, t)
\end{aligned}
\tag{2.227}
$$

satisfy the same relation. When integrating (2.226) over all $\mathbf{x}$, and using Green's theorem as done in Eq. (1.110), we obtain a *global conservation law* that ensures the time independence of the particle number operator

$$
\hat{N} = \int d^3x\, \hat{\rho}(\mathbf{x}, t) = \int d^3x\, \hat{\psi}^\dagger(\mathbf{x}, t)\hat{\psi}(\mathbf{x}, t).
\tag{2.228}
$$

Since this is time-independent, we can use (2.134) to rewrite

$$
\hat{N} = \int d^3x\, \hat{\rho}(\mathbf{x}, 0) = \int d^3x\, \hat{\psi}^\dagger(\mathbf{x}, 0)\hat{\psi}(\mathbf{x}, 0) = \int d^3x\, \hat{a}_\mathbf{x}^\dagger \hat{a}_\mathbf{x},
\tag{2.229}
$$

so that $\hat{N}$ coincides with the particle number operator (2.78). The original form (2.228) is the Heisenberg picture of the particle number operator, which coincides with (2.229), since the particle number is conserved.

2.13 Free-Particle Propagator

The perturbation theory of interacting fields to be developed later in Chapter 10 requires knowledge of an important free-field quantity called the *free-particle propagator*. It is the vacuum expectation of the time-ordered product of two free field operators. As we shall see, the calculation of any observable quantities can be reduced to the calculation of some linear combination of products of free propagators [see Section 7.17.1]. Let us first extend the definition (1.249) of the time-ordered product of n time-dependent operators to allow for fermion field operators. Suppose that the times in an operator product $\hat{A}_n(t_n) \cdots \hat{A}_1(t_1)$ have an order

$$
t_{i_n} > t_{i_{n-1}} > \ldots > t_{i_1}.
\tag{2.230}
$$

Then the time-ordered product of the operators is defined by

$$
\hat{T}\hat{A}_n(t_n) \cdots \hat{A}_1(t_1) \equiv \epsilon_P \hat{A}_{i_n}(t_{i_n}) \cdots \hat{A}_{i_1}(t_{i_1}).
\tag{2.231}
$$

With respect to the definition (1.250), the right hand side carries a sign factor $\epsilon_P = \pm 1$ depending on whether an even or an odd permutation P of the fermion field operators is necessary to reach the time-ordered form. For bosons, $\varepsilon_P \equiv 1$.

The definition of the time-ordered products can be given more concisely using the Heaviside function $\Theta(t)$ of Eq. (1.313).

For two operators, we have

$$\hat{T}\hat{A}(t_1)\hat{B}(t_2) = \Theta(t_1 - t_2)\hat{A}(t_1)\hat{B}(t_2) \pm \Theta(t_2 - t_1)\hat{B}(t_2)\hat{A}(t_1), \qquad (2.232)$$

with the upper and lower sign applying to bosons and fermions, respectively. The free-particle propagator can now be constructed from the field operators as the vacuum expectation value

$$G(\mathbf{x}, t; \mathbf{x}', t') = \langle 0|\hat{T}\hat{\psi}(\mathbf{x}, t)\hat{\psi}^\dagger(\mathbf{x}', t')|0\rangle. \qquad (2.233)$$

Applying the free-field operator equations (2.203) and (2.204), we notice a remarkable property: The free-particle propagator $G(\mathbf{x}, t; \mathbf{x}', t')$ coincides with the *Green function* of the Schrödinger differential operator. Recall that a Green function of a homogeneous differential equation is defined by being the solution of the inhomogeneous equation with a δ-function source (see Section 1.6). This property may easily be verified for the free-particle propagator, which satisfies the differential equations

$$\left(i\hbar\partial_t + \frac{\hbar^2}{2M}\partial_{\mathbf{x}}^2\right)G(\mathbf{x}, t; \mathbf{x}', t') = i\hbar\delta(t - t')\delta^{(3)}(\mathbf{x} - \mathbf{x}'), \qquad (2.234)$$

$$G(\mathbf{x}, t; \mathbf{x}', t')\left(-i\hbar\overset{\leftarrow}{\partial_{t'}} + \frac{\hbar^2}{2M}\overset{\leftarrow 2}{\partial_{\mathbf{x}}}\right) = i\hbar\delta(t - t')\delta^{(3)}(\mathbf{x} - \mathbf{x}'), \qquad (2.235)$$

thus being a Green function of the free-particle Schrödinger equation: The right-hand side follows directly from the fact that the field $\hat{\psi}(\mathbf{x}, t)$ satisfies the Schrödinger equation and the obvious formula

$$\partial_t\Theta(t - t') = \delta(t - t'). \qquad (2.236)$$

With the help of the chain rule of differentiation and Eq. (2.232), we see that

$$\left(i\hbar\partial_t + \frac{\hbar^2}{2M}\partial_{\mathbf{x}}^2\right)\langle 0|\hat{T}\hat{\psi}(\mathbf{x}, t)\hat{\psi}^\dagger(\mathbf{x}', t')|0\rangle$$

$$= i\hbar\left[\partial_t\Theta(t - t')\langle 0|\hat{\psi}(\mathbf{x}, t)\hat{\psi}^\dagger(\mathbf{x}', t')|0\rangle \pm \partial_t\Theta(t' - t)\langle 0|\hat{\psi}^\dagger(\mathbf{x}', t')\hat{\psi}(\mathbf{x}, t)|0\rangle\right]$$

$$= i\hbar\delta(t - t')\langle 0|[\hat{\psi}(\mathbf{x}, t), \hat{\psi}^\dagger(\mathbf{x}', t)]_{\mp}|0\rangle = i\hbar\delta(t - t')\delta^{(3)}(\mathbf{x} - \mathbf{x}'), \qquad (2.237)$$

where the commutation and anticommutation rules (2.138) and (2.197) have been used, together with the unit normalization (2.87) of the vacuum state.

In the theory of differential equations, Green functions are introduced to find solutions for arbitrary inhomogeneous terms. These solutions may be derived from superpositions of δ-function sources. In quantum field theory, the same Green functions serve as propagators to solve inhomogeneous differential equations that involve *field operators*.

Explicitly, the free field propagator is calculated as follows: Since $\hat{\psi}(\mathbf{x}, t)$ annihilates the vacuum, only the first term in the defining Eq. (2.232) contributes, so that we can write

$$G(\mathbf{x}, t; \mathbf{x}', t') = \Theta(t - t')\langle 0|\hat{\psi}(\mathbf{x}, t)\hat{\psi}^\dagger(\mathbf{x}', t')|0\rangle. \qquad (2.238)$$

Inserting the expansion Eq. (2.215) with the wave functions (2.212), and using (2.218), the right-hand side becomes

$$\Theta(t - t') \int d^3p \, d^3p' \, e^{i[(\mathbf{px} - \mathbf{p'x'}) - (\mathbf{p}^2 t/2M - \mathbf{p'}^2 t'/2M)]/\hbar} \langle 0|\hat{a}(\mathbf{p})\hat{a}^\dagger(\mathbf{p'})|0\rangle$$

$$= \Theta(t - t') \int d^3p \, e^{i[\mathbf{p}(\mathbf{x} - \mathbf{x'}) - \mathbf{p}^2(t - t')/2M]/\hbar}. \tag{2.239}$$

By completing the square and using the Gaussian integral

$$\int d^3p \, e^{-ap^2/2\hbar} = \frac{1}{\sqrt{2\pi\hbar a}^3}, \tag{2.240}$$

we find

$$G(\mathbf{x}, t; \mathbf{x'}, t') = \Theta(t - t')\frac{1}{\sqrt{2\pi i\hbar(t - t')/M}^3}e^{iM(\mathbf{x} - \mathbf{x'})^2/2\hbar(t - t')}$$

$$= G(\mathbf{x} - \mathbf{x'}, t - t'). \tag{2.241}$$

The right-hand side is recognized as the usual quantum-mechanical Green function of the free-particle Schrödinger equation of Eq. (1.350). Indeed, the factor after $\Theta(t - t')$ is simply the one-particle matrix element of the time evolution operator

$$\langle 0|\hat{\psi}(\mathbf{x}, t)\hat{\psi}^\dagger(\mathbf{x'}, t')|0\rangle = \langle 0|\hat{\psi}(\mathbf{x})e^{-i\hat{H}(t - t')/\hbar}\hat{\psi}^\dagger(\mathbf{x'})|0\rangle$$

$$= \langle \mathbf{x}|\hat{U}(t, t')|\mathbf{x'}\rangle. \tag{2.242}$$

This is precisely the expression discussed in Eqs. (1.310)–(1.312). It describes the probability amplitude that a single free particle has propagated from $\mathbf{x}$ to $\mathbf{x'}$ in the time $t - t' > 0$. For $t - t' < 0$, G vanishes.

There exists a more useful way of writing the Fourier representation of the propagator than that in Eq. (2.239). It is based on the integral representation (1.319) of the Heaviside function:

$$\Theta(t - t') = \int_{-\infty}^{\infty} dE \, e^{-iE(t - t')/\hbar} \frac{i\hbar}{E + i\eta}. \tag{2.243}$$

As discussed in general in Eqs. (1.317)–(1.319), the $i\eta$ in the denominator ensures the causality. For $t > t'$, the contour of integration can be closed by an infinite semicircle below the energy axis, thereby picking up the pole at $E = -i\eta$, so that we obtain by the residue theorem

$$\Theta(t - t') = 1, \quad t > t'. \tag{2.244}$$

For $t < t'$, on the other hand, the contour may be closed above the energy axis and, since there is no pole in the upper half-plane, we have

$$\Theta(t - t') = 0, \quad t < t'. \tag{2.245}$$

Relation (2.243) can be generalized to

$$\Theta(t - t')e^{-iE_0(t-t')/\hbar} = \int_{-\infty}^{\infty} dE \, e^{-iE(t-t')/\hbar} \frac{i\hbar}{E - E_0 + i\eta}. \qquad (2.246)$$

Using this with $E_0 = \mathbf{p}^2/2M$ we find from (2.239) the integral representation

$$G(\mathbf{x} - \mathbf{x}', t - t') = \int d^3p \int_{-\infty}^{\infty} dE \, e^{i\mathbf{p}(\mathbf{x}-\mathbf{x}')/\hbar - iE(t-t')/\hbar} \frac{i\hbar}{E - \mathbf{p}^2/2M + i\eta}. \qquad (2.247)$$

In this form we can trivially verify the equations of motion (2.234) and (2.235). This expression agrees, of course, with the quantum mechanical time evolution amplitude (1.344).

The Fourier-transformed propagator

$$\begin{aligned} G(\mathbf{p}, E) &= \int d^3x \int_{-\infty}^{\infty} dt \, e^{-i(\mathbf{p}\mathbf{x} - Et)/\hbar} G(\mathbf{x}, t) \\ &= \frac{i\hbar}{E - \mathbf{p}^2/2M + i\eta} \end{aligned} \qquad (2.248)$$

has the property of being singular when the variable E is equal to a physical particle energy $E = \mathbf{p}^2/2M$. This condition is often called the *energy shell* condition. It is a general property of Green functions that their singularities in the energy-momentum variables display the spectra of the particles of the system.

2.14 Collapse of Wave Function

A related Green function can be used to illustrate the much discussed phenomenon of the *collapse of the wave function* in quantum mechanics [10]. If we create a particle at some time t', we create a Schrödinger wave function that fills immediately the entire space. If we annihilate the particle at some later time t, the wave function disappears instantaneously from the entire space. This phenomenon which is hard to comprehend physically is obviously an artifact of the nonrelativistic Schrödinger theory. Let us see how it comes about in the formalism. If we measure the particle density at a time t'' that lies only slightly later than the later time t in the above Green function, we find

$$\begin{aligned} G(\mathbf{z}, t''; \mathbf{x}, t; \mathbf{x}', t') &= \langle 0|\hat{T}\hat{\rho}(\mathbf{z}, t'')\hat{\psi}(\mathbf{x}, t)\hat{\psi}^\dagger(\mathbf{x}', t')|0\rangle \\ &= \langle 0|\hat{T}\hat{\psi}^\dagger(\mathbf{z}, t'')\hat{\psi}(\mathbf{z}, t'')\hat{\psi}(\mathbf{x}, t)\hat{\psi}^\dagger(\mathbf{x}', t')|0\rangle. \end{aligned} \qquad (2.249)$$

The second and the fourth field operators yield a time-ordered Green function $\langle \hat{T}\hat{\psi}(\mathbf{z}, t'')\hat{\psi}^\dagger(\mathbf{x}', t')\rangle = \Theta(t'' - t')G(\mathbf{z}, t''; \mathbf{x}'t')$, which is zero for $t'' > t'$. This is multiplied by the time-ordered Green function of the fist and the third field operators which is $\langle \hat{T}\hat{\psi}^\dagger(\mathbf{z}, t'')\hat{\psi}(\mathbf{x}, t)\rangle = \Theta(t - t'')G(\mathbf{z}, t''; \mathbf{x}\,t)$, and thus vanishes for $t'' > t$. Applying Wick's theorem to (2.249) shows that by the time t'' that is later than t and t', the wave function created at the initial time t' has completely collapsed.

2.15 Quantum Statistics of Free Nonrelativistic Fields

2.15.1 Thermodynamic Quantities

Consider the grand-canonical partition function introduced in Eq. (1.493):

$$Z_G(T,\mu) = \mathrm{Tr}\,(e^{-(\hat{H}-\mu\hat{N})/k_BT}). \tag{2.250}$$

The trace has to be taken over the complete set of basis states (2.219):

$$\sum_{\mathbf{p}_1\mathbf{p}_2\mathbf{p}_3\cdots}\;\sum_{n_{\mathbf{p}_1}n_{\mathbf{p}_2}n_{\mathbf{p}_3}\cdots n_{\mathbf{p}_k}} \langle n_{\mathbf{p}_1}n_{\mathbf{p}_2}n_{\mathbf{p}_3}\cdots|e^{-(E_{n_{\mathbf{p}_1}n_{\mathbf{p}_2}n_{\mathbf{p}_3}\cdots}-\mu\sum_i n_{\mathbf{p}_i})/k_BT}|n_{\mathbf{p}_1}n_{\mathbf{p}_2}n_{\mathbf{p}_3}\cdots\rangle.$$

Using the additivity of the energies of all single-particle states found in Eq. (2.223), this can be written as an infinite product

$$Z_G(T,\mu) = \sum_{\mathbf{p}_1\mathbf{p}_2\mathbf{p}_3\cdots}\;\sum_{n_{\mathbf{p}_1}n_{\mathbf{p}_2}n_{\mathbf{p}_3}\cdots n_{\mathbf{p}_k}} e^{-(\frac{\mathbf{p}_1^2}{2M}-\mu)n_{\mathbf{p}_1}/k_BT}e^{-(\frac{\mathbf{p}_2^2}{2M}-\mu)n_{\mathbf{p}_2}/k_BT}e^{-(\frac{\mathbf{p}_3^2}{2M}-\mu)n_{\mathbf{p}_3}/k_BT}\cdots.$$

$$\tag{2.251}$$

Each Boltzmann factor leads to the partition function associated with the available single-particle momentum $\mathbf{p}_1, \mathbf{p}_2, \dots$. The product is turned into a sum by taking the logarithm of this and considering the grand-canonical free energy

$$F_G(T,\mu) \equiv -k_BT\log Z_G(T,\mu) = -k_BT\sum_{\mathbf{p}}\log\sum_n e^{-(\frac{\mathbf{p}^2}{2M}-\mu)n/k_BT}. \tag{2.252}$$

We now distinguish between Bose and Fermi particles. In the first case, the occupation numbers n_i run over all integers $0, 1, 2, \dots$ up to infinity:

$$\sum_{n=0}^{\infty} e^{-(\frac{\mathbf{p}^2}{2M}-\mu)n/k_BT} = \frac{1}{1-e^{-(\frac{\mathbf{p}^2}{2M}-\mu)/k_BT}}. \tag{2.253}$$

In the second case, n_i can be only zero or one, so that

$$\sum_{n=0}^{1} e^{-(\frac{\mathbf{p}^2}{2M}-\mu)n/k_BT} = 1 + e^{-(\frac{\mathbf{p}^2}{2M}-\mu)/k_BT}. \tag{2.254}$$

Thus we obtain

$$F_G(T,\mu) = \pm k_BT\sum_{\mathbf{p}}\log[1 \mp e^{-(\frac{\mathbf{p}^2}{2M}-\mu)/k_BT}]. \tag{2.255}$$

Because of the frequent appearance of the energy combination $\mathbf{p}^2/2M - \mu$, it will often be useful to define the quantity

$$\xi_{\mathbf{p}} = \frac{\mathbf{p}^2}{2M} - \mu = \varepsilon_{\mathbf{p}} - \mu. \tag{2.256}$$

This will abbreviate calculations in grand-canonical ensembles.

In a large volume, momentum states lie so close to each other that the sum may be approximately evaluated as an integral with the help of the limiting formula

$$\sum_{\mathbf{p}} \xrightarrow[V\to\infty]{} gV \int \frac{d^3p}{(2\pi\hbar)^3} = gV \int d\!\!\!^-{}^3p. \tag{2.257}$$

In writing this we have allowed for a degeneracy number g for each momentum state $\mathbf{p}$. It accounts for extra degrees of freedom of the particles in each momentum state. In the absence of internal quantum numbers, g counts the different spin polarization states. If s denotes the spin, then its third component can run from $-s$ to s so that

$$g = 2s + 1. \tag{2.258}$$

Moreover, the limit (2.257) is certainly valid only for sums over sufficiently smooth functions. We shall see in Section 2.15.3 that the limit fails for a Bose gas near $T = 0$, where the limit requires the more careful treatment in Eq. (2.337).

As an alternative to the momentum integral (2.257), we may integrate over the single-particle energies. With the energy $\varepsilon_{\mathbf{p}} = \mathbf{p}^2/2M$, the relation between the integration measures is

$$
\begin{aligned}
\int d\!\!\!^-{}^3p &= \frac{4\pi}{(2\pi)^3\hbar^3} \int_0^\infty dp\, p^2 \\
&= \frac{1}{\sqrt{2\pi\hbar^2/M}^3} \frac{2}{\sqrt{\pi}} \int_0^\infty d\varepsilon \sqrt{\varepsilon} \equiv \int g_\varepsilon d\varepsilon.
\end{aligned} \tag{2.259}
$$

In the last expression we have introduced the quantity

$$g_\varepsilon \equiv \frac{1}{\sqrt{2\pi\hbar^2/M}^3} \frac{2}{\sqrt{\pi}} \sqrt{\varepsilon}, \tag{2.260}$$

which is the *density of states* per unit energy interval and volume. With the help of this quantity we may write (2.255) as an energy integral

$$F_G(T, \mu, V) = gV \int_0^\infty d\varepsilon\, g_\varepsilon F_\varepsilon(T, \mu), \tag{2.261}$$

where

$$F_\varepsilon(T, \mu) \equiv \pm k_B T \log[1 \mp e^{-(\varepsilon-\mu)/k_B T}] \tag{2.262}$$

is the grand-canonical free energy of an individual single-particle energy state.

According to the thermodynamic rule (1.502), the average particle number is found from the derivative of $F_G(T, \mu, V)$ with respect to the chemical potential. Using (2.255) or the integral representation (2.261), we find

$$
\begin{aligned}
N &= gV \sum_{\mathbf{p}} \frac{1}{e^{(\frac{\mathbf{p}^2}{2M}-\mu)/k_B T} \mp 1} = -gV \int_0^\infty d\varepsilon\, g_\varepsilon \frac{\partial}{\partial\mu} F_\varepsilon(T, \mu) \\
&\equiv gV \int_0^\infty d\varepsilon\, g_\varepsilon f_\varepsilon,
\end{aligned} \tag{2.263}
$$

where

$$f_\varepsilon \equiv -\frac{\partial}{\partial \mu} F_\varepsilon(T, \mu) = \frac{1}{e^{(\varepsilon-\mu)/k_B T} \mp 1} \tag{2.264}$$

are the average Bose and Fermi occupation numbers of a level of energy ε, respectively. They are plotted in Figs. 2.1 and 2.2.
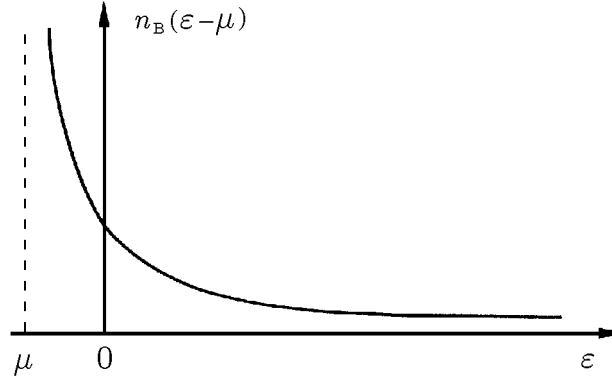
FIGURE 2.1 Average Bose occupation number $n_B(\varepsilon - \mu)$. Note that free bosons have a negative chemical potential μ.
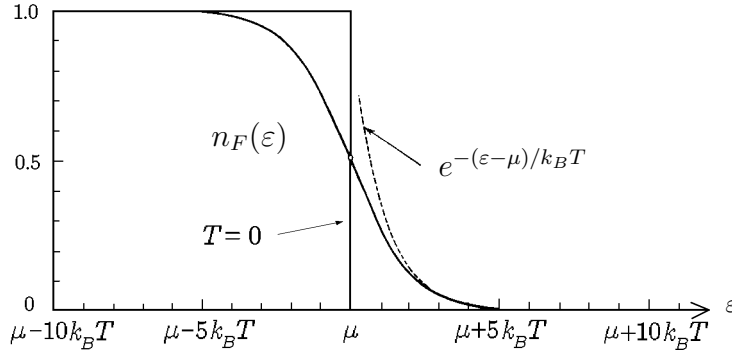
FIGURE 2.2 Average Fermi occupation number $n_F(\varepsilon)$. Fermions have a positive chemical potential μ.

The internal energy of the system can be calculated from the integral

$$
\begin{aligned}
E &= g \int_0^\infty d\varepsilon\, g_\varepsilon f_\varepsilon \varepsilon \\
&= g \frac{V}{\sqrt{2\pi\hbar^2/M}^3} \frac{2}{\sqrt{\pi}} \int_0^\infty \frac{d\varepsilon \sqrt{\varepsilon}\,\varepsilon}{e^{(\varepsilon-\mu)/k_B T} \mp 1}.
\end{aligned} \tag{2.265}
$$

On the other hand, we find by a partial integration of the integral in (2.261):

$$\int_0^\infty d\varepsilon\, \varepsilon^{1/2} \log[e^{(\varepsilon-\mu)/k_B T} \mp 1] = -\frac{2}{3} \int_0^\infty \frac{d\varepsilon\, \varepsilon^{3/2}}{e^{(\varepsilon-\mu)/k_B T} \mp 1}, \tag{2.266}$$

so that the grand-canonical partition function can be rewritten as

$$F_G(T,\mu,V) = g \int_0^\infty d\varepsilon\, g_\varepsilon F_\varepsilon = -\frac{2}{3} g \int_0^\infty d\varepsilon\, g_\varepsilon f_\varepsilon \varepsilon. \tag{2.267}$$

This implies the general thermodynamic relation for a free Bose or Fermi gas:

$$F_G = -\frac{2}{3} E. \tag{2.268}$$

Recalling the definition of the pressure (1.527), we have thus found the *equation of state* for a free Bose or Fermi gas:

$$pV = \frac{2}{3} E. \tag{2.269}$$

To evaluate the energy integral, we introduce the variable $z \equiv \varepsilon/k_B T$ and write (2.263) as

$$N = N(T,\mu) \equiv g \frac{V}{\lambda^3(T)} \frac{1}{\Gamma(3/2)} I_{3/2}^{\mp}\left(\frac{\mu}{k_B T}\right), \tag{2.270}$$

where

$$\lambda(T) \equiv \frac{1}{\sqrt{2\pi\hbar^2/Mk_B T}} \tag{2.271}$$

is the *thermal length* associated with mass M and temperature T, and $I_n^{\mp}(\mu/k_B T)$ denotes the function

$$I_n^{\mp}(\alpha) \equiv \int_0^\infty dz \frac{z^{n-1}}{e^{z-\alpha} \mp 1}. \tag{2.272}$$

After expanding the denominator in a power series, each term can be integrated and leads for bosons to a series representation

$$I_n^-(\alpha) = \Gamma(n) \sum_{k=1}^\infty \frac{e^{k\alpha}}{k^n}. \tag{2.273}$$

The sum can be expressed in terms of the *polylogarithmic function* [8][3]

$$\zeta_n(z) \equiv \sum_{k=1}^\infty \frac{z^k}{k^n} \tag{2.274}$$

as

$$I_n^-(\alpha) = \Gamma(n)\zeta_n(e^\alpha). \tag{2.275}$$

---

[3]A frequently used notation for $\zeta_n(z)$ is $\text{Li}_n(z)$.

The sum in (2.273) converges only for $\alpha < 0$. In the limit $\alpha \to -0$, it has the limit

$$I_n^-(0) = \Gamma(n)\zeta(n), \qquad n > 1, \tag{2.276}$$

where $\zeta(n)$ is *Riemann's zeta function*

$$\zeta(\nu) \equiv \sum_{k=1}^{\infty} \frac{1}{k^\nu}. \tag{2.277}$$

For $n \leq 1$, the function $I_n^-(\alpha)$ diverges like $(-\alpha)^{n-1}$ in the limit $\alpha \to -0$. In the opposite limit $\alpha \to -\infty$, it goes to a constant:

$$I_n^-(\alpha) \to e^\alpha \Gamma(n). \tag{2.278}$$

This limit is needed to find the high-temperature behavior of the free Bose gas at a fixed average particle number N, as we see from Eq. (2.270). For large T, the ratio $\mu/k_B T$ diverges to $-\infty$.

In the case of fermions, the expansions (2.273), (2.275) read

$$I_n^+(\alpha) = \Gamma(n) \sum_{k=1}^{\infty} (-1)^{k-1} \frac{e^{k\alpha}}{k^n} = -\Gamma(n)\zeta_n(-e^\alpha), \tag{2.279}$$

the only difference with respect to bosons being the alternating signs in the sum. For $\alpha = 0$, this becomes

$$I_n^+(0) = \frac{1}{1} - \frac{1}{2^n} + \frac{1}{3^n} - \frac{1}{4^n} + \ldots = \sum_{k=0}^{\infty} \frac{1}{k^n} - 2^{1-n} \sum_{k=0}^{\infty} \frac{1}{k^n} = \left(1 - 2^{1-n}\right) \zeta(n). \tag{2.280}$$

In the opposite limit $\alpha \to -\infty$, the sum yields the same constant as in (2.278):

$$I_n^+(\alpha) \to e^\alpha \Gamma(n). \tag{2.281}$$

At a fixed particle number N, the chemical potential changes with temperature in a way determined by the vanishing of the derivative of (2.270), which yields the equation

$$T\partial_T \frac{\mu}{k_B T} = -3 \frac{I_{3/2}^\mp\left(\frac{\mu}{k_B T}\right)}{I_{1/2}^\mp\left(\frac{\mu}{k_B T}\right)}. \tag{2.282}$$

Here we have used the property

$$\partial_z I_n^\mp(z) = (n-1) I_{n-1}^\mp(z), \tag{2.283}$$

which follows directly from the series expansion (2.273). For large T, we obtain from Eqs. (2.276) and (2.278) the limit

$$T\partial_T \frac{\mu}{k_B T} \xrightarrow[T \to \infty]{} -\frac{3}{2}. \tag{2.284}$$

Relation (2.269) can also be obtained from the general thermodynamic calculation:

$$E - \mu N = -Z_G^{-1} \frac{\partial Z_G}{\partial \beta} = \frac{\partial}{\partial \beta} \beta F_G, \qquad (2.285)$$

which follows directly from (2.250) by differentiating with respect to $\beta = 1/k_B T$.

The grand-canonical free energy is from (2.267), using (2.260), (2.264), (2.271), and (2.272):

$$
\begin{aligned}
F_G(T, \mu, V) = -pV &= -g \frac{V}{\lambda^3(T)} k_B T \frac{2}{3} \frac{1}{\Gamma(3/2)} I_{5/2}^{\mp} \left(\frac{\mu}{k_B T} \right) \\
&= -N(T, \mu) \, k_B T \, \frac{2}{3} \frac{I_{5/2}^{\mp}(\frac{\mu}{k_B T})}{I_{3/2}^{\mp}(\frac{\mu}{k_B T})}. \qquad (2.286)
\end{aligned}
$$

For large T where $\alpha \to -\infty$, the limiting formula (2.278) shows that F_G has the correct Dulong-Petit-like behavior $-N k_B T$, implying the *ideal-gas law*

$$pV = N k_B T. \qquad (2.287)$$

Due to the relation (2.268), the energy is

$$E = N(T, \mu) \, k_B T \, \frac{I_{5/2}^{\mp}(\frac{\mu}{k_B T})}{I_{3/2}^{\mp}(\frac{\mu}{k_B T})}. \qquad (2.288)$$

For large temperatures, this has the correct Dulong-Petit limit of free particles $3 N k_B T / 2$.

We may check the first line in Eq. (2.286) by differentiating it with respect to μ and using the relation (2.283) to reobtain the thermodynamic relation $N = -\partial F_G / \partial \mu$.

According to Eq. (1.520), the entropy S is obtained from the negative derivative of (2.286) with respect to T. This yields

$$S = k_B g \frac{V}{\lambda^3(T)} \frac{2}{\sqrt{\pi}} I_S^{\mp} \left(\frac{\mu}{k_B T} \right) = g k_B N(T, \mu) \frac{2}{3} \frac{I_S^{\mp} \left(\frac{\mu}{k_B T} \right)}{I_{3/2}^{\mp} \left(\frac{\mu}{k_B T} \right)}, \qquad (2.289)$$

where

$$I_S^{\mp}(\alpha) \equiv \frac{5}{2} I_{5/2}^{\mp}(\alpha) - \alpha I_{5/2}^{\mp}{}'(\alpha) = \frac{5}{2} I_{5/2}^{\mp}(\alpha) - \frac{3}{2} \alpha I_{3/2}^{\mp}(\alpha). \qquad (2.290)$$

This agrees with the general thermodynamic relation

$$F_G(T, \mu) = E(T, \mu) - \mu N(T, \mu) - T S(T, \mu). \qquad (2.291)$$

Adiabatic processes are defined by the condition $S/N = $ const. which implies by Eq. (2.290) that the ratio $\mu/k_B T$ is also a constant. Inserting this into (2.270) with (2.271) we find that, at a constant particle number, an adiabatic process satisfies

$$VT^{3/2}|_{\text{adiab}} = \text{const.} \qquad (2.292)$$

Combining this with (2.287) leads to

$$pV^{5/3}|_{\text{adiab}} = \text{const.} \qquad (2.293)$$

The specific heat at a constant volume and particle number is found from the entropy by forming the derivative $C_V = T\partial_T S$ of Eq. (2.289). Using (2.282), this leads to

$$C_V = gk_B N \frac{1}{2}\left[5\frac{I_{5/2}^{\mp}(\alpha)}{I_{3/2}^{\mp}(\alpha)} - 9\frac{I_{3/2}^{\mp}(\alpha)}{I_{1/2}^{\mp}(\alpha)}\right], \qquad \alpha = \frac{\mu}{k_B T}. \qquad (2.294)$$

For large T, we use (2.278) again to show that this becomes a constant

$$C_V \xrightarrow[T\to\infty]{} C_V^{\text{DP}} = g\frac{3}{2}Nk_B, \qquad (2.295)$$

which complies with the classical rule of Dulong and Petit ($k_B/2$ per degree of freedom).

2.15.2 Degenerate Fermi Gas Near $T = 0$

Consider the Fermi gas close to zero temperature which is called the *degenerate limit*. Then the occupation number (2.264) reduces to

$$f_\varepsilon = \left\{\begin{array}{c} 1 \\ 0 \end{array}\right\} \quad \text{for} \quad \left\{\begin{array}{c} \varepsilon < \mu \\ \varepsilon > \mu \end{array}\right\} = \Theta(\varepsilon - \mu). \qquad (2.296)$$

All states with energy lower than μ are filled, all higher states are empty. The chemical potential μ at zero temperature is called Fermi energy ε_{F}:

$$\mu\Big|_{T=0} \equiv \varepsilon_{\text{F}}. \qquad (2.297)$$

The Fermi energy for a given particle number N is found from (2.260), (2.263), and (2.296):

$$N = gV\int_0^\infty d\varepsilon\, g_\varepsilon f_\varepsilon = gV\int_0^{\varepsilon_{\text{F}}} d\varepsilon\, g_\varepsilon = gV\frac{\sqrt{2}M^{3/2}\varepsilon_{\text{F}}^{3/2}}{3\pi^2\hbar^3} = gV\frac{p_{\text{F}}^3}{6\pi^2\hbar^3}, \qquad (2.298)$$

where

$$p_{\text{F}} = \sqrt{2M\varepsilon_{\text{F}}} \equiv \hbar k_{\text{F}} \qquad (2.299)$$

is the Fermi momentum associated with the Fermi energy. Equation (2.298) is solved for ε_{F} by

$$\varepsilon_{\text{F}} = \left(\frac{6\pi^2}{g}\right)^{2/3}\left(\frac{N}{V}\right)^{2/3}\frac{\hbar^2}{2M}, \qquad (2.300)$$

and for the Fermi momentum by

$$p_{\mathrm{F}} \equiv k_{\mathrm{F}}\hbar = \left(\frac{6\pi^2}{g}\right)^{1/3}\left(\frac{N}{V}\right)^{1/3}\hbar. \tag{2.301}$$

In two dimensions, we find

$$\varepsilon_{\mathrm{F}} = \frac{2\pi}{g}\frac{\rho}{M}. \tag{2.302}$$

Note that in terms of the particle number N, the density of states per unit energy interval and volume (2.260) can be written as

$$gg_{\varepsilon} \equiv \frac{3}{2}\frac{N}{V}\frac{1}{\varepsilon_{\mathrm{F}}}\sqrt{\frac{\varepsilon}{\varepsilon_{\mathrm{F}}}}. \tag{2.303}$$

As the gas is heated slightly, there is a softening of the degeneracy in the particle distribution (2.296). In order to study this quantitatively it is useful to define a characteristic temperature associated with the Fermi energy ε_{F}, the so-called *Fermi temperature*

$$T_{\mathrm{F}} \equiv \frac{\varepsilon_{\mathrm{F}}}{k_B} = \frac{1}{k_B}\frac{p_{\mathrm{F}}^2}{2M} = \frac{\hbar^2}{k_B}\frac{k_{\mathrm{F}}^2}{2M}. \tag{2.304}$$

For electrons in a metal, k_{F} is of the order of $1/\text{Å}$. Inserting $M = m_e = 9.109558 \times 10^{-28}$ g, $k_B = 1.380622 \times 10^{-16}$ erg/K, and $\hbar = 6.0545919 \times 10^{-27}$ erg sec, we see that the order of magnitude of T_{F} is

$$T_{\mathrm{F}} \approx 44\,000\,\mathrm{K}. \tag{2.305}$$

Hence the relation

$$T/T_{\mathrm{F}} \ll 1 \tag{2.306}$$

is quite well fulfilled even far above room temperature, and T/T_{F} can be used as an expansion parameter in evaluating the thermodynamic properties of the electron gas at nonzero temperature.

Let us do this to calculate the corrections to the above equations at small T. Eliminating the particle number in (2.270) in favor of the Fermi temperature with the help of Eqs. (2.298) and (2.304), we find the temperature dependence of the chemical potential from the equation

$$1 = \left(\frac{T}{T_{\mathrm{F}}}\right)^{3/2}\frac{3}{2}I_{3/2}^{+}\left(\frac{\mu}{k_B T}\right). \tag{2.307}$$

For $T \to 0$, the chemical potential μ approaches the Fermi energy ε_{F}, so that small T corresponds to a large reduced chemical potential $\bar{\mu} = \mu/k_B T$. Let us derive an expansion for $I_{3/2}^{+}(\bar{\mu})$ in powers of $1/\bar{\mu}$ in this regime. For this we set

$$z - \bar{\mu} \equiv x, \tag{2.308}$$

and write $I_n^+(\bar\mu)$ as

$$I_n^+(\bar\mu) \;=\; \int_{-\bar\mu}^\infty dx \frac{(\bar\mu+x)^{n-1}}{e^x+1} = \int_0^{\bar\mu} dx \frac{(\bar\mu-x)^{n-1}}{e^{-x}+1} + \int_0^\infty dx \frac{(\bar\mu+x)^{n-1}}{e^x+1}. \quad (2.309)$$

In the first integral on the right-hand side we substitute

$$\frac{1}{e^{-x}+1} = 1 - \frac{1}{e^x+1} \qquad (2.310)$$

and obtain

$$I_n^+(\bar\mu) = \int_0^{\bar\mu} dx\, x^{n-1} + \int_0^\infty dx \frac{(\bar\mu+x)^{n-1}-(\bar\mu-x)^{n-1}}{e^x+1} + \int_{\bar\mu}^\infty dx \frac{(\bar\mu-x)^{n-1}}{e^x+1}. \quad (2.311)$$

In the limit $\bar\mu\to\infty$, only the first term survives, whereas the last term

$$L(\bar\mu) \equiv \int_{\bar\mu}^\infty dx \frac{(\bar\mu-x)^{n-1}}{e^x+1} = -(-1)^n \int_0^\infty dx \frac{x^{n-1}}{e^{x+\bar\mu}+1} = (-1)^n \Gamma(n)\zeta_n(-e^{-\bar\mu}) \quad (2.312)$$

is exponentially small, so that it can be ignored in an expansion in powers of $1/\bar\mu$. The second term is expanded as

$$2\sum_{k=\text{odd}}^\infty \binom{n-1}{k} \bar\mu^{n-1-k} \int_0^\infty dx \frac{x^k}{e^x+1} = 2\sum_{k=\text{odd}} \frac{(n-1)!}{(n-1-k)!} \bar\mu^{n-1-k}(1-2^{-k})\zeta(k+1). \quad (2.313)$$

At even positive and odd negative integer arguments, the zeta function is related to the Bernoulli numbers by[4]

$$\zeta(1-2n) = -\frac{B_{2n}}{2n}, \qquad \zeta(2n) = \frac{(2\pi)^{2n}}{2(2n)!}|B_{2n}|. \qquad (2.314)$$

The two equations go over into each other via the identity

$$\zeta(x) = 2^x \pi^{x-1} \sin(\pi x/2)\Gamma(1-x)\zeta(1-x), \qquad (2.315)$$

which can also be written as

$$\zeta(x) = 2^{x-1}\pi^x \zeta(1-x)/\Gamma(x) \cos\frac{x\pi}{2}. \qquad (2.316)$$

The lowest values of $\zeta(k+1)$ occurring in the expansions (2.313) are[5]

$$\zeta(2) = \frac{\pi^2}{6}, \quad \zeta(4) = \frac{\pi^4}{90}, \quad \zeta(6) = \frac{\pi^6}{945}, \qquad (2.317)$$

---

[4]These and the subsequent formulas are found in I.S. Gradshteyn and I.M. Ryzhik, op. cit., Formulas 9.542 and 9.535.

[5]Other often-needed values are $\zeta(0) = -1/2$, $\zeta'(0) = -\log(2\pi)/2$, $\zeta(-2n) = 0$, $\zeta(3) \approx 1.202057$, $\zeta(5) \approx 1.036928, \dots$.

so that $I_n^+(\bar{\mu})$ starts out for large $\bar{\mu}$ like

$$I_n^+(\bar{\mu}) = \frac{1}{n}\bar{\mu}^n + 2(n-1)\frac{1}{2}\zeta(2)\bar{\mu}^{n-2} + 2(n-1)(n-2)(n-3)\frac{7}{8}\zeta(4)\bar{\mu}^{n-4} + \ldots . \quad (2.318)$$

Inserting this with $n = 3/2$ into Eq. (2.307), we find

$$1 = \left(\frac{T}{T_{\mathrm{F}}}\right)^{3/2}\frac{3}{2}\left[\frac{2}{3}\left(\frac{\mu}{k_BT}\right)^{3/2} + \frac{\pi^2}{12}\left(\frac{\mu}{k_BT}\right)^{-1/2} + \frac{7\pi^4}{3\cdot 320} + \left(\frac{\mu}{k_BT}\right)^{-5/2}\ldots\right]. \tag{2.319}$$

From this we derive, by inversion, a small-T/T_{F} expansion of μ/k_BT. Rewriting the latter ratio as a product $\mu/\varepsilon_{\mathrm{F}} \times T_{\mathrm{F}}/T$, we obtain for μ the series

$$\mu = \varepsilon_{\mathrm{F}}\left[1 - \frac{\pi^2}{12}\left(\frac{T}{T_{\mathrm{F}}}\right)^2 + \frac{7\pi^4}{720}\left(\frac{T}{T_{\mathrm{F}}}\right)^4 + \ldots\right]. \tag{2.320}$$

Only exponentially small terms in $e^{-T_{\mathrm{F}}/T}$ coming from the integral $L(\bar{\mu})$ of (2.312) are ignored. Inserting the chemical potential (2.320) into the grand-canonical free energy F_G, we obtain by reexpanding the first line in (2.286):

$$F_G(T,\mu,V) = F_G(0,\mu,V)\left[1 + \frac{5\pi^2}{8}\left(\frac{T}{T_{\mathrm{F}}}\right)^2 - \frac{7\pi^4}{384}\left(\frac{T}{T_{\mathrm{F}}}\right)^4 + \ldots\right], \tag{2.321}$$

where

$$F_G(0,\mu,V) \equiv -\frac{2}{5}gV\frac{\sqrt{2}M^{3/2}}{3\pi^2\hbar^3}\mu^{5/2} = -\frac{2}{5}gV\frac{k_\mu^3}{6\pi^2}\mu. \tag{2.322}$$

Here k_μ is the analog of k_{F}, to which it reduces for $T = 0$ [compare (2.299)]:

$$k_\mu \equiv \frac{1}{\hbar}\sqrt{2M\mu}. \tag{2.323}$$

At $T = 0$ where ε_{F}, we see from (2.299) that

$$F_G(0,\varepsilon_{\mathrm{F}},V) = -\frac{2}{5}N\varepsilon_F. \tag{2.324}$$

This can also be obtained from (2.286) using the limiting behavior (2.281).

By differentiating F_G with respect to the temperature at fixed μ, we obtain the low-temperature behavior of the entropy

$$S = k_B\frac{\pi^2}{2}\frac{T}{T_{\mathrm{F}}}\frac{N}{V} + \ldots , \tag{2.325}$$

and from this the specific heat

$$C_V = T\frac{\partial S}{\partial T}\bigg|_{V,N} = k_B\frac{\pi^2}{2}N\frac{T}{T_{\mathrm{F}}}. \tag{2.326}$$

This is a linear behavior with a slope C_V^{DP} of Eq. (2.295) associated with the high-temperature Dulong-Petit law:

$$C_V = C_V^{\mathrm{DP}} \times \frac{\pi^2}{3g} \frac{T}{T_{\mathrm{F}}}. \tag{2.327}$$

The linear growth is a characteristic feature of the electronic specific heat at low temperature sketched for all temperatures in Fig. 2.3. It is due to the progressive softening of the Fermi distribution with temperature, and this makes a linearly increasing number of electrons thermally excitable. This is directly observable experimentally in metals at low temperature. There the contribution of lattice vibrations are frozen out since they behave like $(T/T_D)^3$. The temperature T_D is the Debye temperature which characterizes the elastic stiffness of a crystal. It ranges typically from $T_D \approx 90\,\mathrm{K}$ in soft metals like lead, over $T_D \approx 389\,\mathrm{K}$ for aluminum, to $T_D \approx 1890\,\mathrm{K}$ for diamonds. The measured experimental slope is usually larger than that for a free electron gas in (2.326). This can be explained mainly by the effect of the lattice which leads to an increased effective mass $M_{\mathrm{eff}} > M$ of the electrons.

Note that the quantity $F_G(0, \mu, V)$ is temperature-dependent via the chemical potential μ. Inserting (2.320) into (2.321), we find the complete T-dependence

$$F_G(T, \mu, V) = F_G(0, \varepsilon_{\mathrm{F}}, V) \left[1 + \frac{5\pi^2}{12} \left(\frac{T}{T_{\mathrm{F}}} \right)^2 - \frac{\pi^4}{16} \left(\frac{k_B T}{\varepsilon_{\mathrm{F}}} \right)^4 + \dots \right] \tag{2.328}$$

with $F_G(0, \varepsilon_{\mathrm{F}}, V)$ given by Eq. (2.324) at $\mu = \varepsilon_{\mathrm{F}}$.

Recalling the relation (2.268), the above equation supplies us also with the low-temperature behavior of the internal energy:

$$E = \frac{3}{5} N \varepsilon_{\mathrm{F}} \left[1 + \frac{5\pi^2}{12} \left(\frac{T}{T_{\mathrm{F}}} \right)^2 - \frac{\pi^4}{16} \left(\frac{T}{T_{\mathrm{F}}} \right)^4 + \dots \right]. \tag{2.329}$$
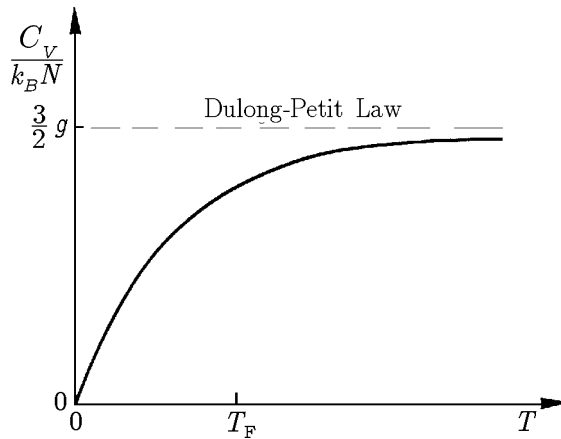

FIGURE 2.3 Temperature behavior of the specific heat of a free Fermi gas.

The first term is the energy of the zero-temperature Fermi sphere. Using the relation $C_V = \partial E/\partial T$, the second term yields once more the leading $T \to 0$ behavior (2.326) of the specific heat.

This behavior of the specific heat can be observed in metals where the conduction electrons behave like a free electron gas. Due to *Bloch's theorem*, a single electron in a perfect lattice behaves just like a free particle. For many electrons, this is still approximately true, if the mass of the electrons is replaced by an effective mass.

Another important macroscopic system, where the behavior (2.326) can be observed, is a liquid consisting of the fermionic isotope ^{3}He. There are two electron spins and an odd number of nucleon spins which make this atom a fermion. The atoms interact strongly in the liquid, but it turns out that these interactions produce a screening effect after which the system may be considered approximately as an almost-free gas of quasiparticles which behave like free fermions whose mass is about 8 times that of the strongly interacting atoms [10].

2.15.3　Degenerate Bose Gas Near $T = 0$

For bosons, the low-temperature discussion is quite different. As we can see from Eq. (2.263), the particle density remains positive for all $\varepsilon \in (0, \infty)$ only if the chemical potential μ is negative. A positive μ would also cause a divergence in the integrals (2.270), (2.272). At high temperatures, the chemical potential has a large negative value, which moves closer to zero as the temperature decreases (see Fig. 2.4, compare also with Fig. 2.1).
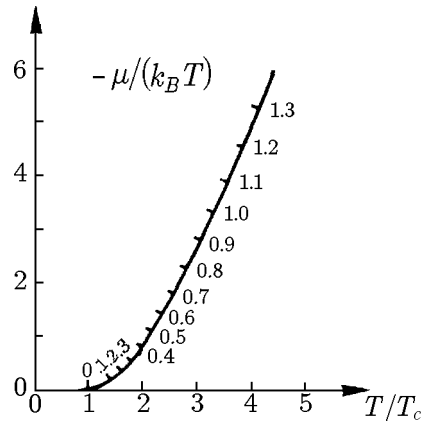
FIGURE 2.4 Temperature behavior of the chemical potential of a free Bose gas.
The chemical potential vanishes at a critical temperature T_c. From Eqs. (2.263), (2.270), and (2.276), this is determined by the equation

$$
\begin{aligned}
\frac{N}{V} &= g \int d^3p \frac{1}{e^{(\frac{\mathbf{p}^2}{2M} - \mu)/k_B T} - 1} = g \int_0^\infty d\varepsilon\, g_\varepsilon f_\varepsilon \\
&= g \frac{V}{\lambda^3(T)} \frac{2}{\sqrt{\pi}} I_{3/2}^- \left(\frac{\mu}{k_B T} \right),
\end{aligned} \tag{2.330}
$$

at $\mu = 0$, where it yields, via Eq. (2.276), the particle density

$$\frac{N}{V} = g\frac{V}{\lambda^3(T)}\zeta(3/2). \tag{2.331}$$

Thus the critical temperature T_c satisfies the equation

$$T_c = [g\zeta(3/2)]^{-2/3}\left(\frac{N}{V}\right)^{2/3}\frac{2\pi\hbar^2}{k_BM}, \tag{2.332}$$

with $\zeta(3/2) = 2.61238\ldots$.

It is interesting to rewrite this equation in natural variables. We may introduce an average distance a between the bosons by the relation $N/V \equiv 1/a^3$. There is an energy associated with it,

$$\varepsilon_a \equiv \frac{\hbar^2}{2Ma^2}, \tag{2.333}$$

and a temperature $T_a \equiv \varepsilon_a/k_B$. In these natural units, the critical temperature (2.332) of the free Bose gas is simply

$$T_c = [g\zeta(3/2)]^{-2/3}4\pi T_a. \tag{2.334}$$

We may rewrite Eq. (2.330) in the form

$$1 = \left(\frac{T}{T_c}\right)^{3/2}\frac{I_{3/2}(\bar{\mu})}{I_{3/2}(0)}, \qquad \bar{\mu} = \frac{\mu}{k_BT}. \tag{2.335}$$

For $\bar{\mu}$ between 0 and 1, this equation yields $T/T_c > 1$, while Eq. (2.294) gives us the associated specific heat. The result is displayed in Fig. 2.5. To understand the figure we must realize what happens in the regime of low temperatures $T < T_c$ where (2.270) has no solution.
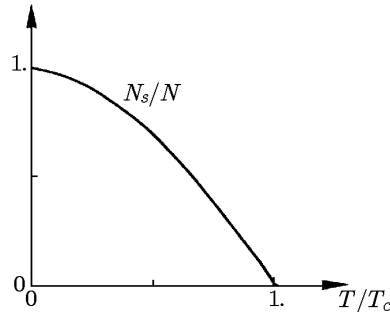

FIGURE 2.5 Temperature behavior of the fraction of zero-momentum bosons in a free Bose gas.

A glance at Eq. (2.331) shows that a phase transition takes place when the average distance a between atoms becomes smaller than the De Broglie wavelength of thermal motion (2.271). In natural units, this may be expressed as

$$\lambda(T) = \frac{1}{\sqrt{4\pi}} \sqrt{\frac{T_a}{T}}. \tag{2.336}$$

For helium, this length scale has roughly the value $5.64\,\text{Å}$.[6]

For $T < T_c$, Eq. (2.330) has no solution even though the physical system can be cooled further. The apparent contradiction has its origin in a failure of the integral approximation (2.257) to replace the sum over momenta for $T < T_c$. The reason is that the state with $\mathbf{p} = 0$ is not properly included in the energy integral over all states in Eq. (2.270). To avoid this we have to write more properly:

$$N = N_{\mathbf{p}=0} + N_{\mathbf{p}\neq 0} \equiv N_s + gV \int_0^\infty d\varepsilon\, g_\varepsilon f_\varepsilon|_{\mu=0}\,, \tag{2.337}$$

where $N_s \equiv N_{\mathbf{p}=0}$ is the number of Bose particles at zero momentum and energy. Below T_c, a finite fraction of all particles N_s/N accumulates in this single degenerate state. It can be calculated from the modified Eq. (2.330):

$$
\begin{aligned}
N - N_s &= Vg \int_0^\infty d\varepsilon\, g_\varepsilon f_\varepsilon|_{\mu=0} \\
&= g \frac{V}{\lambda^3(T)} \frac{2}{\sqrt{\pi}} I_{3/2}^-(0) = N \left(\frac{T}{T_c}\right)^{3/2}.
\end{aligned} \tag{2.338}
$$

Thus we find that the number of degenerate bosons has the temperature behavior

$$N_s = N \left[1 - \left(\frac{T}{T_c}\right)^{3/2} \right], \tag{2.339}$$

which is plotted in Fig. 2.5.

The phenomenon of a macroscopic accumulation of particles in a single state is called *Bose condensation* and plays a central role in the understanding of the phenomenon of *superfluidity* in liquid helium consisting of the bosonic atoms of ^{4}He. In fact, the temperature T_c calculated from Eq. (2.332) is $T_c \sim 3.1\,\text{K}$, which is roughly of the same order as the experimental value[7]

$$T_c^{\mathrm{exp}} \equiv 2.18\text{K}. \tag{2.340}$$

The discrepancy is due to the strong interactions between the ^{4}He atoms in the liquid state, which have all been neglected in deriving Eq. (2.340).

There exists a phenomenological two-fluid description of superfluidity in which the condensate of the $\mathbf{p} = 0$-bosons is identified with the *superfluid component* of

___

[6]See p. 256 in the textbook Ref. [11].

[7]The mass density is $\rho \approx 0.145$ g/cm^3. With the mass of the helium atoms being $M_{{}^4\mathrm{He}} \approx 4m_{\mathrm{p}} \approx 4 \times 1.6762 \times 10^{-24}$g, this implies a volume per atom of $V/N \approx 46.2\text{Å}^3$.
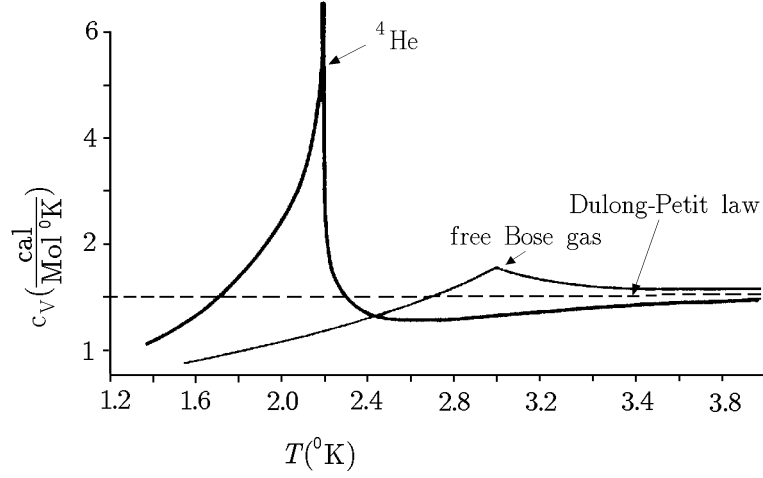
FIGURE 2.6 Temperature behavior of the specific heat of a free Bose gas. For comparison we show the specific heat of the strongly interacting Bose liquid ^{4}He, scaled down by a factor of 2 to match the Dulong-Petit limit of the free Bose gas.

the liquid. This is the reason why we have used the subscript s in (2.338). The complementary piece

$$N_n = N - N_s \qquad (2.341)$$

is usually referred to as the *normal component* of the superfluid.

For $T < T_c$, the energy of the normal liquid is equal to the total energy. Using Eq. (2.288) with $\mu = 0$ we obtain

$$
\begin{aligned}
E = E_n &= g \frac{V}{\lambda^3(T)} \frac{2}{\sqrt{\pi}} k_B T I_{5/2}^-(0) = g \frac{I_{5/2}^-(0)}{I_{3/2}^-(0)} N k_B T \left(\frac{T}{T_c}\right)^{3/2} \\
&\approx g\, 0.7703\, N k_B T \left(\frac{T}{T_c}\right)^{3/2} \equiv E_c \left(\frac{T}{T_c}\right)^{3/2},
\end{aligned} \qquad (2.342)
$$

where we have expressed $I_n^-(0)$ via Eq. (2.276). From this energy we derive the specific heat below T_c:

$$
\begin{aligned}
C_V &= T \frac{\partial S}{\partial T}\Big|_{V,N} = \frac{\partial E}{\partial T}\Big|_{V,N} \\
&= \frac{5}{2} \frac{E}{T} \propto T^{3/2}.
\end{aligned} \qquad (2.343)
$$

Integrating this with respect to the temperature gives the entropy

$$S = \frac{5}{3} \frac{E}{T}, \qquad (2.344)$$

and the free energy $F = E - TS$ takes the simple form

$$F = -\frac{2}{3} E. \qquad (2.345)$$

This is consistent with the general relation (2.268), since for $\mu = 0$ the grand canonical free energy F_G coincides with the free energy F [recall the Euler relation (1.529)].

The special role of the Bose condensate lies in the fact that it provides the system with a particle reservoir, with the relation (2.270) being replaced by Eq. (2.330) and Eq. (2.338).

Inserting (2.342) into (2.343), the low-temperature behavior of the specific heat becomes explicitly

$$C_V = \frac{\partial E}{\partial T} = gk_B N \frac{5}{2} \frac{\Gamma(5/2)\zeta(5/2)}{\Gamma(3/2)\zeta(3/2)} \left(\frac{T}{T_c}\right)^{3/2} \approx gk_B N \, 1.92567 \left(\frac{T}{T_c}\right)^{3/2}. \qquad (2.346)$$

Comparing (2.346) with (2.294) and using the fact that $I_{1/2}(0) = \infty$, we see that at T_c the peak in (2.346) has the same maximal value as in the $T > T_c$ -solution (since $I_{1/2}(0) = \infty$).

As T passes T_c, the chemical potential becomes negative. To calculate the behavior of $-\mu$ in this regime, we use Eq. (2.335), and replace $I_{3/2}^-(\bar{\mu})$ by $I_{3/2}^-(0) + \Delta I_{3/2}^-(\bar{\mu})$ with

$$\Delta I_{3/2}^-(\bar{\mu}) \;=\; \int_0^\infty dz \, z^{1/2} \left(\frac{1}{e^{z-\bar{\mu}} - 1} - \frac{1}{e^z - 1}\right). \qquad (2.347)$$

This function receives its main contribution from $z \approx 0$, where it can be approximated by[8]

$$\Delta I_{3/2}^-(\bar{\mu}) \approx \bar{\mu} \int_0^\infty dz \frac{1}{z^{1/2}(z - \bar{\mu})} = -\pi\sqrt{-\bar{\mu}}. \qquad (2.348)$$

Hence we obtain from (2.335) the relation

$$1 = \left(\frac{T}{T_c}\right)^{3/2} \left[1 + \frac{\Delta I_{3/2}^-\left(\frac{\mu}{k_B T}\right)}{I_{3/2}^-(0)}\right]. \qquad (2.349)$$

Inserting here the small-$\bar{\mu}$ behavior (2.348), we see that, for T slightly above T_c, the negative chemical potential $-\mu$ becomes nonzero behaving like

$$-\mu \approx \frac{1}{\pi^2} k_B T_c \, [I_{3/2}^-(0)]^2 \left[\left(\frac{T}{T_c}\right)^{3/2} - 1\right]^2, \qquad (2.350)$$

where $I_{3/2}^-(0)$ is given by Eq. (2.276).

Let us use this result to find the internal energy slightly above the critical temperature T_c. With the help of relation (2.268) we calculate the derivative of the energy with respect to the chemical potential as

$$\left.\frac{\partial E}{\partial \mu}\right|_{T,V} = -\frac{3}{2} \left.\frac{\partial F_G}{\partial \mu}\right|_{T,V} = \frac{3}{2} gN. \qquad (2.351)$$

---

[8]In general, the small-$\bar{\mu}$ expansion of $I_\nu^-(\bar{\mu}) = \Gamma(n)\zeta_\nu(e^{\bar{\mu}})$ follows from the so-called *Robinson expansion*: $\zeta_\nu(e^{\bar{\mu}}) = \Gamma(1 - \nu)\bar{\mu}^{\nu-1} + \zeta(\nu) + \sum_{k=1}^\infty (-\bar{\mu})^k \zeta(\nu - k)/k!$, derived in Subsec. 2.15.6 of the textbook in Ref. [1].

This allows us to find the internal energy slightly above the critical temperature T_c, where $-\mu$ is small, as

$$
\begin{aligned}
E &\approx E_c + \frac{3}{2}gN\mu \\
&= E_c - \frac{3}{2\pi^2}gNk_BT_c\,[I_{3/2}^-(0)]^2\left[\left(\frac{T}{T_c}\right)^{3/2} - 1\right]^2.
\end{aligned}
\tag{2.352}
$$

Here E_c is the internal energy at the critical point defined in Eq. (2.342). Forming the derivative with respect to the temperature as in (2.343) we see that at T_c the specific heat has a kink. Its slope jumps by

$$
\Delta\left(\frac{\partial C_V}{\partial T}\right) \approx \frac{27}{4\pi^2}[I_{3/2}^-(0)]^2\,gN\frac{k_B}{T_c} \equiv 3.6658\,gN\frac{k_B}{T_c},
\tag{2.353}
$$

the slopes being below T_c from (2.342):

$$
\left(\frac{\partial C_V}{\partial T}\right) = \frac{5}{2}\frac{3}{2}\frac{I_{5/2}(0)}{I_{3/2}(0)}\frac{gNk_B}{T_c} \approx \frac{5}{2}\frac{3}{2}0.7703\frac{gNk_B}{T_c} \approx 2.8885\frac{gNk_B}{T_c}, \quad T \leq T_c, \tag{2.354}
$$

and above T_c from (2.352):

$$
\left(\frac{\partial C_V}{\partial T}\right) = \left\{\frac{5}{2}\frac{3}{2}\frac{I_{5/2}(0)}{I_{3/2}(0)} - \frac{27}{4\pi^2}[I_{3/2}^-(0)]^2\right\}\frac{gNk_B}{T_c} \approx -0.7715\frac{gNk_B}{T_c}, \quad T > T_c. \tag{2.355}
$$

Let us compare the behavior of the specific heat of the free Bose gas with the experimental results for the Bose liquid ^{4}He (see Fig. 2.6). The latter also rises like T^3 for small T, but it has a sharp singularity at $T = T_c$. Considering the crudeness of the free-gas approximation, the similarity of the curves is quite surprising, indicating the physical relevance of the above idealized quantum-statistical description.

2.15.4 High Temperatures

At high temperatures, the particles are distributed over a large volume in phase space, so that the occupation numbers of each energy level are very small. As a consequence, the difference between bosons and fermions disappears, and the distribution functions (2.264) become

$$
f_\varepsilon \equiv -\frac{\partial}{\partial\mu}F_\varepsilon(T,\mu) \approx e^{(\mu-\varepsilon)/k_BT},
\tag{2.356}
$$

for either statistics. The high-temperature limit of the thermodynamic quantities can therefore all be calculated from the fermion expressions. The corresponding limit in the functions $I_n^\mp(\bar\mu)$ in Eq. (2.272) is $\bar\mu \to -\infty$, for which we obtain

$$
I_n^\mp(\bar\mu) \xrightarrow[\bar\mu\to-\infty]{} \int_0^\infty z^n e^{\bar\mu-z} = n!e^{\bar\mu}.
\tag{2.357}
$$

Inserting this into (2.307) for $n = 1/2$, we find that at a fixed particle number N, the chemical potential has the large-T behavior

$$\frac{\mu}{k_B T} \approx \frac{3}{2} \log \left[\frac{T}{T_{\mathrm{F}}} \left(\frac{3\sqrt{\pi}}{4} \right)^{2/3} \right]. \tag{2.358}$$

In the same limit, the grand-canonical free energy (2.286) behaves like

$$F_G(T, \mu, V) \approx -gN(T, \mu) \, k_B T. \tag{2.359}$$

With the definition of the pressure (1.527), this is the equation of state for the *ideal gas*. Using the relation (2.268), we obtain from this the internal energy at a fixed particle number

$$E \approx \frac{3}{2} g N \, k_B T. \tag{2.360}$$

This equation is a manifestation of the *Dulong-Petit law*: Each of the $3N$ degrees of freedom of the system carries an internal energy $k_B T/2$.

The corresponding specific heat per constant unit volume is

$$C_V^{\mathrm{DP}} = \frac{3}{2} g N k_B \tag{2.361}$$

[compare with the fermion formula (2.295)]. The low-temperature behavior (2.346) is related to this by the factor [compare with (2.327)]:

$$C_V \underset{\text{small } T}{\approx} C_V^{\mathrm{DP}} \times 5 \frac{\zeta(5/2)}{\zeta(3/2)} \left(\frac{T}{T_c} \right)^{3/2} \approx C_V^{\mathrm{DP}} \times 1.2838 \left(\frac{T}{T_c} \right)^{3/2}. \tag{2.362}$$

2.16   Noninteracting Bose Gas in a Trap

In 1995, Bose-Einstein condensation was observed in a dilute gas in a way that fits the above simple theoretical description [9]. When ^{87}Rb atoms were cooled down in a magnetic trap to temperatures less than 170 nK, about 50 000 atoms were observed to form a condensate, a kind of "superatom". Such condensates have been set into rotation and shown to become perforated by vortex lines [12, 13, 14] just as in rotating superfluid helium II.

2.16.1   Bose Gas in a Finite Box

Consider first the condensation process in a finite number N of bosons enclosed in a large cubic box of size L. Then the momentum sum in Eq. (2.263) has to be carried out over the discrete momentum vectors $\mathbf{p_n} = \hbar\pi(n_1, n_2, \ldots, n_D)/L$ with $n_i = 1, 2, 3, \ldots$:

$$N = \frac{V_D}{l_{\mathrm{e}}^D(\hbar\beta)} \zeta_{D/2}^{\mathrm{box}}(z) \equiv \sum_{\mathbf{P_n}} \frac{1}{e^{\beta\mathbf{p_n}^2/2M - \beta\mu} - 1}, \tag{2.363}$$

where $z \equiv e^{\mu\beta}$ is the so-called *fugacity*. This can be expressed in terms of the one-dimensional auxiliary partition function of a particle in a one-dimensional "box":

$$Z_1(b) \equiv \sum_{n=1}^{\infty} e^{-bn^2/2}, \quad b \equiv \beta\hbar^2\pi^2/ML^2 = \pi l_e^2(\hbar\beta)/2L^2. \quad (2.364)$$

Using this, we can rewrite (2.363) in the form of a so-called *fugacity expansion*

$$N = \frac{V_D}{l_e^D(\hbar\beta)}\zeta_{D/2}^{\text{box}}(z) \equiv \sum_w Z_1^D(wb)z^w, \quad (2.365)$$

where the function $Z_1(b)$ is related to the *elliptic theta function*

$$\vartheta_3(u, z) \equiv 1 + 2\sum_{n=1}^{\infty} z^{n^2}\cos 2nu \quad (2.366)$$

by $Z_1(b) = [\vartheta_3(0, e^{-b/2}) - 1]/2$. The small-$b$ behavior of this function is easily calculated as follows. We rewrite the sum as a sum over integrals

$$\begin{aligned}
\vartheta_3(0, e^{-b/2}) &= \sum_{k=-\infty}^{\infty} e^{-k^2b/2} = \sum_{m=-\infty}^{\infty}\int_{-\infty}^{\infty} dk\, e^{-k^2b/2+2\pi ikm} \\
&= \sqrt{\frac{2\pi}{b}}\left(1 + 2\sum_{m=1}^{\infty} e^{-2\pi^2m^2/b}\right). \quad (2.367)
\end{aligned}$$

Thus, up to exponentially small corrections, we may replace $\vartheta_3(0, e^{-b/2})$ by $\sqrt{2\pi/b}$, so that for small b (i.e., large $L/\sqrt{\beta}$):

$$Z_1(b) = \sqrt{\frac{\pi}{2b}} - \frac{1}{2} + \mathcal{O}(e^{-2\pi^2/b}). \quad (2.368)$$

For large b, $Z_1(b)$ falls exponentially fast to zero.

In the sum (2.363), the lowest energy level with $\mathbf{p}_{1,\dots,1} = \hbar\pi(1,\dots,1)/L$ plays a special role. Its contribution to the total particle number is the number of particles in the condensate:

$$N_{\text{cond}}(T) = \frac{1}{e^{Db/2-\beta\mu}-1} = \frac{z_D}{1-z_D}, \quad z_D \equiv e^{\beta\mu-Db/2}. \quad (2.369)$$

This number diverges for $z_D \to 1$, where the box function $\zeta_{D/2}^{\text{box}}(z)$ has a pole $1/(Db/2 - \beta\mu)$. This pole prevents $\beta\mu$ from becoming exactly equal to $Db/2$ when solving the equation (2.363) for the particle number in the box.

For a large but finite system near $T = 0$, almost all particles will go into the condensate, so that $Db/2 - \beta\mu$ will be very small, of the order $1/N$, but not zero. The thermodynamic limit can be performed smoothly by defining a regularized function $\bar{\zeta}_{D/2}^{\text{box}}(z)$ in which the lowest (singular) term in the sum (2.363) is omitted. Let us define the number of *normal* particles which have not condensed into the state of

zero momentum as $N_{\mathrm{n}}(T) = N - N_{\mathrm{cond}}(T)$. Then we can rewrite Eq. (2.363) as an equation for the number of normal particles:

$$N_{\mathrm{n}}(T) = \frac{V_D}{l_{\mathrm{e}}^D(\hbar\beta)}\bar\zeta_{D/2}^{\mathrm{box}}(z(\beta)), \qquad (2.370)$$

which reads more explicitly

$$N_{\mathrm{n}}(T) = S_D(z_D) \equiv \sum_{w=1}^{\infty}[Z_1^D(wb)e^{wDb/2} - 1]z_D^w. \qquad (2.371)$$

A would-be critical point may now be determined by setting here $z_D = 1$ and equating the resulting N_{n} with the total particle number N. If N is sufficiently large, we need only the small-b limit of $S_D(1)$ which is calculated in Appendix 2B [see Eq. (2B.14)], so that the associated temperature $T_c^{(1)}$ is determined from the equation

$$N = \sqrt{\frac{\pi}{2b_c}}^3 \zeta(3/2) + \frac{3\pi}{4b_c^{(1)}} \log C_3 b_c + \dots , \qquad (2.372)$$

where $C_3 \approx 0.0186$. In the thermodynamic limit, the critical temperature $T_c^{(0)}$ is obtained by ignoring the second term, yielding

$$N = \sqrt{\frac{\pi}{2b_c^{(0)}}}^3 \zeta(3/2), \qquad (2.373)$$

in agreement with Eq. (2.331) for T_c, if we recall b from (2.364). Using this we rewrite (2.372) as

$$1 \equiv \left(\frac{T_c^{(1)}}{T_c^{(0)}}\right)^{3/2} + \frac{3}{2N}\frac{\pi}{2b_c^{(0)}} \log C_3 b_c^{(0)}. \qquad (2.374)$$

Expressing $b_c^{(0)}$ in terms of N from (2.373), this implies

$$\frac{\delta T_c^{(1)}}{T_c^{(0)}} \approx \frac{1}{\zeta^{2/3}(3/2)N^{1/3}} \log \frac{2}{\pi C_3}\frac{N^{2/3}}{\zeta^{2/3}(3/2)}. \qquad (2.375)$$

Experimentally, the temperature $T_c^{(1)}$ is not immediately accessible. What is easy to find is the place where the condensate density has the largest curvature, i.e., where $d^3 N_{\mathrm{cond}}/dT^3 = 0$. The associated temperature T_c^{exp} is larger than $T_c^{(1)}$ by a factor $1 + \mathcal{O}(1/N)$, so that it does not modify the leading finite-size correction which is of the order $1/N^{1/3}$.

Alternatively we may use the phase space formula

$$N_{\mathrm{n}} = \int d^D x \frac{d^D p}{(2\pi\hbar)^D} \frac{1}{e^{\beta[p^2/2M+V(\mathbf{x})]} - 1} = \sum_{n=1}^{\infty} \int d^D x \frac{d^D p}{(2\pi\hbar)^D} e^{-n\beta[p^2/2M+V(\mathbf{x})]}$$

$$= \sum_{n=1}^{\infty} \frac{1}{\sqrt{2\pi\hbar^2 n\beta/M}^D} \int d^D x \, e^{-n\beta V(\mathbf{x})}, \qquad (2.376)$$

where the spatial integration produces a factor $\sqrt{2\pi/M\omega^2 n\beta}$ so that the right-hand side becomes again $(T/T_c^{(0)})^D N$.

2.16.2 Harmonic and General Power Trap

For a D-dimensional harmonic trap $V = M\omega^2 \mathbf{x}^2/2$, the critical temperature is reached if N_{n} is equal to the total particle number N where

$$k_B T_c^{(0)} = \hbar\omega \left[\frac{N}{\zeta(D)}\right]^{1/D}. \qquad (2.377)$$

This formula has a solution only for $D > 1$.

The equation (2.376) for the particle number can be easily calculated for a more general trap where the potential has the anisotropic power behavior

$$V(\mathbf{x}) = \frac{M}{2}\tilde{\omega}^2 \tilde{a}^2 \sum_{i=1}^{D} \left(\frac{|x_i|}{a_i}\right)^{p_i}. \qquad (2.378)$$

The parameter $\tilde{\omega}$ denotes some frequency parameter, and $\tilde{a}$ the geometric average $\tilde{a} \equiv \left[\Pi_{i=1}^{D} a_i\right]^{1/D}$. Inserting (2.378) into (2.376) we encounter a product of integrals:

$$\prod_{i=1}^{D} \int_{-\infty}^{\infty} dx\, e^{-n\beta M\tilde{\omega}^2\tilde{a}^2(|x_i|/a_i)^{p_i}/2} = \prod_{i=1}^{D} \frac{a_i}{(\beta M\tilde{\omega}^2\tilde{a}^2/2)^{1/p_i}}\Gamma(1+1/p_i), \qquad (2.379)$$

so that the right-hand side of (2.376) becomes $(T/T_c^{(0)})^{\tilde{D}}N$, with the critical temperature

$$k_B T_c^{(0)} = \frac{M\tilde{a}^2\tilde{\omega}^2}{2}\left(\frac{\hbar\tilde{\omega}}{M\tilde{a}^2\tilde{\omega}^2}\right)^{D/\tilde{D}}\left[\frac{N\pi^{D/2}}{\zeta(\tilde{D})\prod_{i=1}^{D}\Gamma(1+1/p_i)}\right]^{1/\tilde{D}}. \qquad (2.380)$$

Here $\tilde{D}$ is the dimensionless parameter

$$\tilde{D} \equiv \frac{D}{2} + \sum_{i=1}^{D}\frac{1}{p_i} \qquad (2.381)$$

that takes over the role of D in the harmonic formula (2.377). A harmonic trap, that has different oscillator frequencies $\omega_1, \ldots, \omega_D$ along the D Cartesian axes, is a special case of (2.378) with $p_i \equiv 2$, $\omega_i^2 = \tilde{\omega}^2\tilde{a}^2/a_i^2$, and $\tilde{D} = D$, and formula (2.380) reduces to (2.377), with ω replaced by the geometric average $\tilde{\omega} \equiv (\omega_1\cdots\omega_D)^{1/D}$ of the frequencies. The parameter $\tilde{a}$ disappears from the formula. A free Bose gas in a box of size $V_D = \prod_{i=1}^{D}(2a_i) = 2^D\tilde{a}^D$ is described by (2.378) in the limit $p_i \to \infty$, where $\tilde{D} = D/2$. Then Eq. (2.380) reduces to

$$k_B T_c^{(0)} = \frac{\pi\hbar^2}{2M\tilde{a}^2}\left[\frac{N}{\zeta(D/2)}\right]^{2/D} = \frac{2\pi\hbar^2}{M}\left[\frac{N}{V_D\zeta(D/2)}\right]^{2/D}, \qquad (2.382)$$

in agreement with Eq. (2.331).

Another interesting limiting case is that of a box of length $L = 2a_1$ in the x-direction with $p_1 = \infty$, and two different oscillators of frequency ω_2 and ω_3 in the

other two directions. To find $T_c^{(0)}$ for such a Bose gas we identify $\tilde{\omega}^2 \tilde{a}^2 / a_{2,3}^2 = \omega_{2,3}^2$ in the potential (2.378), so that $\tilde{\omega}^4 / \tilde{a}^2 = \omega_2^2 \omega_3^2 / a_1^2$, and we obtain

$$k_B T_c^{(0)} = \hbar \tilde{\omega} \left(\frac{\pi \hbar}{2M\tilde{\omega}} \right)^{1/5} \left[\frac{N}{a_1 \zeta(5/2)} \right]^{2/5} = \hbar \tilde{\omega} \left(\frac{2\pi \lambda_{\omega_1} \lambda_{\omega_2}}{L^2} \right)^{1/5} \left[\frac{N}{\zeta(5/2)} \right]^{2/5} . \quad (2.383)$$

2.16.3   Anharmonic Trap in Rotating Bose-Einstein Gas

Another interesting potential can be prepared in the laboratory by rotating a Bose condensate [13] with an angular velocity Ω around the z-axis. The vertical trapping frequency is $\omega_z \approx 2\pi \times 11.0\,\text{Hz} \approx 0.58 \times \text{nK}$, while the horizontal one is $\omega_\perp \approx 6 \times \omega_z$. The centrifugal forces create an additional repulsive harmonic potential, bringing the rotating potential to the form

$$V(\mathbf{x}) = \frac{M\omega_z^2}{2} \left(z^2 + 36\eta r_\perp^2 + \frac{\kappa}{2} \frac{r_\perp^4}{\lambda_{\omega_z}^2} \right) = \frac{\hbar \omega_z}{2} \left(\frac{z^2}{\lambda_{\omega_z}^2} + 36\eta \frac{r_\perp^2}{\lambda_{\omega_z}^2} + \frac{\kappa}{2} \frac{r_\perp^4}{\lambda_{\omega_z}^4} \right), \quad (2.384)$$

where $r_\perp^2 = x^2 + y^2$, $\eta \equiv 1 - \Omega^2/\omega_\perp^2$, $\kappa \approx 0.4$, and $\lambda_{\omega_z} \equiv 3.245\,\mu\text{m} \approx 1.42 \times 10^{-3}\,\text{K}$. For $\Omega > \omega_\perp$, η turns negative and the potential takes the form of a Mexican hat as shown in Fig. 2.7, with a circular minimum at $r_\text{m}^2 = -36\eta \lambda_{\omega_z}^2 / \kappa$. For a large rotation speed Ω, the potential may be approximated by a circular harmonic well, so that we may apply formula (2.383) with $a_1 = 2\pi r_\text{m}$, to obtain the η-independent critical temperature

$$k_B T_c^{(0)} \approx \hbar \omega_z \left(\frac{\kappa}{\pi} \right)^{1/5} \left[\frac{N}{\zeta(5/2)} \right]^{2/5} . \quad (2.385)$$

FIGURE 2.7 Rotating trap potential for $\omega^2 > 0$ and $\omega^2 < 0$, pictured for the case of two components x_1, x_2. The right-hand figure looks like a Mexican hat or the bottom of a champagne bottle.
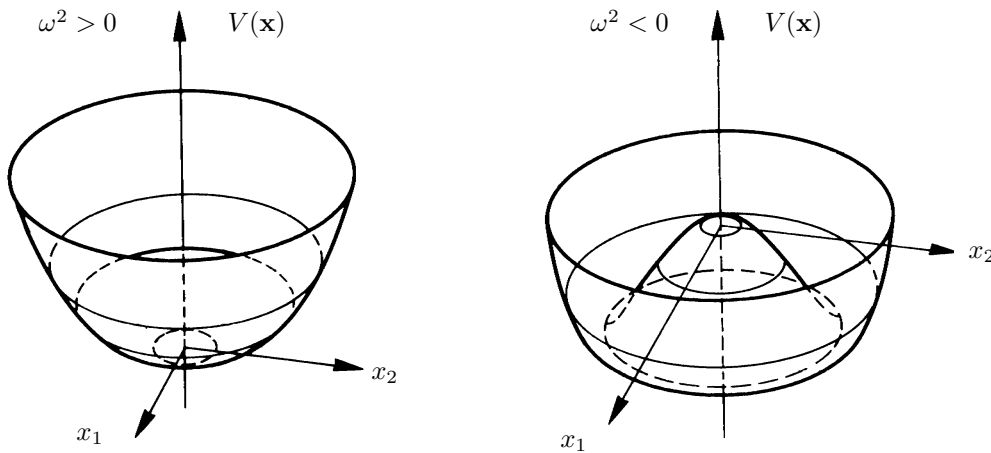
For $\kappa = 0.4$ and $N = 300\,000$, this yields $T_c \approx 53$nK.

At the critical rotation speed $\Omega = \omega_\perp$, the potential is purely quartic $r_\perp = \sqrt{(x^2 + y^2)}$. To estimate $T_c^{(0)}$ we approximate it for a moment by the slightly different potential (2.378) with the powers $p_1 = 2, p_2 = 4, p_3 = 4$, $a_1 = \lambda_{\omega_z}, a_2 = a_3 = \lambda_{\omega_z}(\kappa/2)^{1/4}$, so that formula (2.380) becomes

$$k_B T_c^{(0)} = \hbar\omega_z \left[\frac{\pi^2 \kappa}{16\Gamma^4(5/4)} \right]^{1/5} \left[\frac{N}{\zeta(5/2)} \right]^{2/5}. \tag{2.386}$$

It is easy to change this result so that it holds for the potential $\propto r^4 = (x + y)^4$ rather than $x^4 + y^4$. We use the semiclassical formula for the number of normal particles in the form

$$N_n = \int_{E_{\min}}^\infty dE \, \frac{\rho_{\rm cl}(E)}{e^{E/k_B T} - 1}, \tag{2.387}$$

where $E_{\min}$ is the classical ground state energy, and

$$\rho_{\rm cl}(E) = \left(\frac{M}{2\pi\hbar^2} \right)^{D/2} \frac{1}{\Gamma(D/2)} \int d^D x \, [E - V(\mathbf{x})]^{D/2-1} \tag{2.388}$$

is the semiclassical density of states. For a harmonic trap, the spatial integral can be done, after which the energy integral on the right-hand side of (2.387) yields $[k_B T/\hbar\omega]^D \zeta(D) = (T/T_c^{(0)})^D N$, thus leading back to (2.377). Hence the critical temperature for the potential $\propto r^4 = (x + y)^4$ rather than $x^4 + y^4$ is obtained by multiplying the right-hand side of Eq. (2.387) for N by a factor

$$\frac{2\pi \int r dr dx dy \, e^{-r^4}}{\int dx dy \, e^{-x^4 - y^4}} = \frac{\pi^{3/2}}{\Gamma[5/4]^2}. \tag{2.389}$$

This factor arrives inversely in front of N in Eq. (2.390), so that we obtain the critical temperature of the critically rotating Bose gas:

$$k_B T_c^{(0)} = \hbar\omega_z \left(\frac{4\kappa}{\pi} \right)^{1/5} \left[\frac{N}{\zeta(5/2)} \right]^{2/5}. \tag{2.390}$$

The critical temperature at $\Omega = \omega_\perp$ is therefore by a factor $4^{1/5} \approx 1.32$ larger than at infinite Ω. Actually, this limit is somewhat academic in a semiclassical approximation since it ignores the quantum nature of the oscillator.

For more details see Chapter 7 in the textbook [1].

2.17   Temperature Green Functions of Free Particles

As argued in Section 1.7, all properties of a system in thermodynamic equilibrium are calculable by continuing the quantum theory to imaginary times $t = -i\tau$, with real τ. We shall see later that the calculation of small interaction effects to the

free-particle results, presented in the last section, can be done perturbatively. It involves the analytically continued analog of the free-particle propagator (2.249).

In a grand-canonical ensemble, the relevant quantity is the so called *finite-temperature Green function* or *finite-temperature propagator* of the free particles:

$$
\begin{aligned}
G(\mathbf{x}, \tau; \mathbf{x}'\tau') &= \frac{\operatorname{Tr}\left[e^{-\hat{H}_G/k_B T}\hat{T}_\tau\left(\hat{\psi}(\mathbf{x},\tau)\hat{\psi}^\dagger(\mathbf{x}',\tau')\right)\right]}{\operatorname{Tr}\left(e^{-\hat{H}_G/k_B T}\right)} \\
&= e^{F_G/k_B T}\operatorname{Tr}\left[e^{-\hat{H}_G/k_B T}\hat{T}_\tau\left(\hat{\psi}(\mathbf{x},\tau)\hat{\psi}^\dagger(\mathbf{x}',\tau')\right)\right]. \quad (2.391)
\end{aligned}
$$

Here $\hat{T}_\tau$ is the τ-ordering operator defined in complete analogy to the time-ordering operator $\hat{T}$ in (2.231). The fields $\hat{\psi}(\mathbf{x},\tau)$, $\hat{\psi}^\dagger(\mathbf{x},\tau)$ are defined in analogy to (2.133) and (2.134) via an analytically continued time evolution operator as follows:

$$
\hat{\psi}(\mathbf{x},\tau) = e^{\hat{H}_G\tau/\hbar}a_{\mathbf{x}}e^{-\hat{H}_G\tau/\hbar}, \quad (2.392)
$$

$$
\hat{\psi}^\dagger(\mathbf{x},\tau) = e^{-\hat{H}_G\tau/\hbar}\hat{a}_{\mathbf{x}}^\dagger e^{\hat{H}_G\tau\hbar}. \quad (2.393)
$$

At equal imaginary time, these satisfy canonical commutation relations analogous to (2.205):

$$
\begin{aligned}
[\hat{\psi}(\mathbf{x},\tau),\hat{\psi}(\mathbf{x}',\tau)]_{\mp} &= 0, \\
[\hat{\psi}^\dagger(\mathbf{x},\tau),\hat{\psi}^\dagger(\mathbf{x}',\tau)]_{\mp} &= 0, \quad\quad (2.394) \\
[\hat{\psi}(\mathbf{x},\tau),\hat{\psi}^\dagger(\mathbf{x}',\tau)]_{\mp} &= \delta^{(3)}(\mathbf{x}-\mathbf{x}').
\end{aligned}
$$

The time evolution of these field operators is governed by the grand-canonical Hamiltonian

$$
\hat{H}_G = \hat{H} - \mu\hat{N}. \quad (2.395)
$$

Note that while $\psi_{\mathbf{p}}^\dagger$ in (2.393) at $\tau = 0$ is the Hermitian conjugate of $\psi_{\mathbf{p}}$ in (2.392), this is no longer true for $\tau \neq 0$. The advantages of using these non-Hermitian fields will become apparent later when we discuss perturbation theory.

When it comes to calculating physical phenomena in thermal equilibrium, all Green functions will be needed whose imaginary time τ lies in the interval

$$
\tau \in (0, \hbar/k_B T). \quad (2.396)
$$

Differentiating (2.392) and (2.393) with respect to τ, we obtain the Heisenberg equations

$$
\hat{\partial}_\tau\hat{\psi}(\mathbf{x},\tau) = [\hat{H}_G,\hat{\psi}(\mathbf{x},\tau)], \quad (2.397)
$$

$$
\hat{\partial}_\tau\hat{\psi}^\dagger(\mathbf{x},\tau) = -[\hat{H}_G,\hat{\psi}(\mathbf{x},\tau)]. \quad (2.398)
$$

Using the canonical field commutation relations (2.394), the fields $\hat{\psi}(\mathbf{x},\tau)$ and $\hat{\psi}^\dagger(\mathbf{x},\tau)$ are seen to satisfy the analytically continued Schrödinger equations

$$
\left(-\hbar\partial_\tau + \frac{\hbar^2}{2M}\partial_{\mathbf{x}}^2 + \mu\right)\hat{\psi}(\mathbf{x},\tau) = 0, \quad (2.399)
$$

$$
\hat{\psi}^\dagger(\mathbf{x},\tau)\left(\hbar\overleftarrow{\partial}_\tau + \frac{\hbar^2}{2M}\overleftarrow{\partial}_{\mathbf{x}}^2 + \mu\right) = 0. \quad (2.400)
$$

If we apply these differential operators to the Green function (2.391), we obtain the equation

$$\left(-\hbar\partial_\tau + \frac{\hbar^2}{2M}\partial_{\mathbf{x}}^2 + \mu\right) G(\mathbf{x}, \tau; \mathbf{x}'\tau')$$
$$= e^{F_G/k_B T} \mathrm{Tr}\left\{e^{-\hat{H}_G/k_B T}\delta(\tau - \tau')\left[\hat{\psi}(\mathbf{x}, \tau), \hat{\psi}^\dagger(\mathbf{x}', \tau')\right]\right\}. \qquad (2.401)$$

Using the commutation rule (2.395), this becomes

$$\left(-\hbar\partial_\tau + \frac{\hbar^2}{2M}\partial_{\mathbf{x}}^2 + \mu\right) G(\mathbf{x}, \tau; \mathbf{x}'\tau') = \delta(\tau - \tau')\delta^{(3)}(\mathbf{x} - \mathbf{x}'), \qquad (2.402)$$

which is the general defining equation of a Green function [recall (1.315)].

The plane-wave solutions of Eqs. (2.399) and (2.400) are the analytically-continued versions of the plane-wave solutions (2.206),

$$\begin{aligned}
\hat{\psi}_{\mathbf{p}}(\mathbf{x}, \tau) &= \hat{a}_{\mathbf{p}} e^{(i\mathbf{px} - \xi(\mathbf{p})\tau)/\hbar}, \\
\hat{\psi}_{\mathbf{p}}^\dagger(\mathbf{x}, \tau) &= \hat{a}_{\mathbf{p}}^\dagger e^{(-i\mathbf{px} + \xi(\mathbf{p})\tau)/\hbar},
\end{aligned} \qquad (2.403)$$

where

$$\xi(\mathbf{p}) \equiv \frac{\mathbf{p}^2}{2M} - \mu \qquad (2.404)$$

with particle energies counted from the chemical potential μ rather than from zero. The canonical field operators solving (2.399) and (2.400) have momentum-space expansions of the type (2.215), namely

$$\begin{aligned}
\hat{\psi}(\mathbf{x}, \tau) &= \int \dbar^3 p \, e^{i\mathbf{px}/\hbar - \xi(\mathbf{p})\tau/\hbar} \hat{a}_{\mathbf{p}}, \\
\hat{\psi}^\dagger(\mathbf{x}, \tau) &= \int \dbar^3 p \, e^{-i\mathbf{px}/\hbar + \xi(\mathbf{p})\tau/\hbar} \hat{a}_{\mathbf{p}}^\dagger.
\end{aligned} \qquad (2.405)$$

Inserting these into (2.391), we now calculate the Green function for $\tau > \tau'$:

$$\begin{aligned}
G(\mathbf{x}, \tau; \mathbf{x}', \tau') &= G(\mathbf{x} - \mathbf{x}', \tau - \tau') \\
&= e^{F_G/k_B T} \mathrm{Tr}\left[e^{-\hat{H}_G/k_B T} \hat{\psi}(\mathbf{x}, \tau)\hat{\psi}^\dagger(\mathbf{x}', \tau')\right] \qquad (2.406) \\
&= e^{F_G/k_B T} \int \dbar^3 p \int \dbar^3 p' \, \mathrm{Tr}(e^{-\hat{H}_G/k_B T}\hat{a}_{\mathbf{p}}\hat{a}_{\mathbf{p}'}^\dagger)e^{i[\mathbf{px} - \mathbf{p}'\mathbf{x}']/\hbar - i[\xi(\mathbf{p})\tau - \xi(\mathbf{p}')\tau']/\hbar}.
\end{aligned}$$

Here we observe that the expression

$$e^{F_G/kT}\mathrm{Tr}\left(e^{-\hat{H}_G/k_B T}\hat{a}_{\mathbf{p}}^\dagger\hat{a}_{\mathbf{p}'}\right) = \frac{\mathrm{Tr}\left(e^{-\hat{H}_G/k_B T}\hat{a}_{\mathbf{p}}^\dagger\hat{a}_{\mathbf{p}'}\right)}{\mathrm{Tr}(e^{-\hat{H}_G/k_B T})} \qquad (2.407)$$

is simply the average particle number of Eq. (2.264) for the energy $\xi(\mathbf{p})$:

$$f_{\xi(\mathbf{p})} = \frac{1}{e^{\xi(\mathbf{p})/k_B T} \mp 1}, \qquad (2.408)$$

apart from a Dirac δ-function in the momenta $\delta^{(3)}(\mathbf{p} - \mathbf{p}')$. Hence we find for $\tau > 0$:

$$G(\mathbf{x}, \tau) \equiv \int d^3 p \, e^{i\mathbf{p}\mathbf{x}/\hbar - \xi(\mathbf{p})\tau/\hbar}(1 \pm f_{\xi(\mathbf{p})}). \qquad (2.409)$$

For $\tau < 0$, the operator order is reversed, and we obtain directly

$$G(\mathbf{x}, \tau) \equiv \pm \int d^3 p \, e^{i\mathbf{p}\mathbf{x}/\hbar - \xi(\mathbf{p})\tau/\hbar} f_{\xi(\mathbf{p})}. \qquad (2.410)$$

From these expressions we can derive an important property of the temperature Green function. Using the identity

$$e^{\xi/k_B T} f_\xi = 1 \pm f_\xi, \qquad (2.411)$$

we see that $G(\mathbf{x}, \tau)$ is periodic or antiperiodic under the replacement

$$\tau \to \tau + \frac{\hbar}{k_B T}, \qquad (2.412)$$

depending on whether the particles are bosons or fermions, respectively. Explicitly. the Green function satisfies the relation

$$G(\mathbf{x}, \tau) = \pm G(\mathbf{x}, \tau + \hbar/k_B T), \qquad \tau \in (-\hbar/k_B T, \hbar/k_B T]. \qquad (2.413)$$

At zero imaginary time this reduces to $G(\mathbf{x}, 0) = \pm G(\mathbf{x}, \hbar/k_B T)$, implying that $G(\mathbf{x}, \tau)$ has a Fourier transform

$$G(\mathbf{x}, \tau) = \frac{k_B T}{\hbar} \sum_{\omega_m} e^{-i\omega_m \tau} G(\mathbf{x}, \omega_m) \qquad (2.414)$$

with the frequencies

$$\omega_m \equiv \omega_m = \frac{2\pi}{\hbar\beta} \begin{cases} m & \text{for bosons,} \\ m + \frac{1}{2} & \text{for fermions,} \end{cases} \qquad (2.415)$$

where m runs through all integer values $m = 0, \pm1, \pm2, \ldots$. These are known as *Matsubara frequencies*.

The Fourier components are given by the integrals

$$G(\mathbf{x}, \omega_m) = \int_0^{\hbar/k_B T} d\tau \, e^{i\omega_m \tau} G(\mathbf{x}, \tau). \qquad (2.416)$$

The full Fourier representation in space and imaginary time reads

$$G(\mathbf{x}, \tau) = \frac{k_B T}{\hbar} \sum_{\omega_m} \int d^3 p \, e^{-i\omega_m \tau + i\mathbf{p}\mathbf{x}/\hbar} G(\mathbf{p}, \omega_m), \qquad (2.417)$$

with the components

$$\begin{aligned}
G(\mathbf{p}, \omega_m) &= \int d^3 x \int_0^{\hbar/k_B T} d\tau \, e^{i\omega_m \tau - i\mathbf{p}\mathbf{x}/\hbar} G(\mathbf{x}, \tau) \\
&= \frac{\hbar}{i\hbar\omega_m - \xi(\mathbf{p})}(1 \pm f_{\xi(\mathbf{p})}) \left\{ e^{[i\hbar\omega_m - \xi(\mathbf{p})]/k_B T} - 1 \right\}. \qquad (2.418)
\end{aligned}$$

Inserting (2.408) and the explicit form of the Matsubara frequencies (2.415), we obtain

$$G(\mathbf{p}, \omega_m) = -\frac{\hbar}{i\hbar\omega_m - \xi(\mathbf{p})}. \tag{2.419}$$

Due to a marvelous cancellation, this has become very simple. In fact, the result can be obtained from the Fourier transform (2.248) of the quantum field theoretic Green function $G(\mathbf{p}, E)$ in two steps: First, we continue (2.248) analytically in the energy E to the imaginary off-shell values $E = i\hbar\omega_m$, and second, we shift the single-particle energy from $\varepsilon(\mathbf{p}) = \mathbf{p}^2/2M$ to $\xi(\mathbf{p}) = \varepsilon(\mathbf{p}) - \mu$, this being a trivial consequence of the use of $\hat{H}_G = \hat{H} - \mu\hat{N}$ instead of $\hat{H}$.

As a cross check, let us calculate $G(\mathbf{x}, \tau)$ for a very small negative $\tau = -\eta$ from the Fourier representation (2.417) with the components (2.419) for bosons:

$$G(\mathbf{x}, -\eta) = -\int d^3p\, e^{i\mathbf{p}\mathbf{x}/\hbar}\, \frac{k_B T}{\hbar} \sum_{\omega_m} e^{i\omega_m \eta} \frac{\hbar}{-i\omega_m + \xi(\mathbf{p})}. \tag{2.420}$$

The phase factor $e^{i\omega_m \eta}$ is necessary to ensure convergence of the otherwise logarithmically-divergent sums. The sum can be performed by rephrasing it as the contour integral

$$-k_B T \sum_{\omega_m} e^{i\omega_m \eta} \frac{1}{i\omega_m - \xi(\mathbf{p})} = \mp \frac{k_B T}{2\pi i} \int_C dz \frac{e^{\eta z}}{e^{z/k_B T} \mp 1} \frac{1}{z - \xi}. \tag{2.421}$$

The contour of integration C encircles the imaginary z-axis in the positive sense, thereby enclosing all integer or half-integer valued poles at $z = i\omega_m$. The upper signs on the right-hand side of (2.421) holds for bosons, the lower for fermions.

The closed contour C may be viewed as the result of two straight contours, which lie next to each other: one runs upwards to the right of the imaginary axis and the other that runs downwards to the left of it. The two parts may be closed by infinite semicircles Γ_l and Γ_r at infinity (see Fig. 2.8). These contribute nothing since the right-semicircle is suppressed by an exponential factor $e^{-z/k_B T}$, and the left-hand by a factor $e^{\eta z}$. The two resulting closed contours may now be distorted and shrunk to zero. There is a pole only on the right-hand side, at $z = \xi$, which contributes by Cauchy's residue theorem:

$$\mp k_B T \sum_{\omega_m} e^{i\omega_m \eta} \frac{1}{i\omega_m - \xi(\mathbf{p})} = \pm \frac{1}{e^{\xi(\mathbf{p})/k_B T} \mp 1} = \pm f_{\xi(\mathbf{p})}. \tag{2.422}$$

Via Eq. (2.420) these lead to the Bose and Fermi distribution functions represented by Eq. (2.410) for small negative τ.

In the opposite limit $\tau = +\eta$, the phase factor in the sum would be $e^{-i\omega_n \eta}$. In this case, the sum is converted into the contour integral

$$-k_B T \sum_{\omega_n} e^{i\omega_n \eta} \frac{1}{i\omega_n - \xi(\mathbf{p})} = \pm \frac{k_B T}{2\pi i} \int_C dz \frac{e^{-\eta z}}{e^{-z/k_B T} \mp 1} \frac{1}{z - \xi}, \tag{2.423}$$
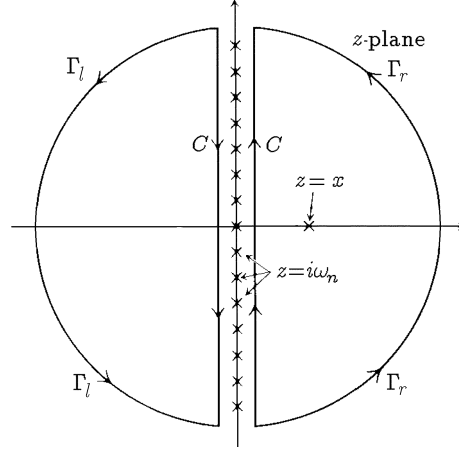
FIGURE 2.8 Contour C in the complex z-plane for evaluating the Matsubara sum (2.422). The semicircles at infinity Γ_l and Γ_r do not contribute. After shrinking the contours, only the pole on the right-hand side contributes via Cauchy's residue theorem.

from which we would find $1 \pm f_{\xi(\mathbf{p})}$, corresponding to Eq. (2.409) for small positive τ.

While the phase factors $e^{\pm i \omega_m \eta}$ are needed to make the logarithmically-divergent sums converge, they become superfluous if the two sums are combined. Indeed, adding the two sums yields

$$-k_B T \sum_{\omega_n} \left[e^{i\omega_n \eta} \frac{1}{i\omega_n - \xi} + e^{-i\omega_n \eta} \frac{1}{i\omega_n - \xi} \right] = -k_B T \sum_{\omega_n} e^{i\omega_n \eta} \left[\frac{1}{i\omega_n - \xi} + \frac{1}{-i\omega_n - \xi} \right]$$

$$= \frac{k_B T}{\hbar} \sum_{\omega_m} \frac{2\xi}{\omega_m^2 + \xi^2} = 1 \pm 2 f_\xi$$

$$= \left\{ \begin{array}{c} \coth(\hbar \xi / k_B T) \\ \tanh(\hbar \xi / k_B T) \end{array} \right\} \text{ for } \left\{ \begin{array}{c} \text{bosons} \\ \text{fermions} \end{array} \right\}. \tag{2.424}$$

The right-hand side is the thermal expectation value of $\hat{a}_{\mathbf{p}} \hat{a}_{\mathbf{p}}^\dagger + \hat{a}_{\mathbf{p}}^\dagger \hat{a}_{\mathbf{p}}$.

2.18   Calculating the Matsubara Sum via Poisson Formula

There exists another way of calculating the Matsubara sum in the finite-temperature propagator (2.417). At very low temperatures, the Matsubara frequencies $\omega_m = 2m\pi k_B T/\hbar$ or $\omega_m = (2m+1)\pi k_B T/\hbar$ move infinitely close to each other, so that the sum over ω_m becomes an integral

$$\frac{k_B T}{\hbar} \sum_{n=-\infty}^{\infty} \to \int_{-\infty}^{\infty} \frac{d\omega_m}{2\pi} \tag{2.425}$$

for Bose and Fermi fields. The propagator (2.417) becomes therefore, with (2.419),

$$
\begin{aligned}
G(\mathbf{x}, \tau) &= \frac{k_B T}{\hbar} \sum_{m=-\infty}^{\infty} \int \dbar^3 p \, e^{-i\omega_m \tau + i\mathbf{p}\mathbf{x}/\hbar} \frac{i}{\omega_m + i\xi(\mathbf{p})/\hbar} \\
&\rightarrow \int_{-\infty}^{\infty} \frac{d\omega_m}{2\pi} \int \dbar^3 p \, e^{-i\omega_m \tau + i\mathbf{p}\mathbf{x}/\hbar} \frac{i}{\omega_m + i\xi(\mathbf{p})/\hbar}.
\end{aligned}
\tag{2.426}
$$

The integral over ω_m can be performed trivially with the help of the residue theorem, as in Eq. (2.243), yielding

$$
G(\mathbf{p}, \tau) = \int_{-\infty}^{\infty} \frac{d\omega_m}{2\pi} e^{-i\omega_m \tau} \frac{i}{\omega_m + i\xi(\mathbf{p})/\hbar} = \Theta(\tau) e^{-\xi(\mathbf{p})\tau/\hbar}.
\tag{2.427}
$$

For finite temperatures we make use of Poisson's summation formula (1.213) to write

$$
\sum_{m=-\infty}^{\infty} f(m) = \int_{-\infty}^{\infty} d\mu \sum_{n=-\infty}^{\infty} e^{2\pi i \mu n} f(\mu),
\tag{2.428}
$$

from which we derive

$$
\sum_{m=-\infty}^{\infty} f(m+1/2) = \int_{-\infty}^{\infty} d\mu \sum_{n=-\infty}^{\infty} (-)^n e^{2\pi i \mu n} f(\mu).
\tag{2.429}
$$

A direct application of this formula shows that

$$
\frac{k_B T}{\hbar} \sum_{m=-\infty}^{\infty} e^{-i\omega_m \tau} \frac{i}{\omega_m + i\xi(\mathbf{p})/\hbar} = \sum_{n=-\infty}^{\infty} \left\{ \begin{matrix} 1 \\ (-1)^n \end{matrix} \right\} \Theta(\tau + n\hbar\beta) e^{-\xi(\mathbf{p})(\tau + n\hbar\beta)/\hbar}.
\tag{2.430}
$$

Thus the finite-temperature Green function is obtained from the zero-temperature function by making it periodic or antiperiodic by forming a simple sum over all periods, with equal or alternating signs. This guarantees the property (2.413). The sum over n on the right-hand side of (2.430) is a geometric series in powers of $e^{-\xi(\mathbf{p})n\hbar\beta}$, which can be performed trivially. For $\tau \in (0, \hbar\beta)$, the Heaviside function forces the sum to run only over positive n, so that we find

$$
G(\mathbf{p}, \tau) = \sum_{n=0}^{\infty} \left\{ \begin{matrix} 1 \\ (-1)^n \end{matrix} \right\} \Theta(\tau + n\hbar\beta) e^{-\xi(\mathbf{p})\tau/\hbar} e^{-n\xi(\mathbf{p})\beta} = \frac{e^{-\xi(\mathbf{p})\tau/\hbar}}{1 \mp e^{-\xi(\mathbf{p})\beta}}.
\tag{2.431}
$$

This can also be rewritten in terms of the Bose and Fermi distribution functions (2.408) as

$$
G(\mathbf{p}, \tau) = e^{-\xi(\mathbf{p})\tau/\hbar} \left(1 \pm f_{\xi(\mathbf{p})} \right).
\tag{2.432}
$$

For free particles with zero chemical potential where $\xi(\mathbf{p}) = \mathbf{p}^2/2M$, the momentum integral can be done at zero temperature as in Eq. (2.239), and we obtain the imaginary-time version of the Schrödinger propagator (2.241):

$$
\begin{aligned}
G(\mathbf{x}, \tau; \mathbf{x}', \tau') &= \Theta(\tau - \tau') \frac{1}{\sqrt{2\pi\hbar^2(\tau - \tau')/M}^3} e^{-M(\mathbf{x}-\mathbf{x}')^2/2\hbar^2(\tau - \tau')} \\
&= G(\mathbf{x} - \mathbf{x}', \tau - \tau').
\end{aligned}
\tag{2.433}
$$

This Gaussian function coincides with the end-to-end distribution of random walk of length proportional to $\hbar(\tau - \tau')$. Thus the quantum-mechanical propagator is a complex version of a particle performing a random walk. The random walk is caused by *quantum fluctuations*. This fluctuation picture of the Schrödinger theory is exhibited best in the path-integral formulation of quantum mechanics.[9] In the imaginary-time formulation of quantum field theory, we describe ensembles of particles. They correspond therefore to ensembles of random walks of fixed length. For this reason, nonrelativistic quantum field theories can be used efficiently to formulate theories of fluctuating polymers. In this context, they are called *disorder field theories*.[10].

2.19   Nonequilibrium Quantum Statistics

The physical systems which can be described by the above imaginary-time Green functions are quite limited. They must be in thermodynamic equilibrium, with a constant temperature enforced by a thermal reservoir. Only then can a partition function and a particle distribution be calculated from an analytic continuation of quantum-mechanical time evolution amplitudes to an imaginary time $t_b - t_a = -i\hbar/k_B T$. In this section we want to go beyond such equilibrium physics and extend the path-integral formalism to nonequilibrium time-dependent phenomena.

2.19.1   Linear Response and Time-Dependent Green Functions for $T \neq 0$

If the deviations of a quantum system from thermal equilibrium are small, the easiest description of nonequilibrium phenomena proceeds via the *theory of linear response*. In operator quantum mechanics, this theory is introduced as follows. First, the system is assumed to have a time-independent Hamiltonian operator $\hat{H}$. The ground state is determined by the Schrödinger equation, evolving as a function of time according to the equation

$$|\Psi_S(t)\rangle = e^{-i\hat{H}t}|\Psi_S(0)\rangle \tag{2.434}$$

(in natural units with $\hbar = 1$, $k_B = 1$). The subscript S denotes the Schrödinger picture.

Next, the system is slightly disturbed by adding to $\hat{H}$ a time-dependent external interaction,

$$\hat{H} \rightarrow \hat{H} + \hat{H}^{\text{ext}}(t), \tag{2.435}$$

where $\hat{H}^{\text{ext}}(t)$ is assumed to set in at some time t_0, i.e., $\hat{H}^{\text{ext}}(t)$ vanishes identically for $t < t_0$. The disturbed Schrödinger ground state has the time dependence

$$|\Psi_S^{\text{dist}}(t)\rangle = e^{-i\hat{H}t}\hat{U}_H(t)|\Psi_S(0)\rangle, \tag{2.436}$$

---

[9]See the textbook Ref. [1].
[10]See the textbooks Refs. [1] and [11].

where $\hat{U}_H(t)$ is the time translation operator in the Heisenberg picture. It satisfies the equation of motion

$$i\dot{\hat{U}}_H(t) = \hat{H}_H^{\mathrm{ext}}(t)\hat{U}_H(t), \tag{2.437}$$

with[11]

$$\hat{H}_H^{\mathrm{ext}}(t) \equiv e^{i\hat{H}t}\hat{H}^{\mathrm{ext}}(t)e^{-i\hat{H}t}. \tag{2.438}$$

To lowest-order perturbation theory, the operator $\hat{U}_H(t)$ is given by

$$\hat{U}_H(t) = 1 - i\int_{t_0}^t dt'\,\hat{H}_H^{\mathrm{ext}}(t') + \cdots. \tag{2.439}$$

In the sequel, we shall assume the onset of the disturbance to lie at $t_0 = -\infty$. Consider an arbitrary time-independent Schrödinger observable $\hat{O}$ whose Heisenberg representation has the time dependence

$$\hat{O}_H(t) = e^{i\hat{H}t}\hat{O}e^{-i\hat{H}t}. \tag{2.440}$$

Its time-dependent expectation value in the disturbed state $|\Psi_S^{\mathrm{dist}}(t)\rangle$ is given by

$$\begin{aligned}
\langle\Psi_S^{\mathrm{dist}}(t)|\hat{O}|\Psi_S^{\mathrm{dist}}(t)\rangle &= \langle\Psi_S(0)|\hat{U}_H^\dagger(t)e^{i\hat{H}t}\hat{O}e^{-i\hat{H}t}\hat{U}_H(t)|\Psi_S(0)\rangle \\
&\approx \langle\Psi_S(0)|\left(1 + i\int_{-\infty}^t dt'\,\hat{H}_H^{\mathrm{ext}}(t') + \ldots\right)\hat{O}_H(t) \\
&\quad \times \left(1 - i\int_{-\infty}^t dt'\,\hat{H}_H^{\mathrm{ext}}(t') + \ldots\right)|\Psi_S(0)\rangle \\
&= \langle\Psi_H|\hat{O}_H(t)|\Psi_H\rangle - i\langle\Psi_H|\int_{-\infty}^t dt'\,\left[\hat{O}_H(t), \hat{H}_H^{\mathrm{ext}}(t')\right]|\Psi_H\rangle + \ldots. \quad (2.441)
\end{aligned}$$

We have identified the time-independent Heisenberg state with the time-dependent Schrödinger state at zero time in the usual manner, i.e., $|\Psi_H\rangle \equiv |\Psi_S(0)\rangle$. Thus the expectation value of $\hat{O}$ deviates from equilibrium by

$$\begin{aligned}
\delta\langle\Psi_S(t)|\hat{O}|\Psi_S(t)\rangle &\equiv \langle\Psi_S^{\mathrm{dist}}(t)|\hat{O}(t)|\Psi_S^{\mathrm{dist}}(t)\rangle - \langle\Psi_S(t)|\hat{O}(t)|\Psi_S(t)\rangle \\
&= -i\int_{-\infty}^t dt'\,\langle\Psi_H|\left[\hat{O}_H(t), \hat{H}_H^{\mathrm{ext}}(t')\right]|\Psi_H\rangle. \quad (2.442)
\end{aligned}$$

If the left-hand side is transformed into the Heisenberg picture, it becomes

$$\delta\langle\Psi_S(t)|\hat{O}|\Psi_S(t)\rangle = \delta\langle\Psi_H|\hat{O}_H(t)|\Psi_H\rangle = \langle\Psi_H|\delta\hat{O}_H(t)|\Psi_H\rangle,$$

---

[11] Note that after the replacements $H \to H_0$, $H_H^{\mathrm{ext}} \to H_I^{\mathrm{int}}$, Eq. (2.437) coincides with the equation for the time evolution operator in the interaction picture to appear in Section 9.1.3. In contrast to that section, however, the present interaction is a nonpermanent artifact to be set equal to zero at the end, and H is the complicated total Hamiltonian, not a simple free one. This is why we do not speak here of an interaction picture.

so that Eq. (2.442) takes the form

$$\langle \Psi_H | \delta \hat{O}_H(t) | \Psi_H \rangle = -i \int_{-\infty}^{t} dt' \, \langle \Psi_H | \left[\hat{O}_H(t), \hat{H}_H^{\text{ext}}(t') \right] | \Psi_H \rangle. \qquad (2.443)$$

It is useful to use the retarded Green function of the operators $\hat{O}_H(t)$ and $\hat{H}_H(t')$ in the state $|\Psi_H\rangle$

$$G_{OH}^R(t, t') \equiv \Theta(t - t') \langle \Psi_H | \left[\hat{O}_H(t), \hat{H}_H(t') \right] | \Psi_H \rangle. \qquad (2.444)$$

Then the deviation from equilibrium is given by the integral

$$\langle \Psi_H | \delta \hat{O}_H(t) | \Psi_H \rangle = -i \int_{-\infty}^{\infty} dt' \, G_{OH}^R(t, t'). \qquad (2.445)$$

Suppose now that the observable $\hat{O}_H(t)$ is capable of undergoing oscillations. Then an external disturbance coupled to $\hat{O}_H(t)$ will in general excite these oscillations. The simplest coupling is a linear one, with an interaction energy

$$\hat{H}^{\text{ext}}(t) = -\hat{O}_H(t) \delta j(t), \qquad (2.446)$$

where $j(t)$ is some external source. Inserting (2.446) into (2.445) yields the linear-response formula

$$\langle \Psi_H | \delta \hat{O}_H(t) | \Psi_H \rangle = i \int_{-\infty}^{\infty} dt' \, G_{OO}^R(t, t') \delta j(t'), \qquad (2.447)$$

where G_{OO}^R is the retarded Green function of two operators $\hat{O}$:

$$G_{OO}^R(t, t') = \Theta(t - t') \langle \Psi_H | \left[\hat{O}_H(t), \hat{O}_H(t') \right] | \Psi_H \rangle. \qquad (2.448)$$

At frequencies where the Fourier transform of $G_{OO}(t, t')$ is singular, the slightest disturbance causes a large response. This is the well-known resonance phenomenon found in any oscillating system. Whenever the external frequency ω hits an eigenfrequency, the Fourier transform of the Green function diverges. Usually, the eigenfrequencies of a complicated N-body system are determined by calculating (2.448) and by finding the singularities in ω.

It is easy to generalize this description to a thermal ensemble at a nonzero temperature. The principal modification consists in the replacement of the ground state expectation by the thermal average

$$\langle \hat{O} \rangle_T \equiv \frac{\text{Tr} \left(e^{-\hat{H}/T} \hat{O} \right)}{\text{Tr} \left(e^{-\hat{H}/T} \right)}.$$

Using the free energy

$$F = -T \log \text{Tr} \left(e^{-\hat{H}/T} \right),$$

this can also be written as

$$\langle \hat{O} \rangle_T = e^{F/T} \text{Tr}\,(e^{-\hat{H}/T}\hat{O}). \tag{2.449}$$

In a grand-canonical ensemble, $\hat{H}$ must be replaced by $\hat{H} - \mu\hat{N}$ and F by its grand-canonical version F_G (see Section 1.16). At finite temperatures, the linear-response formula (2.447) becomes

$$\delta\langle\hat{O}(t)\rangle_T = i \int_{-\infty}^{\infty} dt'\, G_{OO}^R(t,t')\delta j(t'), \tag{2.450}$$

where $G_{OO}^R(t,t')$ is the *retarded Green function at nonzero temperature* defined by [recall (1.313)]

$$G_{OO}^R(t,t') \equiv G_{OO}^R(t-t') \equiv \Theta(t-t')\,e^{F/T}\text{Tr}\left\{e^{-\hat{H}/T}\left[\hat{O}_H(t),\hat{O}_H(t')\right]\right\}. \tag{2.451}$$

In a realistic physical system, there are usually many observables, say $\hat{O}_H^i(t)$ for $i = 1, 2, \ldots, l$, which perform coupled oscillations. Then the relevant retarded Green function is some $l \times l$ matrix

$$G_{ij}^R(t,t') \equiv G_{ij}^R(t-t') \equiv \Theta(t-t')\,e^{F/T}\text{Tr}\left\{e^{-\hat{H}/T}\left[\hat{O}_H^i(t),\hat{O}_H^j(t')\right]\right\}. \tag{2.452}$$

After a Fourier transformation and diagonalization, the singularities of this matrix render the important physical information on the resonance properties of the system.

The retarded Green function at $T \neq 0$ occupies an intermediate place between the real-time Green function of field theories at $T = 0$, and the imaginary-time Green function used before to describe thermal equilibria at $T \neq 0$. The Green function (2.452) depends both on the real time and on the temperature via an imaginary time.

2.19.2 Spectral Representations of Green Functions for $T \neq 0$

The retarded Green functions are related to the imaginary-time Green functions of equilibrium physics by an analytic continuation. For two arbitrary operators $\hat{O}_H^1$, $\hat{O}_H^2$, the latter is defined by the thermal average

$$G_{12}(\tau, 0) \equiv G_{12}(\tau) \equiv e^{F/T}\text{Tr}\left[e^{-\hat{H}/T}\hat{T}_\tau\hat{O}_H^1(\tau)\hat{O}_H^2(0)\right], \tag{2.453}$$

where $\hat{O}_H(\tau)$ is the *imaginary-time Heisenberg operator*

$$\hat{O}_H(\tau) \equiv e^{\hat{H}\tau}\hat{O}e^{-\hat{H}\tau}. \tag{2.454}$$

To see the relation between $G_{12}(\tau)$ and the retarded Green function $G_{12}^R(t)$, we take a complete set of states $|n\rangle$, insert them between the operators $\hat{O}^1$, $\hat{O}^2$, and expand $G_{12}(\tau)$ for $\tau \geq 0$ into the spectral representation

$$G_{12}(\tau) = e^{F/T}\sum_{n,n'}e^{-E_n/T}e^{(E_n-E_{n'})\tau}\langle n|\hat{O}^1|n'\rangle\langle n'|\hat{O}^2|n\rangle. \tag{2.455}$$

Since $G_{12}(\tau)$ is periodic under $\tau \to \tau + 1/T$, its Fourier representation contains only the discrete Matsubara frequencies $\omega_m = 2\pi m T$:

$$
\begin{aligned}
G_{12}(\omega_m) &= \int_0^{1/T} d\tau \, e^{i\omega_m \tau} G_{12}(\tau) \\
&= e^{F/T} \sum_{n,n'} e^{-E_n/T} \left(1 - e^{(E_n - E_{n'})/T} \right) \langle n|\hat{O}^1|n'\rangle\langle n'|\hat{O}^2|n\rangle \\
&\qquad\qquad\qquad\qquad \times \frac{-1}{i\omega_m - E_{n'} + E_n}.
\end{aligned}
\tag{2.456}
$$

The retarded Green function satisfies no periodic (or antiperiodic) boundary condition. It possesses Fourier components with *all* real frequencies ω:

$$
\begin{aligned}
G_{12}^R(\omega) &= \int_{-\infty}^{\infty} dt \, e^{i\omega t} \, \Theta(t) e^{F/T} \mathrm{Tr} \left\{ e^{-\hat{H}/T} \left[\hat{O}_H^1(t), \hat{O}_H^2(0) \right]_{\mp} \right\} \\
&= e^{F/T} \int_0^{\infty} dt \, e^{i\omega t} \sum_{n,n'} \Big[\ e^{-E_n/T} e^{i(E_n - E_{n'})t} \langle n|\hat{O}^1|n'\rangle\langle n'|\hat{O}^2|n\rangle \\
&\qquad\qquad \mp e^{-E_n/T} e^{-i(E_n - E_{n'})t} \langle n|\hat{O}^2|n'\rangle\langle n'|\hat{O}^1|n\rangle \Big].
\end{aligned}
\tag{2.457}
$$

In the second sum we exchange n and n' and perform the integral, after having attached to ω an infinitesimal positive-imaginary part $i\eta$ to ensure convergence. The result is

$$
\begin{aligned}
G_{12}^R(\omega) &= e^{F/T} \sum_{n,n'} e^{-E_n/T} \left[1 - e^{(E_n - E_{n'})/T} \right] \langle n|\hat{O}^1|n'\rangle\langle n'|\hat{O}^2|n\rangle \\
&\qquad\qquad\qquad \times \frac{i}{\omega - E_{n'} + E_n + i\eta}.
\end{aligned}
\tag{2.458}
$$

By comparing this with (2.456), we see that the thermal Green functions are obtained from the retarded ones by the replacement (for a discussion see [15])

$$
\frac{i}{\omega - E_{n'} + E_n + i\eta} \to \frac{-1}{i\omega_m - E_{n'} + E_n}.
\tag{2.459}
$$

A similar procedure holds for fermion operators $\hat{O}^i$ (which are not observable). There are only two changes with respect to the boson case. First, in the Fourier expansion of the imaginary-time Green functions, the bosonic Matsubara frequencies ω_m in (2.456) become fermionic. Second, in the definition of the retarded Green functions (2.452), the commutator is replaced by an anticommutator, i.e., the retarded Green function of fermion operators $\hat{O}_H^i$ is defined by

$$
G_{ij}^R(t,t') \equiv G_{ij}^R(t - t') \equiv \Theta(t - t') e^{F/T} \mathrm{Tr} \left\{ e^{-\hat{H}/T} \left[\hat{O}_H^i(t), \hat{O}_H^j(t') \right]_+ \right\}.
\tag{2.460}
$$

These changes produce an opposite sign in front of the $e^{(E_n - E_{n'})/T}$-term in both of the formulas (2.456) and (2.458). Apart from that, the relation between the two Green functions is again given by the replacement rule (2.459).

At this point it is customary to introduce the *spectral function*

$$\rho_{12}(\omega') = \left(1 \mp e^{-\omega'/T}\right) e^{F/T}$$

$$\times \sum_{n,n'} e^{-E_n/T} 2\pi \delta(\omega - E_{n'} + E_n)\langle n|\hat{O}^1|n'\rangle\langle n'|\hat{O}^2|n\rangle, \qquad (2.461)$$

where the upper and the lower sign hold for bosons and fermions, respectively. Under an interchange of the two operators it behaves like

$$\rho_{12}(\omega') = \mp\rho_{12}(-\omega'). \qquad (2.462)$$

Using this spectral function, we may rewrite the Fourier-transformed retarded and thermal Green functions as the following spectral integrals:

$$G_{12}^R(\omega) = \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \rho_{12}(\omega') \frac{i}{\omega - \omega' + i\eta}, \qquad (2.463)$$

$$G_{12}(\omega_m) = \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \rho_{12}(\omega') \frac{-1}{i\omega_m - \omega'}. \qquad (2.464)$$

These equations show how the imaginary-time Green functions arise from the retarded Green functions by a simple analytic continuation in the complex frequency plane to the discrete Matsubara frequencies, $\omega \to i\omega_m$. The inverse problem is not solvable. It is impossible to reconstruct the retarded Green functions in the entire upper half-plane of ω from the imaginary-time Green functions defined only at the Matsubara frequencies ω_m. The problem is solvable only approximately if other information is available [16]. For instance, the sum rules for canonical fields, which will be derived later in Eq. (2.499) with the ensuing asymptotic condition (2.500), are sufficient to make the continuation unique [17].

Going back to the time variables t and τ, the Green functions are

$$G_{12}^R(t) = \Theta(t) \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \rho_{12}(\omega') e^{-i\omega' t}, \qquad (2.465)$$

$$G_{12}(\tau) = \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \rho_{12}(\omega') T \sum_{\omega_m} e^{-i\omega_m \tau} \frac{-1}{i\omega_m - \omega'}. \qquad (2.466)$$

The sum over even or odd Matsubara frequencies on the right-hand side of $G_{12}(\tau)$ was evaluated before as [recall (2.422)]

$$T\sum_n e^{-i\omega_m \tau} \frac{-1}{i\omega_m - \omega} = G_{\omega,e}^p(\tau) = e^{-\omega(\tau - 1/2T)} \frac{1}{2\sin(\omega/2T)}$$

$$= e^{-\omega\tau}(1 + f_\omega), \qquad (2.467)$$

and

$$T\sum_n e^{-i\omega_m \tau} \frac{-1}{i\omega_m - \omega} = G_{\omega,e}^a(\tau) = e^{-\omega(\tau - 1/2T)} \frac{1}{2\cos(\omega/2T)}$$

$$= e^{-\omega\tau}(1 - f_\omega), \qquad (2.468)$$

with the Bose and Fermi distribution functions (2.422)

$$f_\omega = \frac{1}{e^{\omega/T} \mp 1}, \qquad (2.469)$$

respectively.

2.20   Other Important Green Functions

In studying the dynamics of systems at finite temperature, several other Green functions are useful. Let us derive their spectral functions and general properties.

By complete analogy with the retarded Green functions for bosonic and fermionic operators, we may introduce their counterparts, the so-called *advanced Green functions* (compare page 39):

$$G_{12}^A(t,t') \equiv G_{12}^A(t-t') = -\Theta(t'-t)e^{F/T}\mathrm{Tr}\left\{ e^{-\hat{H}/T}\left[\hat{O}_H^1(t), \hat{O}_H^2(t')\right]_\mp \right\}. \quad (2.470)$$

Their Fourier transforms have the spectral representation

$$G_{12}^A(\omega) = \int_{-\infty}^\infty \frac{d\omega'}{2\pi}\, \rho_{12}(\omega')\frac{i}{\omega - \omega' - i\eta}, \qquad (2.471)$$

differing from the retarded case (2.463) only by the sign of the $i\eta$-term. This makes the Fourier transforms vanish for $t > 0$, so that the time-dependent Green function has the spectral representation [compare (2.465)]

$$G_{12}^A(t) = -\Theta(-t)\int_{-\infty}^\infty \frac{d\omega}{2\pi}\, \rho_{12}(\omega)e^{-i\omega t}. \qquad (2.472)$$

By subtracting retarded and advanced Green functions, we obtain the thermal expectation value of commutator or anticommutator:

$$C_{12}(t,t') = e^{F/T}\mathrm{Tr}\left\{ e^{-\hat{H}/T}\left[\hat{O}_H^1(t), \hat{O}_H^2(t')\right]_\mp \right\} = G_{12}^R(t,t') - G_{12}^A(t,t'). \quad (2.473)$$

Note the simple relations:

$$\begin{aligned} G_{12}^R(t,t') &= \Theta(t-t')C_{12}(t,t'), & (2.474)\\ G_{12}^A(t,t') &= -\Theta(t'-t)C_{12}(t,t'). & (2.475) \end{aligned}$$

When inserting into (2.473) the spectral representations (2.463) and (2.472) of $G_{12}^R(t)$ and $G_{12}^A(t)$ and using the identity (1.337),

$$\frac{i}{\omega - \omega' + i\eta} - \frac{i}{\omega - \omega' - i\eta} = 2\frac{\eta}{(\omega-\omega')^2 + \eta^2} = 2\pi\delta(\omega-\omega'), \qquad (2.476)$$

we obtain the spectral integral representation for the commutator function:[12]

$$C_{12}(t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \, \rho_{12}(\omega) e^{-i\omega t}. \tag{2.477}$$

Thus a knowledge of the commutator function $C_{12}(t)$ determines directly the spectral function $\rho_{12}(\omega)$ by its Fourier components

$$C_{12}(\omega) = \rho_{12}(\omega). \tag{2.478}$$

An important role in studying the dynamics of a system in a thermal environment is played by the time-ordered Green functions. They are defined by

$$G_{12}(t, t') \equiv G_{12}(t - t') = e^{F/T} \mathrm{Tr} \left[e^{-\hat{H}/T} \, \hat{T} \hat{O}_H^1(t) \hat{O}_H^2(t') \right]. \tag{2.479}$$

Inserting intermediate states as in (2.456) we find the spectral representation

$$
\begin{aligned}
G_{12}(\omega) &= \int_{-\infty}^{\infty} dt \, e^{i\omega t} \, \Theta(t) \; e^{F/T} \mathrm{Tr} \left\{ e^{-\hat{H}/T} \hat{O}_H^1(t) \hat{O}_H^2(0) \right\} \\
&+ \int_{-\infty}^{\infty} dt \, e^{i\omega t} \, \Theta(-t) e^{F/T} \mathrm{Tr} \left\{ e^{-\hat{H}/T} \hat{O}_H^2(t) \hat{O}_H^1(0) \right\} \\
&= e^{F/T} \int_0^{\infty} dt \, e^{i\omega t} \sum_{n,n'} e^{-E_n/T} e^{i(E_n - E_{n'})t} \; \langle n|\hat{O}^1|n'\rangle \langle n'|\hat{O}^2|n\rangle \\
&\pm \; e^{F/T} \int_{-\infty}^{0} dt \, e^{i\omega t} \sum_{n,n'} e^{-E_n/T} e^{-i(E_n - E_{n'})t} \langle n|\hat{O}^2|n'\rangle \langle n'|\hat{O}^1|n\rangle .
\end{aligned} \tag{2.480}
$$

Interchanging again n and n', this can be written in terms of the spectral function (2.461) as

$$G_{12}(\omega) = \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \rho_{12}(\omega') \left[\frac{1}{1 \mp e^{-\omega'/T}} \frac{i}{\omega - \omega' + i\eta} + \frac{1}{1 \mp e^{\omega'/T}} \frac{i}{\omega - \omega' - i\eta} \right]. \tag{2.481}$$

Let us also write down the spectral decomposition of a further operator expression complementary to $C_{12}(t)$ of (2.473), in which boson or fermion fields appear with the "wrong" commutator:

$$A_{12}(t - t') \equiv e^{F/T} \mathrm{Tr} \left\{ e^{-\hat{H}/T} \left[\hat{O}_H^1(t), \hat{O}_H^2(t') \right]_{\pm} \right\}. \tag{2.482}$$

This function characterizes the size of fluctuations of the operators O_H^1 and O_H^2. Inserting intermediate states, we find

$$
\begin{aligned}
A_{12}(\omega) &= \int_{-\infty}^{\infty} dt \, e^{i\omega t} e^{F/T} \mathrm{Tr} \left\{ e^{-\hat{H}/T} \left[\hat{O}_H^1(t), \hat{O}_H^2(0) \right]_{\pm} \right\} \\
&= e^{F/T} \int_{-\infty}^{\infty} dt \, e^{i\omega t} \sum_{n,n'} \left[\; e^{-E_n/T} e^{i(E_n - E_{n'})t} \langle n|\hat{O}^1|n'\rangle \langle n'|\hat{O}^2|n\rangle \right. \\
&\qquad\qquad \left. \pm e^{-E_n/T} e^{-i(E_n - E_{n'})t} \langle n|\hat{O}^2|n'\rangle \langle n'|\hat{O}^1|n\rangle \right].
\end{aligned} \tag{2.483}
$$

---

[12]Due to the relation (2.474), the same representation is found by dropping the factor $\Theta(t)$ in (2.465).

In the second sum we exchange n and n' and perform the integral, which now runs over the entire time interval and therefore gives a δ-function:

$$
\begin{aligned}
A_{12}(\omega) \;=\; & e^{F/T} \sum_{n,n'} e^{-E_n/T} \left[1 \pm e^{(E_n - E_{n'})/T} \right] \langle n|\hat{O}^1|n'\rangle \langle n'|\hat{O}^2|n\rangle \\
& \times 2\pi \delta(\omega - E_{n'} + E_n).
\end{aligned} \tag{2.484}
$$

In terms of the spectral function (2.461), this has the simple form

$$
A_{12}(\omega) \;=\; \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \tanh^{\mp 1} \frac{\omega'}{2T} \rho_{12}(\omega') \, 2\pi \delta(\omega - \omega') = \tanh^{\mp 1} \frac{\omega}{2T} \rho_{12}(\omega). \tag{2.485}
$$

Thus the expectation value (2.482) of the "wrong" commutator has the time dependence

$$
A_{12}(t, t') \equiv A_{12}(t - t') = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \rho_{12}(\omega) \tanh^{\mp 1} \frac{\omega}{2T} e^{-i\omega(t - t')}. \tag{2.486}
$$

There exists another way of writing the spectral representation of the various Green functions. For retarded and advanced Green functions G_{12}^R, G_{12}^A, we decompose in the spectral representations (2.463) and (2.471) according to the rule (1.338):

$$
\frac{i}{\omega - \omega' \pm i\eta} = i \left[\frac{\mathcal{P}}{\omega - \omega'} \mp i\pi \delta(\omega - \omega') \right], \tag{2.487}
$$

where $\mathcal{P}$ indicates principal value integration across the singularity, leading to

$$
G_{12}^{R,A}(\omega) = i \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \rho_{12}(\omega') \left[\frac{\mathcal{P}}{\omega - \omega'} \mp i\pi \delta(\omega - \omega') \right]. \tag{2.488}
$$

Inserting (2.487) into (2.481) we find the alternative representation of the time-ordered Green function

$$
G_{12}(\omega) \;=\; i \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \rho_{12}(\omega') \left[\frac{\mathcal{P}}{\omega - \omega'} - i\pi \tanh^{\mp 1} \frac{\omega}{2T} \delta(\omega - \omega') \right]. \tag{2.489}
$$

The term proportional to $\delta(\omega - \omega')$ in the spectral representation is commonly referred to as the *absorptive* or *dissipative part* of the Green function. The first term proportional to the principal value is called the *dispersive* or *fluctuation part*.

The relevance of the spectral function $\rho_{12}(\omega')$ in determining both the *fluctuation part* as well as the *dissipative part* of the time-ordered Green function is the content of the important *fluctuation-dissipation theorem*. In more detail, this may be restated as follows: The common spectral function $\rho_{12}(\omega')$ which appears in the commutator function in (2.477), in the retarded Green function in (2.463), and in the *fluctuation part* of the time-ordered Green function in (2.489) determines, after multiplication by a factor $\tanh^{\mp 1}(\omega'/2T)$, the *dissipative part* of the time-ordered Green function in Eq. (2.489).

The three Green functions $-iG_{12}(\omega)$, $-iG_{12}^R(\omega)$, and $-iG_{12}^A(\omega)$ have the same real parts. By comparing Eqs. (2.463) and (2.464), we see that retarded and advanced

Green functions are simply related to the imaginary-time Green function via an analytic continuation. The spectral decomposition (2.489) shows that this is not true for the time-ordered Green function, due to the extra factor $\tanh^{\mp 1}(\omega/2T)$ in the absorptive term.

Another representation of the time-ordered Green function is useful. It is obtained by expressing $\tan^{\mp 1}$ in terms of the Bose and Fermi distribution functions (2.469) as $\tan^{\mp 1} = 1 \pm 2 f_\omega$. Then we can decompose

$$G_{12}(\omega) \;\; = \;\; \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \, \rho_{12}(\omega') \left[\frac{i}{\omega - \omega' + i\eta} \pm 2\pi f_\omega \, \delta(\omega - \omega') \right]. \qquad (2.490)$$

2.21 Hermitian Adjoint Operators

If the two operators $\hat{O}_H^1(t)$, $\hat{O}_H^2(t)$ are Hermitian adjoint to each other,

$$\hat{O}_H^2(t) = [\hat{O}_H^1(t)]^\dagger, \qquad (2.491)$$

the spectral function (2.461) can be rewritten as

$$\begin{aligned} \rho_{12}(\omega') \;\; = \;\; & (1 \mp e^{-\omega'/T}) e^{F/T} \\ & \times \sum_{n,n'} e^{-E_n/T} 2\pi \delta(\omega' - E_{n'} + E_n) |\langle n|\hat{O}_H^1(t)|n'\rangle\|^2. \end{aligned} \qquad (2.492)$$

This shows that

$$\begin{aligned} \rho_{12}(\omega')\omega' \;\; &\geq 0 \qquad \text{for bosons,} \\[6pt] \rho_{12}(\omega') \;\; &\geq 0 \qquad \text{for fermions.} \end{aligned} \qquad (2.493)$$

This property makes it possible to derive several useful inequalities between various diagonal Green functions.

Under the condition (2.491), the expectation values of anticommutators and commutators satisfy the time-reversal relations

$$\begin{aligned} G_{12}^A(t,t') \;\; &= \;\; \mp G_{21}^R(t',t)^*, & (2.494) \\ A_{12}(t,t') \;\; &= \;\; \pm A_{21}(t',t)^*, & (2.495) \\ C_{12}(t,t') \;\; &= \;\; \mp C_{21}(t',t)^*, & (2.496) \\ G_{12}(t,t') \;\; &= \;\; \pm G_{21}(t',t)^*. & (2.497) \end{aligned}$$

Examples are the corresponding functions for creation and annihilation operators which will be treated in detail below. More generally, these properties hold for any interacting nonrelativistic particle fields $\hat{O}_H^1(t) = \hat{\psi}_{\mathbf{p}}(t)$, $\hat{O}_H^2(t) = \hat{\psi}_{\mathbf{p}}^\dagger(t)$ of a specific momentum $\mathbf{p}$.

Such operators satisfy, in addition, the canonical equal-time commutation rules at each momentum:

$$\left[\hat{\psi}_{\mathbf{p}}(t), \hat{\psi}_{\mathbf{p}}^\dagger(t) \right] = 1. \qquad (2.498)$$

Using (2.473) and (2.477), we derive from this the *spectral function sum rule*:

$$\int_{-\infty}^{\infty} \frac{d\omega'}{2\pi}\rho_{12}(\omega') = 1. \tag{2.499}$$

For a canonical free field with $\rho_{12}(\omega') = 2\pi\delta(\omega'-\omega)$, this sum rule is of course trivially fulfilled. In general, the sum rule ensures the large-ω behavior of imaginary-time Green functions of canonically conjugate field operators, the retarded expressions depending on real time, and the advanced expressions to be the same as for a free particle, i.e.,

$$G_{12}(\omega_m) \xrightarrow[\omega_m\to\infty]{} \frac{i}{\omega_m}, \quad G_{12}^{R,A}(\omega) \xrightarrow[\omega\to\infty]{} \frac{1}{\omega}. \tag{2.500}$$

2.22   Harmonic Oscillator Green Functions for $T \neq 0$

As an example, consider a single harmonic oscillator of frequency Ω or, equivalently, a free particle at a point in the second-quantized field formalism. We shall start with the second representation.

2.22.1   Creation Annihilation Operators

The operators $\hat{O}_H^1(t)$ and $\hat{O}_H^2(t)$ are the creation and annihilation operators in the Heisenberg picture

$$\hat{a}_H^\dagger(t) = \hat{a}^\dagger e^{i\Omega t}, \quad \hat{a}_H(t) = \hat{a}e^{-i\Omega t}. \tag{2.501}$$

The eigenstates of the Hamilton operator

$$\hat{H} = \frac{1}{2}\left(\hat{p}^2 + \Omega^2\hat{x}^2\right) = \frac{\omega}{2}\left(\hat{a}^\dagger\hat{a} + \hat{a}\hat{a}^\dagger\right) = \omega\left(\hat{a}^\dagger\hat{a} \pm \frac{1}{2}\right) \tag{2.502}$$

are

$$|n\rangle = \frac{1}{\sqrt{n!}}(\hat{a}^\dagger)^n|0\rangle, \tag{2.503}$$

with the eigenvalues $E_n = (n \pm 1/2)\Omega$ for $n = 0, 1, 2, 3, \ldots$ or $n = 0, 1$, if $\hat{a}^\dagger$ and $\hat{a}$ commute or anticommute, respectively. In the second-quantized field interpretation the energies are $E_n = n\Omega$ and the final Green functions are the same. The spectral function $\rho_{12}(\omega')$ is trivial to calculate. The Schrödinger operator $\hat{O}^2 = \hat{a}^\dagger$ can connect the state $|n\rangle$ only to $\langle n+1|$, with the matrix element $\sqrt{n+1}$. The operator $\hat{O}^1 = \hat{a}$ does the opposite. Hence we have

$$\rho_{12}(\omega') = 2\pi\delta(\omega' - \Omega)(1 \mp e^{-\Omega/T})e^{F/T}\sum_{n=0}^{\infty,0} e^{-(n\pm1/2)\Omega/T}(n+1). \tag{2.504}$$

Now we make use of the explicit partition functions of the oscillator whose paths satisfy periodic and antiperiodic boundary conditions:

$$Z_\Omega \equiv e^{-F/T} = \sum_{n=0}^{\infty,1} e^{-(n\pm 1/2)\Omega/T} = \left\{ \begin{array}{cc} [2\sinh(\Omega/2T)]^{-1} & \text{bosons} \\ 2\cosh(\Omega/2T) & \text{fermions} \end{array} \right\}. \quad (2.505)$$

These allow us to calculate the sums in (2.504) as follows

$$\sum_{n=0}^{\infty} e^{-(n+1/2)\Omega/T}(n+1) = \left(-T\frac{\partial}{\partial\Omega} + \frac{1}{2}\right)e^{-F/T} = \left(1 \mp e^{-\Omega/T}\right)^{-1} e^{-F/T},$$

$$\sum_{n=0}^{0} e^{-(n-1/2)\Omega/T}(n+1) = e^{\Omega/2T} = \left(1 + e^{-\Omega/T}\right)^{-1} e^{-F/T}. \quad (2.506)$$

The spectral function $\rho_{12}(\omega')$ of the single oscillator quantum of frequency Ω is therefore given by

$$\rho_{12}(\omega') = 2\pi\delta(\omega' - \Omega). \quad (2.507)$$

With it, the retarded and imaginary-time Green functions become

$$G_\Omega^R(t,t') = \Theta(t-t')e^{-\Omega(t-t')}, \quad (2.508)$$

$$G_\Omega(\tau,\tau') = -T\sum_{m=-\infty}^{\infty} e^{-i\omega_m(\tau-\tau')} \frac{1}{i\Omega_m - \Omega} \quad (2.509)$$

$$= e^{-\Omega(\tau-\tau')} \left\{ \begin{array}{c} 1 \pm n_\Omega \\ \pm n_\Omega \end{array} \right. \quad \text{for} \quad \tau \begin{array}{c} \geq \\ < \end{array} \tau', \quad (2.510)$$

with the average particle number f_Ω of (2.469). The commutation function, for instance, is by (2.477) and (2.507):

$$C_{12}(t,t') = e^{-i\Omega(t-t')}, \quad (2.511)$$

and the correlation function of the "wrong commutator" is from (2.486) and (2.507):

$$A_\Omega(t,t') = \tanh^{\mp 1} \frac{\Omega}{2T} e^{-i\Omega(t-t')}. \quad (2.512)$$

Of course, these harmonic-oscillator expressions could have been obtained directly by starting from the defining operator equations. For example, the commutator function

$$C_\Omega(t,t') = e^{F/T}\text{Tr}\left\{e^{-\hat{H}/T}[\hat{a}_H(t), \hat{a}_H^\dagger(t')]_\mp\right\} \quad (2.513)$$

turns into (2.511) by using the commutation rule at different times:

$$[\hat{a}_H(t), \hat{a}_H^\dagger(t')] = e^{-i\Omega(t-t')}, \quad (2.514)$$

which follows from (2.501). Since the right-hand side is a *c*-number, the thermodynamic average is trivial:

$$e^{F/T}\mathrm{Tr}\left(e^{-\hat{H}/T}\right) = 1. \tag{2.515}$$

After this, the relations (2.474) and (2.475) determine the retarded and advanced Green functions

$$G_{\Omega}^{R}(t-t') = \Theta(t-t')e^{-i\Omega(t-t')}, \quad G_{\Omega}^{A}(t-t') = -\Theta(t'-t)e^{-i\Omega(t-t')}. \tag{2.516}$$

For the Green function at imaginary times

$$G_{\Omega}(\tau,\tau') \equiv e^{F/T}\mathrm{Tr}\left[e^{-\hat{H}/T}\hat{T}_{\tau}\hat{a}_{H}(\tau)\hat{a}_{H}^{\dagger}(\tau')\right], \tag{2.517}$$

the expression (2.510) is found using [see (2.518)]

$$\begin{aligned}
\hat{a}_{H}^{\dagger}(\tau) &\equiv e^{\hat{H}\tau}\hat{a}^{\dagger}e^{-\hat{H}\tau} = \hat{a}^{\dagger}e^{\Omega\tau}, \\
\hat{a}_{H}(\tau) &\equiv e^{\hat{H}\tau}\hat{a}e^{-\hat{H}\tau} = \hat{a}e^{-\Omega\tau},
\end{aligned} \tag{2.518}$$

and the summation formula (2.506).

The "wrong" commutator function (2.512) can, of course, be immediately derived from the definition

$$A_{12}(t-t') \equiv e^{F/T}\mathrm{Tr}\left\{e^{-\hat{H}/T}\left[\hat{a}_{H}(t),\hat{a}_{H}^{\dagger}(t')\right]_{\pm}\right\} \tag{2.519}$$

using (2.501) and inserting intermediate states.

For the temporal behavior of the time-ordered Green function we find from (2.481):

$$G_{\Omega}(\omega) = \left(1 \mp e^{-\Omega/T}\right)^{-1}G_{\Omega}^{R}(\omega) + \left(1 \mp e^{\Omega/T}\right)^{-1}G_{\Omega}^{A}(\omega), \tag{2.520}$$

and from this by a Fourier transformation:

$$\begin{aligned}
G_{\Omega}(t,t') &= \left(1 \mp e^{-\Omega/T}\right)^{-1}\Theta(t-t')e^{-i\Omega(t-t')} - \left(1 \mp e^{\Omega/T}\right)^{-1}\Theta(t'-t)e^{-i\Omega(t-t')} \\
&= \left[\Theta(t-t') \pm (e^{\Omega/T} \mp 1)^{-1}\right]e^{-i\Omega(t-t')} = \left[\Theta(t-t') \pm f_{\Omega}\right]e^{-i\Omega(t-t')}.
\end{aligned} \tag{2.521}$$

The same result is easily obtained by directly evaluating the defining equation using (2.501) and inserting intermediate states:

$$\begin{aligned}
G_{\Omega}(t,t') &\equiv G_{\Omega}(t-t') = e^{F/T}\mathrm{Tr}\left[e^{-\hat{H}/T}\,\hat{T}\hat{a}_{H}(t)\hat{a}_{H}^{\dagger}(t')\right] \\
&= \Theta(t-t')\langle\hat{a}\,\hat{a}^{\dagger}\rangle e^{-i\Omega(t-t')} \pm \Theta(t'-t)\langle\hat{a}^{\dagger}\,\hat{a}\rangle e^{-i\Omega(t-t')} \\
&= \Theta(t-t')(1 \pm f_{\Omega})e^{-i\Omega(t-t')} \pm \Theta(t'-t)f_{\Omega}e^{-i\Omega(t-t')},
\end{aligned} \tag{2.522}$$

which is the same as (2.521). For the correlation function with a and $a^{\dagger}$ interchanged,

$$\bar{G}_{\Omega}(t,t') \equiv G_{\Omega}(t-t') = e^{F/T}\mathrm{Tr}\left[e^{-\hat{H}/T}\,\hat{T}\hat{a}_{H}^{\dagger}(t)\hat{a}_{H}(t')\right], \tag{2.523}$$

we find in this way

$$\begin{aligned}
\bar{G}_{\Omega}(t,t') &= \Theta(t-t')\langle\hat{a}^{\dagger}\,\hat{a}\rangle e^{-i\Omega(t-t')} \pm \Theta(t'-t)\langle\hat{a}\,\hat{a}^{\dagger}\rangle e^{-i\Omega(t-t')} \\
&= \Theta(t-t')f_{\Omega}e^{-i\Omega(t-t')} \pm \Theta(t'-t)(1 \pm f_{\Omega})e^{-i\Omega(t-t')}
\end{aligned} \tag{2.524}$$

in agreement with (2.497).

2.22.2   Real Field Operators

From the above expressions it is easy to construct the corresponding Green functions for the position operators of the harmonic oscillator $\hat{x}(t)$. It will be useful to keep the discussion more general by admitting oscillators which are not necessarily mass points in space but can be field variables. Thus we shall use, instead of $\hat{x}(t)$, the symbol $\varphi(t)$, and call this a field variable. We decompose the field as

$$\hat{x}(t) = \sqrt{\frac{\hbar}{2M\Omega}} \left(\hat{a} e^{-i\Omega t} + \hat{a}^{\dagger} e^{i\Omega t} \right), \tag{2.525}$$

using in this section physical units. The commutator function (2.473) is directly

$$C(t,t') \equiv \langle [\hat{\varphi}(t), \hat{\varphi}(t')]_{\mp} \rangle_{\rho} = -\frac{\hbar}{2M\Omega} 2i \sin \Omega(t-t'), \tag{2.526}$$

implying a spectral function [recall (2.477)]

$$\rho(\omega') = \frac{1}{2M\Omega} 2\pi \left[\delta(\omega' - \Omega) - \delta(\Omega' + \Omega) \right]. \tag{2.527}$$

The real operator $\hat{\varphi}(t)$ behaves like the difference of a particle of frequency Ω and $-\Omega$, with an overall factor $1/2M\Omega$. It is then easy to find the retarded and advanced Green functions of the operators $\hat{\varphi}(t)$ and $\hat{\varphi}(t')$:

$$G^R(t,t') = \frac{\hbar}{2M\Omega} \left[G^R_{\Omega}(t,t') - G^R_{-\Omega}(t,t') \right] = -\frac{\hbar}{2M\Omega} \Theta(t-t') \, 2i \sin \Omega(t-t'), \tag{2.528}$$

$$G^A(t,t') = \frac{\hbar}{2M\Omega} \left[G^A_{\Omega}(t,t') - G^A_{-\Omega}(t,t') \right] = \frac{\hbar}{2M\Omega} \Theta(t-t') \, 2i \sin \Omega(t'-t). \tag{2.529}$$

From the spectral representation (2.486), we obtain for the "wrong commutator"

$$A(t,t') = \langle [\hat{\varphi}(t), \hat{\varphi}(t')]_{\mp} \rangle = \frac{\hbar}{2M\Omega} \coth^{\pm 1} \frac{\Omega}{2k_B T} 2 \cos \Omega(t-t'). \tag{2.530}$$

The relation with (2.526) is again a manifestation of the fluctuation-dissipation theorem (2.486).

    The average of these two functions yields the time-dependent correlation function at finite temperature, containing only the product of the operators:

$$G^P(t,t') \equiv \langle \hat{\varphi}(t) \hat{\varphi}(t') \rangle = \frac{\hbar}{2M\Omega} \left[(1 \pm 2f_{\Omega}) \cos \Omega(t-t') - i \sin \Omega(t-t') \right], \tag{2.531}$$

with the average particle number f_{Ω} of (2.469). In the limit of zero temperature where $f_{\Omega} \equiv 0$, this reduces to

$$G^P(t,t') = \langle \hat{\varphi}(t) \hat{\varphi}(t') \rangle = \frac{\hbar}{2M\Omega} e^{-i\Omega(t-t')}. \tag{2.532}$$

The time-ordered Green function is obtained from this by the obvious relation

$$G(t, t') = \Theta(t - t')G^P(t, t') \pm \Theta(t' - t)G^P(t', t) = \frac{1}{2}\left[A(t, t') + \epsilon(t - t')C(t, t')\right],$$
(2.533)

where $\epsilon(t - t')$ is the step function of Eq. (1.323). Explicitly, the time-ordered Green function is

$$G(t, t') \equiv \langle \hat{T}\hat{\varphi}(t)\hat{\varphi}(t')\rangle = \frac{\hbar}{2M\Omega}\left[(1 \pm 2f_\Omega)\cos\Omega|t - t'| - i\sin\Omega|t - t'|\right], \quad (2.534)$$

which reduces for $T \to 0$ to

$$G(t, t') = \langle \hat{T}\hat{\varphi}(t)\hat{\varphi}(t')\rangle = \frac{\hbar}{2M\Omega}e^{-i\Omega|t - t'|}. \tag{2.535}$$

Thus, as a mnemonic rule, a finite temperature is introduced into a zero-temperature Green function by simply multiplying the real part of the exponential function by a factor $1 \pm 2f_\Omega$. This is another way of stating the *fluctuation-dissipation theorem*.

There is another way of writing the time-ordered Green function (2.534) in the bosonic case:

$$G(t, t') \equiv \langle \hat{T}\hat{\varphi}(t)\hat{\varphi}(t')\rangle = \frac{\hbar}{2M\Omega}\frac{\cosh\left[\frac{\Omega}{2}\left(\hbar\beta - i|t - t'|\right)\right]}{\sinh\frac{\hbar\Omega\beta}{2}}. \tag{2.536}$$

For $t - t' > 0$, this coincides precisely with the periodic Green function $G_e^p(\tau, \tau') = G_e^p(\tau - \tau')$ at imaginary-times $\tau > \tau'$ [see (2.431)], if τ and τ' are continued analytically to it and it', respectively. Decomposing (2.534) into real and imaginary parts, we see by comparison with (2.533) that anticommutator and commutator functions are the doubled real and imaginary parts of the time-ordered Green function:

$$A(t, t') = 2\operatorname{Re}G(t, t'), \qquad C(t, t') = 2i\operatorname{Im}G(t, t'). \tag{2.537}$$

In the fermionic case, the hyperbolic functions cosh and sinh in numerator and denominator are simply interchanged, and the result coincides with the analytically continued antiperiodic imaginary-time Green function [see again (2.431)].

For real fields $\hat{\varphi}(t)$, the time-reversal properties (2.494)–(2.497) of the Green functions become

$$\begin{aligned}
G^A(t, t') &= \mp G^R(t', t), & (2.538) \\
A(t, t') &= \pm A(t', t), & (2.539) \\
C(t, t') &= \mp C(t', t), & (2.540) \\
G(t, t') &= \pm G(t', t). & (2.541)
\end{aligned}$$

Appendix 2A   Permutation Group and Representations on n-Particle Wave Functions

A permutation of n particles is given by

$$P = \begin{pmatrix} 1 & 2 & \dots & n \\ p(1) & p(2) & \dots & p(n) \end{pmatrix}, \tag{2A.1}$$

where $p(i)$ are all possible one-to-one mappings of the integers $1, 2, 3, \dots, n$ onto themselves. In the notation (2A.1) the order of the columns is irrelevant, i.e., the same permutation can be written in any other form in which the columns are interchanged with each other, for example:

$$P = \begin{pmatrix} 2 & 1 & \dots & n \\ p(2) & p(1) & \dots & p(n) \end{pmatrix}. \tag{2A.2}$$

Given n particles at positions $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n$, the permutation P may be taken to change the position $\mathbf{x}_1$ to $\mathbf{x}_{p(1)}$, $\mathbf{x}_2$ to $\mathbf{x}_{p(2)}$, etc., i.e., we define P to act directly on the indices:

$$P\mathbf{x}_i \equiv \mathbf{x}_{p(i)}. \tag{2A.3}$$

Given an n-particle wave function $\psi(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n; t)$, it behaves under P as follows:

$$\begin{aligned} P\psi(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n; t) &= \psi(P\mathbf{x}_1, P\mathbf{x}_2, \dots, P\mathbf{x}_n; t) \\ &= \psi(\mathbf{x}_{p(1)}, \mathbf{x}_{p(2)}, \dots, \mathbf{x}_{p(n)}; t). \end{aligned} \tag{2A.4}$$

There exists a different but equivalent definition of permutations, to be denoted by P', in which the variables $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n$ of the wave functions are taken from their places $1, 2, \dots, n$ in the list of arguments of $\psi(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n; t)$ and moved to the positions $p(1), p(2), \dots, p(n)$ in this list, i.e.,

$$P'\psi(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n; t) \equiv \psi(\dots, \mathbf{x}_1, \dots, \mathbf{x}_2, \dots; t), \tag{2A.5}$$

where $\mathbf{x}_1$ is now at position $p(1)$, $\mathbf{x}_2$ at position $p(2)$, etc. The difference between the two definitions is seen in the simple example:

$$\begin{pmatrix} 1 & 2 & 3 \\ 2 & 3 & 1 \end{pmatrix} \psi(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3; t) = \psi(\mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_1; t), \tag{2A.6}$$

to be compared with

$$\begin{pmatrix} 1 & 2 & 3 \\ 2 & 3 & 1 \end{pmatrix}' \psi(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3; t) = \psi(\mathbf{x}_3, \mathbf{x}_1, \mathbf{x}_2; t). \tag{2A.7}$$

In the following we shall use only the first definition, but all statements to be derived would hold as well if we use the second one throughout the remainder of this appendix.

For n elements there are $n!$ different permutations P. Given any two permutations

$$P = \begin{pmatrix} 1 & \dots & n \\ p(1) & \dots & p(n) \end{pmatrix}$$

and

$$Q = \begin{pmatrix} 1 & \dots & n \\ q(1) & \dots & q(n) \end{pmatrix},$$

a product is defined by rewriting Q as

$$Q = \begin{pmatrix} p(1) & \dots & p(n) \\ q(p(1)) & \dots & q(p(n)) \end{pmatrix}$$

and setting

$$
\begin{aligned}
QP &\equiv \begin{pmatrix} p(1) & \dots & p(n) \\ q(p(1)) & \dots & q(p(n)) \end{pmatrix} \begin{pmatrix} 1 & \dots & n \\ p(1) & \dots & p(n) \end{pmatrix} \\
&\equiv \begin{pmatrix} 1 & \dots & n \\ q(p(1)) & \dots & q(p(n)) \end{pmatrix}.
\end{aligned} \tag{2A.8}
$$

Every element has an inverse. Indeed, if we apply first P and multiply it by

$$
P^{-1} \equiv \begin{pmatrix} p(1) & \dots & p(n) \\ 1 & \dots & n \end{pmatrix}, \tag{2A.9}
$$

the operation $P^{-1}P$ returns all elements to their original places:

$$
P^{-1}P = \begin{pmatrix} p(1) & \dots & p(n) \\ 1 & \dots & n \end{pmatrix} \begin{pmatrix} 1 & \dots & n \\ p(1) & \dots & p(n) \end{pmatrix} = \begin{pmatrix} 1 & \dots & n \\ 1 & \dots & n \end{pmatrix} \equiv I. \tag{2A.10}
$$

The right-hand side is defined as the *identity permutation I*.

It can easily be checked that for three permutations PQR, the product is associative:

$$
P(QR) = (PQ)R. \tag{2A.11}
$$

Thus the $n!$ permutations of n elements form a group, also called the *symmetric group S_n*.

If P is such that only two elements $p(i)$ are different from i, it can be written as

$$
T_{ij} = \left\{ \begin{matrix} 1 & 2 & \dots & i & \dots & j & \dots & n \\ 1 & 2 & \dots & p(i) & \dots & p(j) & \dots & n \end{matrix} \right\}. \tag{2A.12}
$$

It is called a *transposition*, also denoted in short by (i, j). Only the elements i and j are interchanged. Every permutation can be decomposed into a product of transpositions. There are many ways of doing this. However, each permutation decomposes either into an even or an odd number of transpositions. Therefore each permutation can be characterized by this property. As mentioned on p. 86, it is called the *parity of the permutation*. It is useful to introduce the function

$$
\epsilon_P = \left\{ \begin{matrix} 1 \\ -1 \end{matrix} \right\} \quad \text{for} \quad \left\{ \begin{matrix} P = \text{even} \\ P = \text{odd} \end{matrix} \right\}, \tag{2A.13}
$$

which indicates the parity. This function satisfies the identity

$$
\epsilon_{PQ} \equiv \epsilon_P \epsilon_Q. \tag{2A.14}
$$

Indeed, if P and Q are decomposed into transpositions,

$$
P = \prod_{(ij)} T_{(ij)}, \qquad n \text{ factors}, \tag{2A.15}
$$

$$
Q = \prod_{(i'j')} T_{(i'j')}, \quad m \text{ factors},
$$

then the product

$$
PQ = \prod_{(ij)} \prod_{(i'j')} T_{(ij)} T_{(i'j')} \tag{2A.16}
$$

contains $n \times m$ transpositions. This number is even if n and m are both even or odd, and odd, if one of them is odd and the other even. Since the identity is trivially even, the inverse P^{-1} of a permutation has the same parity as P itself, i.e.,

$$
\epsilon_{P^{-1}} = \epsilon_P. \tag{2A.17}
$$

Let us find the irreducible representations of the permutation group on the Hilbert space of n-particle wave functions. The permutation on this space is defined by (2A.4). The irreducible representations can be classified with the help of so-called *Young tableaux*. These are arrays of n boxes of the form

$$\boxed{1}\boxed{2}\boxed{3}\boxed{4}\boxed{5}\boxed{6}\ \boxed{7}\boxed{8}\boxed{9}\boxed{\cdot}\boxed{\cdot}$$

(2A.18)

The boxes are filled successively with the numbers 1 to n. The numbers of boxes in the rows $m_1, m_2, m_3, \ldots$ are ordered as

$$m_1 \geq m_2 \geq m_3 \geq \ldots \qquad \sum_{k=1}^{n} m_k = n.$$

Each tableau defines a symmetry type of a set of wave functions on which the group of permutations is represented irreducibly. The symmetry types are constructed as follows. Let p_i be all permutations of the numbers i in the row (including the identity), and let q_j be the corresponding operations in the column j. Then we define the operations P and Q as

$$
\begin{aligned}
P &= \prod_i \left(\sum p_i \right), \\
Q &= \prod_j \left(\sum \epsilon_{q_j} q_j \right).
\end{aligned}
$$

The product is taken over all rows i or all columns j, and ϵ_q is the parity function (2A.13). Now apply the operation QP to the *indices* of the wave function $\psi(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n)$.

As an example, take the Hilbert space of three-particle wave functions. There are three different Young tableaux corresponding to the following irreducible representations of S_3:

$$\boxed{1}\boxed{2}\boxed{3} \qquad P = \sum p \text{ (sum over all 6 elements of } S_3\text{)}, \ Q = 1 \qquad (2A.19)$$

$$\begin{array}{l}\boxed{1}\boxed{2}\\ \boxed{3}\end{array} \qquad P = 1 + (1,2), \quad Q = 1 - (1,3) \qquad (2A.20)$$

$$\begin{array}{l}\boxed{1}\\ \boxed{2}\\ \boxed{3}\end{array} \qquad P = 1, \ Q = \sum \epsilon_q q \text{ (sum over all 6 elements of } S_3\text{)}. \qquad (2A.21)$$

The wave functions associated with these have the form

$$
\begin{aligned}
\boxed{1}\boxed{2}\boxed{3}\ \psi(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3) &= \psi(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3) + \psi(\mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_1) \\
&+\ \psi(\mathbf{x}_3, \mathbf{x}_1, \mathbf{x}_2) + \psi(\mathbf{x}_1, \mathbf{x}_3, \mathbf{x}_2) \\
&+\ \psi(\mathbf{x}_2, \mathbf{x}_1, \mathbf{x}_3) + \psi(\mathbf{x}_3, \mathbf{x}_2, \mathbf{x}_1),
\end{aligned}
$$

(2A.22)

$$
\begin{aligned}
\begin{array}{l}\boxed{1}\boxed{2}\\ \boxed{3}\end{array}\ \psi(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3) &= \psi(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3) + \psi(\mathbf{x}_2, \mathbf{x}_1, \mathbf{x}_3) \\
&-\ \psi(\mathbf{x}_3, \mathbf{x}_2, \mathbf{x}_1) - \psi(\mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_1),
\end{aligned}
$$

(2A.23)

$$
\begin{aligned}
\begin{array}{l}\boxed{1}\\ \boxed{2}\\ \boxed{3}\end{array}\ \psi(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3) &= \psi(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3) + \psi(\mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_1) \\
&+\ \psi(\mathbf{x}_3, \mathbf{x}_1, \mathbf{x}_2) - \psi(\mathbf{x}_1, \mathbf{x}_3, \mathbf{x}_2) \\
&-\ \psi(\mathbf{x}_2, \mathbf{x}_1, \mathbf{x}_3) - \psi(\mathbf{x}_3, \mathbf{x}_2, \mathbf{x}_1).
\end{aligned}
$$

(2A.24)

These wave functions are easily normalized by dividing them by the square root of the number of terms in each expression, i.e., $\sqrt{6}, 2, \sqrt{6}$, in the three cases. The horizontal array leads to the completely symmetrized wave function, the vertical array to the completely antisymmetrized one. The second tableau results in a mixed symmetry.

Four-particle wave functions are classified with the following tableaux:

$$\boxed{1}\boxed{2}\boxed{3}\boxed{4} + \begin{array}{c}\boxed{1}\boxed{2}\boxed{3}\\\boxed{4}\end{array} + \begin{array}{c}\boxed{1}\boxed{2}\\\boxed{3}\boxed{4}\end{array} + \begin{array}{c}\boxed{1}\boxed{2}\\\boxed{3}\\\boxed{4}\end{array} + \begin{array}{c}\boxed{1}\\\boxed{2}\\\boxed{3}\\\boxed{4}\end{array}. \tag{2A.25}$$

Consider, for instance, the third of these

$$\begin{array}{c}\boxed{1}\boxed{2}\\\boxed{3}\boxed{4}\end{array}.$$

This stands for the permutation operator QP with

$$P = (1 + (3,4))\,(1 + (1,2)), \qquad Q = (1 - (2,4))\,(1 - (1,3)), \tag{2A.26}$$

so that

$$
\begin{aligned}
P\psi(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4) ={}& \psi(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4) + \psi(\mathbf{x}_2, \mathbf{x}_1, \mathbf{x}_3, \mathbf{x}_4) \\
& + \psi(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_4, \mathbf{x}_3) + \psi(\mathbf{x}_2, \mathbf{x}_1, \mathbf{x}_4, \mathbf{x}_3), \\
QP\psi(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4) ={}& \psi(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4) - \psi(\mathbf{x}_3, \mathbf{x}_2, \mathbf{x}_1, \mathbf{x}_4) \\
& - \psi(\mathbf{x}_1, \mathbf{x}_4, \mathbf{x}_3, \mathbf{x}_2) + \psi(\mathbf{x}_3, \mathbf{x}_4, \mathbf{x}_1, \mathbf{x}_2) \\
& + \psi(\mathbf{x}_2, \mathbf{x}_1, \mathbf{x}_3, \mathbf{x}_4) - \psi(\mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_1, \mathbf{x}_4) \\
& - \psi(\mathbf{x}_4, \mathbf{x}_1, \mathbf{x}_3, \mathbf{x}_2) + \psi(\mathbf{x}_4, \mathbf{x}_3, \mathbf{x}_1, \mathbf{x}_2) \\
& + \psi(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_4, \mathbf{x}_3) - \psi(\mathbf{x}_3, \mathbf{x}_2, \mathbf{x}_4, \mathbf{x}_1) \\
& - \psi(\mathbf{x}_1, \mathbf{x}_4, \mathbf{x}_2, \mathbf{x}_3) + \psi(\mathbf{x}_3, \mathbf{x}_4, \mathbf{x}_2, \mathbf{x}_1) \\
& + \psi(\mathbf{x}_2, \mathbf{x}_1, \mathbf{x}_4, \mathbf{x}_3) - \psi(\mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4, \mathbf{x}_1) \\
& - \psi(\mathbf{x}_4, \mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3) + \psi(\mathbf{x}_4, \mathbf{x}_3, \mathbf{x}_2, \mathbf{x}_1).
\end{aligned}
\tag{2A.28}
$$

There exists an altertive but mathematically equivalent prescription of forming the wave functions of different symmetry types based on the permutations P' introduced in (2A.5). Instead of performing the permutations on the indices, one exchanges the positions of the arguments in the wave functions to produce $\psi(\mathbf{x}_1, \ldots, \mathbf{x}_i, \ldots, \mathbf{x}_j, \ldots, \mathbf{x}_n)$. As an example, take the tableaux

$$\begin{array}{c}\boxed{1}\boxed{2}\\\boxed{3}\end{array},$$

whose associated wave function was written down in (2A.23). The alternative wave function would be

$$\begin{array}{c}\boxed{1}\boxed{2}\\\boxed{3}\end{array}' \quad \psi(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3) = \psi(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3) + \psi(\mathbf{x}_2, \mathbf{x}_1, \mathbf{x}_3) - \psi(\mathbf{x}_3, \mathbf{x}_2, \mathbf{x}_1) - \psi(\mathbf{x}_3, \mathbf{x}_1, \mathbf{x}_2), \tag{2A.29}$$

with the last two terms differing from those in (2A.23).

The following formula specifies the dimensionality with which the group elements of the permutation group are represented for these symmetry classes:

$$d = \frac{n!}{\prod_{i,j} h_{ij}}, \tag{2A.30}$$

where h_{ij} is the number of boxes to the right of the position ij, plus the number of boxes below the position ij in the tableau, plus 1 for the box on the position ij itself.

As a useful check for the calculated dimensions we may use the *dimensionality theorem*, by which the squares of the dimensions d of all inequivalent, irreducible, unitary representations add up to the order of the group, here $n!$:

$$\sum d^2 = n! \; . \tag{2A.31}$$

This is a direct consequence of the *great orthogonality theorem* of such representations for any finite group.

For the permutation group at hand, one has the additional property that the defining representation contains each irreducible representation with a multiplicity equal to its dimension.

For three particles, the symmetric and antisymmetric representations

$$\boxed{1}\boxed{2}\boxed{3}$$

and

$$\begin{array}{c}\boxed{1}\\\boxed{2}\\\boxed{3}\end{array}$$

are $3!/3 \times 2 \times 1 = 1$-dimensional. The mixed representation

$$\begin{array}{c}\boxed{1}\boxed{2}\\\boxed{3}\end{array}$$

is $3!/3 \times 1 \times 1 = 2$-dimensional. These dimensions fulfill the dimensionality formula (2A.31):

$$1^2 + 1^1 + 2^2 = 3! \; . \tag{2A.32}$$

Similarly, one has for four particles the dimensionalities

$$\boxed{1}\boxed{2}\boxed{3}\boxed{4} \quad d = \frac{4!}{4 \times 3 \times 2 \times 1} = 1,$$

$$\begin{array}{c}\boxed{1}\boxed{2}\boxed{3}\\\boxed{4}\end{array} \quad d = \frac{4!}{4 \times 2 \times 1 \times 1} = 3,$$

$$\begin{array}{c}\boxed{1}\boxed{2}\\\boxed{3}\boxed{4}\end{array} \quad d = \frac{4!}{3 \times 2 \times 2 \times 1} = 2,$$

$$\begin{array}{c}\boxed{1}\boxed{2}\\\boxed{3}\\\boxed{4}\end{array} \quad d = \frac{4!}{4 \times 1 \times 2 \times 1} = 3, \tag{2A.33}$$

$$\begin{array}{c}\boxed{1}\\\boxed{2}\\\boxed{3}\\\boxed{4}\end{array} \quad d = \frac{4!}{4 \times 3 \times 2 \times 1} = 1.$$

Again we check that these dimensions fulfill the dimensionality formula (2A.31):

$$1^2 + 3^2 + 2^2 + 3^2 + 1^2 = 4! \; . \tag{2A.34}$$

Appendix 2B   Treatment of Singularities in Zeta-Function

Here we show how to evaluate the sums which determine the would-be critical temperatures of a Bose gas in a box and in a harmonic trap.

2B.1   Finite Box

According to Eqs. (2.364), (2.369), and (2.371), the relation between temperature $T = \hbar^2\pi^2/bML^2k_B$ and the fugacity z_D at a fixed particle number N in a finite D-dimensional box is determined by the equation

$$N = N_{\rm n}(T) + N_{\rm cond}(T) = S_D(z_D) + \frac{z_D}{1 - z_D}. \tag{2B.1}$$

Here $S_D(z_D)$ is the subtracted infinite sum

$$S_D(z_D) \equiv \sum_{w=1}^{\infty} [Z_1^D(wb)e^{wDb/2} - 1]z_D^w, \tag{2B.2}$$

containing the Dth power of a one-particle partition function in the box $Z_1(b) = \sum_{k=1}^{\infty} e^{-bk^2/2}$. The would-be critical temperature is found by equating this sum at $z_D = 1$ with the total particle number N. We shall rewrite $Z_1(b)$ as

$$Z_1(b) = e^{-b/2}\left[1 + e^{-3b/2}\sigma_1(b)\right], \tag{2B.3}$$

where $\sigma_1(b)$ is related to the elliptic theta function (2.366) by

$$\sigma_1(b) \equiv \sum_{k=2}^{\infty} e^{-(k^2-4)b/2} = \frac{e^{2b}}{2}\left[\vartheta_3(0, e^{-b/2}) - 1 - 2e^{-b/2}\right]. \tag{2B.4}$$

According to Eq. (2.368), this has the small-b behavior

$$\sigma_1(b) = \sqrt{\frac{\pi}{2b}}e^{2b} - e^{3b/2} - \frac{1}{2}e^{2b} + \dots \, . \tag{2B.5}$$

The omitted terms are exponentially small as long as $b < 1$ [see the sum over m in Eq. (2.367)]. For large b, these terms become important to ensure an exponentially fast falloff like $e^{-3b/2}$. Inserting (2B.3) into (2B.2), we find

$$S_D(1) \equiv D\sum_{w=1}^{\infty}\left[\sigma_1(wb)e^{-3wb/2} + \frac{D-1}{2}\sigma_1^2(wb)e^{-6wb/2} + \frac{(D-1)(D-2)}{6}\sigma_1^3(wb)e^{-9wb/2}\right]. \tag{2B.6}$$

Inserting here the small-b expression (2B.5), we obtain

$$S_2(1) \equiv \sum_{w=1}^{\infty}\left(\frac{\pi}{2wb}e^{wb} - \sqrt{\frac{\pi}{2wb}}e^{wb} + \frac{1}{4}e^{wb} - 1\right) + \dots \, , \tag{2B.7}$$

$$S_3(1) \equiv \sum_{w=1}^{\infty}\left(\sqrt{\frac{\pi}{2wb}}^{3}e^{3wb/2} - \frac{3}{2}\frac{\pi}{2wb}e^{3wb/2} + \frac{3}{4}\sqrt{\frac{\pi}{2wb}}e^{3wb/2} - \frac{1}{8}e^{3wb/2} - 1\right) + \dots \, , \tag{2B.8}$$

the dots indicating again exponentially small terms. The sums are convergent only for negative b, this being a consequence of the approximate nature of these expressions. If we evaluate them in this regime, the sums produce polylogarithmic functions

$$\zeta_\nu(z) \equiv \sum_{w=1}^{\infty}\frac{z^w}{w^\nu}, \tag{2B.9}$$

and we find, using the property at the origin,[13]

$$\zeta(0) = -1/2, \qquad \zeta'(0) = -\frac{1}{2}\log 2\pi, \tag{2B.10}$$

---

[13]I.S. Gradshteyn and I.M. Ryzhik, op. cit., Formula 9.541.4.

which imply $\sum_{w=1}^{\infty} 1 = \zeta(0) = -1/2$, $\quad -\sum_{w=1}^{\infty} \log w = \zeta'(0) = -\frac{1}{2}\log 2\pi$, such that

$$S_2(1) = \zeta_1(e^b) - \sqrt{\frac{\pi}{2b}}\zeta_{1/2}(e^b) + \frac{1}{4}\zeta_0(e^b) - \zeta(0) + \dots . \tag{2B.11}$$

$$S_3(1) = \sqrt{\frac{\pi}{2b}}^3 \zeta_{3/2}(e^{3b/2}) - \frac{3}{2}\frac{\pi}{2b}\zeta_1(e^{3b/2}) + \frac{3}{4}\sqrt{\frac{\pi}{2b}}\zeta_1(e^{3b/2}) - \frac{1}{8}\zeta_0(e^{3b/2}) - \zeta(0) + \dots . \tag{2B.12}$$

These expressions can now be expanded in powers of b with the help of the Robinson expansion given in the footnote on p. 8. Afterwards, b is continued analytically to positive values and we obtain

$$S_2(1) = -\frac{\pi}{2b}\log(C_2 b) - \sqrt{\frac{\pi}{2b}}\zeta(1/2) + \frac{1}{8}(3 - 2\pi) + \mathcal{O}(b^{1/2}), \tag{2B.13}$$

$$S_3(1) = \sqrt{\frac{\pi}{2b}}^3 \zeta(3/2) + \frac{3\pi}{4b}\log(C_3 b) + \frac{3}{4}\sqrt{\frac{\pi}{2b}}\zeta(1/2)(1 + \pi) + \frac{9}{16}(1 + \pi) + \mathcal{O}(b^{1/2}). \tag{2B.14}$$

The constants $C_{2,3}, C'_{2,3}$ inside the logarithms turn out to be complex, implying that the limiting expressions (2B.7) and (2B.8) cannot be used reliably. A proper way to proceed goes as follows: We subtract from $S_D(1)$ terms which remove the small-b singularities by means of modifications of (2B.7) and (2B.8) which have the same small-b expansion up to b^0:

$$\tilde{S}_2(1) \equiv \sum_{w=1}^{\infty} \left(\frac{\pi}{2wb} - \sqrt{\frac{\pi}{2wb}} + \frac{4\pi - 3}{4} \right) e^{-wb} + \dots , \tag{2B.15}$$

$$\tilde{S}_3(1) \equiv \sum_{w=1}^{\infty} \left[\sqrt{\frac{\pi}{2wb}}^3 - \frac{3}{2}\frac{\pi}{2wb} + \frac{3}{4}(1 + 2\pi)\sqrt{\frac{\pi}{2wb}} - \frac{9}{8}(1 + 2\pi) \right] e^{-3wb/2} + \dots . \tag{2B.16}$$

In these expressions, the sums over w can be performed for positive b, yielding

$$\tilde{S}_2(1) \equiv \frac{\pi}{2b}\zeta_1(e^{-b}) - \sqrt{\frac{\pi}{2b}}\zeta_{1/2}(e^{-b}) + \frac{4\pi - 3}{4}\zeta_0(e^{-b}) + \dots , \tag{2B.17}$$

$$\tilde{S}_3(1) \equiv \sqrt{\frac{\pi}{2b}}^3 \zeta_{3/2}(e^{-3b/2}) - \frac{3}{2}\frac{\pi}{2b}\zeta_1(e^{-3b/2}) + \frac{3}{4}(1 + 2\pi)\sqrt{\frac{\pi}{2b}}\zeta_{1/2}(e^{-3b/2})$$
$$- \frac{9}{8}(1 + 2\pi)\zeta_0(e^{-3b/2}) + \dots . \tag{2B.18}$$

Inserting again the Robinson expansion in the footnote on p. 8, we obtain once more the above expansions (2B.13) and (2B.14), but now with the well-determined real constants

$$\tilde{C}_2 = e^{3/2\pi - 2 + \sqrt{2}} \approx 0.8973, \qquad \tilde{C}_3 = \frac{3}{2}e^{-2 + 1/\sqrt{3} - 1/\pi} \approx 0.2630. \tag{2B.19}$$

The subtracted expressions $S_D(1) - \tilde{S}_D(1)$ are smooth near the origin, so that the leading small-b behavior of the sums over these can simply be obtained from a numeric integral over w:

$$\int_0^{\infty} dw[S_2(1) - \tilde{S}_2(1)] = -\frac{1.1050938}{b}, \quad \int_0^{\infty} dw[S_3(1) - \tilde{S}_3(1)] = 3.0441. \tag{2B.20}$$

These modify the constants $\tilde{C}_{2,3}$ to

$$C_2 = 1.8134, \quad C_3 = 0.9574. \tag{2B.21}$$

The corrections to the sums over $S_D(1) - \tilde{S}_D(1)$ are of order b^0 and higher. They were already included in the expansions (2B.13) and (2B.14), which only were unreliable as far as $C_{2,3}$ is concerned.

Let us calculate from (2B.14) the finite-size correction to the critical temperature by equating $S_3(1)$ with N. Expressing this in terms of $b_c^{(0)}$ via (2.373), and introducing the ratio $\hat{b}_c \equiv b_c/b_c^{(0)}$ which is close to unity, we obtain the expansion in powers of the small quantity $2b_c^{(0)}/\pi = [\zeta(3/2)/N]^{2/3}$:

$$\hat{b}_c^{3/2} = 1 + \sqrt{\frac{2b_c^{(0)}}{\pi}} \frac{3\sqrt{\hat{b}_c}}{2\zeta(3/2)} \log(C_3 b_c^{(0)}\hat{b}_c) + \frac{2b_c^{(0)}}{\pi} \frac{3}{4\zeta(3/2)}\zeta(1/2)(1+\pi)\hat{b}_c + \dots . \quad (2B.22)$$

To lowest order, the solution is simply

$$\hat{b}_c = 1 + \sqrt{\frac{2b_c^{(0)}}{\pi}} \frac{1}{\zeta(3/2)} \log(C_3 b_c^{(0)}) + \dots , \quad (2B.23)$$

yielding the would-be critical temperature to first order in $1/N^{1/3}$ as stated in (2.375). To next order we insert, into the last term, the zero-order solution $\hat{b}_c \approx 1$, and into the second term, the first-order solution (2B.23). This leads to

$$
\begin{aligned}
\hat{b}_c^{3/2} &= 1 + \frac{3}{2}\sqrt{\frac{2b_c^{(0)}}{\pi}} \frac{1}{\zeta(3/2)} \log(C_3 b_c^{(0)}) \\
&+ \frac{2b_c^{(0)}}{\pi} \frac{3}{4\zeta(3/2)} \left\{ \zeta(1/2)(1+\pi) + \frac{1}{\zeta(3/2)} \left[2\log(C_3 b_c^{(0)}) + \log^2(C_3 b_c^{(0)}) \right] \right\} + \dots . \quad (2B.24)
\end{aligned}
$$

Replacing $b_c^{(0)}$ by $(2/\pi)\,[\zeta(3/2)/N]^{2/3}$, we obtain the ratio $(T_c^{(0)}/T_c)^{3/2}$ between finite- and infinite-size critical temperatures T_c and $T_c^{(0)}$. The first and second-order corrections are plotted in Fig. 2.9, together with precise results from a numeric solution of the equation $N = S_3(1)$.
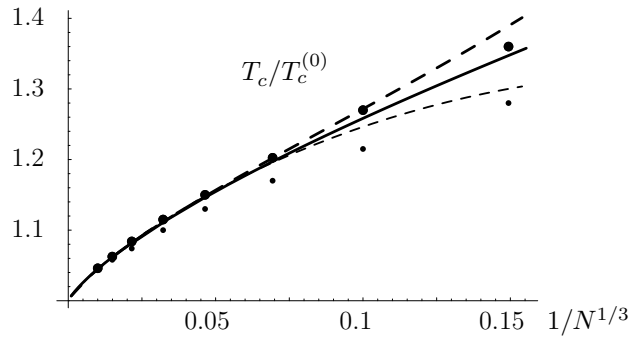

FIGURE 2.9 Finite-size corrections to the critical temperature for $N > 300$, calculated once from the formula $N = S_3(1)$ (solid curve), and once from the expansion (2B.24) (short-dashed up to the order $[b_c^{(0)}]^{1/2} \propto 1/N^{1/3}$, long-dashed up to the order $b_c^{(0)} \propto 1/N^{2/3}$). The fat dots show the peaks in the second derivative $d^2 N_{\mathrm{cond}}(T)/dT^2$. The small dots show the corresponding values for canonical ensembles, for comparison.

2B.2 Harmonic Trap

The sum relevant for the would-be phase transition in a harmonic trap is

$$S_D(b, z_D) = \sum_{w=1}^{\infty} \left[\frac{1}{(1-e^{-wb})^D} - 1 \right] z_D^w, \quad (2B.25)$$

which determines the number of normal particles in the harmonic trap via

$$N_{\mathrm{n}}(T) = Z_{\omega}(\beta)\bar{\zeta}_D(\beta\hbar\omega; z_D) \equiv S_D(\beta\hbar\omega, z_D). \qquad (2\mathrm{B}.26)$$

We consider only the point $z_D = 1$ which determines the critical temperature by the condition $N_{\mathrm{n}} = N$. Restricting ourselves to the physical cases $D = 1, 2, 3$, we rewrite the sum as

$$S_D(b, 1) = \sum_{w=1}^{\infty} D \left[e^{-wb} - \frac{(D-1)}{2} e^{-2wb} + \frac{(D-1)(D-2)}{6} e^{-3wb} \right] \frac{1}{(1 - e^{-wb})^D}. \qquad (2\mathrm{B}.27)$$

According to the method developed in the evaluation of the Robinson expansion in the footnote on p. 8, we obtain such a sum in two steps. First we go to small b where the sum reduces to an integral over w. After this we calculate the difference between sum and integral by a naive power series expansion.

As it stands, the sum (2B.27) cannot be converted into an integral due to singularities at $w = 0$. These must first be removed by subtractions. Thus we decompose $S_D(b, 1)$ into a subtracted sum plus a remainder as

$$S_D(b, 1) = \bar{S}_D(b, 1) + \Delta_D S_D(b, 1) + b\frac{D}{2}\Delta_{D-1} S_D(b, 1) + b^2 \frac{D(3D-1)}{24}\Delta_{D-2} S_D(b, 1). \qquad (2\mathrm{B}.28)$$

Here

$$\begin{aligned}
\bar{S}_D(b, 1) &= \sum_{w=1}^{\infty} D \left[e^{-wb} - \frac{D-1}{2} e^{-2wb} + \frac{(D-1)(D-2)}{6} e^{-3wb} \right] \\
&\times \left[\frac{1}{(1 - e^{-wb})^D} - \frac{1}{w^D b^D} - \frac{D}{2w^{D-1}b^{D-1}} - \frac{D(3D-1)}{24w^{D-2}b^{D-2}} \right]
\end{aligned} \qquad (2\mathrm{B}.29)$$

is the subtracted sum and

$$\Delta_{D'} S_D(b, 1) \equiv \frac{D}{b^D} \left[\zeta_{D'}(e^{-b}) - \frac{D-1}{2}\zeta_{D'}(e^{-2b}) + \frac{(D-1)(D-2)}{6}\zeta_{D'}(e^{-3b}) \right] \qquad (2\mathrm{B}.30)$$

collects the remainders. The subtracted sum can now be done in the limit of small b as an integral over w, using the well-known integral formula for the Beta function:

$$\int_0^{\infty} dx \frac{e^{-ax}}{(1 - e^{-x})^b} = B(a, 1 - b) = \frac{\Gamma(a)\Gamma(1-b)}{\Gamma(1 + a - b)}. \qquad (2\mathrm{B}.31)$$

This yields the small-b contributions to the subtracted sums

$$\begin{aligned}
\bar{S}_1(b, 1) &\underset{b\to 0}{\to} \frac{1}{b}\left(\gamma - \frac{7}{12}\right) \equiv s_1, \\
\bar{S}_2(b, 1) &\underset{b\to 0}{\to} \frac{1}{b}\left(\gamma + \log 2 - \frac{9}{8}\right) \equiv s_2, \\
\bar{S}_3(b, 1) &\underset{b\to 0}{\to} \frac{1}{b}\left(\gamma + \log 3 - \frac{19}{24}\right) \equiv s_3,
\end{aligned} \qquad (2\mathrm{B}.32)$$

where $\gamma = 0.5772\ldots$ is the *Euler-Mascheroni number*. The remaining sum-minus-integral is obtained by a series expansion of $1/(1 - e^{-wb})^D$ in powers of b and performing the sums over w using the formula:

$$\left(\sum_{n=1}^{\infty} - \int_0^{\infty}\right) \frac{e^{n\beta\hbar\omega}}{n^{\nu}} = \sum_{k=1}^{\infty} \frac{1}{k!}(-\beta\hbar\omega)^k \zeta(\nu - k) \equiv \bar{\zeta}_{\nu}(e^{\beta\hbar\omega}). \qquad (2\mathrm{B}.33)$$

However, due to the subtractions, the corrections are all small of order $(1/b^D)\mathcal{O}(b^3)$. They will be ignored here. Thus we obtain

$$S_D(b,1) = \frac{s_D}{b^D} + \Delta S_D(b,1) + \frac{1}{b^D}\mathcal{O}(b^3). \tag{2B.34}$$

We now expand $\Delta_{D'}S_D(b,1)$ using Robinson's formula stated in the footnote on p. 8 up to b^2/b^D and find

$$\Delta_{D'}S_1(b,1) = \frac{1}{b}\zeta_{D'}(e^{-b}), \tag{2B.35}$$

$$\Delta_{D'}S_2(b,1) = \frac{1}{b^2}\left[2\zeta_{D'}(e^{-b}) - \zeta_{D'}(e^{-2b})\right], \tag{2B.36}$$

$$\Delta_{D'}S_3(b,1) = \frac{1}{b^3}\left[3\zeta_{D'}(e^{-b}) - 3\zeta_{D'}(e^{-2b}) + \zeta_{D'}(e^{-3b})\right], \tag{2B.37}$$

where

$$\zeta_1(e^{-b}) = -\log\left(1 - e^{-b}\right) = -\log b + \frac{b}{2} - \frac{b^2}{24} + \dots ,$$

$$\zeta_2(e^{-b}) = \zeta(2) + b(\log b - 1) - \frac{b^2}{4} + \dots , \tag{2B.38}$$

$$\zeta_3(e^{-b}) = \zeta(3) - \frac{b}{6}\zeta(2) - \frac{b^2}{2}\left(\log b - \frac{3}{2}\right) + \dots . \tag{2B.39}$$

The results are

$$S_1(b,1) = \frac{1}{b}\left[(-\log b + \gamma) + \frac{b}{4} - \frac{b^2}{144} + \dots\right],$$

$$S_2(b,1) = \frac{1}{b^2}\left[\zeta(2) - b\left(\log b - \gamma + \frac{1}{2}\right) + \frac{7b^2}{24} + \dots\right], \tag{2B.40}$$

$$S_3(b,1) = \frac{1}{b^3}\left[\zeta(3) + \frac{3b}{2}\zeta(2) - b^2\left(\log b - \gamma + \frac{19}{24}\right) + \dots\right].$$

Note that the calculation cannot be shortened by simply expanding the factor $1/(1 - e^{-wb})^D$ in the unsubtracted sum (2B.27) in powers of w, which would yield the result (2B.28) without the first term $\bar{S}_1(b,1)$, and thus without the integrals (2B.32).

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