Mirum, quod divina natura dedit agros
It's wonderful that divine nature has given us fields
VARRO (116 BC–27 BC)

7

Many Particle Orbits – Statistics and Second Quantization

Realistic physical systems usually contain groups of identical particles such as specific atoms or electrons. Focusing on a single group, we shall label their orbits by $\mathbf{x}^{(\nu)}(t)$ with $\nu = 1, 2, 3, \ldots, N$. Their Hamiltonian is invariant under the group of all $N!$ permutations of the orbital indices ν. Their Schrödinger wave functions can then be classified according to the irreducible representations of the permutation group.

Not all possible representations occur in nature. In more than two space dimensions, there exists a *superselection rule*, whose origin is yet to be explained, which eliminates all complicated representations and allows only for the two simplest ones to be realized: those with complete symmetry and those with complete antisymmetry. Particles which appear always with symmetric wave functions are called *bosons*. They all carry an integer-valued spin. Particles with antisymmetric wave functions are called *fermions*[1] and carry a spin whose value is half-integer.

The symmetric and antisymmetric wave functions give rise to the characteristic statistical behavior of fermions and bosons. Electrons, for example, being spin-1/2 particles, appear only in antisymmetric wave functions. The antisymmetry is the origin of the famous *Pauli exclusion principle*, allowing only a single particle of a definite spin orientation in a quantum state, which is the principal reason for the existence of the *periodic system* of elements, and thus of matter in general. The atoms in a gas of helium, on the other hand, have zero spin and are described by symmetric wave functions. These can accommodate an infinite number of particles in a single quantum state giving rise to the famous phenomenon of Bose-Einstein condensation. This phenomenon is observable in its purest form in the absence of interactions, where at zero temperature all particles condense in the ground state. In interacting systems, Bose-Einstein statistics can lead to the stunning quantum state of superfluidity.

The particular association of symmetry and spin can be explained within relativistic quantum field theories in spaces with more than two dimensions where it is shown to be intimately linked with the *locality* and *causality* of the theory.

[1] Had M. Born as editor of Zeitschrift für Physik not kept a paper by P. Jordan in his suitcase for half a year in 1925, they would be called *jordanons*. See the bibliographical notes by B. Schroer (hep-th/0303241).

In two dimensions there can be particles with an exceptional statistical behavior. Their properties will be discussed in Section 7.5. In Chapter 16, such particles will serve to explain the fractional quantum Hall effect.

The problem to be solved in this chapter is how to incorporate the statistical properties into a path integral description of the orbits of a many-particle system. Afterwards we describe the formalism of *second quantization* or *field quantization* in which the path integral of *many* identical particle orbits is abandoned in favor of a path integral over a *single fluctuating field* which is able to account for the statistical properties in a most natural way.

7.1 Ensembles of Bose and Fermi Particle Orbits

For bosons, the incorporation of the statistical properties into the orbital path integrals is quite easy. Consider, for the moment, distinguishable particles. Their many-particle time evolution amplitude is given by the path integral

$$(\mathbf{x}_b^{(1)}, \dots, \mathbf{x}_b^{(N)}; t_b | \mathbf{x}_a^{(1)}, \dots, \mathbf{x}_a^{(N)}; t_a) = \prod_{\nu=1}^{N} \left[\int \mathcal{D}^D x^{(\nu)} \right] e^{i\mathcal{A}^{(N)}/\hbar}, \tag{7.1}$$

with an action of the typical form

$$\mathcal{A}^{(N)} = \int_{t_a}^{t_b} dt \left\{ \sum_{\nu=1}^{N} \left[\frac{M^{(\nu)}}{2} \dot{\mathbf{x}}^{(\nu)2} - V(\mathbf{x}^{(\nu)}) \right] - \frac{1}{2} \sum_{\nu \neq \nu'=1}^{N} V_{\text{int}}(\mathbf{x}^{(\nu)} - \mathbf{x}^{(\nu')}) \right\}, \tag{7.2}$$

where $V(\mathbf{x}^{(\nu)})$ is some common background potential for all particles interacting via the pair potential $V_{\text{int}}(\mathbf{x}^{(\nu)} - \mathbf{x}^{(\nu')})$. We shall ignore interactions involving more than two particles at the same time, for simplicity.

If we want to apply the path integral (7.1) to indistinguishable particles of spin zero, we merely have to *add* to the sum over all paths $\mathbf{x}^{(\nu)}(t)$ running to the final positions $\mathbf{x}_b^{(\nu)}$ the sum of all paths running to the indistinguishable permuted final positions $\mathbf{x}_b^{(p(\nu))}$. The amplitude for n bosons reads therefore

$$(\mathbf{x}_b^{(1)}, \dots, \mathbf{x}_b^{(N)}; t_b | \mathbf{x}_a^{(1)}, \dots, \mathbf{x}_a^{(N)}; t_a) = \sum_{p(\nu)} (\mathbf{x}_b^{(p(1))}, \dots, \mathbf{x}_b^{(p(N))}; t_b | \mathbf{x}_a^{(1)}, \dots, \mathbf{x}_a^{(N)}; t_a), \tag{7.3}$$

where $p(\nu)$ denotes the $N!$ permutations of the indices ν. For bosons of higher spin, the same procedure applies to each subset of particles with equal spin orientation.

A similar discussion holds for fermions. Their Schrödinger wave function requires complete antisymmetrization in the final positions. Correspondingly, the amplitude (7.1) has to be summed over all permuted final positions $\mathbf{x}_b^{(p(\nu))}$, with an extra minus sign for each odd permutation $p(\nu)$. Thus, the path integral involves both *sums and differences* of paths. So far, the measure of path integration has always been a true *sum* over paths. For this reason it will be preferable to attribute the alternating sign to an interaction between the orbits, to be called a *statistics interaction*. This interaction will be derived in Section 7.4.

For the statistical mechanics of Bose- and Fermi systems consider the imaginary-time version of the amplitude (7.3):

$$(\mathbf{x}_b^{(1)},\ldots,\mathbf{x}_b^{(N)};\hbar\beta|\mathbf{x}_a^{(1)},\ldots,\mathbf{x}_a^{(N)};0)=\sum_{p(\nu)}\epsilon_{p(\nu)}(\mathbf{x}_b^{(p(1))},\ldots,\mathbf{x}_b^{(p(N))};\hbar\beta|\mathbf{x}_a^{(1)},\ldots,\mathbf{x}_a^{(N)};0), \tag{7.4}$$

where $\epsilon_{p(\nu)}=\pm 1$ is the parity of even and odd permutations $p(\nu)$, to be used for Bosons and Fermions, respectively. Its spatial trace integral yields the partition function of N-particle orbits:

$$Z^{(N)}=\frac{1}{N!}\int d^Dx^{(1)}\cdots d^Dx^{(N)}\,(\mathbf{x}^{(1)},\ldots,\mathbf{x}^{(N)};\hbar\beta|\mathbf{x}^{(1)},\ldots,\mathbf{x}^{(N)};0). \tag{7.5}$$

A factor $1/N!$ accounts for the indistinguishability of the permuted final configurations.

For free particles, each term in the sum (7.4) factorizes:

$$(\mathbf{x}_b^{(p(1))},\ldots,\mathbf{x}_b^{(p(N))};\hbar\beta|\mathbf{x}_a^{(1)},\ldots,\mathbf{x}_a^{(N)};0)_0=(\mathbf{x}_b^{(p(1))}\hbar\beta|\mathbf{x}_a^{(1)}0)_0\cdots(\mathbf{x}_b^{(p(N))}\hbar\beta|\mathbf{x}_a^{(N)}0)_0, \tag{7.6}$$

where each factor has a path integral representation

$$(\mathbf{x}_b^{(p(\nu))}\hbar\beta|\mathbf{x}_a^{(\nu)}\,0)_0=\int_{\mathbf{x}^{(\nu)}(0)=\mathbf{x}_a^{(\nu)}}^{\mathbf{x}^{(\nu)}(\hbar\beta)=\mathbf{x}_b^{(p(\nu))}}\mathcal{D}^Dx^{(\nu)}\exp\left[-\frac{1}{\hbar}\int_0^{\hbar\beta}d\tau\frac{M}{2}\dot{\mathbf{x}}^{(\nu)2}(\tau)\right], \tag{7.7}$$

which is solved by the imaginary-time version of (2.74):

$$(\mathbf{x}_b^{(p(\nu))}\hbar\beta|\mathbf{x}_a^{(\nu)}\,0)_0=\frac{1}{\sqrt{2\pi\hbar^2\beta/M}^D}\exp\left\{-\frac{1}{\hbar}\frac{M}{2}\frac{\left[\mathbf{x}_b^{(p(\nu))}-\mathbf{x}_a^{(\nu)}\right]^2}{\hbar\beta}\right\}. \tag{7.8}$$

The partition function can therefore be rewritten in the form

$$Z_0^{(N)}=\frac{1}{\sqrt{2\pi\hbar^2\beta/M}^{ND}}\frac{1}{N!}\int d^Dx^{(1)}\cdots d^Dx^{(N)}\sum_{p(\nu)}\epsilon_{p(\nu)}\prod_{\nu=1}^{N}\exp\left\{-\frac{1}{\hbar}\frac{M}{2}\frac{\left[\mathbf{x}^{(p(\nu))}-\mathbf{x}^{(\nu)}\right]^2}{\hbar\beta}\right\}. \tag{7.9}$$

This is a product of Gaussian convolution integrals which can easily be performed as before when deriving the time evolution amplitude (2.76) for free particles with the help of Formula (2.75). Each convolution integral simply extends the temporal length in the fluctuation factor by $\hbar\beta$. Due to the indistinguishability of the particles, only a few paths will have their end points connected to their own initial points, i.e., they satisfy periodic boundary conditions in the interval $(0,\hbar\beta)$. The sum over permutations connects the final point of some paths to the initial point of a different path, as illustrated in Fig. 7.1. Such paths satisfy periodic boundary conditions on an interval $(0,w\hbar\beta)$, where w is some integer number. This is seen most clearly by drawing the paths in Fig. 7.1 in an extended zone scheme shown in Fig. 7.2, which

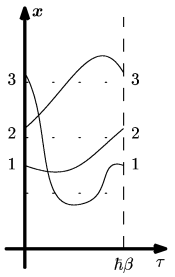

Figure 7.1 Paths summed in partition function (7.9). Due to indistinguishability of particles, final points of one path may connect to initial points of another.

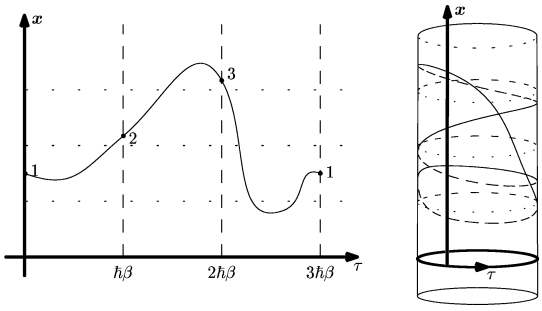

Figure 7.2 Periodic representation of paths summed in partition function (7.9), once in extended zone scheme, and once on D-dimensional hypercylinder embedded in $D+1$ dimensions. The paths are shown in Fig. 7.1. There is now only one closed path on the cylinder. In general there are various disconnected parts of closed paths.

is reminiscent of Fig. 6.1. The extended zone scheme can, moreover, be placed on a hypercylinder, illustrated in the right-hand part of Fig. 7.2. In this way, all paths decompose into mutually disconnected groups of closed paths winding around the cylinder, each with a different *winding number* w [1]. An example for a connected path which winds three times 3 around the D-dimensional cylinder contributes to the partition function a factor [using Formula (2.75)]:

$$\Delta Z_0^{(N)3} = \frac{1}{\sqrt{2\pi\hbar^2\beta/M}^{3D}} \int d^D x^{(1)} d^D x^{(2)} d^D x^{(3)} \exp\left\{-\frac{1}{\hbar}\frac{M}{2}\frac{\left[\mathbf{x}^{(3)}-\mathbf{x}^{(2)}\right]^2}{\hbar\beta}\right\}$$
$$\times \exp\left\{-\frac{1}{\hbar}\frac{M}{2}\frac{\left[\mathbf{x}^{(2)}-\mathbf{x}^{(1)}\right]^2}{\hbar\beta}\right\} \exp\left\{-\frac{1}{\hbar}\frac{M}{2}\frac{\left[\mathbf{x}^{(1)}-\mathbf{x}^{(3)}\right]^2}{\hbar\beta}\right\} = \frac{V_D}{\sqrt{2\pi\hbar^2 3\beta/M}^{D}}. \quad (7.10)$$

For cycles of length w the contribution is

$$\Delta Z_0^{(N)\,w} = Z_0(w\beta)\,, \quad (7.11)$$

where $Z_0(w\beta)$ is the partition function of a free particle in a D-dimensional volume V_D for an imaginary-time interval $w\hbar\beta$:

$$Z_0(w\beta) = \frac{V_D}{\sqrt{2\pi\hbar^2 w\beta/M}^D}. \tag{7.12}$$

In terms of the thermal de Broglie length $l_e(\hbar\beta) \equiv \sqrt{2\pi\hbar^2\beta/M}$ associated with the temperature $T = 1/k_B\beta$ [recall (2.353)], this can be written as

$$Z_0(w\beta) = \frac{V_D}{l_e^D(w\hbar\beta)}. \tag{7.13}$$

There is an additional factor $1/w$ in Eq. (7.11), since the number of connected windings of the total $w!$ closed paths is $(w-1)!$. In group theoretic language, it is the number of *cycles* of length w, usually denoted by $(1, 2, 3, \ldots, w)$, plus the $(w-1)!$ permutations of the numbers $2, 3, \ldots, w$. They are illustrated in Fig. 7.3 for $w = 2$, 3, 4. In a decomposition of all $N!$ permutations as products of cycles, the number of elements consisting of C_1, C_2, C_3, ... cycles of length 1, 2, 3, ... contains

$$M(C_1, C_2, \ldots, C_N) = \frac{N!}{\prod_{w=1}^N C_w! w^{C_w}} \tag{7.14}$$

elements [2].

With the knowledge of these combinatorial factors we can immediately write down the canonical partition function (7.9) of N bosons or fermions as the sum of all orbits around the cylinder, decomposed into cycles:

$$Z_0^{(N)}(\beta) = \frac{1}{N!}\sum_{p(\nu)} \epsilon_{p(\nu)} M(C_1, \ldots, C_N) \prod_{\substack{w=1 \\ N=\Sigma_w w C_w}}^{N} \Big[Z_0(w\beta)\Big]^{C_w} \quad . \tag{7.15}$$

The sum can be reordered as follows:

$$Z_0^{(N)} = \frac{1}{N!} \sum_{\substack{C_1,\ldots,C_N \\ N=\Sigma_w w C_w}} M(C_1, \ldots, C_N)\, \epsilon_{w,C_1,\ldots,C_n} \prod_{w=1}^{N} \Big[Z_0(w\beta)\Big]^{C_w} \quad . \tag{7.16}$$

The parity $\epsilon_{w,C_1,\ldots,C_n}$ of permutations is equal to $(\pm 1)^{\Sigma_w(w+1)C_w}$. Inserting (7.14), the sum (7.16) can further be regrouped to

$$\begin{aligned} Z_0^{(N)}(\beta) &= \sum_{\substack{C_1,\ldots,C_N \\ N=\Sigma_w w C_w}} \frac{1}{\prod_{w=1}^N C_w!\, w^{C_w}} (\pm 1)^{\Sigma_w(w+1)C_w} \prod_{w=1}^{N} \Big[Z_0(w\beta)\Big]^{C_w} \\ &= \sum_{\substack{C_1,\ldots,C_N \\ N=\Sigma_w w C_w}} \prod_{w=1}^{N} \frac{1}{C_w!} \left[(\pm 1)^{w-1} \frac{Z_0(w\beta)}{w}\right]^{C_w} \quad . \end{aligned} \tag{7.17}$$

For $N = 0$, this formula yields the trivial partition function $Z_0^{(0)}(\beta) = 1$ of the no-particle state, the *vacuum*. For $N = 1$, i.e., a single particle, we find $Z_0^{(1)}(\beta) = Z_0(\beta)$.

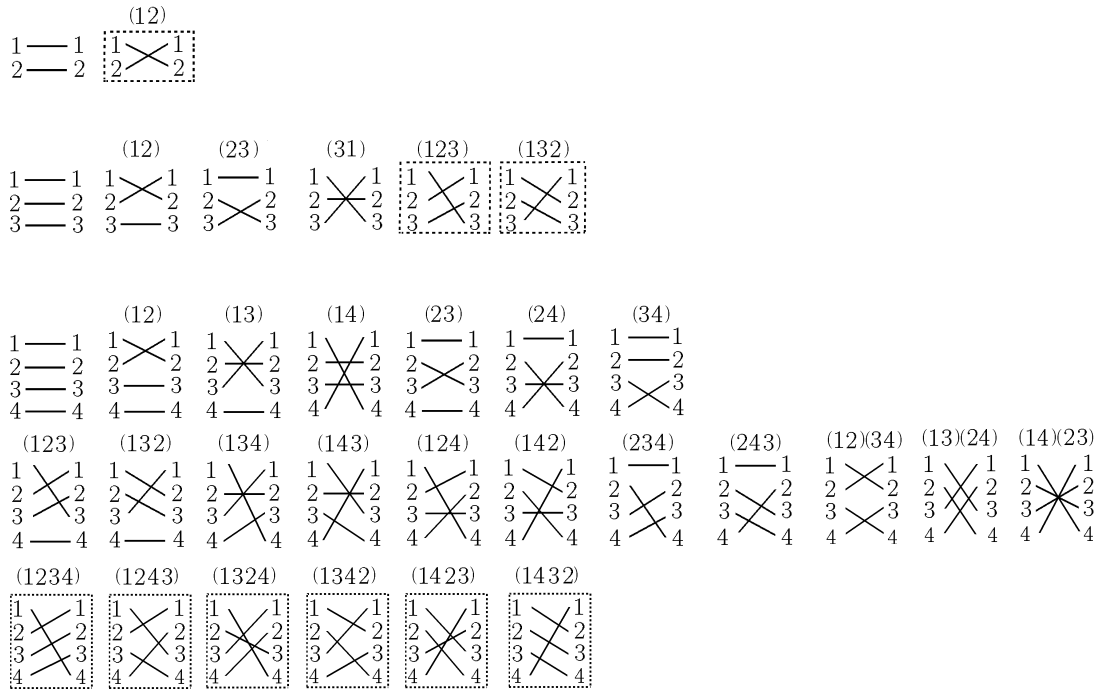

Figure 7.3 Among the $w!$ permutations of the different windings around the cylinder, $(w-1)!$ are connected. They are marked by dotted frames. In the cycle notation for permutation group elements, these are (12) for two elements, (123), (132) for three elements, (1234), (1243), (1324), (1342), (1423), (1432) for four elements. The cycles are shown on top of each graph, with trivial cycles of unit length omitted. The graphs are ordered according to a decreasing number of cycles.

The higher $Z_0^{(N)}$ can be written down most efficiently if we introduce a characteristic temperature

$$T_c^{(0)} \equiv \frac{2\pi\hbar^2}{k_B M}\left[\frac{N}{V_D \zeta(D/2)}\right]^{2/D}, \tag{7.18}$$

and measure the temperature T in units of $T_c^{(0)}$, defining a reduced temperature $t \equiv T/T_c^{(0)}$. Then we can rewrite $Z_0^{(1)}(\beta)$ as $t^{D/2}V_D$. Introducing further the N-dependent variable

$$\tau_N \equiv \left[\frac{N}{\zeta(D/2)}\right]^{2/D} t, \tag{7.19}$$

we find $Z_0^{(1)} = \tau_1^{D/2}$. A few low-N examples are for bosons and fermions:

$$\begin{aligned} Z_0^{(2)} &= \pm 2^{-1-D/2}\tau_2^{D/2} + \tau_2^D, \\ Z_0^{(3)} &= \pm 3^{-1-D/2}\tau_3^{D/2} + 2^{-1-D/2}\tau_3^D \pm 3^{-1}2^{-1}\tau_3^{3D/2}, \\ Z_0^{(4)} &= \pm 2^{-2-D}\tau_4^{D/2} + (2^{-3-D} + 3^{-1-D/2})\,\tau_4^D \pm 2^{-2-\frac{D}{2}}\tau_4^{3D/2} + 3^{-1}2^{-3}\tau_4^{2D}. \end{aligned} \tag{7.20}$$

From $Z_0^{(N)}(\beta)$ we calculate the specific heat [recall (2.602)] of the free canonical ensemble:

$$C_0^{(N)} = T\frac{d^2}{dT^2}[T\log Z_0^{(N)}] = \tau_N \frac{d^2}{d\tau_N^2}[\tau_N \log Z_0^{(N)}], \tag{7.21}$$

and plot it [3] in Fig. 7.4 against t for increasing particle number N. In the limit $N \to \infty$, the curves approach a limiting form with a phase transition at $T = T_c^{(0)}$, which will be derived from a grand-canonical ensemble in Eqs. (7.67) and (7.70).

The partition functions can most easily be calculated with the help of a recursion relation [4, 5], starting from $Z_0^{(0)} \equiv 1$:

$$Z_0^{(N)}(\beta) = \frac{1}{N}\sum_{n=1}^{N}(\pm 1)^{n-1} Z_0(n\beta) Z_0^{(N-n)}(\beta). \tag{7.22}$$

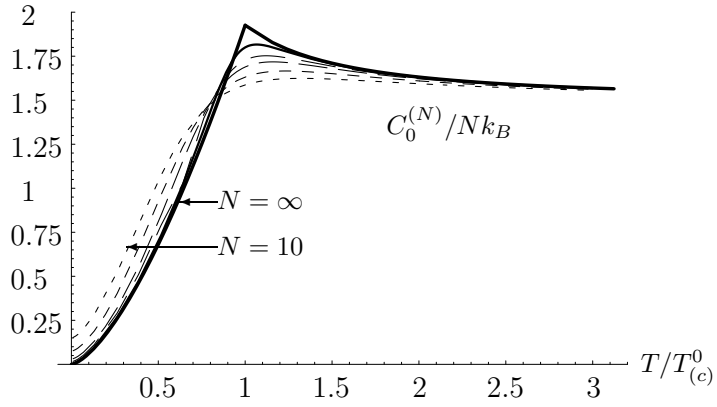

Figure 7.4 Plot of the specific heat of free Bose gas with $N = 10, 20, 50, 100, 500, \infty$ particles. The curve approaches for large T the Dulong-Petit limit $3k_BN/2$ corresponding to the three harmonic kinetic degrees of freedom in the classical Hamiltonian $\mathbf{p}^2/2M$. There are no harmonic potential degrees of freedom.

This relation is proved with the help of the grand-canonical partition function which is obtained by forming the sum over all canonical partition functions $Z_0^{(N)}(\beta)$ with a weight factor z^N:

$$Z_{G\,0}(\beta) \equiv \sum_{N=0}^{\infty} Z_0^{(N)}(\beta)\, z^N. \tag{7.23}$$

The parameter z is the Boltzmann factor of one particle with the chemical potential μ:

$$z = z(\beta) \equiv e^{\beta\mu}. \tag{7.24}$$

It is called the *fugacity* of the ensemble. Inserting the cycle decompositions (7.17), the sum becomes

$$Z_{G\,0}(\beta) \;=\; \sum_{\substack{C_1,\ldots,C_N \\ N=\Sigma_w w C_w}} \prod_{w=1}^{N} \frac{1}{C_w!}\left[(\pm 1)^{w-1}\frac{Z_0(w\beta)e^{w\beta\mu}}{w}\right]^{C_w}. \tag{7.25}$$

The right-hand side may be rearranged to

$$\begin{aligned} Z_{G\,0}(\beta) &= \prod_{w=1}^{\infty} \sum_{C_w=0}^{\infty} \frac{1}{C_w!} \left[(\pm 1)^{w-1} \frac{Z_0(w\beta) e^{w\beta\mu}}{w} \right]^{C_w} \\ &= \exp\left[\sum_{w=1}^{\infty} (\pm 1)^{w-1} \frac{Z_0(w\beta)}{w} e^{w\beta\mu} \right]. \end{aligned} \tag{7.26}$$

From this we read off the grand-canonical free energy [recall (1.545)] of noninteracting identical particles

$$F_G(\beta) \equiv -\frac{1}{\beta} \log Z_{G\,0}(\beta) = -\frac{1}{\beta} \sum_{w=1}^{\infty} (\pm 1)^{w-1} \frac{Z_0(w\beta)}{w} e^{w\beta\mu}. \tag{7.27}$$

This is simply the sum of the contributions (7.11) of connected paths to the canonical partition function which wind $w = 1, 2, 3, \ldots$ times around the cylinder [1, 6]. Thus we encounter the same situation as observed before in Section 3.20: the free energy of any quantum-mechanical system can be obtained from the perturbation expansion of the partition function by keeping only the connected diagrams.

The canonical partition function is obviously obtained from (7.27) by forming the derivative:

$$Z_0^{(N)}(\beta) = \frac{1}{N!} \frac{\partial^N}{\partial z^N} Z_{G\,0}(\beta) \bigg|_{z=0}. \tag{7.28}$$

It is now easy to derive the recursion relation (7.22). From the explicit form (7.27), we see that

$$\frac{\partial}{\partial z} Z_{G\,0} = -\left(\frac{\partial}{\partial z} \beta F_G \right) Z_{G\,0}\ . \tag{7.29}$$

Applying to this $N-1$ more derivatives yields

$$\frac{\partial^{N-1}}{\partial z^{N-1}} \left[\frac{\partial}{\partial z} Z_{G\,0} \right] = -\sum_{l=0}^{N-1} \frac{(N-1)!}{l!(N-l-1)!} \left(\frac{\partial^{l+1}}{\partial z^{l+1}} \beta F_G \right) \frac{\partial^{N-l-1}}{\partial z^{N-l-1}} Z_{G0}\ .$$

To obtain from this $Z_0^{(N)}$ we must divide this equation by $N!$ and evaluate the derivatives at $z = 0$. From (7.27) we see that the $l+1$st derivative of the grand-canonical free energy is

$$\frac{\partial^{l+1}}{\partial z^{l+1}} \beta F_G \bigg|_{z=0} = -(\pm 1)^l\, l!\, Z_0((l+1)\beta). \tag{7.30}$$

Thus we obtain

$$\frac{1}{N!} \frac{\partial^N}{\partial z^N} Z_{G\,0} \bigg|_{z=0} = \frac{1}{N} \sum_{l=0}^{N-1} (\pm 1)^l\, Z_0((l+1)\beta) \frac{1}{(N-l-1)!} \frac{\partial^{N-l-1}}{\partial z^{N-l-1}} Z_{G0} \bigg|_{z=0}\ .$$

Inserting here (7.28) and replacing $l \to n-1$ we obtain directly the recursion relation (7.22).

The grand-canonical free energy (7.27) may be simplified by using the property

$$Z_0(w\beta) = Z_0(\beta)\frac{1}{w^{D/2}} \tag{7.31}$$

of the free-particle partition function (7.12), to remove a factor $1/\sqrt{w}^D$ from $Z_0(w\beta)$. This brings (7.27) to the form

$$F_G = -\frac{1}{\beta}Z_0(\beta)\sum_{w=1}^{\infty}(\pm 1)^{w-1}\frac{e^{w\beta\mu}}{w^{D/2+1}}. \tag{7.32}$$

The average number of particles is found from the derivative with respect to the chemical potential[2]

$$N = -\frac{\partial}{\partial\mu}F_G = Z_0(\beta)\sum_{w=1}^{\infty}(\pm 1)^{w-1}\frac{e^{w\beta\mu}}{w^{D/2}}. \tag{7.33}$$

The sums over w converge certainly for negative or vanishing chemical potential μ, i.e., for fugacities smaller than unity. In Section 7.3 we shall see that for fermions, the convergence extends also to positive μ.

If the particles have a nonzero spin S, the above expressions carry a multiplicity factor $g_S = 2S + 1$, which has the value 2 for electrons.

The grand-canonical free energy (7.32) will now be studied in detail thereby revealing the interesting properties of many-boson and many-fermion orbits, the ability of the former to undergo *Bose-Einstein condensation*, and of the latter to form a *Fermi sphere* in momentum space.

7.2 Bose-Einstein Condensation

We shall now discuss the most interesting phenomenon observable in systems containing a large number of bosons, the Bose-Einstein condensation process.

7.2.1 Free Bose Gas

For bosons, the above thermodynamic functions (7.32) and (7.33) contain the functions

$$\zeta_\nu(z) \equiv \sum_{w=1}^{\infty}\frac{z^w}{w^\nu}. \tag{7.34}$$

These start out for small z like z, and increase for $z \to 1$ to $\zeta(\nu)$, where $\zeta(z)$ is Riemann's zeta function (2.521). The functions $\zeta_\nu(z)$ are called *Polylogarithmic functions* in the mathematical literature [7], where they are denoted by $\mathrm{Li}_\nu(z)$.

[2] In grand-canonical ensembles, one always deals with the average particle number $\langle N\rangle$ for which one writes N in all thermodynamic equations [recall (1.551)]. This should be no lead to confusion.

They are related to the *Hurwitz zeta function* $\zeta(\nu,a,z) \equiv \sum_{w=0}^{\infty} z^w/(w+a)^\nu$ as $\zeta_\nu(z) = z\zeta(\nu,1,z)$. The functions $\phi(z,\nu,a) = \zeta(\nu,a,z)$ are also known as *Lerch functions*.

In terms of the functions $\zeta_\nu(z)$, and the explicit form (7.12) of $Z_0(\beta)$, we may write F_G and N of Eqs. (7.32) and (7.33) simply as

$$F_G = -\frac{1}{\beta} Z_0(\beta)\zeta_{D/2+1}(z) = -\frac{1}{\beta}\frac{V_D}{l_{\rm e}^D(\hbar\beta)}\zeta_{D/2+1}(z), \tag{7.35}$$

$$N = Z_0(\beta)\zeta_{D/2}(z) = \frac{V_D}{l_{\rm e}^D(\hbar\beta)}\zeta_{D/2}(z). \tag{7.36}$$

The most interesting range where we want to know the functions $\zeta_\nu(z)$ is for negative small chemical potential μ. There the convergence is very slow and it is useful to find a faster-convergent representation. As in Subsection 2.15.6 we rewrite the sum over w for $z = e^{\beta\mu}$ as an integral plus a difference between sum and integral

$$\zeta_\nu(e^{\beta\mu}) \equiv \int_0^\infty dw \frac{e^{w\beta\mu}}{w^\nu} + \left(\sum_{w=1}^{\infty} - \int_0^\infty dw\right)\frac{e^{w\beta\mu}}{w^\nu}. \tag{7.37}$$

The integral yields $\Gamma(1-\nu)(-\beta\mu)^{\nu-1}$, and the remainder may be expanded sloppily in powers of μ to yield the Robinson expansion (2.581):

$$\zeta_\nu(e^{\beta\mu}) = \Gamma(1-\nu)(-\beta\mu)^{\nu-1} + \sum_{k=0}^{\infty}\frac{1}{k!}(\beta\mu)^k\zeta(\nu-k). \tag{7.38}$$

There exists a useful integral representation for the functions $\zeta_\nu(z)$:

$$\zeta_\nu(z) \equiv \frac{1}{\Gamma(\nu)} i_\nu(\beta\mu), \tag{7.39}$$

where $i_\nu(\alpha)$ denotes the integral

$$i_\nu(\alpha) \equiv \int_0^\infty d\varepsilon \frac{\varepsilon^{\nu-1}}{e^{\varepsilon-\alpha}-1}, \tag{7.40}$$

containing the Bose distribution function (3.93):

$$n_\varepsilon^{\rm b} = \frac{1}{e^{\varepsilon-\alpha}-1}. \tag{7.41}$$

Indeed, by expanding the denominator in the integrand in a power series

$$\frac{1}{e^{\varepsilon-\alpha}-1} = \sum_{w=1}^{\infty} e^{-w\varepsilon}e^{w\alpha}, \tag{7.42}$$

and performing the integrals over ε, we obtain directly the series (7.34).

It is instructive to express the grand-canonical free energy F_G in terms of the functions $i_\nu(\alpha)$. Combining Eqs. (7.35) with (7.39) and (7.40), we obtain

$$F_G = -\frac{1}{\beta} Z_0(\beta)\frac{i_{D/2+1}(\beta\mu)}{\Gamma(D/2+1)} = -\frac{1}{\beta\Gamma(D/2+1)}\frac{V_D}{\sqrt{2\pi\hbar^2\beta/M}^D}\int_0^\infty d\varepsilon\,\frac{\varepsilon^{D/2}}{e^{\varepsilon-\beta\mu}-1}. \tag{7.43}$$

The integral can be brought to another form by partial integration, using the fact that

$$\frac{1}{e^{\varepsilon-\beta\mu}-1}=\frac{\partial}{\partial\varepsilon}\log(1-e^{-\varepsilon+\beta\mu}). \tag{7.44}$$

The boundary terms vanish, and we find immediately:

$$F_G=\frac{1}{\beta\Gamma(D/2)}\frac{V_D}{\sqrt{2\pi\hbar^2\beta/M}^D}\int_0^\infty d\varepsilon\,\varepsilon^{D/2-1}\log(1-e^{-\varepsilon+\beta\mu}). \tag{7.45}$$

This expression is obviously equal to the sum over momentum states of oscillators with energy $\hbar\omega_{\mathbf{p}}\equiv\mathbf{p}^2/2M$, evaluated in the thermodynamic limit $N\to\infty$ with fixed particle density N/V, where the momentum states become continuous:

$$F_G=\frac{1}{\beta}\sum_{\mathbf{p}}\log(1-e^{-\beta\hbar\omega_{\mathbf{p}}+\beta\mu}). \tag{7.46}$$

This is easily verified if we rewrite the sum with the help of formula (1.558) for the surface of a unit sphere in D dimensions and a change of variables to the reduced particle energy $\varepsilon=\beta\mathbf{p}^2/2M$ as an integral

$$\begin{aligned}\sum_{\mathbf{p}}\;&\to\;V_D\int\frac{d^Dp}{(2\pi\hbar)^D}=V_DS_D\frac{1}{(2\pi\hbar)^D}\int dp\,p^{D-1}=V_DS_D\frac{(2M/\beta)^{D/2}}{(2\pi\hbar)^D}\frac{1}{2}\int d\varepsilon\,\varepsilon^{D/2-1}\\&=\;\frac{1}{\Gamma(D/2)}\frac{V_D}{\sqrt{2\pi\hbar^2\beta/M}^D}\int_0^\infty d\varepsilon\,\varepsilon^{D/2-1}.\end{aligned} \tag{7.47}$$

Another way of expressing this limit is

$$\sum_{\mathbf{p}}\to\int_0^\infty d\varepsilon\,N_\varepsilon, \tag{7.48}$$

where N_ε is the reduced *density of states* per unit energy interval:

$$N_\varepsilon\equiv\frac{1}{\Gamma(D/2)}\frac{V_D}{\sqrt{2\pi\hbar^2\beta/M}^D}\,\varepsilon^{D/2-1}. \tag{7.49}$$

The free energy of each oscillator (7.46) differs from the usual harmonic oscillator expression (2.485) by a missing ground-state energy $\hbar\omega_{\mathbf{p}}/2$. The origin of this difference will be explained in Sections 7.7 and 7.14.

The particle number corresponding to the integral representations (7.45) and (7.46) is

$$N=-\frac{\partial}{\partial\mu}F_G=\frac{1}{\Gamma(D/2)}\frac{V_D}{\sqrt{2\pi\hbar^2\beta/M}^D}\int_0^\infty d\varepsilon\frac{\varepsilon^{D/2-1}}{e^{\varepsilon-\beta\mu}-1}\approx\sum_{\mathbf{p}}\frac{1}{e^{\beta\hbar\omega_{\mathbf{p}}-\beta\mu}-1}. \tag{7.50}$$

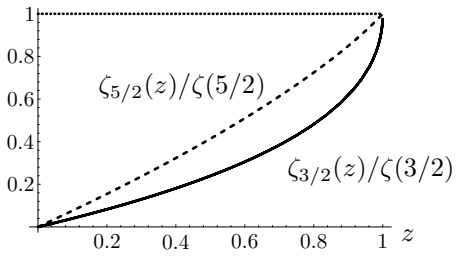

Figure 7.5 Plot of functions $\zeta_\nu(z)$ for $\nu = 3/2$ and $5/2$ appearing in Bose-Einstein thermodynamics.

For a given particle number N, Eq. (7.36) allows us to calculate the fugacity as a function of the inverse temperature, $z(\beta)$, and from this the chemical potential $\mu(\beta) = \beta^{-1} \log z(\beta)$. This is most simply done by solving Eq. (7.36) for β as a function of z, and inverting the resulting function $\beta(z)$. The required functions $\zeta_\nu(z)$ are shown in Fig. 7.5.

There exists a solution $z(\beta)$ only if the total particle number N is smaller than the characteristic function defined by the right-hand side of (7.36) at unit fugacity $z(\beta) = 1$, or zero chemical potential $\mu = 0$:

$$N < \frac{V_D}{l_{\rm e}^D(\hbar\beta)}\zeta(D/2). \tag{7.51}$$

Since $l_{\rm e}(\hbar\beta)$ decreases with increasing temperature, this condition certainly holds at sufficiently high T. For decreasing temperature, the solution exists only as long as the temperature is higher than the critical temperature $T_c = 1/k_B\beta_c$, determined by

$$N = \frac{V_D}{l_{\rm e}^D(\hbar\beta_c)}\zeta(D/2). \tag{7.52}$$

This determines the critical density of the atoms. The de Broglie length at the critical temperature will appear so frequently that we shall abbreviate it by ℓ_c:

$$l_{\rm e}(\hbar\beta_c) = \ell_c \equiv \left[\frac{N}{V_D\zeta(D/2)}\right]^{-1/D}. \tag{7.53}$$

The critical density is reached at the characteristic temperature $T_c^{(0)}$ introduced in Eq. (7.18). Note that for a two-dimensional system, Eq. (7.18) yields $T_c^{(0)} = 0$, due to $\zeta(1) = \infty$, implying the nonexistence of a condensate. One can observe, however, definite experimental signals for the vicinity of a transition. In fact, we have neglected so far the interaction between the atoms, which is usually repulsive. This will give rise to a special type of phase transition called Kosterlitz-Thouless transition. For a discussion of this transition see other textbooks [8].

By combining (7.18) with (7.36) we obtain an equation for the temperature dependence of z above T_c:

$$1 = \left(\frac{T}{T_c}\right)^{D/2} \frac{\zeta_{D/2}(z(T))}{\zeta(D/2)}, \quad T > T_c. \tag{7.54}$$

This is solved most easily by calculating T/T_c as a function of $z = e^{\beta\mu}$. Since for small z, all functions $\eta_\nu(z)$ behave like z, the high-temperature-behavior of z is $z \approx \zeta(D/2)(T_c/T)^{D/2}$

If the temperature drops below T_c, the system can no longer accommodate all particles N in a normal state. A certain fraction of them, say $N_{\rm cond}(T)$, is forced to condense in the ground state of zero momentum, forming the so-called *Bose-Einstein condensate*. The condensate acts like a particle reservoir with a chemical potential zero.

Both phases can be described by the single equation for the number of normal particles, i.e., those outside the condensate:

$$N_{\rm n}(T) = \frac{V_D}{l_{\rm e}^D(\hbar\beta)} \zeta_{D/2}(z(\beta)). \tag{7.55}$$

For $T > T_c$, all particles are normal and the relation between μ and the temperature is found from the equation $N_{\rm n}(T) = N$, where (7.55) reduces to (7.36). For $T < T_c$, however, the chemical potential vanishes so that $z = 1$ and (7.55) reduces to

$$N_{\rm n}(T) = \frac{V_D}{l_{\rm e}^D(\hbar\beta)} \zeta_{D/2}(1), \tag{7.56}$$

which yields the temperature dependence of the number of normal particles:

$$\frac{N_{\rm n}(T)}{N} = \left(\frac{T}{T_c}\right)^{D/2}, \quad T < T_c. \tag{7.57}$$

The density of particles in the condensate is therefore given by

$$\frac{N_{\rm cond}(T)}{N} = 1 - \frac{N_{\rm n}(T)}{N} = 1 - \left(\frac{T}{T_c}\right)^{D/2}. \tag{7.58}$$

We now calculate the internal energy which is, according to the general thermodynamic relation (1.553), given by

$$E = F_G + TS + \mu N = F_G - T\partial_T F_G + \mu N = \partial_\beta(\beta F_G) + \mu N. \tag{7.59}$$

Expressing N as $-\partial F_G/\partial\mu$, we can also write

$$E = F_G + (\beta\partial_\beta - \mu\partial_\mu) F_G. \tag{7.60}$$

Inserting (7.35) we see that only the β-derivative of the prefactor contributes since $(\beta\partial_\beta - \mu\partial_\mu)$ applied to any function of $z = e^{\beta\mu}$ vanishes. Thus we obtain directly

$$E = -\frac{D}{2} F_G, \tag{7.61}$$

which becomes with (7.35) and (7.36):

$$E = \frac{D}{2\beta} Z_0(\beta)\zeta_{D/2+1}(z) = \frac{D}{2}\frac{\zeta_{D/2+1}(z)}{\zeta_{D/2}(z)} N k_B T. \tag{7.62}$$

The entropy is found using the thermodynamic relation (1.574):

$$S = \frac{1}{T}\left(E - \mu N - F_G\right) = \frac{1}{T}\left(-\frac{D+2}{2}F_G - \mu N\right), \tag{7.63}$$

or, more explicitly,

$$S = k_B\left[\frac{D+2}{2}Z_0(\beta)\zeta_{D/2+1}(z) - \beta\mu N\right] = k_B N\left[\frac{D+2}{2}\frac{\zeta_{D/2+1}(z)}{\zeta_{D/2}(z)} - \beta\mu\right]. \tag{7.64}$$

For $T < T_c$, the entropy is given by (7.64) with $\mu = 0$, $z = 1$ and N replaced by the number $N_{\rm n}$ of normal particles of Eq. (7.57):

$$S_< = k_B N\left(\frac{T}{T_c}\right)^{D/2}\frac{(D+2)}{2}\frac{\zeta_{D/2+1}(1)}{\zeta_{D/2}(1)}, \quad T < T_c. \tag{7.65}$$

The particles in the condensate do not contribute since they are in a unique state. They do not contribute to E and F_G either since they have zero energy and $\mu = 0$. Similarly we find from (7.62):

$$E_< = \frac{D}{2}\,N k_B T\left(\frac{T}{T_c}\right)^{D/2}\frac{\zeta_{D/2+1}(1)}{\zeta_{D/2}(1)} = \frac{D}{D+2}TS_<, \quad T < T_c. \tag{7.66}$$

The specific heat C at a constant volume in units of k_B is found for $T < T_c$ from (7.65) via the relation $C = T\partial_T S|_N$ [recall (2.602)]:

$$C = k_B N\left(\frac{T}{T_c}\right)^{D/2}\frac{(D+2)D}{4}\frac{\zeta_{D/2+1}(1)}{\zeta_{D/2}(1)}, \quad T < T_c. \tag{7.67}$$

For $T > T_c$, the chemical potential at fixed N satisfies the equation

$$\beta\partial_\beta(\beta\mu) = \frac{D}{2}\frac{\zeta_{D/2}(z)}{\zeta_{D/2-1}(z)}. \tag{7.68}$$

This follows directly from the vanishing derivative $\beta\partial_\beta N = 0$ implied by the fixed particle number N. Applying the derivative to Eq. (7.36) and using the relation $z\partial_z\zeta_\nu(z) = \zeta_{\nu-1}(z)$, as well as $\beta\partial_\beta f(z) = z\partial_z f(z)\,\beta\partial_\beta(\beta\mu)$, we obtain

$$\begin{aligned}\beta\partial_\beta N &= [\beta\partial_\beta Z_0(\beta)]\zeta_{D/2}(z) + Z_0(\beta)\beta\partial_\beta\zeta_{D/2}(z)\\ &= -\frac{D}{2}Z_0(\beta)\zeta_{D/2}(z) + Z_0(\beta)\,\zeta_{D/2-1}(z)\beta\partial_\beta(\beta\mu) = 0,\end{aligned} \tag{7.69}$$

thus proving (7.68).

The specific heat C at a constant volume in units of k_B is found from the derivative $C = T\partial_T S|_N = -\beta^2 \partial_\beta E|_N$, using once more (7.68):

$$C = k_B N \left[\frac{(D+2)D}{4} \frac{\zeta_{D/2+1}(z)}{\zeta_{D/2}(z)} - \frac{D^2}{4} \frac{\zeta_{D/2}(z)}{\zeta_{D/2-1}(z)} \right], \quad T > T_c. \tag{7.70}$$

At high temperatures, C tends to the Dulong-Petit limit $Dk_BN/2$ since for small z all $\zeta_\nu(z)$ behave like z.

Consider now the physical case $D = 3$, where the second denominator in (7.70) contains $\zeta_{1/2}(z)$. As the temperature approaches the critical point from above, z tends to unity from below and $\zeta_{1/2}(z)$ diverges. Thus $1/\zeta_{1/2}(1) = 0$ and the second term in (7.70) disappears, yielding a maximal value in three dimensions

$$C_{\max} = k_B N \frac{15}{4} \frac{\zeta_{5/2}(1)}{\zeta_{3/2}(1)} \approx k_B N \, 1.92567. \tag{7.71}$$

This value is the same as the critical value of Eq. (7.67) below T_c. The specific heat is therefore continuous at T_c. It shows, however, a marked kink. To calculate the jump in the slope we calculate the behavior of the thermodynamic quantities for $T \gtrsim T_c$. As T passes T_c from below, the chemical potential starts becoming smaller than zero, and we can expand Eq. (7.54)

$$1 = \left(\frac{T}{T_c} \right)^{3/2} \left[1 + \frac{\Delta\zeta_{3/2}(z)}{\zeta_{3/2}(1)} \right], \tag{7.72}$$

where the symbol Δ in front of a quantity indicates that the same quantity at zero chemical potential is subtracted. Near T_c, we can approximate

$$\left(\frac{T}{T_c} \right)^{3/2} - 1 \approx -\frac{\Delta\zeta_{3/2}(z)}{\zeta_{3/2}(1)}. \tag{7.73}$$

We now use the Robinson expansion (7.38) to approximate for small negative μ:

$$\zeta_{3/2}(e^{\beta\mu}) = \Gamma(-1/2)(-\beta\mu)^{1/2} + \zeta(3/2) + \beta\mu\zeta(1/2) + \dots \, , \tag{7.74}$$

with $\Gamma(-1/2) = -2\sqrt{\pi}$. The right-hand side of (7.73) becomes therefore $-\Delta\zeta_{3/2}(z)/\zeta_{3/2}(1) = -2\sqrt{\pi}/\zeta(3/2)(-\beta\mu)^{1/2}$. Inserting this into Eq. (7.73), we obtain the temperature dependence of $-\mu$ for $T \gtrsim T_c$:

$$-\mu \approx \frac{1}{4\pi} k_B T_c \, \zeta^2(3/2) \left[\left(\frac{T}{T_c} \right)^{3/2} - 1 \right]^2. \tag{7.75}$$

The leading square-root term on the right-hand side of (7.74) can also be derived from the integral representation (7.40) which receives for small α its main contribution from $\alpha \approx 0$, where $\Delta i_{3/2}(\alpha)$ can be approximated by

$$\Delta i_{3/2}(\alpha) = \int_0^\infty dz \, z^{1/2} \left(\frac{1}{e^{z-\alpha}-1} - \frac{1}{e^z - 1} \right) \approx \alpha \int_0^\infty dz \frac{1}{z^{1/2}(z-\alpha)} = -\pi\sqrt{-\alpha}. \tag{7.76}$$

Using the relation (7.61) for $D = 3$, we calculate the derivative of the energy with respect to the chemical potential from

$$\frac{\partial E}{\partial \mu}\Big|_{T,V} = -\frac{3}{2}\frac{\partial F_G}{\partial \mu}\Big|_{T,V}. \tag{7.77}$$

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

$$E \approx E_< + \frac{3}{2}N\mu = E_< - \frac{3}{8\pi}Nk_BT_c\,\zeta^2(3/2)\left[\left(\frac{T}{T_c}\right)^{3/2} - 1\right]^2. \tag{7.78}$$

Forming the derivative of this with respect to the temperature we find that the slope of the specific heat below and above T_c jumps at T_c by

$$\Delta\left(\frac{\partial C}{\partial T}\right) \approx \frac{27}{16\pi}\zeta^2(3/2)\,N\frac{k_B}{T_c} \equiv 3.6658\,N\frac{k_B}{T_c}, \tag{7.79}$$

the individual slopes being from (7.66) with $D = 3$ (using $\partial C/\partial T = \partial^2 E/\partial T^2$):

$$\left(\frac{\partial C_<}{\partial T}\right) = \frac{15}{4}\frac{3}{2}\frac{\zeta(5/2)}{\zeta(3/2)}\frac{Nk_B}{T_c} \approx 2.8885\frac{Nk_B}{T_c}, \quad T < T_c, \tag{7.80}$$

and from (7.78):

$$\left(\frac{\partial C_>}{\partial T}\right) = \left(\frac{\partial C_<}{\partial T}\right) - \Delta\left(\frac{\partial C}{\partial T}\right) \approx -0.7715\frac{Nk_B}{T_c}, \quad T > T_c. \tag{7.81}$$

The specific heat of the three-dimensional Bose gas is plotted in Fig. 7.6, where it is compared with the specific heat of superfluid helium for the appropriate atomic parameters $n = 22.22$ nm^{-3}, $M = 6.695 \times 10^{-27}$ kg, where the critical temperature is $T_c \approx 3.145$K, which is somewhat larger than $T_c \approx 2.17$ K of helium.

There are two major disagreements due to the strong interactions in helium. First, the small-T behavior is $(T/T_c)^{3/2}$ rather than the physical $(T/T_c)^3$ due to phonons. Second, the Dulong-Petit limit of an interacting system is closer to that of harmonic oscillators which is twice as big as the free-particle case. Recall that according to the Dulong-Petit law (2.603), C receives a contribution $Nk_BT/2$ per *harmonic* degree of freedom, potential as well as kinetic. Free particle energies are only harmonic in the momentum.

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". Recently, such condensates have been set into rotation and shown to become perforated by vortex lines [10] just like rotating superfluid helium II.

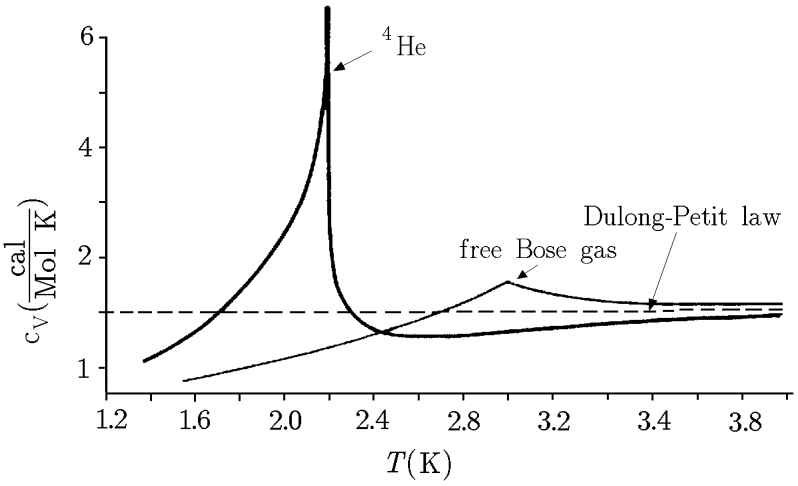

Figure 7.6 Specific heat of ideal Bose gas with phase transition at T_c. For comparison, we have also plotted the specific heat of superfluid helium for the same atomic parameters. The experimental curve is reduced by a factor 2 to have the same Dulong-Petit limit as free bosons.

7.2.2 Bose Gas in Finite Box

The condensation process can be understood better by studying a system in which there is a large but finite number of bosons enclosed in a large cubic box of size L. Then the sum on the right-hand side of Eq. (7.50) gives the contribution of the discrete momentum states to the total particle number. This implies that the function $\zeta_{D/2}(z)$ in Eq. (7.36) has to be replaced by a function $\zeta^{\text{box}}_{D/2}(z)$ defined by the sum over the discrete momentum vectors $\mathbf{p_n} = \hbar\pi(n_1, n_2, \ldots, n_D)/L$ with $n_i = 1, 2, 3, \ldots$:

$$N = \frac{V_D}{l_{\text{e}}^D(\hbar\beta)}\zeta^{\text{box}}_{D/2}(z) = \sum_{\mathbf{p_n}} \frac{1}{e^{\beta \mathbf{p}_\mathbf{n}^2/2M - \beta\mu} - 1}. \tag{7.82}$$

This can be expressed in terms of the one-dimensional auxiliary partition function of a particle in a one-dimensional "box":

$$Z_1(b) \equiv \sum_{n=1}^{\infty} e^{-bn^2/2}, \qquad b \equiv \beta\hbar^2\pi^2/ML^2 = \pi l_{\text{e}}^2(\hbar\beta)/2L^2, \tag{7.83}$$

as

$$N = \frac{V_D}{l_{\text{e}}^D(\hbar\beta)}\zeta^{\text{box}}_{D/2}(z) = \sum_w Z_1^D(wb) z^w. \tag{7.84}$$

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

$$\vartheta_3(u, z) \equiv 1 + 2\sum_{n=1}^{\infty} z^{n^2} \cos 2nu \tag{7.85}$$

by $Z_1(b) = [\vartheta_3(0, e^{-b/2}) - 1]/2$. The small-$b$ behavior of this function is easily calculated following the technique of Subsection 2.15.6. We rewrite the sum with the help of Poisson's summation formula (1.205) as a sum over integrals

$$\begin{aligned} \vartheta_3(0, e^{-b/2}) &= \sum_{k=-\infty}^{\infty} e^{-k^2 b/2} = \sum_{m=-\infty}^{\infty} \int_{-\infty}^{\infty} dk\, e^{-k^2 b/2 + 2\pi i k m} \\ &= \sqrt{\frac{2\pi}{b}} \left(1 + 2 \sum_{m=1}^{\infty} e^{-2\pi^2 m^2/b}\right). \end{aligned} \tag{7.86}$$

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 $L/\sqrt{\beta}$):

$$Z_1(b) = \sqrt{\frac{\pi}{2b}} - \frac{1}{2} + \mathcal{O}(e^{-2\pi^2/b}). \tag{7.87}$$

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

In the sum (7.82), the lowest energy level with $\mathbf{p}_{1,\ldots,1} = \hbar\pi(1, \ldots, 1)/L$ plays a special role. Its contribution to the total particle number is the number of particles in the condensate:

$$N_{\rm cond}(T) = \frac{1}{e^{Db/2 - \beta\mu} - 1} = \frac{z_D}{1 - z_D}, \qquad z_D \equiv e^{\beta\mu - Db/2}. \tag{7.88}$$

This number diverges for $z_D \to 1$, where the box function $\zeta^{\rm box}_{D/2}(z)$ has a pole $1/(Db/2 - \beta\mu)$. This pole prevents $\beta\mu$ from becoming exactly equal to $Db/2$ when solving the equation (7.82) 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 $\bar{\zeta}^{\rm box}_{D/2}(z)$ in which the lowest, singular term in the sum (7.82) is omitted. Let us define the number of *normal* particles which have not condensed into the state of zero momentum as $N_{\rm n}(T) = N - N_{\rm cond}(T)$. Then we can rewrite Eq. (7.82) as an equation for the number of normal particles

$$N_{\rm n}(T) = \frac{V_D}{l_{\rm e}^D(\hbar\beta)} \bar{\zeta}^{\rm box}_{D/2}(z(\beta)), \tag{7.89}$$

which reads more explicitly

$$N_{\rm n}(T) = S_D(z_D) \equiv \sum_{w=1}^{\infty} [Z_1^D(wb) e^{wDb/2} - 1] z_D^w. \tag{7.90}$$

A would-be critical point may now be determined by setting here $z_D = 1$ and equating the resulting $N_{\rm n}$ 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 7A

[see Eq. (7A.12)], so that the associated temperature $T_c^{(1)}$ is determined from the equation

$$N = \sqrt{\frac{\pi}{2b_c}}^3 \zeta(3/2) + \frac{3\pi}{4b_c^{(1)}} \log C_3 b_c + \dots \ , \tag{7.91}$$

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

$$N = \sqrt{\frac{\pi}{2b_c^{(0)}}}^3 \zeta(3/2), \tag{7.92}$$

in agreement with Eq. (7.52), if we recall b from (7.83). Using this we rewrite (7.91) as

$$1 \equiv \left(\frac{T_c^{(1)}}{T_c^{(0)}}\right)^{3/2} + \frac{3}{2N}\frac{\pi}{2b_c^{(0)}} \log C_3 b_c^{(0)}. \tag{7.93}$$

Expressing $b_c^{(0)}$ in terms of N from (7.92), this implies

$$\frac{\delta T_c^{(1)}}{T_c^{(0)}} \approx \frac{1}{\zeta^{2/3}(3/2) N^{1/3}} \log \frac{2}{\pi C_3} \frac{N^{2/3}}{\zeta^{2/3}(3/2)}. \tag{7.94}$$

Experimentally, the temperature $T_c^{(1)}$ is not immediatly accessible. What is easy to find is the place where the condensate density has the largest curvature, i.e., where $d^3 N_{\rm cond}/dT^3 = 0$. The associated temperature $T_c^{\rm exp}$ 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 to order in $1/N^{1/3}$. The proof is given in Appendix 7B.

7.2.3 Effect of Interactions

Superfluid helium has a lower transition temperature than the ideal Bose gas. This should be expected since the atomic repulsion impedes the condensation process of the atoms in the zero-momentum state. Indeed, a simple perturbative calculation based on a potential whose Fourier transform behaves for small momenta like

$$\tilde{V}(\mathbf{k}) = g\left[1 - r_{\rm eff}^2 \mathbf{k}^2/6 + \dots\right] \tag{7.95}$$

gives a negative shift $\Delta T_c \equiv T_c - T_c^{(0)}$ proportional to the particle density [11]:

$$\frac{\Delta T_c}{T_c^{(0)}} = -\frac{1}{3\hbar^2} M r_{\rm eff}^2 g \frac{N}{V}, \tag{7.96}$$

where V is the three-dimensional volume. When discussing the interacting system we shall refer to the previously calculated critical temperature of the free system as $T_c^{(0)}$. This result follows from the fact that for small g and $r_{\rm eff}$, the free-particle energies $\epsilon_0(\mathbf{k}) = \hbar^2\mathbf{k}^2/2M$ are changed to $\epsilon(\mathbf{k}) = \epsilon(0) + \hbar^2\mathbf{k}^2/2M^*$ with a renormalized inverse effective mass $1/M^* = [1 - M r_{\rm eff}^2 g N/3\hbar^2 V]/M$. Inserting this into Eq. (7.18), from

which we may extract the equation for the temperature shift $\Delta T_c/T_c^{(0)} = M/M^* - 1$, we obtain indeed the result (7.96). The parameter $r_{\rm eff}$ is called the *effective range* of the potential. The parameter g in (7.95) can be determined by measuring the s-wave *scattering length* a in a two-body scattering experiment. The relation is obtained from a solution of the Lippmann-Schwinger equation (1.525) for the T-matrix. In a dilute gas, this yields in three dimensions

$$g = \frac{2\pi\hbar^2}{M/2}\, a. \tag{7.97}$$

The denominator $M/2$ is the reduced mass of the two identical bosons. In $D = 2$ dimensions where g has the dimension energy×length^D, Eq. (7.97) is replaced by [12, 13, 14, 15, 17]

$$g = \frac{\pi^{D/2-1}}{2^{2-D}\Gamma(1-D/2)(na^D)^{D-2} + \Gamma(D/2-1)}\frac{2\pi\hbar^2}{M/2}a^{D-2} \equiv \gamma(D, na^D)\frac{2\pi\hbar^2}{M/2}a^{D-2}. \tag{7.98}$$

In the limit $D \to 2$, this becomes

$$g = -\frac{2\pi\hbar^2/M}{\ln(e^\gamma na^2/2)}, \tag{7.99}$$

where γ is the Euler-Mascheroni constant. The logarithm in the denominator implies that the effective repulsion decreases only very slowly with decreasing density [16].

For a low particle density N/V, the effective range $r_{\rm eff}$ becomes irrelevant and the shift ΔT_c depends on the density with a lower power $(N/V)^{\kappa/3}$, $\kappa < 3$. The low-density limit can be treated by keeping in (7.95) only the first term corresponding to a pure δ-function repulsion

$$V(\mathbf{x} - \mathbf{x}') = g\,\delta^{(3)}(\mathbf{x} - \mathbf{x}'). \tag{7.100}$$

For this interaction, the lowest-order correction to the energy is in D dimensions

$$\Delta E = g\int d^D x\, n^2(\mathbf{x}), \tag{7.101}$$

where $n(\mathbf{x})$ is the local particle density. For a homogeneous gas, this changes the grand-canonical free energy from (7.35) to

$$F_G = -\frac{1}{\beta}\frac{V_D}{l_{\rm e}^D(\hbar\beta)}\zeta_{D/2+1}(z) + g\,V_D\left[\frac{\zeta_{D/2}(z)}{l_{\rm e}^D(\hbar\beta)}\right]^2 + \mathcal{O}(g^2), \tag{7.102}$$

where we have substituted $n(\mathbf{x})$ by the constant density N/V_D of Eq. (7.36). We now introduce a length parameter α proportional to the coupling constant g:

$$g \equiv \frac{2}{\beta}\,\frac{\alpha}{l_{\rm e}(\hbar\beta)}l_{\rm e}^D(\hbar\beta). \tag{7.103}$$

In three dimensions, α coincides in the dilute limit (small na^D) with the s-wave scattering length a of Eq. (7.97). In in D dimensions, the relation is

$$\alpha = \gamma(D, na^D) \left[\frac{a}{l_{\rm e}(\hbar\beta)}\right]^{D-3} a. \tag{7.104}$$

In two dimensions, this has the limit

$$\alpha = -\frac{l_{\rm e}(\hbar\beta)}{\ln(e^\gamma na^2/2)}. \tag{7.105}$$

We further introduce the reduced dimensionless coupling parameter $\hat{\alpha} \equiv \alpha/l_{\rm e}(\hbar\beta) = \gamma(D, na^D)\,[a/l_{\rm e}(\hbar\beta)]^{D-2}$, for brevity [recall (7.104)]. In terms of $\hat{\alpha}$, the grand-canonical free energy (7.102) takes the form

$$F_G \;=\; -\frac{1}{\beta}\frac{V_D}{l_{\rm e}^D(\hbar\beta)}\left\{\zeta_{D/2+1}(z) - 2\hat{\alpha}[\zeta_{D/2}(z)]^2\right\} + \mathcal{O}(\alpha^2). \tag{7.106}$$

A second-order perturbation calculation extends this by a term [18, 19]

$$\Delta F_G \;=\; -\frac{1}{\beta}\frac{V_D}{l_{\rm e}^D(\hbar\beta)}\left\{8\hat{\alpha}^2 h_D(z)\right\}, \tag{7.107}$$

where $h_D(z) = h_D^{(1)}(z) + h_D^{(2)}(z)$ is the sum of two terms. The first is simply

$$h_D^{(1)}(z) \equiv [\zeta_{D/2}(z)]^2\zeta_{D/2-1}(z), \tag{7.108}$$

the second has been calculated only for $D = 3$:

$$h_3^{(2)}(z) \equiv \sum_{n_1,n_2,n_3=1}^{\infty} \frac{z^{n_1+n_2+n_3}}{\sqrt{n_1n_2n_3}(n_1+n_2)(n_1+n_3)}. \tag{7.109}$$

The associated particle number is

$$N = \frac{V_D}{l_{\rm e}^D(\hbar\beta)}\left\{\zeta_{D/2}(z) - 4\hat{\alpha}\zeta_{D/2-1}(z)\zeta_{D/2}(z) + 8\hat{\alpha}^2 z\frac{dh_D(z)}{dz}\right\} + \mathcal{O}(\alpha^3). \tag{7.110}$$

For small α, we may combine the equations for F_G and N and derive the following simple relation between the shift in the critical temperature and the change in the particle density caused by the interaction

$$\frac{\Delta T_c}{T_c^{(0)}} \approx -\frac{2}{D}\frac{\Delta n}{n}, \tag{7.111}$$

where Δn is the change in the density at the critical point caused by the interaction. The equation is correct to lowest order in the interaction strength.

The calculation of $\Delta T_c/T_c^{(0)}$ in three dimensions has turned out to be a difficult problem. The reason is that the perturbation series for the right-hand side of (7.111) is found to be an expansion in powers $(T - T_c^{(0)})^{-n}$ which needs a strong-coupling

evaluation for $T \to T_c^{(0)}$. Many theoretical papers have given completely different result, even in sign, and Monte Carlo data to indicate sign and order of magnitude. The ideal tool for such a calculation, field theoretic variational perturbation theory, has only recently been developed [20], and led to a result in rough agreement with Monte Carlo data [21]. Let us briefly review the history.

All theoretical results obtained in the literature have the generic form

$$\frac{\Delta T_c}{T_c^{(0)}} = c[\zeta(3/2)]^{\kappa/3} \left[\frac{a}{\ell_c}\right]^{\kappa} = c\, a^{\kappa} \left(\frac{N}{V}\right)^{\kappa/3}, \tag{7.112}$$

where the right-hand part of the equation follows from the middle part via Eq. (7.53). In an early calculation [22] based on the δ-function potential (7.100), κ was found to be $1/2$, with a downward shift of T_c. More recent studies, however, have lead to the opposite sign [23]–[38]. The exponents κ found by different authors range from $\kappa = 1/2$ [23, 18, 31] to $\kappa = 3/2$ [19]. The most recent calculations yield $\kappa = 1$ [24]–[28], i.e., a direct proportionality of $\Delta T_c/T_c^{(0)}$ to the s-wave scattering length a, a result also found by Monte Carlo simulations [29, 30, 38], and by an extrapolation of experimental data measured in the strongly interacting superfluid ^{4}He after diluting it with the help of Vycor glass [40]. As far as the proportionality constant c is concerned, the literature offers various values which range for $\kappa = 1$ from $c = 0.34 \pm 0.03$ [29] to $c = 5.1$ [40]. A recent negative value $c \approx -0.93$ [41] has been shown to arise from a false assumption on the relation between canonical and grand-canonical partition function [42]. An older Monte Carlo result found $c \approx 2.3$ [30] lies close to the theoretical results of Refs. [23, 27, 28], who calculated $c_1 \approx -8\zeta(1/2)/3\zeta^{1/3}(3/2) \approx 2.83$, $8\pi/3\zeta^{4/3}(3/2) \approx 2.33$, 1.9, respectively, while the extrapolation of the experimental data on ^{4}He in Vycor glass favored $c = 5.1$, near the theoretical estimate $c = 4.66$ of Stoof [24]. The latest Monte Carlo data, however, point towards a smaller value $c \approx 1.32 \pm 0.02$, close to theoretical numbers 1.48 and 1.14 in Refs. [35, 39] and 1.14 ± 0.11 in Ref. [21].

There is no space here to discuss in detail how the evaluation is done. We only want to point out an initially surprising result that in contrast to a potential with a finite effective range in (7.96), the δ-function repulsion (7.100) with a pure phase shift causes no change of T_c linear $an^{1/D}$ if only the first perturbative correction to the grand-canonical free energy in Eq. (7.106) is taken into account. A simple nonperturbative approach which shows this goes as follows: We observe that the one-loop expression for the free energy may be considered as the extremum with respect to σ of the variational expression

$$F_G^{\sigma} = -\frac{1}{\beta}\frac{V_D}{l_{\rm e}^D(\hbar\beta)}\left[\zeta_{D/2+1}(ze^{\sigma}) - \frac{\sigma^2}{8\hat{\alpha}}\right], \tag{7.113}$$

which is certainly correct to first order in a. We have introduced the reduced dimensionless coupling parameter $\hat{\alpha} \equiv \alpha/l_{\rm e}(\hbar\beta) = \gamma(D, na^D)\,[a/l_{\rm e}(\hbar\beta)]^{D-2}$, for brevity [recall (7.104)]. The extremum lies at $\sigma = \Sigma$ which solves the implicit equation

$$\Sigma \equiv -4\hat{\alpha}\zeta_{D/2}(ze^{\Sigma}). \tag{7.114}$$

The extremal free energy is

$$F_G^\Sigma = -\frac{1}{\beta}\frac{V_D}{l_{\rm e}^D(\hbar\beta)}\left\{\zeta_{D/2+1}(Z) - 2\hat{\alpha}[\zeta_{D/2}(Z)]^2\right\}, \quad Z \equiv ze^\Sigma. \tag{7.115}$$

The equation for the particle number, obtained from the derivative of the free energy (7.113) with respect to $-\mu$, reads

$$N = \frac{V_D}{l_{\rm e}^D(\hbar\beta)}\zeta_{D/2}(Z), \tag{7.116}$$

and fixes Z. This equation has the same form as in the free case (7.36), so that the phase transition takes place at $Z = 1$, implying the same transition temperature as in the free system to this order. As discussed above, a nonzero shift (7.112) can only be found after summing up many higher-order Feynman diagrams which all diverge at the critical temperature.

Let us also point out that the path integral approach is not an adequate tool for discussing the condensed phase below the critical temperature, for which infinitely many particle orbits are needed. In the condensed phase, a quantum field theoretic formulation is more appropriate (see Section 7.6). The result of such a discussion is that due to the positive value of c in (7.112), the phase diagram has an unusual shape shown in Fig. 7.7. The nose in the phase transition curve implies that the system can undergo Bose-Einstein condensation slightly *above* $T_c^{(0)}$ if the interaction is *increased* (see Ref. [43]).

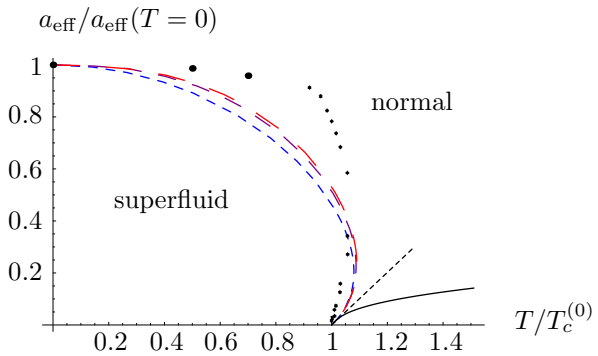

Figure 7.7 Reentrant transition in phase diagram of Bose-Einstein condensation for different interaction strengths. Curves were obtained in Ref. [43] from a variationally improved one-loop approximation to field-theoretic description with properly imposed positive slope at $T_c^{(0)}$ (dash length increasing with order of variational perturbation theory). Short solid curve and dashed straight line starting at $T_c^{(0)}$ are due to Ref. [38] and [21]. Diamonds correspond to the Monte-Carlo data of Ref. [29] and dots stem from Ref. [44], both scaled to their critical value $a_{\rm eff}(T=0) \approx 0.63$.

An important consequence of a repulsive short-range interaction is a change in the particle excitation energies below T_c. It was shown by Bogoliubov [46] that this changes the energy from the quadratic form $\epsilon(\mathbf{p}) = \mathbf{p}^2/2M$ to

$$\epsilon(\mathbf{p}) = \sqrt{\epsilon^2(\mathbf{p}) + 2gn\epsilon(\mathbf{p})}, \tag{7.117}$$

which starts linearly like $\epsilon(\mathbf{p}) = \sqrt{gn/M}|\mathbf{p}| = \hbar\sqrt{4\pi an/M}|\mathbf{p}|$ for small $\mathbf{p}$, the slope defining the second sound velocity. In the strongly interacting superfluid helium, the momentum dependence has the form shown in Fig. 7.8. It was shown by Bogoliubov

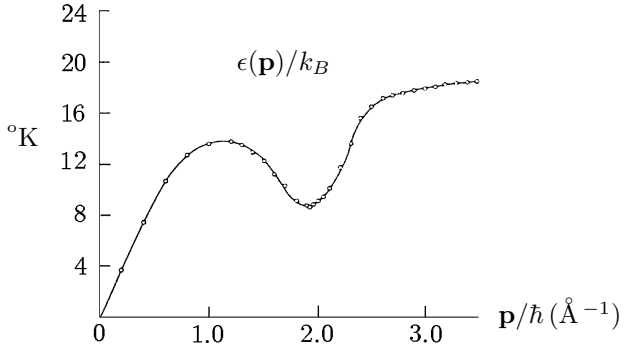

Figure 7.8 Energies of elementary excitations of superfluid ^{4}He measured by neutron scattering showing excitation energy of NG bosons [after R.A. Cowley and A.D. Woods, Can. J. Phys *49*, 177 (1971)].

[46] that a system in which $\epsilon(\mathbf{p}) > v_c\,|\mathbf{p}|$ for some finite critical velocity v_c will display superfluidity as long as it moves with velocity $\mathbf{v} = \partial\epsilon(\mathbf{p})/\partial\mathbf{p}$ smaller than v_c. This follows by forming the free energy in a frame moving with velocity $\mathbf{v}$. It is given by the Legendre transform:

$$f \equiv \epsilon(\mathbf{p}) - \mathbf{v}\cdot\mathbf{p}, \tag{7.118}$$

which has a minimum at $\mathbf{p} = 0$ if as long as $|\mathbf{v}| < v_c$, implying that the particles do not move. Seen from the moving frame, they keep moving with a constant velocity $-\mathbf{v}$, without slowing down. This is in contrast to particles with the free spectrum $\epsilon(\mathbf{p}) = \mathbf{p}^2/2M$ for which f has a minimum at $\mathbf{p} = M\mathbf{v}$, implying that these particles always move with the same velocity as the moving frame. Note that the second sound waves of long wavelength have an energy $\epsilon(\mathbf{p} = c|\mathbf{p}|$ just like light waves in the vacuum, with light velocity exchanged by the sound velocity. Even though the superfluid is nonrelativistic, the sound waves behave like relativistic particles. This phenomenon is known from the sound waves in crystals which behave similar to relativistic massless particles. In fact, the Debye theory of specific heat is very similar to Planck's black-body theory, except that the lattice size appears explicitly as a short-wavelength cutoff. It has recently been speculated that the relativistically invariant world we observe is merely the long-wavelength limit of a

world crystal whose lattice constant is very small [47], of the order of the Planck length $\ell_{\rm P} \approx 8.08 \times 10^{-33}\,{\rm cm}$.

7.2.4 Bose-Einstein Condensation in Harmonic Trap

In a harmonic magnetic trap, the path integral (7.7) of the individual orbits becomes

$$(\mathbf{x}_b^{(p(\nu))}\hbar\beta|\mathbf{x}_a^{(\nu)}\,0)_\omega = \int_{\mathbf{x}^{(\nu)}(\tau_a)=\mathbf{x}_a^{(\nu)}}^{\mathbf{x}^{(p(\nu))}(\tau_b)=\mathbf{x}_b^{(\nu)}} \mathcal{D}^D x^{(\nu)} \exp\left\{-\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau \frac{M}{2}\left[\dot{\mathbf{x}}^{(\nu)2} + \omega^2 \mathbf{x}^{(\nu)2}\right]\right\}, \quad (7.119)$$

and is solved by [recall (2.411)]

$$\begin{aligned}(\mathbf{x}_b^{(p(\nu))}\hbar\beta|\mathbf{x}_a^{(\nu)}\,0)_\omega = {} & \frac{1}{\sqrt{2\pi\hbar/M}^D}\sqrt{\frac{\omega}{\sinh\beta\hbar\omega}}^D \\ & \times \exp\left\{-\frac{1}{2\hbar}\frac{M\omega}{\sinh\beta\hbar\omega}[(\mathbf{x}_b^{(p(\nu))\,2} + \mathbf{x}_a^{(\nu)\,2})\cosh\beta\hbar\omega - 2\mathbf{x}_b^{(p(\nu))}\mathbf{x}_a^{(\nu)}]\right\}.\end{aligned} \quad (7.120)$$

The partition function (7.5) can therefore be rewritten in the form

$$\begin{aligned}Z_\omega^{(N)} = {} & \sqrt{\frac{M\omega}{2\pi\hbar\sinh\beta\hbar\omega}}^{ND} \frac{1}{N!}\int d^D x^{(1)} \cdots d^D x^{(N)} \\ & \times \sum_{p(\nu)} \exp\left\{-\frac{1}{2\hbar}\frac{M\omega}{\sinh\beta\hbar\omega}[(\mathbf{x}^{(p(\nu))\,2} + \mathbf{x}^{(\nu)\,2})\cosh\beta\hbar\omega - 2\mathbf{x}^{(p(\nu))}\mathbf{x}^{(\nu)}]\right\}. \end{aligned} \quad (7.121)$$

7.2.5 Thermodynamic Functions

With the same counting arguments as before we now obtain from the connected paths, which wind some number $w = 1, 2, 3, \ldots$ times around the cylinder, a contribution to the partition function

$$\Delta Z_\omega^{(N)\,w} = Z_\omega(w\beta)\frac{1}{w} = \int d^D x\, z_\omega(w\beta;\mathbf{x})\,\frac{1}{w}, \quad (7.122)$$

where

$$Z_\omega(\beta) = \frac{1}{[2\sinh(\beta\hbar\omega/2)]^D} \quad (7.123)$$

is the D-dimensional harmonic partition function (2.407), and $z_\omega(w\beta;\mathbf{x})$ the associated density [compare (2.333) and (2.412)]:

$$z_\omega(\beta;\mathbf{x}) = \sqrt{\frac{\omega M}{2\pi\hbar\sinh\beta\hbar\omega}}^D \exp\left[-\frac{M\omega}{\hbar}\tanh\frac{\beta\hbar\omega}{2}\ \mathbf{x}^2\right]. \quad (7.124)$$

Its spatial integral is the partition function of a free particle at an imaginary-time interval β [compare (2.412)]. The sum over all connected contributions (7.122) yields the grand-canonical free energy

$$F_G = -\frac{1}{\beta}\sum_{w=1}^{\infty} Z_\omega(w\beta)\frac{e^{w\beta\mu}}{w} = -\frac{1}{\beta}\sum_{w=1}^{\infty}\int d^D x\, z_\omega(w\beta;\mathbf{x})\frac{e^{w\beta\mu}}{w}. \quad (7.125)$$

Note the important difference between this and the free-boson expression (7.27). Whereas in (7.27), the winding number appeared as a factor $w^{-D/2}$ which was removed from $Z_0(w\beta)$ by writing $Z_0(w\beta) = Z_0(\beta)/w^{D/2}$ which lead to (7.32), this is no longer possible here. The average number of particles is thus given by

$$N = -\frac{\partial}{\partial\mu}F_G = \sum_{w=1}^{\infty} Z_\omega(w\beta)e^{w\beta\mu} = \int d^D x \sum_{w=1}^{\infty} z_\omega(w\beta;\mathbf{x})e^{w\beta\mu}. \tag{7.126}$$

Since $Z_\omega(w\beta) \approx e^{-wD\hbar\omega\beta/2}$ for large w, the sum over w converges only for $\mu < D\hbar\omega/2$. Introducing the fugacity associated with the ground-state energy

$$z_D(\beta) = e^{-(D\hbar\omega/2-\mu)\beta} = e^{-D\beta\hbar\omega/2}z, \tag{7.127}$$

by analogy with the fugacity (7.24) of the zero-momentum state, we may rewrite (7.126) as

$$N = -\frac{\partial}{\partial\mu}F_G = Z_\omega(\beta)\zeta_D(\beta\hbar\omega; z_D). \tag{7.128}$$

Here $\zeta_D(\beta\hbar\omega; z_D)$ are generalizations of the functions (7.34):

$$\zeta_D(\beta\hbar\omega; z_D) \equiv \sum_{w=1}^{\infty}\left[\frac{\sinh(\omega\hbar\beta/2)}{\sinh(w\omega\hbar\beta/2)}\right]^D e^{w\beta\mu} = Z_\omega^{-1}(\beta)\sum_{w=1}^{\infty}\frac{1}{(1-e^{-2w\beta\hbar\omega})^{D/2}}z_D^w, \tag{7.129}$$

which reduce to $\zeta_D(z)$ in the trapless limit $\omega \to 0$, where $z_D \to z$. Expression (7.128) is the closest we can get to the free-boson formula (7.36).

We may define local versions of the functions $\zeta_D(\beta\hbar\omega; z_D)$ as in Eq.(7.124):

$$\zeta_D(\beta\hbar\omega; z_D; \mathbf{x}) \equiv Z_\omega^{-1}(\beta)\sum_{w=1}^{\infty}\frac{1}{(1-e^{-2w\beta\hbar\omega})^{D/2}}\left(\frac{\omega M}{\pi\hbar}\right)^{D/2} e^{-M\omega\tanh(w\beta\hbar\omega/2)\mathbf{x}^2/\hbar}z_D^w, \tag{7.130}$$

in terms of which the particle number (7.128) reads

$$N = -\frac{\partial}{\partial\mu}F_G = \int d^D x\, n_\omega(\mathbf{x}) \equiv Z_\omega(\beta)\int d^D x\, \zeta_D(\beta\hbar\omega; z_D; \mathbf{x}), \tag{7.131}$$

and the free energy (7.125) becomes

$$F_G = \int d^D x\, f(\mathbf{x}) \equiv -\frac{1}{\beta}Z_\omega(\beta)\int d^D x \int_0^{z_D}\frac{dz}{z}\,\zeta_D(\beta\hbar\omega; z; \mathbf{x}). \tag{7.132}$$

For small trap frequency ω, the function (7.130) has a simple limiting form:

$$\zeta_D(\beta\hbar\omega; z_D; \mathbf{x}) \overset{\omega\approx 0}{\approx} \left(\frac{\beta\hbar\omega}{2\pi}\right)^{D/2}\frac{1}{\lambda_\omega^D}\sum_{w=1}^{\infty}\frac{1}{w^{D/2}}e^{-w\beta(M\omega^2\mathbf{x}^2/2-\mu)}, \tag{7.133}$$

where λ_ω is the oscillator length scale $\sqrt{\hbar/M\omega}$ of Eq. (2.303). Together with the prefactor $Z_\omega(\hbar\beta)$ in (7.131), which for small ω becomes $Z_\omega(\hbar\beta) \approx 1/(\beta\hbar\omega)^D$, this yields the particle density

$$n_0(\beta; z; \mathbf{x}) = \frac{1}{l_{\rm e}^D(\hbar\beta)}\sum_{w=1}^{\infty}\frac{1}{w^{D/2}}e^{-w\beta[V(\mathbf{x})-\mu]} = \frac{1}{l_{\rm e}^D(\hbar\beta)}\zeta_{D/2}(e^{-\beta[V(\mathbf{x})-\mu]}), \tag{7.134}$$

where $V(\mathbf{x}) = M\omega^2\mathbf{x}^2/2$ is the oscillator potential and $l_{\rm e}(\hbar\beta)$ the thermal length scale (2.353). There is only one change with respect to the corresponding expression for the density in the homogeneous gas [compare (7.36)]: the fugacity $z = e^{\beta\mu}$ in the argument by the *local fugacity*

$$z(\mathbf{x}) \equiv e^{-\beta[V(\mathbf{x})-\mu]}. \tag{7.135}$$

The function $\zeta_D(\beta\hbar\omega; z_D)$ starts out like z_D, and diverges for $z_D \to 1$ like $[2\sinh(\beta\hbar\omega/2)]^D/(z_D-1)$. This divergence is the analog of the divergence of the box function (7.82) which reflects the formation of a condensate in the discrete ground state with particle number [compare (7.88)]

$$N_{\rm cond} = \frac{1}{e^{D\beta\hbar\omega/2-\beta\mu}-1}. \tag{7.136}$$

This number diverges for $\mu \to D\hbar\omega/2$ or $z_D \to 1$.

In a box with a finite the number of particles, Eq. (7.36) for the particle number was replaced by the equation for the normal particles (7.89) containing the regularized box functions $\bar{\zeta}^{\rm box}_{D/2}(z)$. In the thermodynamic limit, this turned into the function $\zeta_{D/2}(z)$ in which the momentum sum was evaluated as an integral. The present functions $\zeta_D(\beta\hbar\omega; z_D)$ governing the particle number in the harmonic trap play precisely the role of the previous box functions, with a corresponding singular term which has to be subtracted, thus defining a regularized function

$$\bar{\zeta}_D(\beta\hbar\omega; z_D) \equiv \zeta_D(\beta\hbar\omega; z_D) - Z_\omega^{-1}(\beta)\frac{z_D}{1-z_D} = Z_\omega^{-1}(\beta)S_D(\beta\hbar\omega; z_D), \tag{7.137}$$

where $S(\beta\hbar\omega, z_D)$ is the sum

$$S(\beta\hbar\omega, z_D) \equiv \sum_{w=1}^{\infty}\left[\frac{1}{(1-e^{-w\beta\hbar\omega})^D}-1\right]z_D^w \tag{7.138}$$

The local function (7.130) has a corresponding divergence and can be regularized by a similar subtraction.

The sum (7.138) governs directly the number of *normal* particles

$$N_{\rm n}(T) = Z_\omega(\beta)\bar{\zeta}_D(\beta\hbar\omega; z_D) \equiv S_D(\beta\hbar\omega, z_D). \tag{7.139}$$

The replacement of the singular equation (7.128) by the regular (7.139) of completely analogous to the replacement of the singular (7.82) by the regular (7.89) in the box.

7.2.6 Critical Temperature

Bose-Einstein condensation can be observed as a proper phase transition in the thermodynamic limit, in which N goes to infinity, at a constant average particle density in the trap defined by $N/\lambda_\omega^D \propto N\omega^D$. In this limit, ω goes to zero and the sum (7.139) becomes $\zeta_D(z_D)/\beta\hbar\omega^D$. The associated particle equation

$$N_{\rm n} = \frac{1}{(\beta\hbar\omega)^D}\zeta_D(z_D) \tag{7.140}$$

can be solved only as long as $z_D < 1$. Above T_c, this equation determines z_D as a function of T from the condition that all particles are normal, $N_\mathrm{n} = N$. Below T_c, it determines the temperature dependence of the number of normal particles by inserting $z_D = 1$, where

$$N_\mathrm{n} = \frac{1}{(\beta\hbar\omega)^D}\zeta(D). \tag{7.141}$$

The particles in the ground state from a condensate, whose fraction is given by $N_\mathrm{cond}(T)/N \equiv 1 - N_\mathrm{n}(T)/N$. This is plotted in Fig. 7.9 as a function of the temperature for a total particle number $N = 40\,000$.

The critical point with $T = T_c$, $\mu = \mu_c = D\omega/2$ is reached if N_n is equal to the total particle number N where

$$k_B T_c^{(0)} = \hbar\omega \left[\frac{N}{\zeta(D)}\right]^{1/D}. \tag{7.142}$$

This formula has a solution only for $D > 1$.

Inserting (7.142) back into (7.162), we may re-express the normal fraction as a function of the temperature as follows:

$$\frac{N_\mathrm{n}^{(0)}}{N} \approx \left(\frac{T}{T_c^{(0)}}\right)^D, \tag{7.143}$$

and the condensate fraction as

$$\frac{N_\mathrm{cond}^{(0)}}{N} \approx 1 - \left(\frac{T}{T_c^{(0)}}\right)^D. \tag{7.144}$$

Including the next term in (7.162), the condensate fraction becomes

$$\frac{N_\mathrm{cond}^{(0)}}{N} \approx 1 - \left(\frac{T}{T_c^{(0)} + \delta T_c}\right)^D. \tag{7.145}$$

It is interesting to re-express the critical temperature (7.142) in terms of the particle density at the origin which is at the critical point, according to Eq. (7.134),

$$n_0(\mathbf{0}) = \frac{1}{l_\mathrm{e}^D(\hbar\beta_c)}\zeta(D/2), \tag{7.146}$$

where we have shortened the notation on an obvious way. From this we obtain

$$k_B T_c^{(0)} = \frac{2\pi\hbar^2}{M}\left[\frac{n_0(\mathbf{0})}{\zeta(D/2)}\right]^{2/D}. \tag{7.147}$$

Comparing this with the critical temperature *without a trap* in Eq. (7.18) we see that both expressions agree if we replace N/V by the uniform density $n_0(\mathbf{0})$. As an

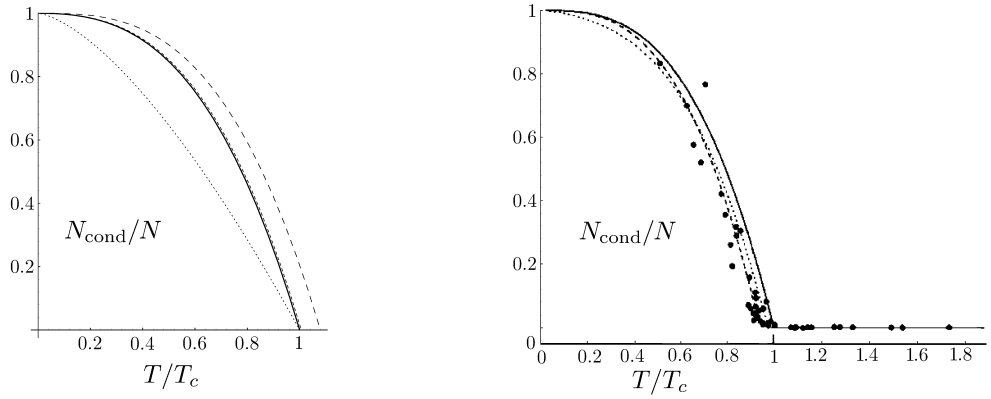

Figure 7.9 Condensate fraction $N_{\rm cond}/N \equiv 1 - N_{\rm n}/N$ as function of temperature for total number of N particles. The long- and short-dashed curves on the left-hand show the zeroth and first-order approximations (7.144) and (7.163). The dotted curve displays the free-boson behavior (7.58). The right-hand figure shows experimental data for 40 000 ^{87}Rb atoms near T_c by Ensher *et. al.*, Phys. Rev. Lett. *77*, 4984 (1996). The solid curve describes noninteracting Bose gas in a harmonic trap [cf. (7.144)]. The dotted curve corrects for finite-N effects [cf. (7.163)]. The dashed curve is the best fit to the data. The transition lies at $T_c \approx 280\,$nK, about 3% below the dotted curve.

obvious generalization, we conclude that Bose condensation in *any* trap will set in when the density at the lowest point reaches the critical value determined by (7.147) [and (7.18)].

Note the different power D and argument in $\zeta(D)$ in Eq. (7.142) in comparison with the free-boson argument $D/2$ in Eq. (7.18). This has the consequence that in contrast to the free Bose gas, the gas in a trap can form a condensate in two dimensions. There is now, however, a problem in $D = 1$ dimension where (7.142) gives a vanishing transition temperature. The leading-order expression (7.142) for critical temperature can also be calculated from a simple statistical consideration. For small ω, the density of states available to the bosons is given by the classical expression (4.216):

$$\rho_{\rm cl}(E) = \left(\frac{M}{2\pi\hbar^2}\right)^{D/2} \frac{1}{\Gamma(D/2)} \int d^D x\, [E - V(\mathbf{x})]^{D/2-1}. \tag{7.148}$$

The number of normal particles is given by the equation

$$N_{\rm n} = \int_{E_{\rm min}}^{\infty} dE\, \frac{\rho_{\rm cl}(E)}{e^{E/k_B T} - 1}, \tag{7.149}$$

where $E_{\rm min}$ is the classical ground state energy. For a harmonic trap, the spatial integral in (7.148) can be done and is proportional to E^D, after which the integral over E in (7.149) yields $[k_B T/\hbar\omega]^D \zeta(D) = (T/T_c^{(0)})^D N$, in agreement with (7.143).

Alternatively we may use the phase space formula

$$N_{\rm n} = \int d^D x \frac{d^D p}{(2\pi\hbar)^D} \frac{1}{e^{\beta[p^2/2M+V(\mathbf{x})]}-1} = \sum_{n=1}^{\infty} \int d^D x \frac{d^D p}{(2\pi\hbar)^D} e^{-n\beta[p^2/2M+V(\mathbf{x})]}$$
$$= \sum_{n=1}^{\infty} \frac{1}{\sqrt{2\pi\hbar^2 n\beta/M}^D} \int d^D x\, e^{-n\beta V(\mathbf{x})}, \tag{7.150}$$

where the spatial integration produces a factor $\sqrt{2\pi/M\omega^2 n\beta}$ so that the right-hand side becomes again $(T/T_c^{(0)})^D N$.

7.2.7 More General Anisotropic Trap

The equation (7.150) for the particle number can be easily calculated for a more general trap where the potential has the anisotropic power behavior

$$V(\mathbf{x}) = \frac{M}{2}\tilde{\omega}^2\tilde{a}^2 \sum_{i=1}^{D} \left(\frac{|x_i|}{a_i}\right)^{p_i}, \tag{7.151}$$

where $\tilde{\omega}$ is some frequency parameter and $\tilde{a}$ is the geometric average $\tilde{a} \equiv \left[\Pi_{i=1}^D a_i\right]^{1/D}$. Inserting (7.151) into (7.150) we encounter a product of integrals

$$\prod_{i=1}^{D} \int_{-\infty}^{\infty} dx\, e^{-n\beta M\tilde{\omega}^2\tilde{a}^2(|x_i|/a_i)^{p_i}/2} = \prod_{i=1}^{D} \frac{a_i}{(\beta M\tilde{\omega}^2\tilde{a}^2/2)^{1/p_i}} \Gamma(1+1/p_i), \tag{7.152}$$

so that the right-hand side of (7.150) becomes $(T/T_c^{(0)})^{\tilde{D}} N$, with the critical temperature

$$k_B T_c^{(0)} = \frac{M\tilde{a}^2\tilde{\omega}^2}{2} \left(\frac{\hbar\tilde{\omega}}{M\tilde{a}^2\tilde{\omega}^2}\right)^{D/\tilde{D}} \left[\frac{N\pi^{D/2}}{\zeta(\tilde{D})\prod_{i=1}^D \Gamma(1+1/p_i)}\right]^{1/\tilde{D}}, \tag{7.153}$$

where $\tilde{D}$ is the dimensionless parameter

$$\tilde{D} \equiv \frac{D}{2} + \sum_{i=1}^{D} \frac{1}{p_i}. \tag{7.154}$$

which takes over the role of D in the harmonic formula (7.142). A harmonic trap with different oscillator frequencies $\omega_1, \ldots, \omega_D$ along the D Cartesian axes, is a special case of (7.151) with $p_i \equiv 2$, $\omega_i^2 = \tilde{\omega}^2\tilde{a}^2/a_i^2$ and $\tilde{D} = D$, and formula (7.153) reduces to (7.142) with ω replaced by the geometric average of the frequencies $\tilde{\omega} \equiv (\omega_1 \cdots \omega_D)^{1/D}$. 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 (7.151) in the limit $p_i \to \infty$ where $\tilde{D} = D/2$. Then Eq. (7.153) reduces to

$$k_B T_c^{(0)} = \frac{\pi\hbar^2}{2M\tilde{a}^2} \left[\frac{N}{\zeta(D/2)}\right]^{2/D} = \frac{2\pi\hbar^2}{M} \left[\frac{N}{V_D\zeta(D/2)}\right]^{2/D}, \tag{7.155}$$

in agreement with (7.53) and (7.18).

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 (7.151), so that $\tilde{\omega}^4/\tilde{a}^2 = \omega_2^2\omega_3^2/a_1^2$, and obtain

$$k_B T_c^{(0)} = \hbar\tilde{\omega}\left(\frac{\pi\hbar}{2M\tilde{\omega}}\right)^{1/5}\left[\frac{N}{a_1\zeta(5/2)}\right]^{2/5} = \hbar\tilde{\omega}\left(\frac{2\pi\lambda_{\omega_1}\lambda_{\omega_2}}{L^2}\right)^{1/5}\left[\frac{N}{\zeta(5/2)}\right]^{2/5}. \quad (7.156)$$

7.2.8 Rotating Bose-Einstein Gas

Another interesting potential can be prepared in the laboratory by rotating a Bose condensate [48] with an angular velocity Ω around the z-axis. The vertical trapping frequencies is $\omega_z \approx 2\pi \times 11.0\,\mathrm{Hz} \approx 0.58\times\,\mathrm{nK}$, 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

$$V(\mathbf{x}) = \frac{M\omega_z^2}{2}\left(z^2 + 36\eta r_\perp^2 + \frac{\kappa}{2}\frac{r_\perp^4}{\lambda_{\omega_z}^2}\right) = \frac{\hbar\omega_z}{2}\left(\frac{z^2}{\lambda_{\omega_z}^2} + 36\eta\frac{r_\perp^2}{\lambda_{\omega_z}^2} + \frac{\kappa}{2}\frac{r_\perp^4}{\lambda_{\omega_z}^4}\right), \quad (7.157)$$

where $r_\perp^2 = x^2 + y^2$, $\eta \equiv 1 - \Omega^2/\omega_\perp^2$, $\kappa \approx 0.4$, and $\lambda_{\omega_z} \equiv 3.245\,\mu\mathrm{m} \approx 1.42 \times 10^{-3}\,\mathrm{K}$. For $\Omega > \omega_\perp$, η turns negative and the potential takes the form of a Mexican hat as shown in Fig. 3.13, with a circular minimum at $r_\mathrm{m}^2 = -36\eta\lambda_{\omega_z}^2/\kappa$. For large rotation speed, the potential may be approximated by a circular harmonic well, so that we may apply formula (7.156) with $a_1 = 2\pi r_\mathrm{m}$, to obtain the η-independent critical temperature

$$k_B T_c^{(0)} \approx \hbar\omega_z\left(\frac{\kappa}{\pi}\right)^{1/5}\left[\frac{N}{\zeta(5/2)}\right]^{2/5}. \quad (7.158)$$

For $\kappa = 0.4$ and $N = 300\,000$, this yields $T_c \approx 53\mathrm{nK}$.

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 (7.151) 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 (7.153) becomes

$$k_B T_c^{(0)} = \hbar\omega_z\left[\frac{\pi^2\kappa}{16\Gamma^4(5/4)}\right]^{1/5}\left[\frac{N}{\zeta(5/2)}\right]^{2/5}. \quad (7.159)$$

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 multiply the right-hand side of equation (7.149) for N by a factor

$$\frac{2\pi\int r dr dx dy\, e^{-r^4}}{\int dx dy\, e^{-x^4-y^4}} = \frac{\pi^{3/2}}{\Gamma[5/4]^2}. \quad (7.160)$$

This factor arrives inversely in front of N in Eq. (7.161), so that we obtain the critical temperature in the critically rotating Bose gas

$$k_B T_c^{(0)} = \hbar\omega_z \left(\frac{4\kappa}{\pi}\right)^{1/5} \left[\frac{N}{\zeta(5/2)}\right]^{2/5}. \tag{7.161}$$

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 the quantum nature of the oscillator should be accounted for.

7.2.9 Finite-Size Corrections

Experiments never take place in the thermodynamic limit. The particle number is finite and for comparison with the data we must calculate finite-size corrections coming from finite N where ll $\omega \approx 1/N^{1/D}$ is small but nonzero. The transition is no longer sharp and the definition of the critical temperature is not precise. As in the thermodynamic limit, we shall identify it by the place where $z_D = 1$ in Eq. (7.139) for $N_{\rm n} = N$. For $D > 3$, the corrections are obtained by expanding the first term in the sum (7.138) in powers of ω and performing the sums over w and subtracting $\zeta(0)$ for the sum $\sum_{w=1}^{\infty} 1$:

$$\begin{aligned} N_{\rm n}(T_c) = {} & \frac{1}{(\beta\hbar\omega)^D}\left[\zeta(D) + \frac{\beta\hbar\omega}{2} D\zeta(D-1) + \frac{(\omega\hbar\beta)^2}{24} D(3D-1)\zeta(D-2) + \dots\right] \\ & - \quad \zeta(0). \end{aligned} \tag{7.162}$$

The higher expansion terms contain logarithmically divergent expressions, for instance in one dimension the first term $\zeta(1)$, and in three dimensions $\zeta(D-2) = \zeta(1)$. These indicate that the expansion powers of $\beta\hbar\omega$ is has been done improperly at a singular point. Only the terms whose ζ-function have a positive argument can be trusted. A careful discussion along the lines of Subsection 2.15.6 reveals that $\zeta(1)$ must be replaced by $\zeta_{\rm reg}(1) = -\log(\beta\hbar\omega) + \text{const.}$, similar to the replacement (2.590). The expansion is derived in Appendix 7A.

For $D > 1$, the expansion (7.162) can be used up to the $\zeta(D-1)$ terms and yields the finite-size correction to the number of normal particles

$$\frac{N_{\rm n}}{N} = \left(\frac{T}{T_c^{(0)}}\right)^D + \frac{D}{2}\frac{\zeta(D-1)}{\zeta^{1-1/D}(D)}\frac{1}{N^{1/D}}. \tag{7.163}$$

Setting $N_{\rm n} = N$, we obtain a shifted critical temperature by a relative amount

$$\frac{\delta T_c}{T_c^{(0)}} = -\frac{1}{2}\frac{\zeta(D-1)}{\zeta^{(D-1)/D}(D)}\frac{1}{N^{1/D}} + \dots. \tag{7.164}$$

In three dimensions, the first correction shifts the critical temperature $T_c^{(0)}$ downwards by 2% for 40 000 atoms.

Note that correction (7.164) has no direct ω-dependence whose size enters only implicitly via $T_c^{(0)}$ of Eq. (7.142). In an anisotropic harmonic trap, the temperature

shift would carry a dimensionless factor $\tilde{\omega}/\bar{\omega}$ where $\bar{\omega}$ is the arithmetic mean $\bar{\omega} \equiv \left(\sum_{i=1}^{D} \omega_i\right)/D$.

The higher finite-size corrections for smaller particle numbers are all calculated in Appendix 7A. The result can quite simply be deduced by recalling that according to the Robinson expansion (2.583), the first term in the naive, wrong power series expansion of $\zeta_\nu(e^{-b}) = \sum_{w=1}^{\infty} e^{-wb}/w^\nu = \sum_{k=0}^{\infty}(-b)^k\zeta(\nu-k)/k!$ is corrected by changing the leading term $\zeta(\nu)$ to $\Gamma(1-\nu)(-b)^{\nu-1} + \zeta(\nu)$ which remains finite for all positive integer ν. Hence we may expect that the correct equation for the critical temperature is obtained by performing this change in Eq. (7.162) on each $\zeta(\nu)$. This expectation is confirmed in Appendix 7A. It yields for $D = 3, 2, 1$ the equations for the number of particles in the excited states

$$N_{\rm n} = \frac{1}{\beta\hbar\omega}\left[-(\log\beta\hbar\omega - \gamma) - \frac{\beta\hbar\omega}{2}\zeta(0) + \frac{(\beta\hbar\omega)^2}{12}\zeta(-1) + \ldots\right], \tag{7.165}$$

$$N_{\rm n} = \frac{1}{(\beta\hbar\omega)^2}\left[\zeta(2) - \beta\hbar\omega\left(\log\beta\hbar\omega - \gamma + \frac{1}{2}\right) - \frac{7(\beta\hbar\omega)^2}{12}\zeta(0) + \ldots\right], \tag{7.166}$$

$$N_{\rm n} = \frac{1}{(\beta\hbar\omega)^3}\left[\zeta(3) + \frac{3\beta\hbar\omega}{2}\zeta(2) - (\beta\hbar\omega)^2\left(\log\beta\hbar\omega - \gamma + \frac{19}{24}\right) + \ldots\right], \tag{7.167}$$

where $\gamma = 0.5772\ldots$ is the Euler-Mascheroni number (2.469). Note that all nonlogarithmic expansion terms coincide with those of the naive expansion (7.162).

These equations may be solved for β at $N_{\rm n} = N$ to obtain the critical temperature of the would-be phase transition.

Once we study the position of would-be transitions at finite size, it makes sense to include also the case $D = 1$ where the thermodynamic limit has no transition at all. There is a strong increase of number of particles in the ground state at a "critical temperature" determined by equating Eq. (7.165) with the total particle number N, which yields

$$k_B T_c^{(0)} = \hbar\omega N \frac{1}{(-\log\beta\hbar\omega + \gamma)} \approx \hbar\omega N \frac{1}{\log N}, \qquad D = 1. \tag{7.168}$$

Note that this result can also be found also from the divergent naive expansion (7.162) by inserting for the divergent quantity $\zeta(1)$ the dimensionally regularized expression $\zeta_{\rm reg}(1) = -\log(\beta\hbar\omega)$ of Eq. (2.590).

7.2.10 Entropy and Specific Heat

By comparing (7.126) with (7.125) we see that the grand-canonical free energy can be obtained from $N_{\rm n}$ of Eq. (7.162) by a simple multiplication with $-1/\beta$ and an increase of the arguments of the zeta-functions $\zeta(\nu)$ by one unit. Hence we have, up to first order corrections in ω

$$F_G(\beta, \mu_c) = -\frac{1}{\beta(\beta\hbar\omega)^D}\left[\,\zeta(D+1) + \beta\hbar\omega\frac{D}{2}\zeta(D) + \ldots\right]. \tag{7.169}$$

From this we calculate immediately the entropy $S = -\partial_T F_G = k_B \beta^2 \partial_\beta F_G$ as

$$S = -k_B(D+1)\beta F_G = k_B(D+1)\frac{1}{(\beta\hbar\omega)^D}\left[\,\zeta(D+1) + \beta\hbar\omega\frac{D}{2}\zeta(D) + \ldots\right]. \quad (7.170)$$

In terms of the lowest-order critical temperature (7.142), this becomes

$$S = k_B N(D+1)\left\{\left(\frac{T}{T_c^{(0)}}\right)^D \frac{\zeta(D+1)}{\zeta(D)} + \frac{D}{2}\left[\frac{\zeta(D)}{N}\right]^{1/D}\left(\frac{T}{T_c^{(0)}}\right)^{D-1} + \ldots\right\}. \quad (7.171)$$

From this we obtain the specific heat $C = T\partial_T S$ below T_c:

$$C = k_B N(D+1)\left\{D\left(\frac{T}{T_c^{(0)}}\right)^D \frac{\zeta(D+1)}{\zeta(D)} + \frac{D(D-1)}{2}\left[\frac{\zeta(D)}{N}\right]^{1/D}\left(\frac{T}{T_c^{(0)}}\right)^{D-1} + \ldots\right\}. \quad (7.172)$$

At the critical temperature, this has the maximal value

$$C_{\max} \approx k_B N(D+1) D\frac{\zeta(D+1)}{\zeta(D)}\left\{1 + \left[\frac{D-1}{2}\frac{\zeta^{1+1/D}(D)}{\zeta(D+1)} - \frac{D}{2}\frac{\zeta(D-1)}{\zeta^{1-1/D}(D)}\right]\frac{1}{N^{1/D}}\right\}. \quad (7.173)$$

In three dimensions, the lowest two approximations have their maximum at

$$C_{\max}^{(0)} \approx k_B N\, 10.805, \qquad C_{\max}^{(1)} \approx k_B N\, 9.556. \quad (7.174)$$

Above T_c, we expand the total particle number (7.126) in powers of ω as in (7.162). The fugacity of the ground state is now different from unity:

$$N(\beta,\mu) = \frac{1}{(\beta\hbar\omega)^D}\left[\zeta_D(z_D) + \beta\hbar\omega\frac{D}{2}\zeta_{D-1}(z_D) + \ldots\right]. \quad (7.175)$$

The grand-canonical free energy is

$$F_G(\beta,\mu) = -\frac{1}{\beta(\beta\hbar\omega)^D}\left[\,\zeta_{D+1}(z_D) + \beta\hbar\omega\frac{D}{2}\zeta_D(z_D) + \ldots\right], \quad (7.176)$$

and the entropy

$$S(\beta,\mu) = k_B\frac{1}{(\beta\hbar\omega)^D}\left\{(D+1)\zeta_{D+1}(z_D) + \frac{1}{2}\left(\beta\hbar\omega D^2 - 2\beta\mu\right)\zeta_D(z_D) + \ldots\right\}. \quad (7.177)$$

The specific heat C is found from the derivative $-\beta\partial_\beta S|_N$ as

$$C(\beta,\mu) = k_B\frac{1}{(\beta\hbar\omega)^D}\left\{(D+1)D\,\zeta_{D+1}(z_D) + \frac{1}{2}\left[D\left(D^2+1\right)\beta\hbar\omega - D\beta\mu - \beta\partial_\beta(\beta\mu)\right]\zeta_D(z_D) + \ldots\right\}. \quad (7.178)$$

The derivative $\beta\partial_\beta(\beta\mu)$ is found as before from the condition: $\partial N(\beta,\mu(\beta))/\partial\beta = 0$, implying

$$0 = \frac{1}{(\beta\hbar\omega)^D}\left\{-\left[D\zeta_D(z_D)+\beta\hbar\omega\frac{D}{2}(D-1)\zeta_{D-1}(z_D)\right]\right.$$
$$\left.+\left[\zeta_{D-1}(z_D)+\beta\hbar\omega\frac{D}{2}\zeta_{D-2}(z_D)\right]\left[\beta\partial_\beta(\beta\mu)-\beta\hbar\omega\frac{D}{2}\right]+\ldots\right\}, \quad (7.179)$$

so that we obtain

$$\beta\partial_\beta(\beta\mu) = D\frac{\zeta_D(z_D)+\beta\hbar\omega\frac{D}{2}\zeta_{D-2}(z_D)+\ldots}{\zeta_{D-1}(z_D)+\beta\hbar\frac{D}{2}\omega\zeta_{D-2}(z_D)+\ldots}. \quad (7.180)$$

Let us first consider the lowest approximation, where

$$N(\beta,\mu) \approx \frac{1}{(\beta\hbar\omega)^D}\zeta_D(z), \quad (7.181)$$

$$F_G(\beta,\mu) \approx -\frac{1}{\beta}\frac{1}{(\beta\hbar\omega)^D}\zeta_{D+1}(z) = -N\frac{1}{\beta}\frac{\zeta_{D+1}(z)}{\zeta_D(z)}, \quad (7.182)$$

$$S(\beta,\mu) \approx \frac{1}{T}\left[\frac{D+1}{\beta}\frac{1}{(\beta\hbar\omega)^D}\zeta_{D+1}(z)-\mu N\right] = Nk_B\left[\frac{D+1}{(\beta\hbar\omega)^D}\frac{\zeta_{D+1}(z)}{\zeta_D(z)}-\beta\mu\right], \quad (7.183)$$

so that from (7.60)

$$E(\beta,\mu) \approx \frac{D}{\beta}\frac{1}{(\beta\hbar\omega)^D}\zeta_{D+1}(z) = N\frac{D}{\beta}\frac{\zeta_{D+1}(z)}{\zeta_D(z)}. \quad (7.184)$$

The chemical potential at fixed N satisfies the equation

$$\beta\partial_\beta(\beta\mu) = D\frac{\zeta_D(z)}{\zeta_{D-1}(z)}. \quad (7.185)$$

The specific heat at a constant volume is

$$C = k_B N\left[(D+1)D\frac{\zeta_{D+1}(z)}{\zeta_D(z)}-D^2\frac{\zeta_D(z)}{\zeta_{D-1}(z)}\right]. \quad (7.186)$$

At high temperatures, C tends to the Dulong-Petit limit DNk_B since for small z all $\zeta_\nu(z)$ behave like z. This is twice a big as the Dulong-Petit limit of the free Bose gas since there are twice as many harmonic modes.

As the temperature approaches the critical point from above, z tends to unity from below and we obtain a maximal value in three dimensions

$$C^{(0)}_{\max} = k_B N\left[12\frac{\zeta_4(1)}{\zeta_3(1)}-9\frac{\zeta_3(1)}{\zeta_2(1)}\right] \approx k_B N\, 4.22785. \quad (7.187)$$

The specific heat for a fixed large number N of particles in a trap has a much sharper peak than for the free Bose gas. The two curves are compared in Fig. 7.10, where we also show how the peak is rounded for different finite numbers N.[3]

[3]P.W. Courteille, V.S. Bagnato, and V.I. Yukalov, Laser Physics *2*, 659 (2001).

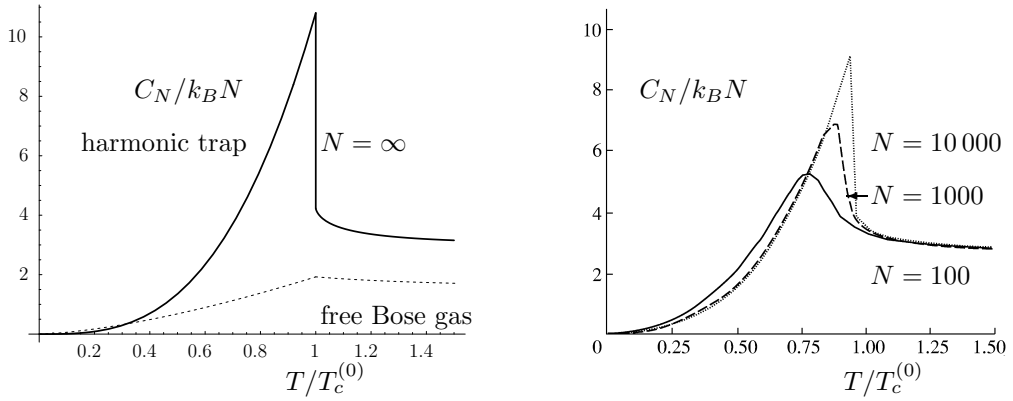

Figure 7.10 Peak of specific heat for infinite (left-hand plot) and various finite numbers 100, 1000, 10 000 of particles N (right-hand plots) in harmonic trap. The large-N curve is compared with that of a free Bose gas.

7.2.11 Interactions in Harmonic Trap

Let us now study the effect of interactions on a Bose gas in an isotropic harmonic trap. This is most easily done by adding to the free part (7.132) the interaction (7.101) with $n(\mathbf{x})$ taken from (7.131), to express the grand-canonical free energy by analogy with (7.102) as

$$F_G = \int d^D x \left\{ -\frac{1}{\beta} Z_\omega(\beta) \int_0^{z_D} \frac{dz}{z} \zeta_D(\beta\hbar\omega; z; \mathbf{x}) + g\, [Z_\omega(\beta)\zeta_D(\beta\hbar\omega; z_D; \mathbf{x})]^2 \right\}. \tag{7.188}$$

Using the relation (7.103), this takes a form more similar to (7.106):

$$F_G = -\frac{1}{\beta} Z_\omega(\beta) \int d^D x \left\{ \int_0^{z_D} \frac{dz}{z} \zeta_D(\beta\hbar\omega; z; \mathbf{x}) - 2\hat{a}\, l_{\rm e}^D(\hbar\beta) Z_\omega(\beta)\, [\zeta_D(\beta\hbar\omega; z_D; \mathbf{x})]^2 \right\}. \tag{7.189}$$

As in Eq. (7.113), we now construct the variational free energy to be extremized with respect to the local parameter $\sigma(\mathbf{x})$. Moreover, we shall find it convenient to express $\zeta(z)$ as $\int_0^z (dz'/z')\zeta(z')$. This leads to the variational expression

$$F_G^\sigma = -\frac{1}{\beta} Z_\omega(\beta) \int d^3x \left[\int_0^{z_D e^{\sigma(\mathbf{x})}} \frac{dz}{z} \zeta_D(\beta\hbar\omega; z; \mathbf{x}) - \frac{\sigma^2(\mathbf{x})}{8\tilde{a}} \right], \tag{7.190}$$

where $z_D = e^{-(D\hbar\omega/2-\mu)\beta} = e^{-D\beta\hbar\omega/2} z$ and

$$\tilde{a} \equiv \hat{a}\, l_{\rm e}^D(\hbar\beta) Z_\omega(\beta) = \frac{a}{l_{\rm e}(\hbar\beta)}\, l_{\rm e}^D(\hbar\beta) Z_\omega(\beta). \tag{7.191}$$

The extremum lies at $\sigma(\mathbf{x}) = \Sigma(\mathbf{x})$ where by analogy with (7.114):

$$\Sigma(\mathbf{x}) \equiv -4\tilde{a}\zeta_D(\beta\hbar\omega; z_D e^{\Sigma(\mathbf{x})}; \mathbf{x}). \tag{7.192}$$

For a small trap frequency ω, we use the function $\zeta_D(\beta\hbar\omega; z_D; \mathbf{x})$ in the approximate form (7.133), written as

$$\zeta_D(\beta\hbar\omega; z_D; \mathbf{x}) \equiv \sum_{w=1}^{\infty} \sqrt{\frac{\omega^2 M\beta}{2\pi w}}^D z_D^w e^{-Mw\beta\omega^2\mathbf{x}^2/2}. \tag{7.193}$$

In this approximation, Eq. (7.192) becomes

$$\Sigma(\mathbf{x}) \overset{\omega\approx 0}{\approx} -4\tilde{a} \sum_{w=1}^{\infty} \sqrt{\frac{\omega^2 M\beta}{2\pi w}}^D z_D^w \, e^{w\Sigma(\mathbf{x})} e^{-Mw\beta\omega^2\mathbf{x}^2/2}. \tag{7.194}$$

For small $\tilde{a}$, $\Sigma(\mathbf{x})$ is also small, so that the factor $e^{w\Sigma(\mathbf{x})}$ on the right-hand side is close to unity and can be omitted. This will be inserted into the equation for the particle number above T_c:

$$N = \int d^D x \, n(\mathbf{x}) = Z_\omega(\beta) \int d^D x \, \bar{\zeta}_D(\beta\hbar\omega; z_D e^{\Sigma(\mathbf{x})}; \mathbf{x}). \tag{7.195}$$

Recall that in the thermodynamic limit for $D > 1$ where the phase transition properly exists, $\zeta_D(\beta\hbar\omega; z_D; \mathbf{x})$ and $\bar{\zeta}_D(\beta\hbar\omega; z_D; \mathbf{x})$ coincide, due to (7.139) and (7.141).

From (7.195) we may derive the following equation for the critical temperature as a function of z_D:

$$1 = \frac{Z_\omega(\beta)}{Z_\omega(\beta_c^{(0)})} \int d^D x \frac{\bar{\zeta}_D(\beta\hbar\omega; z_D e^{\Sigma(\mathbf{x})}; \mathbf{x})}{\bar{\zeta}_D(\beta_c^{(0)}\hbar\omega; 1)}, \tag{7.196}$$

where $T_c^{(0)}$ is the critical temperature in the trap *without* the repulsive interaction. The critical temperature T_c of the interacting system is reached if the second argument of $\bar{\zeta}_D(\beta\hbar\omega; z_D e^{\Sigma(\mathbf{x})}; \mathbf{x})$ hits the boundary of the unit convergence radius of the expansion (7.130) for $\mathbf{x} = 0$, i.e., if $z_D e^{\Sigma(\mathbf{0})} = 1$. Thus we find the equation for T_c:

$$1 = \frac{Z_\omega(\beta_c)}{Z_\omega(\beta_c^{(0)})} \int d^D x \frac{\bar{\zeta}_D(\beta_c\hbar\omega; e^{\Sigma_c(\mathbf{x})-\Sigma_c(\mathbf{0})}; \mathbf{x})}{\bar{\zeta}_D(\beta_c^{(0)}\hbar\omega; 1)}, \tag{7.197}$$

where the subscript of $\Sigma_c(\mathbf{x})$ indicates that β in (7.194) has been set equal to β_c. In particular, $\tilde{a}$ contained in $\Sigma_c(\mathbf{x})$ is equal to $\tilde{a}_c \equiv a/\ell_c$. Since this is small by assumption, we expand the numerator of (7.197) as

$$1 \approx \frac{Z_\omega(\beta_c)}{Z_\omega(\beta_c^{(0)})} \left\{ 1 + \frac{1}{\bar{\zeta}_D(\beta_c^{(0)}\hbar\omega; 1)} \int d^D x \, \Delta\bar{\zeta}_D(\beta_c^{(0)}\hbar\omega; 1; \mathbf{x}) \right\}, \tag{7.198}$$

where the integral has the explicit small-ω form

$$\int d^D x \sum_{w=1}^{\infty} \sqrt{\frac{\omega^2 M\beta_c^{(0)}}{2\pi w}}^D e^{-Mw\beta_c^{(0)}\omega^2\mathbf{x}^2/2} \left(e^{w[\Sigma_c(\mathbf{x})-\Sigma_c(\mathbf{0})]} - 1 \right). \tag{7.199}$$

In the subtracted term we have used the fact that for small ω, $\bar{\zeta}_D(\beta_c^{(0)}\hbar\omega; 1) \approx \bar{\zeta}_D(\beta_c\hbar\omega; 1) \approx \zeta(D)$ is independent of β [see (7.139) and (7.141)].

Next we approximate near $T_c^{(0)}$:

$$\frac{Z_\omega(\beta_c)}{Z_\omega(\beta_c^{(0)})} \equiv 1 + D\frac{\Delta T_c}{T_c^{(0)}} \frac{\beta_c^{(0)}\hbar\omega/2}{\tanh(\beta_c^{(0)}\hbar\omega/2)} \overset{\omega\approx 0}{\approx} 1 + D\frac{\Delta T_c}{T_c^{(0)}}, \tag{7.200}$$

such that Eq. (7.198) can be solved for $\Delta T_c/T_c^{(0)}$:

$$\frac{\Delta T_c}{T_c^{(0)}} \approx -\frac{1}{D}\frac{1}{\zeta(D)}\int d^D x\, \Delta\bar{\zeta}_D(\beta_c^{(0)}\hbar\omega; 1; \mathbf{x}). \tag{7.201}$$

On the right-hand side, we now insert (7.199) with the small quantity $\Sigma_c(\mathbf{x})$ approximated by Eq. (7.194) at $\beta_c^{(0)}$, in which the factor $e^{w\Sigma_c(\mathbf{x})}$ on the right-hand side is replaced by 1, and find for the integral (7.199):

$$-4\tilde{a}_c \int d^D x \sum_{w=1}^{\infty} \sqrt{\frac{\omega^2 M\beta_c^{(0)}}{2\pi w}}^D e^{-Mw\beta_c^{(0)}\omega^2\mathbf{x}^2/2}\; w \sum_{w'=1}^{\infty} \sqrt{\frac{\omega^2 M\beta_c^{(0)}}{2\pi w'}}^D \left(e^{Mw'\beta_c^{(0)}\omega^2\mathbf{x}^2/2} - 1\right).$$

The integral leads to

$$-4\tilde{a}_c \sqrt{\frac{\omega^2 M\beta_c^{(0)}}{2\pi}}^D \sum_{w,w'=1}^{\infty} \frac{1}{w^{D/2-1}w'^{D/2}} \left[\frac{1}{(w+w')^{D/2}} - \frac{1}{w^{D/2}}\right] \equiv -4\hat{a}_c S(D), \tag{7.202}$$

where $S(D)$ abbreviates the double sum, whose prefactor has been simplifies to $-4\hat{a}_c$ using (7.191) and the fact that for small ω, $Z_\omega(\beta_c^{(0)}) \approx (\omega\hbar\beta_c^{(0)})^{-D}$. For $D = 3$, the double sum has the value $S(3) \approx 1.2076 - \zeta(2)\zeta(3/2) \approx -3.089$. Inserting everything into (7.201), we obtain for small a and small ω the shift in the critical temperature

$$\frac{\Delta T_c}{T_c^{(0)}} \approx \frac{4\hat{a}_c}{D}\frac{S(D)}{\zeta(D)} \underset{D=3}{\approx} -3.427\frac{a}{\ell_c}. \tag{7.203}$$

In contrast to the free Bose gas, where a small δ-function repulsion does not produce any shift using the same approximation as here [recall (7.116)], and only a high-loop calculation leads to an upwards shift proportional to a, the critical temperature of the trapped Bose gas is shifted *downwards*. We can express ℓ_c in terms of the length scale $\lambda_\omega \equiv \sqrt{\hbar/M\omega}$ associated with the harmonic oscillator [recall Eq. (2.303)] and rewrite $\ell_c = \lambda_\omega\sqrt{2\pi\beta_c\hbar\omega}$. Together with the relation (7.142), we find

$$\frac{\Delta T_c}{T_c^{(0)}} \approx -3.427\frac{1}{\sqrt{2\pi}[\zeta(3)]^{1/6}}\frac{a}{\lambda_\omega}N^{1/6} \approx -1.326\,\frac{a}{\lambda_\omega}N^{1/6}. \tag{7.204}$$

Note that since ω is small, the temperature shift formula (7.201) can also be expressed in terms of the zero-ω density (7.134) as

$$\Delta T_c \overset{\omega,\tilde{a}\approx 0}{\approx} 2g\,\frac{\int d^3x\,[\partial_\mu n_0(\mathbf{x})]\,[n_0(\mathbf{x}) - n_0(\mathbf{0})]}{\int d^3x\,\partial_T n_0(\mathbf{x})}, \tag{7.205}$$

where we have omitted the other arguments β and z of $n_0(\beta; z; \mathbf{x})$, for brevity. To derive this formula we rewrite the grand-canonical free energy (7.190) as

$$F_G = -\frac{1}{\beta}\int d^3x \left[\int_0^{ze^{\beta\nu(\mathbf{x})}} \frac{dz'}{z'} n_0(\beta; z'; \mathbf{x}) - \beta\frac{\nu^2(\mathbf{x})}{4g}\right], \tag{7.206}$$

so that the particle number equation Eq. (7.195) takes the form

$$N = \int d^3x\, n_0(\beta; ze^{\beta\nu(\mathbf{x})}; \mathbf{x}). \tag{7.207}$$

Extremizing F_G in $\nu(\mathbf{x})$ yields the self-consistent equation

$$\nu(\mathbf{x}) = -2g n_0(\beta; ze^{\beta\nu(\mathbf{x})}; \mathbf{x}). \tag{7.208}$$

As before, the critical temperature is reached for $ze^{\beta\nu(\mathbf{0})} = 1$, implying that

$$N = \int d^3x\, n_0(\beta_c; ze^{-2\beta g[n_0(\mathbf{x})-n_0(\mathbf{0})]}; \mathbf{x}). \tag{7.209}$$

In the exponent we have omitted again the arguments β and z of $n_0(\beta; z; \mathbf{x})$. If we now impose the condition of constant N, $\Delta N = (\Delta T_c \partial_T + \Delta\mu\partial_\mu)N = 0$, and insert $\Delta\mu = -2g[n_0(\mathbf{x}) - n_0(\mathbf{0})]$, we find (7.205). Inserting into (7.205) the density (7.134) for the general trap (7.151), we find the generalization of (7.203):

$$\frac{\Delta T_c}{T_c^{(0)}} \approx \frac{4\hat{a}_c}{\tilde{D}}\frac{1}{\zeta(\tilde{D})}\sum_{w,w'=1}^{\infty}\frac{1}{w^{D/2-1}w'^{D/2}}\left[\frac{1}{(w+w')^{\tilde{D}-D/2}} - \frac{1}{w^{\tilde{D}-D/2}}\right], \tag{7.210}$$

which vanishes for the homogeneous gas, as concluded before on the basis of Eq. (7.116).

Let us compare the result (7.204) with the experimental temperature shift for ^{87}Rb in a trap with a critical temperature $T_c \approx 280\,\mathrm{nK}$ which lies about 3% below the noninteracting Bose gas temperature (see Fig. 7.9). Its thermal de Broglie length is calculated best in atomic units. Then the fundamental length scale is the Bohr radius $a_H = \hbar/M_p c\alpha$, where M_p is the proton mass and $\alpha \approx 1/137.035$ the fine-structure constant. The fundamental energy scale is $E_H = M_e c^2\alpha^2$. Writing now the thermal de Broglie length at the critical temperature as

$$\frac{a}{\ell_c} = \frac{2\pi\hbar^2}{Mk_BT_c} = \sqrt{2\pi}\sqrt{\frac{E_H}{k_BT_c}}\sqrt{\frac{M_e}{87M_p}}a_H, \tag{7.211}$$

we estimate with $\sqrt{E_H/k_BT_c} \approx \sqrt{27.21\,\mathrm{eV}/(280\times10^{-9}/11\,604.447\,\mathrm{eV})} \approx 1.06\times10^6$ and $\sqrt{M_e/87M_p} \approx \sqrt{0.511\mathrm{eV}/(87\times938.27\mathrm{eV})} \approx 0.002502$ such that $\ell_c \approx 6646 a_H$.

The triplet s-wave scattering length of ^{87}Rb is $a \approx (106 \pm 4)\, a_H$ such that we find from (7.203)

$$\frac{\Delta T_c}{T_c^{(0)}} \approx -5.4\%, \tag{7.212}$$

which is compatible with the experimentally data of the trap in Fig. 7.9.

Let us finally mention recent studies of more realistic systems in which bosons in a trap interact with longer-range interactions [45].

7.3 Gas of Free Fermions

For fermions, the thermodynamic functions (7.32) and (7.33) contain the functions

$$\zeta_\nu^{\rm f}(z) \equiv \sum_{w=1}^{\infty} (-1)^{w-1} \frac{z^w}{w^\nu}, \tag{7.213}$$

which starts out for small z like z. For $z = 1$, this becomes

$$\zeta_\nu^{\rm f}(1) = \frac{1}{1} - \frac{1}{2^\nu} + \frac{1}{3^\nu} - \frac{1}{4^\nu} + \ldots = \sum_{k=0}^{\infty} \frac{1}{k^\nu} - 2^{1-\nu} \sum_{k=0}^{\infty} \frac{1}{k^\nu} = \left(1 - 2^{1-\nu}\right) \zeta(\nu). \tag{7.214}$$

In contrast to $\zeta_\nu(z)$ in Eq. (7.34) this function is perfectly well-defined for all chemical potentials by analytic continuation. The reason is the alternating sign in the series (7.213). The analytic continuation is achieved by expressing $\zeta_\nu^{\rm f}(z)$ as an integral by analogy with (7.39), (7.40):

$$\zeta_n^{\rm f}(z) \equiv \frac{1}{\Gamma(n)}\, i_n^{\rm f}(\alpha), \tag{7.215}$$

where $i_n^{\rm f}(\alpha)$ are the integrals

$$i_n^{\rm f}(\alpha) \equiv \int_0^\infty d\varepsilon \frac{\varepsilon^{n-1}}{e^{\varepsilon-\alpha}+1}. \tag{7.216}$$

In the integrand we recognize the Fermi distribution function of Eq. (3.111), in which $\omega\hbar\beta$ is replaced by $\varepsilon - \alpha$:

$$n_\varepsilon^{\rm f} = \frac{1}{e^{\varepsilon-\alpha}+1}. \tag{7.217}$$

The quantity ε plays the role of a reduced energy $\varepsilon = E/k_BT$, and α is a reduced chemical potential $\alpha = \mu/k_BT$.

Let us also here express the grand-canonical free energy F_G in terms of the functions $i_n^{\rm f}(\alpha)$. Combining Eqs. (7.32), (7.213), and (7.216) we obtain for fermions with $g_S = 2S+1$ spin orientations:

$$F_G = -\frac{1}{\beta} Z_0(\beta) \frac{g_S}{\Gamma(D/2+1)}\, i_{D/2+1}^{\rm f}(\beta\mu) = -\frac{1}{\beta\Gamma(D/2+1)} \frac{g_S V_D}{\sqrt{2\pi\hbar^2\beta/M}^D} \int_0^\infty d\varepsilon\, \frac{\varepsilon^{D/2}}{e^{\varepsilon-\beta\mu}+1}, \tag{7.218}$$

and the integral can be brought by partial integration to the form

$$F_G = -\frac{1}{\beta\Gamma(D/2)} \frac{g_S V_D}{\sqrt{2\pi\hbar^2\beta/M}^D} \int_0^\infty d\varepsilon\, \varepsilon^{D/2-1} \log(1 + e^{-\varepsilon+\beta\mu}). \tag{7.219}$$

Recalling Eq. (7.47), this can be rewritten as a sum over momenta of oscillators with energy $\hbar\omega_{\mathbf{p}} \equiv \mathbf{p}^2/2M$:

$$F_G = -\frac{g_S}{\beta} \sum_{\mathbf{p}} \log(1 + e^{-\beta\hbar\omega_{\mathbf{p}}+\beta\mu}). \tag{7.220}$$

This free energy will be studied in detail in Section 7.14.

The particle number corresponding to the integral representations (7.219) and (7.220) is

$$N=-\frac{\partial}{\partial\mu}F_G=\frac{1}{\Gamma(D/2)}\frac{g_S V_D}{\sqrt{2\pi\hbar^2\beta/M}^D}\int_0^\infty d\varepsilon\frac{\varepsilon^{D/2-1}}{e^{\varepsilon+\beta\mu}-1}=g_S\sum_{\mathbf{p}}\frac{1}{e^{\beta\hbar\omega_{\mathbf{p}}+\beta\mu}-1}. \quad (7.221)$$

Recalling the reduced density of states, this may be written with the help of the Fermi distribution function $n_\omega^{\rm f}$ of Eq. (7.217) as

$$N=g_S V_D\int_0^\infty d\varepsilon\, N_\varepsilon\, n_\varepsilon^{\rm f}. \quad (7.222)$$

The Bose function contains a pole at $\alpha=0$ which prevents the existence of a solution for positive α. In the analytically continued fermionic function (7.215), on the other hand, the point $\alpha=0$ is completely regular.

Consider now a Fermi gas close to zero temperature which is called the degenerate limit. Then the reduced variables $\varepsilon=E/k_BT$ and $\alpha=\mu/k_BT$ become very large and the distribution function (7.217) reduces to

$$n_\varepsilon^{\rm f} \;=\; \left\{\begin{array}{ll} 1 & \text{for } \varepsilon<\alpha \\ 0 & \text{for } \varepsilon>\alpha \end{array}\right\}=\Theta(\varepsilon-\alpha). \quad (7.223)$$

All states with energy E lower than the chemical potential μ are filled, all higher states are empty. The chemical potential μ at zero temperature is called *Fermi energy* $E_{\rm F}$:

$$\mu\Big|_{T=0}\equiv E_{\rm F}. \quad (7.224)$$

The Fermi energy for a given particle number N in a volume V_D is found by performing the integral (7.222) at $T=0$:

$$N=g_S V_D\int_0^{E_{\rm F}}d\varepsilon N_\varepsilon=\frac{1}{\Gamma(D/2+1)}\frac{g_S V_D E_F^{D/2}}{\sqrt{2\pi\hbar^2/M}^D}=\frac{1}{\Gamma(D/2+1)}\frac{g_S V_D}{\sqrt{4\pi}^D}\left(\frac{p_F}{\hbar}\right)^D, \quad (7.225)$$

where

$$p_{\rm F}\equiv\sqrt{2ME_{\rm F}} \quad (7.226)$$

is the *Fermi momentum* associated with the Fermi energy. Equation (7.225) is solved for $E_{\rm F}$ by

$$E_{\rm F}=\frac{2\pi\hbar^2}{M}\left[\frac{\Gamma(D/2+1)}{g_S}\right]^{2/D}\left(\frac{N}{V_D}\right)^{2/D}, \quad (7.227)$$

and for the Fermi momentum by

$$p_{\rm F}=2\sqrt{\pi}\hbar\left[\frac{\Gamma(D/2+1)}{g_S}\right]^{1/D}\left(\frac{N}{V_D}\right)^{1/D}\hbar. \quad (7.228)$$

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

$$N_\varepsilon \equiv \frac{d}{2}\frac{N}{V_D}\sqrt{\frac{k_BT}{E_{\rm F}}}^{D/2}\varepsilon^{D/2-1}. \tag{7.229}$$

As the gas is heated slightly, the degeneracy in the particle distribution function in Eq. (7.223) softens. The degree to which this happens is governed by the size of the ratio $kT/E_{\rm F}$. It is useful to define a characteristic temperature, the so-called *Fermi temperature*

$$T_{\rm F} \equiv \frac{E_{\rm F}}{k_B} = \frac{1}{k_B}\frac{{p_{\rm F}}^2}{2M}. \tag{7.230}$$

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

$$T_{\rm F} \approx 44\,000\text{K}. \tag{7.231}$$

Hence, even far above room temperatures the relation $T/T_{\rm F} \ll 1$ is quite well fulfilled and can be used as an expansion parameter in evaluating the thermodynamic properties of the electron gas at nonzero temperature.

Let us calculate the finite-T effects in $D = 3$ dimensions. From Eq. (7.225) we obtain

$$N = N(T,\mu) \equiv \frac{g_S V}{l_{\rm e}^3(\hbar\beta)}\frac{2}{\sqrt{\pi}}\, i^{\rm f}_{3/2}\left(\frac{\mu}{k_BT}\right). \tag{7.232}$$

Expressing the particle number in terms of the Fermi energy with the help of Eq. (7.225), we obtain for the temperature dependence of the chemical potential an equation analogous to (7.54):

$$1 = \left(\frac{k_BT}{E_{\rm F}}\right)^{3/2}\frac{3}{2}\, i^{\rm f}_{3/2}\left(\frac{\mu}{k_BT}\right). \tag{7.233}$$

To evaluate this equation, we write the integral representation (7.216) as

$$\begin{aligned} i^{\rm f}_n(\alpha) &= \int_{-\alpha}^{\infty} dx \frac{(\alpha+x)^{n-1}}{e^x+1} \\ &= \int_0^{\alpha} dx \frac{(\alpha-x)^{n-1}}{e^{-x}+1} + \int_0^{\infty} dx \frac{(\alpha+x)^{n-1}}{e^x+1}. \end{aligned} \tag{7.234}$$

where $\varepsilon = x+\alpha$. In the first integral we substitute $1/(e^{-x}+1) = 1 - 1/(e^x+1)$, and obtain

$$i^{\rm f}_n(\alpha) = \int_0^{\alpha} dx\, x^{n-1} + \int_0^{\infty} dx \frac{(\alpha+x)^{n-1}-(\alpha-x)^{n-1}}{e^x+1} + \int_{\alpha}^{\infty} dx \frac{(\alpha-x)^{n-1}}{e^x+1}. \tag{7.235}$$

In the limit $\alpha\to\infty$, only the first term survives, whereas the last term is exponentially small, so that it can be ignored in a series expansion in powers of $1/\alpha$. The second term is expanded in such a series:

$$2\sum_{k=\text{odd}}^{\infty}\binom{n-1}{k}\alpha^{n-1-k}\int_0^\infty dx\frac{x^k}{e^x+1}=2\sum_{k=\text{odd}}\frac{(n-1)!}{(n-1-k)!}\alpha^{n-1-k}(1-2^{-k})\zeta(k+1). \tag{7.236}$$

In the last equation we have used the integral formula for Riemann's ζ-function[4]

$$\int_0^\infty dx\frac{x^{\nu-1}}{e^{\mu x}+1}=\mu^{-\nu}(1-2^{1-\nu})\zeta(\nu). \tag{7.237}$$

At even positive and odd negative integer arguments, the zeta function is related to the Bernoulli numbers by Eq. (2.569). The lowest values of $\zeta(x)$ occurring in the expansion (7.236) are $\zeta(2)$, $\zeta(4),\ldots$, whose values were given in (2.571), so that the expansion of $i_n^{\rm f}(\alpha)$ starts out like

$$i_n^{\rm f}(\alpha)=\frac{1}{n}\alpha^n+2(n-1)\frac{1}{2}\zeta(2)\alpha^{n-2}+2(n-1)(n-2)(n-3)\frac{7}{8}\zeta(4)\alpha^{n-4}+\ldots\ . \tag{7.238}$$

Inserting this into Eq. (7.233) where $n=3/2$, we find the low-temperature expansion

$$1=\left(\frac{k_BT}{E_{\rm F}}\right)^{3/2}\frac{3}{2}\left[\frac{2}{3}\left(\frac{\mu}{k_BT}\right)^{3/2}+\frac{\pi^2}{12}\left(\frac{\mu}{k_BT}\right)^{-1/2}+\frac{7\pi^4}{3\cdot 320}\left(\frac{\mu}{k_BT}\right)^{-5/2}\ldots\right], \tag{7.239}$$

implying for μ the expansion

$$\mu=E_{\rm F}\left[1-\frac{\pi^2}{12}\left(\frac{k_BT}{E_{\rm F}}\right)^2+\frac{7\pi^4}{720}\left(\frac{k_BT}{E_{\rm F}}\right)^4+\ldots\right]. \tag{7.240}$$

These expansions are asymptotic. They have a zero radius of convergence, diverging for any T. They can, however, be used for calculations if T is sufficiently small or at all T after a variational resummation à la Section 5.18.

We now turn to the grand-canonical free energy F_G. In terms of the function (7.216), this reads

$$F_G=-\frac{1}{\beta}\frac{g_SV}{l_{\rm e}^3(\hbar\beta)}\frac{1}{\Gamma(5/2)}\,i_{5/2}^{\rm f}(\alpha). \tag{7.241}$$

Using again (7.238), this has the expansion

$$F_G(T,\mu,V)=F_G(0,\mu,V)\left[1+\frac{5\pi^2}{8}\left(\frac{k_BT}{\mu}\right)^2-\frac{7\pi^4}{384}\left(\frac{k_BT}{\mu}\right)^4+\ldots\right], \tag{7.242}$$

where

$$F_G(0,\mu,V)\quad\equiv\quad-\frac{2}{5}g_SV\frac{\sqrt{2}M^{3/2}}{3\pi^2\hbar^3}\,(\mu)^{3/2}\,\mu=-\frac{2}{5}N\left(\frac{\mu}{E_F}\right)^{3/2}\mu.$$

[4] I.S. Gradshteyn and I.M. Ryzhik, *op. cit.*, Formula 3.411.3.

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

$$S = k_B \frac{\pi^2}{2} \frac{k_B T}{E_{\rm F}} N + \dots \ . \tag{7.243}$$

From this we find a specific heat at constant volume

$$C = T \frac{\partial S}{\partial T}\Big|_{V,N} \overset{T \approx 0}{\approx} S = k_B \frac{\pi^2}{2} \frac{k_B T}{E_{\rm F}} N + \dots \ . \tag{7.244}$$

This grows linearly with increasing temperature and saturates at the constant value $3k_BN/2$ which obeys the Dulong-Petit law of Section 2.12 corresponding to three kinetic and no potential harmonic degrees of freedom in the classical Hamiltonian $\mathbf{p}^2/2M$. See Fig. 7.11 for the full temperature behavior. The linear behavior is

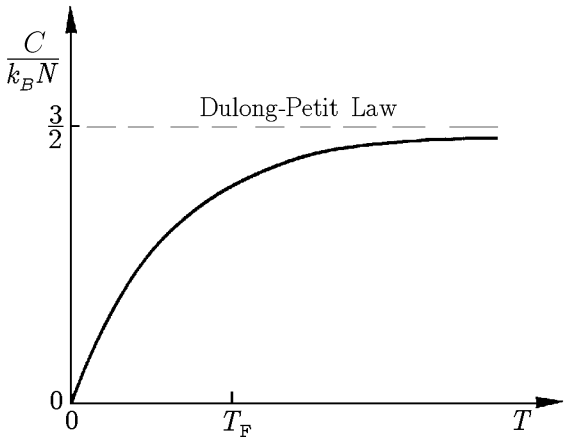

Figure 7.11 Temperature behavior of specific heat of free Fermi gas. As in the free Bose gas, the Dulong-Petit rule gives a high-temperature limit $3k_BN/2$ for the three harmonic kinetic degrees of freedom in the classical Hamiltonian $\mathbf{p}^2/2M$. There are no harmonic potential degrees of freedom.

due to the progressive softening near the surface of the Fermi distribution which makes more and more electrons thermally excitable. It is detected experimentally in metals at low temperature where the contribution of lattice vibrations freezes out as $(T/T_D)^3$. Here T_D is the Debye temperature which characterizes the elastic stiffness of the crystal and ranges from $T_D \approx 90$K in soft metals like lead over $T_D \approx 389$K for aluminum to $T_D \approx 1890$K for diamond. The experimental size of the slope is usually larger than the free electron gas value in (7.244). This can be explained mainly by the interactions with the lattice which result in a large effective mass $M_{\rm eff} > M$.

Note that the quantity $F_G(0, \mu, V)$ is temperature dependent via the chemical potential μ. Inserting (7.240) into (7.242) we find the complete T-dependence

$$F_G(T, \mu, V) = F_G(0, E_{\rm F}, V) \left[1 + \frac{5\pi^2}{12} \left(\frac{k_B T}{E_{\rm F}} \right)^2 - \frac{\pi^4}{16} \left(\frac{k_B T}{E_F} \right)^4 + \dots \right], \tag{7.245}$$

where

$$F_G(0, E_{\rm F}, V) = -\frac{2}{5} N E_{\rm F}. \tag{7.246}$$

As in the boson gas, we have a relation (7.61) between energy and grand-canonical free energy:

$$E = -\frac{3}{2} F_G, \tag{7.247}$$

such that equation (7.245) supplies us with the low-temperature behavior of the internal energy:

$$E = \frac{3}{5} N E_{\rm F} \left[1 + \frac{5\pi^2}{12} \left(\frac{k_B T}{E_F} \right)^2 - \frac{\pi^4}{16} \left(\frac{k_B T}{E_F} \right)^4 + \dots \right]. \tag{7.248}$$

The first term is the energy of the zero-temperature Fermi sphere. Using the relation $c_V = \partial E / V \partial T$, the second term yields once more the leading $T \to 0$ -behavior (7.244) of 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 (7.244) 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. Also there the strong interactions in the liquid produce a screening effect which raises to an effective value of the mass to 8 times that of the atom.

7.4 Statistics Interaction

First, we consider only two identical particles; the generalization to n particles will be obvious. For simplicity, we ignore the one-body potentials $V(\mathbf{x}^{(\nu)})$ in (7.2) since they cause only inessential complications. The total orbital action is then

$$\mathcal{A} = \int_{t_a}^{t_b} dt \left[\frac{M^{(1)}}{2} \dot{\mathbf{x}}^{(1)2} + \frac{M^{(2)}}{2} \dot{\mathbf{x}}^{(2)2} - V_{\rm int}(\mathbf{x}^{(1)} - \mathbf{x}^{(2)}) \right]. \tag{7.249}$$

The standard change of variables to center-of-mass and relative coordinates

$$\mathbf{X} = (M^{(1)}\mathbf{x}^{(1)} + M^{(2)}\mathbf{x}^{(2)})/(M^{(1)} + M^{(2)}), \qquad \mathbf{x} = (\mathbf{x}^{(1)} - \mathbf{x}^{(2)}), \tag{7.250}$$

respectively, separates the action into a free center-of-mass and a relative action

$$\mathcal{A} = \mathcal{A}_{\rm CM} + \mathcal{A}_{\rm rel} = \int_{t_a}^{t_b} dt \frac{M}{2} \dot{\mathbf{X}}^2 + \int_{t_a}^{t_b} dt \left[\frac{\mu}{2} \dot{\mathbf{x}}^2 - V_{\rm int}(\mathbf{x}) \right], \tag{7.251}$$

with a total mass $M = M^{(1)} + M^{(2)}$ and a reduced mass $\mu = M^{(1)} M^{(2)} / (M^{(1)} + M^{(2)})$. Correspondingly, the time evolution amplitude of the two-body system factorizes

into that of an ordinary free particle of mass M, $(\mathbf{X}_b t_b|\mathbf{X}_a t_a)$, and a relative amplitude $(\mathbf{x}_b t_b|\mathbf{x}_a t_a)$. The path integral for the center-of-mass motion is solved as in Chapter 2. Only the relative amplitude is influenced by the particle statistics and needs a separate treatment for bosons and fermions.

First we work in one dimension only. Many of the formulas arising in this case are the same as those of Section 6.2, where we derived the path integral for a particle moving in a half-space $x = r > 0$; only the interpretation is different. We take care of the indistinguishability of the particles by restricting x to the positive semiaxis $x = r \geq 0$; the opposite vector $-x$ describes an identical configuration. The completeness relation of local states reads therefore

$$\int_0^\infty dr|r\rangle\langle r| = 1. \tag{7.252}$$

To write down the orthogonality relation, we must specify the bosonic or fermionic nature of the wave functions. Since these are symmetric or antisymmetric, respectively, we express $\langle r_b|r_a\rangle$ in terms of the complete set of functions with these symmetry properties:

$$\langle r_b|r_a\rangle = 2\int_0^\infty \frac{dp}{\pi\hbar} \left\{ \begin{array}{ll} \cos pr_b/\hbar & \cos pr_a/\hbar \\ \sin pr_b/\hbar & \sin pr_a/\hbar \end{array} \right\}. \tag{7.253}$$

This may be rewritten as

$$\langle r_b|r_a\rangle = \int_{-\infty}^\infty \frac{dp}{2\pi\hbar} \left(e^{ip(r_b-r_a)/\hbar} \pm e^{ip(r_b+r_a)/\hbar}\right) = \delta(r_b - r_a) \pm \delta(r_b + r_a). \tag{7.254}$$

The infinitesimal time evolution amplitude of relative motion is then, in the canonical formulation,

$$\begin{aligned} (r_n\,\epsilon|r_{n-1}\,0) &= \langle r_n|e^{-i\epsilon\hat{H}_{\rm rel}/\hbar}|r_{n-1}\rangle \\ &= \int_{-\infty}^\infty \frac{dp}{2\pi\hbar} \left(e^{ip(r_n-r_{n-1})/\hbar} \pm e^{ip(r_n+r_{n-1})/\hbar}\right) e^{-i\epsilon H_{\rm rel}(p,r_n)/\hbar}, \end{aligned} \tag{7.255}$$

where $H_{\rm rel}(p,x)$ is the Hamiltonian of relative motion associated with the action $\mathcal{A}_{\rm rel}$ in Eq. (7.251). By combining $N+1$ factors, we find the time-sliced amplitude

$$\begin{aligned} (r_b t_b|r_a t_a) = \prod_{n=1}^N \left[\int_0^\infty dr_n\right] \prod_{n=1}^{N+1} \left[\int_{-\infty}^\infty \frac{dp_n}{2\pi\hbar}\right] \\ \times \left\{\exp\left[\frac{i}{\hbar}\sum_{n=1}^{N+1} p_n(r_n - r_{n-1})\right] \pm \exp\left[\frac{i}{\hbar}\sum_{n=1}^{N+1} p_n(r_n + r_{n-1})\right]\right\} e^{-\frac{i}{\hbar}\epsilon\sum_{n=1}^{N+1} H_{\rm rel}(p_n,r_n)}, \end{aligned} \tag{7.256}$$

valid for bosons and fermions, respectively. By extending the radial integral over the entire space it is possible to remove the term after the ±sign by writing

$$\begin{aligned} (r_b t_b|r_a t_a) = \sum_{x_b=\pm r_b} \prod_{n=1}^N \left[\int_{-\infty}^\infty dx_n\right] \prod_{n=1}^{N+1} \left[\int_{-\infty}^\infty \frac{dp_n}{2\pi\hbar}\right] \\ \times \exp\left\{\frac{i}{\hbar}\sum_{a=1}^{N+1} [p_n(x_n - x_{n-1}) - \epsilon H_{\rm rel}(p_n,x_n) + \hbar\pi(\sigma(x_n) - \sigma(x_{n-1}))]\right\}, \end{aligned} \tag{7.257}$$

where the function $\sigma(x)$ vanishes identically for bosons while being equal to

$$\sigma(x) = \Theta(-x) \tag{7.258}$$

for fermions, where $\Theta(x)$ is the Heaviside function (1.313). As usual, we have identified $x_b \equiv x_{N+1}$ and $x_a \equiv x_0$ which is equal to r_a. The final sum over $x_b = \pm r_b$ accounts for the indistinguishability of the two orbits. The phase factors $e^{i\pi\sigma(x_n)}$ give the necessary minus signs when exchanging two fermion positions.

Let us use this formula to calculate explicitly the path integral for a free two-particle relative amplitude. In the bosonic case with a vanishing σ-term, we simply obtain the free-particle amplitude summed over the final positions $\pm r_b$:

$$(r_b t_b | r_a t_a) = \frac{1}{\sqrt{2\pi\hbar i(t_b - t_a)/\mu}} \left\{ \exp\left[\frac{i}{\hbar} \frac{\mu}{2} \frac{(r_b - r_a)^2}{t_b - t_a} \right] + (r_b \to -r_b) \right\}. \tag{7.259}$$

For fermions, the phases $\sigma(x_n)$ in (7.257) cancel each other successively, except for the boundary term

$$e^{i\pi(\sigma(x_b) - \sigma(x_a))}. \tag{7.260}$$

When summing over $x_b = \pm r_b$ in (7.257), this causes a sign change of the term with $x_b = -r_b$ and leads to the antisymmetric amplitude

$$(r_b t_b | r_a t_a) = \frac{1}{\sqrt{2\pi\hbar i(t_b - t_a)/\mu}} \left\{ \exp\left[\frac{i}{\hbar} \frac{\mu}{2} \frac{(r_b - r_a)^2}{(t_b - t_a)} \right] - (r_b \to -r_b) \right\}. \tag{7.261}$$

Let us also write down the continuum limit of the time-sliced action (7.257). It reads

$$\mathcal{A} = \mathcal{A}_{\rm rel} + \mathcal{A}_{\rm f} = \int_{t_a}^{t_b} dt \left[p\dot{x} - H_{\rm rel}(p, x) + \hbar\pi \dot{x}(t) \partial_x \sigma(x(t)) \right]. \tag{7.262}$$

The last term is the desired Fermi statistics interaction. It can also be written as

$$\mathcal{A}_{\rm f} = -\hbar\pi \int_{t_a}^{t_b} dt \dot{x}(t) \delta(x(t)) = \hbar\pi \int_{t_a}^{t_b} dt \partial_t \Theta(-x(t)). \tag{7.263}$$

The right-hand expression shows clearly the pure boundary character of $\mathcal{A}_{\rm f}$, which does not change the equations of motion. Such an interaction is called a *topological interaction*.

Since the integrals in (7.257) over x and p now cover the *entire* phase space and $\sigma(x)$ enters only at the boundaries of the time axis, it is possible to add to the action any potential $V_{\rm int}(r)$. As long as the ordinary path integral can be performed, also the path integral with the additional σ-terms in (7.257) can be done immediately.

It is easy to generalize this result to any number of fermion orbits $x^{(\nu)}(t)$, $\nu = 1, \ldots, n$. The statistics interaction is then $\sum_{\nu<\nu'} \mathcal{A}_{\rm f}[x^{(\nu,\nu')}]$ with the distance vectors $x^{(\nu,\nu')} \equiv x^{(\nu)} - x^{(\nu')}$. When summing over all permuted final positions, the

many-fermion wave functions become antisymmetric. The amplitude is given by the generalization of Eq. (7.257):

$$(x_b^{(\nu_b)};t_b|x_a^{(\nu_a)};t_a)=\sum_{p(\nu_b)}\prod_{\nu=1}^{n}\left\{\prod_{n=1}^{N}\left[\int_{-\infty}^{\infty}dx_n^{(\nu)}\right]\prod_{n=1}^{N+1}\left[\int_{-\infty}^{\infty}\frac{dp_n^{(\nu)}}{2\pi\hbar}\right]\right\}$$
$$\times\exp\left(\frac{i}{\hbar}\sum_{n=1}^{N+1}\left\{\sum_{\nu=1}^{n}\left[p_n^{(\nu)}(x_n^{(\nu)}-x_{n-1}^{(\nu)})-\epsilon H_{\rm rel}(p_n^{(\nu)},x_n^{(\nu)})\right]\right.\right.$$
$$\left.\left.+\hbar\pi\sum_{\nu<\nu'}\left[\sigma(x_n^{(\nu,\nu')})-\sigma(x_{n-1}^{(\nu,\nu')})\right]\right\}\right),\quad(7.264)$$

where $\Sigma_{p(\nu_b)}$ denotes the sum over all permutations of the final positions. The phases $\exp[i\pi\sigma(x)]$ produce the complete antisymmetry for fermions.

Consider now two particles moving in a two-dimensional space. Let the relative motion be described in terms of polar coordinates. For distinguishable particles, the scalar product of localized states is

$$\begin{aligned}\langle r_b\varphi_b|r_a\varphi_a\rangle &= \int_0^\infty dkk\sum_{m=-\infty}^{\infty}i_m(kr_b)i_m(kr_a)\frac{1}{2\pi}e^{im(\varphi_b-\varphi_a)}\\ &= \frac{1}{\sqrt{r_br_a}}\delta(r_b-r_a)\delta(\varphi_b-\varphi_a).\end{aligned}\quad(7.265)$$

This follows straightforwardly by expanding the exponentials $e^{i\mathbf{kx}}=e^{ikr\cos\varphi}$ in the scalar product

$$\langle\mathbf{x}_b|\mathbf{x}_a\rangle=\int\frac{d^2k}{(2\pi)^2}e^{i\mathbf{kx}_b}e^{-i\mathbf{kx}_a}=\delta^{(2)}(\mathbf{x}_b-\mathbf{x}_a)\quad(7.266)$$

into Bessel functions, according to the well-known formula[5]

$$e^{a\cos\varphi}=\sum_{m=-\infty}^{\infty}i_m(a)e^{im\varphi},\quad(7.267)$$

and by rewriting $\delta^{(2)}(\mathbf{x}_b-\mathbf{x}_a)$ as $(r_br_a)^{-1/2}\delta(r_b-r_a)\delta(\varphi_b-\varphi_a)$. For indistinguishable particles, the angle φ is restricted to a half-space, say $\varphi\in[0,\pi)$. When considering bosons or fermions, the phase factor $e^{im(\varphi_b-\varphi_a)}$ must be replaced by $e^{im(\varphi_b-\varphi_a)}\pm e^{im(\varphi_b+\pi-\varphi_a)}$, respectively. In the product of such amplitudes in a time-sliced path integral, the $\pm$-terms in (7.256) can again be accounted for by completing the half-space in φ to the full space $[-\pi,\pi)$ and introducing the field $\sigma(\varphi)$. By including a Hamiltonian and returning to Euclidean coordinates x_1,x_2, we arrive at the relative amplitude

$$(\mathbf{x}_bt_b|\mathbf{x}_at)=\int\mathcal{D}^2x\int\frac{\mathcal{D}^2p}{2\pi}\left\{\exp\left[\frac{i}{\hbar}\mathcal{A}_{\rm rel}+\frac{i}{\hbar}\mathcal{A}_{\rm f}\right]+(\mathbf{x}_b\to-\mathbf{x}_b)\right\},\quad(7.268)$$

with an obvious time slicing as in (7.257).

[5]I.S. Gradshteyn and I.M. Ryzhik, op. cit., Formula 6.633.1.

The Fermi statistics interaction $\mathcal{A}_{\rm f}$ looks in polar coordinates just like (7.263), but with x replaced by φ:

$$\mathcal{A}_{\rm f} = \hbar\pi \int_{t_a}^{t_b} dt \dot{\varphi}(t) \partial_\varphi \sigma(\varphi(t)). \tag{7.269}$$

Adapting the step function $\sigma(\varphi)$ to the periodic nature of the variable φ, we continue this function periodically in φ. Equivalently, we replace it by a step function $\sigma_{\rm p}(\varphi)$ which jumps by one unit at every integer multiple of π and write

$$\mathcal{A}_{\rm f} = \hbar \int_{t_a}^{t_b} dt\, \dot{\mathbf{x}}(t) \cdot \mathbf{a}(\mathbf{x}(t)), \tag{7.270}$$

with a vector potential

$$\mathbf{a}(\mathbf{x}) \equiv \pi \boldsymbol{\nabla} \sigma_{\rm p}(\varphi). \tag{7.271}$$

When calculating particle distributions or partition functions which satisfy periodic boundary conditions, this coupling is invariant under local gauge transformations of the vector potential

$$\mathbf{a}(\mathbf{x}) \to \mathbf{a}(\mathbf{x}) + \boldsymbol{\nabla} \Lambda(\mathbf{x}), \tag{7.272}$$

with smooth and single-valued functions $\Lambda(\mathbf{x})$, i.e., with $\Lambda(\mathbf{x})$ satisfying the integrability condition of Schwarz:

$$(\partial_i \partial_j - \partial_j \partial_i) \Lambda(\mathbf{x}) = 0. \tag{7.273}$$

Taking advantage of gauge invariance, we can in (7.271) replace $\sigma_{\rm p}(\varphi)$ by *any* function of $\mathbf{x}$ as long as it changes by one unit when going from φ_b to $\varphi_b + \pi$. A convenient choice is

$$\sigma_{\rm p}(\mathbf{x}) = \frac{1}{\pi}\varphi(\mathbf{x}) \equiv \frac{1}{\pi} \arctan \frac{x_2}{x_1}. \tag{7.274}$$

With this, the statistics interaction (7.270) becomes

$$\mathcal{A}_{\rm f} = \hbar \int_{t_a}^{t_b} dt \dot{\mathbf{x}} \partial_{\mathbf{x}} \varphi(\mathbf{x}) = \hbar \int_{t_a}^{t_b} dt \epsilon_{ij} \frac{x_i \dot{x}_j}{\mathbf{x}^2}, \tag{7.275}$$

where ϵ_{ij} is the antisymmetric unit tensor of Levi-Civita in two dimensions.

Just like the expression (7.263), this is a purely topological interaction. By comparison with (7.270), we identify the vector potential of the statistics interaction as

$$a_i(\mathbf{x}) = \partial_i \varphi = -\epsilon_{ij} \frac{x_j}{\mathbf{x}^2}. \tag{7.276}$$

The Fermi statistics remains obviously in operation if we choose, instead of the vector potential (7.276), an arbitrary odd multiple of it:

$$a_i(\mathbf{x}) = \partial_i \varphi = -(2n+1) \epsilon_{ij} \frac{x_j}{\mathbf{x}^2}, \qquad n = 0, \pm 1, \pm 2, \ldots. \tag{7.277}$$

The even multiples

$$a_i(\mathbf{x}) = \partial_i \varphi = -2n\epsilon_{ij}\frac{x_j}{\mathbf{x}^2}, \qquad n = 0, \pm 1, \pm 2, \ldots, \tag{7.278}$$

on the other hand, give rise to Bose statistics.

For more than two particles, the amplitude (7.268) is generalized to the two-dimensional analog of Eq. (7.264). In one and two space dimensions we have thus succeeded in taking care of the indistinguishability of the particles and the fermionic nature by the simple statistics interaction terms (7.263) and (7.275). The indistinguishability of the particles requires that the path integral over all paths from the initial point $\mathbf{x}_a$ to the final point $\mathbf{x}_b$ has to be extended by those paths which run to the reflected point $-\mathbf{x}_b$. The statistics interaction guarantees the antisymmetry of the resulting amplitude.

7.5 Fractional Statistics

The above considerations raise an important question. Is it possible that particles with an arbitrary real multiple of the statistical gauge interaction (7.275) exist in nature? Such particles would show an unusual statistical behavior. If the prefactor is denoted by μ_0 and the statistics interaction reads

$$\mathcal{A}_{\mathrm{f}} = \hbar\mu_0 \int_{t_a}^{t_b} dt\, \dot{\mathbf{x}} \cdot \boldsymbol{\nabla}\varphi(\mathbf{x}) = \hbar\mu_0 \int_{t_a}^{t_b} dt \epsilon_{ij}\frac{x_i \dot{x}_j}{\mathbf{x}^2}, \tag{7.279}$$

an interchange of the orbital endpoints in the path integral gives rise to a phase factor $e^{i\pi\mu_0}$. If μ_0 is even or odd, the amplitude describes bosons or fermions, respectively. For rational values of μ_0, however, the particles are neither one nor the other. They are called *anyons*. The phase of the amplitude returns to its initial value only after the particles have been rotated around each other several times. The statistical behavior of such particles will be studied in detail in Section 16.2. There we shall see that for two ordinary particles, an anyonic statistical behavior can be generated by a magnetic interaction. An interaction of the form (7.279) arises from an infinitesimally thin magnetic flux tube of strength $\Phi = \mu_0\Phi_0$ with $\Phi_0 = 2\pi\hbar c/e$. Indeed, the magnetic interaction is given by the gauge-invariant expression

$$\mathcal{A}_{\mathrm{mg}} = \frac{e}{c}\int_{t_a}^{t_b} dt\, \dot{\mathbf{x}}(t)\mathbf{A}(\mathbf{x}(t)), \tag{7.280}$$

and the vector potential of a thin magnetic flux tube of flux Φ reads

$$A_i(\mathbf{x}) = \frac{\Phi}{2\pi}\partial_i\varphi = -\Phi\epsilon_{ij}\frac{x_j}{\mathbf{x}^2}. \tag{7.281}$$

For the flux $\Phi_0 = 2\pi\hbar c/e$ or an odd multiple thereof, the magnetic interaction coincides with the statistics interaction of two fermions (7.275). Bose statistics holds if Φ is zero or an even multiple of Φ_0. The magnetic field can be chosen

to produce any value of μ_0. This analogy will permit us to calculate the second virial coefficient of a gas of anyons in Section 16.3. There we shall also see that the statistical parameter μ_0 determines the behavior of the wave functions near the origin. While the wave functions of bosons and fermions carry either even or odd azimuthal angular momenta m, respectively, and vanish like $|\mathbf{x}|^m$ for $|\mathbf{x}| \to 0$, those of anyons can carry any integer m, behaving like $|\mathbf{x}|^{|m+\mu_0|}$ with a noninteger exponent.

We shall demonstrate in Section 16.2 that flux tubes whose flux Φ is an integer multiple of Φ_0, i.e., those with a flux corresponding to Fermi or Bose statistics, have a vanishing scattering amplitude with respect to particles of charge e (*Aharonov-Bohm effect*).

Such flux tubes can be used as a theoretical artifact to construct the vector potential of a magnetic monopole. Although magnetic fields can have no sources, a monopole can be brought in from infinity inside an infinitely thin tube of flux $\Phi = n\Phi_0$ (n = integer), called a *Dirac string*. Since this cannot be detected by any electromagnetic scattering experiment the endpoint of the string behaves like a magnetic monopole.[6] In an important aspect, the analogy between the magnetic and statistics interaction is not perfect and the present path integral is different from the one governing the magnetic scattering amplitude: The magnetic scattering amplitude deals with two different particles, one with an electric and the other with a magnetic charge. The paths are therefore summed with a fixed endpoint. In the statistics case, on the other hand, the sum includes the final point $\mathbf{x}_b$ and the reflected point $-\mathbf{x}_b$.

For this reason, the magnetic analogy can be used to impose arbitrary statistics only upon two particles and not upon an ensemble of many identical particles. The analogy has nevertheless been useful to guide recent theoretical developments, in particular the explanation of the fractional quantum Hall effect (to be discussed in Sections 16.13–16.12).

Particles in two dimensions with fractional statistics have recently become a source of inspiration in field theory, leading to many new and interesting insights.

7.6 Second-Quantized Bose Fields

We have seen above that the path integral of a system with many identical particles can become quite cumbersome to handle. Fortunately, there exists a much simpler and more efficient path integral description of many-particle systems. In the Schrödinger formulation of quantum mechanics, it is possible to generalize the single-particle Schrödinger equation to an arbitrary and *variable* number of particles by letting the complex Schrödinger fields $\psi(\mathbf{x}, t)$ be *field operators* rather than complex c-numbers. These are denoted by $\hat{\psi}(\mathbf{x}, t)$ and postulated to satisfy the harmonic-oscillator commutation relations at each point $\mathbf{x}$ in space. To impose properly such

[6] See also the discussion in H. Kleinert, Int. J. Mod. Phys. A *7*, 4693 (1992) (`http://www.physik.fu-berlin.de/~kleinert/203`); Phys. Lett. B *246*, 127 (1990) (*ibid.*`http/205`).

local quantization rules, space is discretized into little cubes of volume ϵ^3, centered around the points $\mathbf{x_n} = \epsilon(n_1, n_2, n_3)$, with $n_{1,2,3}$ running through all integers. If we omit the subscripts $\mathbf{n}$, for brevity, the quantization rules are

$$\begin{aligned} [\hat{\psi}(\mathbf{x},t), \hat{\psi}^\dagger(\mathbf{x}',t)] &= \delta_{\mathbf{x}\mathbf{x}'}, \\ [\hat{\psi}^\dagger(\mathbf{x},t), \hat{\psi}^\dagger(\mathbf{x}',t)] &= 0, \\ [\hat{\psi}(\mathbf{x},t), \hat{\psi}(\mathbf{x}',t)] &= 0. \end{aligned} \tag{7.282}$$

The commutativity of the operators at different places ensures the independence of the associated oscillators. Imposing the conditions (7.282) is referred to as *second quantization* or *field quantization*. One also speaks of a *quantization of particle number*. The commutation relations generate an infinite-dimensional Hilbert space at each space point $\mathbf{x}$. Applying the operator $\hat{\psi}^\dagger(\mathbf{x},t)$ n times to the ground state of the harmonic oscillator $|0\rangle_\mathbf{x}$ at $\mathbf{x}$ creates states with n excitations at $\mathbf{x}$:

$$|n,\mathbf{x}\rangle = \frac{1}{\sqrt{n!}}[\hat{\psi}^\dagger(\mathbf{x},0)]^n|0\rangle. \tag{7.283}$$

These states are interpreted as states describing n particles at the point $\mathbf{x}$. The ground state of all oscillators is

$$|0\rangle \equiv \prod_\mathbf{x} |0\rangle_\mathbf{x}\,. \tag{7.284}$$

It is called the *vacuum state* of the system. The total number of particles at each time is measured by the operator

$$\hat{N}(t) = \sum_\mathbf{x} \hat{\psi}^\dagger(\mathbf{x},t)\hat{\psi}(\mathbf{x},t). \tag{7.285}$$

The simplest classical action, whose quantum theory has the above structure, describes an ensemble of free bosons with a chemical potential μ:

$$\mathcal{A}[\psi^*,\psi] = \sum_\mathbf{x} \int_{t_a}^{t_b} dt\, \left[\psi^*(i\hbar\partial_t + \mu)\psi(\mathbf{x},t) - \frac{\hbar^2}{2M}\psi^*\nabla_\mathbf{x}\overline{\nabla}_\mathbf{x}\psi(\mathbf{x},t)\right]. \tag{7.286}$$

The symbols $\nabla_\mathbf{x}, \overline{\nabla}_\mathbf{x}$ denote the difference operators on the discretized three-dimensional space, each component ∇_i, $\overline{\nabla}_i$ being defined in the same way as the difference operators ∇, $\overline{\nabla}$ on the sliced time axis in Eqs. (2.97). The eigenvalues on a plane wave of momentum $\mathbf{p}$ are

$$-i\hbar\nabla_i e^{i\mathbf{p}\mathbf{x}/\hbar} = P_i e^{i\mathbf{p}\mathbf{x}/\hbar}, \quad -i\hbar\overline{\nabla}_i e^{i\mathbf{p}\mathbf{x}/\hbar} = \bar{P}_i e^{i\mathbf{p}\mathbf{x}/\hbar}, \tag{7.287}$$

with

$$P_i = -i\frac{\hbar}{\epsilon}\left[e^{i\epsilon p_i/\hbar} - 1\right], \quad \bar{P}_i = P_i^*. \tag{7.288}$$

By Fourier decomposing the field

$$\psi(\mathbf{x},t) = \sqrt{\frac{\epsilon^3}{V}}\sum_\mathbf{p} e^{i\mathbf{p}\mathbf{x}/\hbar}a_\mathbf{p}(t), \tag{7.289}$$

the difference operators $\nabla_{\mathbf{x}}$, $\overline{\nabla}_{\mathbf{x}}$ are diagonalized and the action is decomposed into a direct sum of fields $a^*_{\mathbf{p}}(t)$, $a_{\mathbf{p}}(t)$ of a fixed momentum $\mathbf{p}$,

$$\mathcal{A}[a^*, a] = \hbar \sum_{\mathbf{p}} \int_{t_a}^{t_b} dt \, \left[a^*_{\mathbf{p}}(t) i\partial_t a_{\mathbf{p}}(t) - \omega(\mathbf{p}) a^*_{\mathbf{p}}(t) a_{\mathbf{p}}(t) \right], \tag{7.290}$$

where $\omega(\mathbf{p})$ denotes the single-particle frequencies

$$\omega(\mathbf{p}) \equiv \frac{1}{\hbar} \left[\frac{|\mathbf{P}|^2}{2M} - \mu \right], \tag{7.291}$$

with

$$|\mathbf{P}|^2 \equiv \frac{\hbar^2}{\epsilon^2} \sum_i 2 \left[1 - \cos\left(\frac{\epsilon p_i}{\hbar} \right) \right]. \tag{7.292}$$

The extremization of (7.286) gives the field equation

$$\left(i\hbar\partial_t + \mu + \frac{\hbar^2}{2M} \nabla_{\mathbf{x}} \overline{\nabla}_{\mathbf{x}} \right) \psi(\mathbf{x}, t) = 0. \tag{7.293}$$

This is the ordinary free-particle Schrödinger equation (the *first-quantized* field equation), apart from a constant shift in the energy by the chemical potential μ. Recall that the chemical potential guarantees a fixed average particle number which, in experiments, is enforced by contact with an appropriate particle reservoir (see Section 1.17). In momentum space, the field equation reads

$$[i\partial_t - \omega(\mathbf{p})] a_{\mathbf{p}}(t) = 0.$$

Knowing the general relation between the operator and the path integral description of quantum mechanics, we expect that the above rules of second quantization of operators can be accounted for by assuming the field variables ${a^*}_{\mathbf{p}}(t)$ and $a_{\mathbf{p}}(t)$ in the action to be fluctuating c-number variables and summing over all their configurations with an amplitude $\exp\{(i/\hbar)\mathcal{A}[a^*, a]\}$. The precise form of this path integral can be inferred from the oscillator nature of the commutation relations (7.282). After the Fourier transform (7.289), the components $\hat{a}_{\mathbf{p}}(t), \hat{a}^\dagger_{\mathbf{p}}(t)$ satisfy

$$\begin{aligned} [\hat{a}_{\mathbf{p}}(t), \hat{a}^\dagger_{\mathbf{p}'}(t)] &= \delta_{\mathbf{p}\mathbf{p}'}, \\ [\hat{a}^\dagger_{\mathbf{p}}(t), \hat{a}^\dagger_{\mathbf{p}'}(t)] &= 0, \\ [\hat{a}_{\mathbf{p}}(t), \hat{a}_{\mathbf{p}'}(t)] &= 0. \end{aligned} \tag{7.294}$$

Since the oscillators at different momenta $\mathbf{p}$ are independent of each other and since the action is a direct sum, we may drop the subscript $\mathbf{p}$ in the sequel and consider fields of a single momentum only.

The commutators (7.294) are the same as those of a harmonic oscillator, of course, obtained from the usual canonical commutators

$$[\hat{p}, \hat{x}] = -i\hbar \tag{7.295}$$

by the canonical transformation

$$\hat{a}^\dagger = \sqrt{M/2\hbar\omega}(\omega\hat{x} - i\hat{p}/M), \quad \hat{a} = \sqrt{M/2\hbar\omega}(\omega\hat{x} + i\hat{p}/M). \tag{7.296}$$

Note that within the present context, the oscillator momentum $\hat{p}$ is the conjugate momentum of the field operator and has no relation to the particle momentum $\mathbf{p}$ (there exists a field operator for each particle momentum $\mathbf{p}$). The transformation (7.296) changes the Hamiltonian of the harmonic oscillator

$$\hat{H}_\omega = \frac{1}{2M}\hat{p}^2 + \frac{M\omega^2}{2}\hat{x}^2 \tag{7.297}$$

into the creation and annihilation operator form

$$\hat{H}_\omega = \frac{\hbar\omega}{2}(\hat{a}^\dagger\hat{a} + \hat{a}\,\hat{a}^\dagger). \tag{7.298}$$

The classical action in the canonical form

$$\mathcal{A}[p,q] = \int_{t_a}^{t_b} dt\ [p\dot{q} - H_\omega(p,q)] \tag{7.299}$$

turns into

$$\mathcal{A}[a^*,a] = \hbar\int_{t_a}^{t_b} dt\,(a^* i\partial_t a - \omega a^* a). \tag{7.300}$$

If one wants to describe quantum statistics, one has to replace $t \to -i\tau$ and use the Euclidean action (with $\beta = 1/k_B T$)

$$\mathcal{A}_{\rm e}[a^*,a] = \hbar\int_0^{\hbar\beta} d\tau\,(a^*\partial_\tau a + \omega a^* a), \tag{7.301}$$

which coincides precisely with the action (7.290) for particles of a single momentum.

7.7 Fluctuating Bose Fields

We set up a path integral formulation which replaces this second-quantized operator structure. Since we have studied the harmonic oscillator extensively in real and imaginary time and since we know how to go back and forth between quantum-mechanical and -statistical expressions, we consider here only the case of imaginary time with the Euclidean action (7.301). For simplicity, we calculate only the partition function. The extension to density matrices is straightforward. Correlation functions will be discussed in detail in Chapter 18.

Since the action (7.300) of the harmonic oscillator is merely a rewritten canonical action (7.299), the partition function of the harmonic oscillator is given by the path integral [see (2.339)]

ref(2.339) lab(2.187) est(2.220)

$$Z_\omega = \oint \mathcal{D}x(\tau)\int\frac{\mathcal{D}p(\tau)}{2\pi\hbar}\exp\left[-\int_0^{\hbar\beta} d\tau\,(a^*\partial_\tau a + \omega a^* a)\right], \tag{7.302}$$

where the quantum-mechanical trace requires the orbits $x(\tau)$ to be periodic in $\tau \to \tau + \hbar\beta$, with a Fourier expansion

$$x(\tau) = \frac{1}{\sqrt{\hbar\beta}} \sum_{m=-\infty}^{\infty} x_m e^{-i\omega_m \tau}, \quad \omega_m = 2\pi m/\hbar\beta. \tag{7.303}$$

The momentum integrations are unrestricted.

If the momentum states were used as the diagonal basis for the derivation of the path integral, the measure would be $\int \mathcal{D}x \oint (\mathcal{D}p/2\pi\hbar)$. Then $p(\tau)$ is periodic under $\tau \to \tau + \hbar\beta$ and the $x(\tau)$-integrations are unrestricted. This would give a different expression at the time-sliced level; the continuum limit $\epsilon \to 0$, however, would be the same.

Since the explicit conjugate variables in the action are now a and a^*, it is customary to express the measure of the path integral in terms of these variables and write

$$Z_\omega \equiv \oint \frac{\mathcal{D}a^*(\tau)\mathcal{D}a(\tau)}{\pi} \exp\left\{-\int_0^{\hbar\beta} d\tau \, (a^*\partial_\tau a + \omega a^* a)\right\}, \tag{7.304}$$

where $\oint \mathcal{D}a^*\mathcal{D}a$ stands for the measure

$$\oint \mathcal{D}a^*\mathcal{D}a = \oint_{-\infty}^{\infty} \mathcal{D}\,\mathrm{Re}\, a \int_{-\infty}^{\infty} \mathcal{D}\,\mathrm{Im}\, a \ . \tag{7.305}$$

With the action being the time-sliced oscillator action, the result of the path integration in the continuum limit is known from (2.409) to be

ref(2.409)
lab(2.240)
est(2.280)

$$Z_\omega = \frac{1}{2\sinh(\hbar\omega\beta/2)}. \tag{7.306}$$

In the context of second quantization, this is not really the desired result. For large β, the partition function (7.306) behaves like

$$Z_\omega \to e^{-\hbar\omega\beta/2}, \tag{7.307}$$

exhibiting in the exponent the oscillator ground-state energy $E_0 = \hbar\omega/2$. In the second-quantized interpretation, however, the ground state is the no-particle state. Hence its energy should be zero. In the operator formulation, this can be achieved by an appropriate operator ordering, choosing the Hamiltonian operator to be

$$\hat{H} = \hbar\omega \hat{a}^\dagger \hat{a}, \tag{7.308}$$

rather than the oscillator expression (7.298). In the path integral, the same goal is achieved by suitably time-slicing the path integral (7.304) and writing

$$Z_\omega^N = \prod_{n=0}^{N} \left[\int \frac{da_n^* da_n}{\pi}\right] \exp\left\{-\frac{1}{\hbar}\mathcal{A}_\omega^N\right\}, \tag{7.309}$$

with the sliced action

$$\mathcal{A}_\omega^N = \hbar \sum_{n=1}^{N} \left[a_n^*(a_n - a_{n-1}) + \epsilon\omega a_n^* a_{n-1} \right]. \tag{7.310}$$

Expressed in terms of the difference operator, it reads

$$\mathcal{A}_\omega^N = \hbar\epsilon \sum_{n=1}^{N} a_n^* \left[(1-\epsilon\omega)\overline{\nabla} + \omega \right] a_n. \tag{7.311}$$

The $a(\tau)$-orbits are taken to be periodic functions of τ, with a Fourier expansion

$$a(\tau) = \frac{1}{\sqrt{\hbar\beta}} \sum_{m=-\infty}^{\infty} a_m e^{-i\omega_m \tau}, \quad \omega_m = 2\pi m/\hbar\beta. \tag{7.312}$$

Note that in contrast to the coefficients x_m in expansion (7.303), a_m and a_{-m} are *independent* of each other, since $a(\tau)$ is complex. The periodicity of $a(\tau)$ arises as follows: In the time-sliced path integral derived in the x-basis with integration variables $x_0, \ldots, x_{N+1}$ and $p_1, \ldots, p_{N+1}$, we introduce a fictitious momentum variable p_0 which is set identically equal to p_{N+1}. Then the time-sliced $\int_0^{\hbar\beta} d\tau p\dot{x}$ term, $\sum_{n=1}^{N+1} p_n \overline{\nabla} x_n$, can be replaced by $-\sum_{n=1}^{N+1} x_n \nabla p_n$ [see the rule of partial integration on the lattice, Eq. (2.103)] or by $-\sum_{n=1}^{N+1} x_n \overline{\nabla} p_n$. The first term in the time-sliced action (7.310) arises by symmetrizing the above two lattice sums.

In order to perform the integrals in (7.309), we make use of the Gaussian formula valid for $\mathrm{Re}\, A > 0$,

$$\int \frac{da_n^*\, da_n}{\pi} e^{-a_n^* A_n a_n} = \frac{1}{A_n}, \qquad \mathrm{Re}\, A_n > 0. \tag{7.313}$$

By taking a product of N of these, we have

$$\prod_{n=0}^{N} \left[\int \frac{da_n^*\, da_n}{\pi} \right] e^{-\sum_n a_n^* A_n a_n} = \prod_{n=1}^{N+1} \frac{1}{A_n}, \qquad \mathrm{Re}\, A_n > 0. \tag{7.314}$$

This is obviously a special case of the matrix formula

$$Z = \prod_{n=0}^{N} \left[\int \frac{da_n^*\, da_n}{\pi} \right] e^{-\sum_{n,m} a_n^* A_{nm} a_m} = \frac{1}{\det A}, \tag{7.315}$$

in which the matrix $A = A^d$ has only diagonal elements with a positive real part. Now we observe that the measure of integration is certainly invariant under any unitary transformation of the components a_n:

$$a_n \to \sum_{n'} U_{n,n'}\, a_{n'}. \tag{7.316}$$

So is the determinant of A:

$$\det A \to \det\left(U\, A^d\, U^\dagger\right) = \det A^d. \tag{7.317}$$

But then formula (7.315) holds for any matrix A which can be diagonalized by a unitary transformation and has only eigenvalues with a positive real part. In the present case, the possibility of diagonalizing A is guaranteed by the fact that A satisfies $AA^\dagger = A^\dagger A$, i.e., it is a *normal* matrix. This property makes the Hermitian and anti-Hermitian parts of A commute with each other, allowing them to be diagonalized simultaneously.

In the partition function (7.309), the $(N+1) \times (N+1)$ matrix A has the form

$$A = \epsilon(1-\epsilon\omega)\overline{\nabla} + \epsilon\omega = \begin{pmatrix} 1 & 0 & 0 & \dots & 0 & -1+\epsilon\omega \\ -1+\epsilon\omega & 1 & 0 & \dots & 0 & 0 \\ 0 & -1+\epsilon\omega & 1 & \dots & 0 & 0 \\ 0 & 0 & -1+\epsilon\omega & \dots & 0 & 0 \\ \vdots & & & & & \vdots \\ 0 & 0 & 0 & \dots & -1+\epsilon\omega & 1 \end{pmatrix}. \tag{7.318}$$

This matrix acts on a complex vector space. Its determinant can immediately be calculated by a repeated expansion along the first row [recall the calculations of the determinants (2.204) and (2.418)], giving

$$\det_{N+1} A = 1 - (1-\epsilon\omega)^{N+1}. \tag{7.319}$$

Hence we obtain the time-sliced partition function

$$Z_\omega^N = \frac{1}{\det_{N+1}[\epsilon(1-\epsilon\omega)\overline{\nabla} + \epsilon\omega]} = \frac{1}{1-(1-\epsilon\omega)^{N+1}}. \tag{7.320}$$

It is useful to introduce the auxiliary frequency

$$\bar{\omega}_{\rm e} \equiv -\frac{1}{\epsilon}\log(1-\epsilon\omega). \tag{7.321}$$

The subscript e records the Euclidean nature of the time [in analogy with the frequencies $\tilde{\omega}_{\rm e}$ of Eq. (2.399)]. In terms of $\bar{\omega}_{\rm e}$, Z_ω^N takes the form

ref(2.399)
lab(2.230)
est(2.270)

$$Z_\omega^N = \frac{1}{1-e^{-\beta\hbar\bar{\omega}_{\rm e}}}. \tag{7.322}$$

This is the well-known partition function of Bose particles for a single state of energy $\bar{\omega}_{\rm e}$. It has the expansion

$$Z_\omega = 1 + e^{-\beta\hbar\bar{\omega}_{\rm e}} + e^{-2\beta\hbar\bar{\omega}_{\rm e}} + \dots\ , \tag{7.323}$$

in which the nth term exhibits the Boltzmann factor for an occupation of a particle state by n particles, in accordance with the Hamiltonian operator

$$\hat{H}_\omega = \hbar\bar{\omega}_{\rm e}\hat{N} = \hbar\bar{\omega}_{\rm e} a^\dagger a. \tag{7.324}$$

In the continuum limit $\epsilon \to 0$, the auxiliary frequency tends to ω,

$$\bar{\omega}_{\rm e} \xrightarrow{\epsilon \to 0} \omega, \tag{7.325}$$

and Z_ω^N reduces to

$$Z_\omega = \frac{1}{1 - e^{-\beta\hbar\omega}}. \tag{7.326}$$

The generalization of the partition function to a system with a time-dependent frequency $\Omega(\tau)$ reads

$$Z_\omega^N = \prod_{n=0}^{N} \left[\int \frac{da_n^\dagger da_n}{\pi} \right] \exp\left\{ -\frac{1}{\hbar} \mathcal{A}^N \right\}, \tag{7.327}$$

with the sliced action

$$\mathcal{A}_\omega^N = \hbar \sum_{n=1}^{N} \left[a_n^*(a_n - a_{n-1}) + \epsilon \Omega_n a_n^* a_{n-1} \right], \tag{7.328}$$

or, expressed in terms of the difference operator $\overline{\nabla}$,

$$\mathcal{A}_\omega^N = \hbar\epsilon \sum_{n=1}^{N} a_n^* \left[(1 - \epsilon\Omega_n)\overline{\nabla} + \Omega_n \right] a_n. \tag{7.329}$$

The result is

$$Z_\omega^N = \frac{1}{\det_{N+1}[\epsilon(1-\epsilon\Omega)\overline{\nabla} + \epsilon\Omega]} = \frac{1}{1 - \prod_{n=0}^{N}(1 - \epsilon\Omega_n)}. \tag{7.330}$$

Here we introduce the auxiliary frequency

$$\bar{\Omega}_{\rm e} \equiv -\frac{1}{(N+1)\epsilon} \sum_{n=0}^{N} \log(1 - \epsilon\Omega_n), \tag{7.331}$$

which brings Z_ω^N to the form

$$Z_\omega^N = \frac{1}{1 - e^{-\beta\hbar\bar{\Omega}_{\rm e}}}. \tag{7.332}$$

For comparison, let us also evaluate the path integral directly in the continuum limit. Then the difference operator (7.318) becomes the differential operator

$$(1 - \epsilon\omega)\overline{\nabla} + \omega \to \partial_\tau + \omega, \tag{7.333}$$

acting on periodic complex functions $e^{-i\omega_m\tau}$ with the Matsubara frequencies ω_m. Hence the continuum partition function of a harmonic oscillator could be written as

$$\begin{aligned} Z_\omega &= \oint \frac{\mathcal{D}a^*\mathcal{D}a}{\pi} \exp\left[-\int_0^{\hbar\beta} d\tau \, (a^*\partial_\tau a + \omega a^* a) \right] \\ &= \mathcal{N}_\omega \frac{1}{\det(\partial_\tau + \omega)}. \end{aligned} \tag{7.334}$$

The normalization constant is fixed by comparison with the time-sliced result. The operator $\partial_\tau + \omega$ has the eigenvalues $-i\omega_m + \omega$. The product of these is calculated by considering the ratios with respect to the $\omega = 0$ -values

$$\prod_{m=-\infty,\neq 0}^{\infty} \frac{-i\omega_m + \omega}{-i\omega_m} = \frac{\sinh(\hbar\omega\beta/2)}{\hbar\omega\beta/2}. \tag{7.335}$$

This product is the ratio of functional determinants

$$\frac{\det(\partial_\tau + \omega)}{\det{}'(\partial_\tau)} = \omega \frac{\sinh(\hbar\omega\beta/2)}{\hbar\omega\beta/2}, \tag{7.336}$$

where the prime on the determinant with $\omega = 0$ denotes the omission of the zero frequency $\omega_0 = 0$ in the product of eigenvalues; the prefactor ω accounts for this.

Note that this ratio formula of continuum fluctuation determinants gives naturally only the harmonic oscillator partition function (7.306), not the second-quantized one (7.322). Indeed, after fixing the normalization factor $\mathcal{N}_\omega$ in (7.334), the path integral in the continuum formulation can be written as

$$\begin{aligned} Z_\omega &= \oint \frac{\mathcal{D}a^*\mathcal{D}a}{\pi} \exp\left[-\int_0^{\hbar\beta} d\tau\, (a^*\partial_\tau a + \omega a^* a)\right] \\ &= \frac{k_B T}{\hbar} \frac{\det{}'(\partial_\tau)}{\det(\partial_\tau + \omega)} = \frac{1}{2\sinh(\hbar\omega\beta/2)}. \end{aligned} \tag{7.337}$$

In the continuum, the relation with the oscillator fluctuation factor can be established most directly by observing that in the determinant, the operator $\partial_\tau + \omega$ can be replaced by the conjugate operator $-\partial_\tau + \omega$, since all eigenvalues come in complex-conjugate pairs, except for the $m = 0$ -value, which is real. Hence the determinant of $\partial_\tau + \omega$ can be substituted everywhere by

$$\det(\partial_\tau + \omega) = \det(-\partial_\tau + \omega) = \sqrt{\det(-\partial_\tau^2 + \omega^2)}, \tag{7.338}$$

rewriting the partition function (7.337) as

$$\begin{aligned} Z_\omega &= \frac{k_B T}{\hbar} \frac{\det{}'(\partial_\tau)}{\det(\partial_\tau + \omega)} \\ &= \frac{k_B T}{\hbar} \left[\frac{\det{}'(-\partial_\tau^2)}{\det(-\partial_\tau^2 + \omega^2)}\right]^{1/2} = \frac{1}{2\sinh(\hbar\omega\beta/2)}, \end{aligned} \tag{7.339}$$

where the second line contains precisely the oscillator expressions (2.396). ref(2.396)

A similar situation holds for an arbitrary time-dependent frequency where the partition function is lab(2.227) est(2.268)

$$\begin{aligned} Z_{\Omega(\tau)} &= \oint \frac{\mathcal{D}a^*(\tau)\mathcal{D}a(\tau)}{\pi} \exp\left\{-\int_0^{\hbar\beta} d\tau\, \left[a^\dagger \partial_\tau a + \Omega(\tau) a^\dagger a\right]\right\} \\ &= \frac{k_B T}{\hbar} \left[\frac{\det{}'(-\partial_\tau^2)}{\det(-\partial_\tau^2 + \Omega^2(\tau))}\right]^{1/2} = \frac{1}{2\sinh(\hbar\omega\beta/2)} \left[\frac{\det(-\partial_\tau^2 + \omega^2)}{\det(-\partial_\tau^2 + \Omega^2(\tau))}\right]^{1/2}. \end{aligned} \tag{7.340}$$

While the oscillator partition function can be calculated right-away in the continuum limit after forming ratios of eigenvalues, the second-quantized path integral depends sensitively on the choice $a_n^\dagger a_{n-1}$ in the action (7.310). It is easy to verify that the alternative slicings $a_{n+1}^\dagger a_n$ and $a_n^\dagger a_n$ would have led to the partition functions $[e^{\beta\hbar\omega}-1]^{-1}$ and $[2\sinh(\hbar\omega\beta/2)]^{-1}$, respectively. The different time slicings produce obviously the same physics as the corresponding time-ordered Hamiltonian operators $\hat{H} = \hat{T}\hat{a}^\dagger(t)\hat{a}(t')$ in which t' approaches t once from the right, once from the left, and once symmetrically from both sides.

It is easy to decide which of these mathematically possible approaches is the physically correct one. Classical mechanics is invariant under canonical transformations. So is Schrödinger theory. Certainly we want path integrals have the same invariance. Since the classical actions (7.300) and (7.301) arise from oscillator actions by the canonical transformation (7.296), the associated partition functions must be the same. This fixes the time-slicing of the harmonic oscillator to the symmetric one with the partition function (7.339), and the general result (7.340).

Another argument in favor of this symmetric ordering of the harmonic oscillator was given in Subsection 2.15.4. We shall see in Section 10.6 that in order to ensure invariance of path integrals under coordinate transformations, which is guaranteed in Schrödinger theory, path integrals should be defined by dimensional regularization. In this framework, the symmetric result (7.340) emerges.

It must be pointed out, however, that the correctness of the symmetric ordering for the oscillator action not true for arbitrary actions with an ordering ambiguity, as will be discussed in detail in Subsection (10.3.1). In fact, there exists to my knowledge no general rule how to translate the procedure of dimensional regularization into an operator-ordering language.

It is also worth noting that the symmetric result (7.339) gives rise to an important and poorly understood physical problem in many-body theory. Since *each* harmonic oscillator in the world has a ground-state energy ω implied by the limiting form (7.307), *each* momentum state of *each* particle field in the world contributes an energy $\hbar\omega/2$ to the vacuum energy. If all these $\hbar\omega/2$ are summed up, they produce a divergence in the cosmological constant, thus eliminating the existence of our universe. Somehow, the infinities of the free oscillators must be canceled by short-range interactions, and it may well be that we shall never possess a theory how this precisely happens. The present quantum feld theories assume only interactions which are completely local. This is certainly a simplification, but it has the advantage that the effect of interactions can be calculated perturbatively order by order in the interaction strength. Moreover, if the local Lagrangian is suitably chosen, the infinities coming from the local interactions are such that our ignorance about their true short-distance behavior does not matter. The results depend only on the experimentally measured parameters, such as mass and coupling strength. Such local Lagrangians are called *renormalizable*. In a renormalizable theory, it is a fundamental rule that all infinities can be subtracted and absorbed in the initial parameters of the action to fit the experimentally observed parameters. The total

energy of all zero-point oscillations is one of these infinities which can be absorbed in the vaccum energy to fit the exerimetally observed cosmlogical constant.

Some people want to ignore this subtraction freedom and get a finite sum over zero-point energies right at the free-field level. The only way to achieve this is by imagining the universe to contains for each Bose field a Fermi field which, as we shall see in Eq. (7.427), contributes a negative vacuum energy to the ground state. Some people have therefore proposed that the world is described by a theory with a broken *supersymmetry*, where an underlying action contains fermions and bosons completely symmetrically. Unfortunately, all elementary particle theories proposed so far possess completely unphysical particle spectra.

There are, however, important mathematical properties of supersymmetry with interesting applications. One of them plays a crucial role in the context of gauge fixing in nonabelian gauge theories, where a residual supersymmetry (the so-called BRST-symmetry) is important for renormalization. The other occurs in the context of disorder and will be presented in Section 18.16.

7.8 Coherent States

As long as we calculate the partition function of the harmonic oscillator in the variables $a^*(\tau)$ and $a(\tau)$, the path integrals do not differ from those of the harmonic-oscillator (except for the possibly absent ground-state energy). The situation changes if we want to calculate the path integral (7.334) for specific initial and final values $a_a = a(\tau_a)$ and $a_b = a(\tau_b)$, implying also $a_a^* = a^*(\tau_a)$ and $a_b^* = a^*(\tau_b)$ by complex conjugation. In the definition of the canonical path integral in Section 2.1 we had to choose between measures (2.46) and (2.47), depending on which of the two completeness relations

$$\int dx\, |x\rangle\langle x| = 1, \qquad \int \frac{dp}{2\pi}\, |p\rangle\langle p| = 1 \tag{7.341}$$

we wanted to insert into the factorized operator version of the Boltzmann factor $e^{-\beta\hat{H}}$ into products of $e^{-\epsilon\hat{H}}$. The time-sliced path integral (7.309), on the other hand, runs over $a^*(\tau)$ and $a(\tau)$ corresponding to an apparent completeness relation

$$\int dx \int \frac{dp}{2\pi}\, |x\, p\rangle\langle x\, p| = 1. \tag{7.342}$$

This resolution of the identity is at first sight surprising, since in a quantum-mechanical system *either* x *or* p can be specified, but not both. Thus we expect (7.342) to be structurally different from the completeness relations in (7.341). In fact, (7.342) may be called an *overcompleteness relation*.

In order to understand this, we form coherent states [49] similar to those used earlier in Eq. (3A.5):

$$|z\rangle \equiv e^{z\hat{a}^\dagger - z^*\hat{a}}|0\rangle, \qquad \langle z| \equiv \langle 0|e^{-z\hat{a}^\dagger + z^*\hat{a}}. \tag{7.343}$$

The Baker-Campbell-Hausdorff formula (2.9) allows us to rewrite

$$e^{z\hat{a}^\dagger - z^*\hat{a}} = e^{z^* z[\hat{a}^\dagger,\hat{a}]/2} e^{z\hat{a}^\dagger} e^{-z^*\hat{a}} = e^{-z^* z/2} e^{z\hat{a}^\dagger} e^{-z^*\hat{a}}. \tag{7.344}$$

Since $\hat{a}$ annihilates the vacuum state, we may expand

$$|z\rangle = e^{-z^* z/2} e^{z\hat{a}^\dagger}|0\rangle = e^{-z^* z/2} \sum_{n=0}^{\infty} \frac{z^n}{\sqrt{n!}} |n\rangle. \tag{7.345}$$

The states $|n\rangle$ and $\langle n|$ can be recovered from the coherent states $|z\rangle$ and $\langle z|$ by the operations:

$$|n\rangle = \left[|z\rangle e^{z^* z/2} \overleftarrow{\partial}_z^n\right]_{z=0} \frac{1}{\sqrt{n!}}, \qquad \langle n| = \frac{1}{\sqrt{n!}} \left[\partial_{z^*}^n e^{z^* z/2} \langle z|\right]_{z=0}. \tag{7.346}$$

For an operator $\hat{\mathcal{O}}$, the trace can be calculated from the integral over the diagonal elements

$$\mathrm{tr}\,\hat{\mathcal{O}} = \int \frac{dz^* dz}{\pi} \langle z|\hat{\mathcal{O}}|z\rangle = \int \frac{dz^* dz}{\pi} e^{-z^* z} \sum_{m,n=0}^{\infty} \frac{z^{*m}}{\sqrt{m!}} \frac{z^n}{\sqrt{n!}} \langle m|\hat{\mathcal{O}}|n\rangle. \tag{7.347}$$

Setting $z = re^{i\phi}$, this becomes

$$\mathrm{tr}\,\hat{\mathcal{O}} = \int dr^2 \left[\frac{d\phi}{2\pi} e^{-i(m-n)\phi}\right] e^{-r^2} \sum_{m,n=0}^{\infty} \left(r^2\right)^{(m+n)/2} \frac{1}{\sqrt{m!}} \frac{1}{\sqrt{n!}} \langle m|\hat{\mathcal{O}}|n\rangle. \tag{7.348}$$

The integral over ϕ gives a Kronecker symbol $\delta_{m,n}$ and the integral over r^2 cancels the factorials, so that we remain with the diagonal sum

$$\mathrm{tr}\,\hat{\mathcal{O}} = \int dr^2\, e^{-r^2} \sum_{n=0}^{\infty} \left(r^2\right)^n \frac{1}{n!} \langle n|\hat{\mathcal{O}}|n\rangle = \sum_{n=0}^{\infty} \langle n|\hat{\mathcal{O}}|n\rangle. \tag{7.349}$$

The sum on the right-hand side of (7.345) allows us to calculate immediately the scalar product of two such states:

$$\langle z_1|z_2\rangle = e^{-z_1^* z_1/2 - z_2^* z_2/2 + z_1^* z_2}. \tag{7.350}$$

The coherent states (7.343) with $z = (x + ip)/\sqrt{2}$ have precisely the property (7.342), i.e., we may identify:

$$|x\, p\rangle \equiv |z\rangle, \qquad \text{where} \quad z \equiv (x + ip)/\sqrt{2}. \tag{7.351}$$

Then (7.345) can be written as

$$|x\, p\rangle = e^{-(x^2+p^2)/4} \sum_{n=0}^{\infty} \frac{(x + ip)^n}{\sqrt{2^n n!}} |0\rangle, \tag{7.352}$$

and

$$\int dx\,\frac{dp}{2\pi}\,|x\,p\rangle\langle x\,p| = \int dx\frac{dp}{2\pi}\,|x\,p\rangle\langle x\,p|e^{-(x^2+p^2)/2}\sum_{m,n=0}^{\infty}\frac{(x-ip)^m}{\sqrt{2^m m!}}\frac{(x+ip)^n}{\sqrt{2^n n!}}|m\rangle\langle n|. \tag{7.353}$$

Setting $(x-ip)/\sqrt{2}\equiv re^{i\phi}$, this can be rewritten as

$$\int dx\,\frac{dp}{2\pi}\,|x\,p\rangle\langle x\,p| = \int dr^2\left[\frac{d\phi}{2\pi}e^{-i(m-n)\phi}\right]e^{-r^2}\sum_{m,n=0}^{\infty}\left(r^2\right)^{(m+n)/2}\frac{1}{\sqrt{m!}}\frac{1}{\sqrt{n!}}|m\rangle\langle n|. \tag{7.354}$$

The angular integration enforces $m=n$, and the integrals over r^2 cancel the factorials, as in (7.348), thus proving the resolution of the identity (7.342), which can also be written as

$$\int\frac{dz^*dz}{\pi}\,|z\rangle\langle z| = 1. \tag{7.355}$$

This resolution of the identity can now be inserted into a product decomposition of a Boltzmann operator

$$\langle z_b|e^{-\beta\hat{H}_\omega}|z_a\rangle = \langle z_b|e^{-\beta\hat{H}_\omega/(N+1)}e^{-\beta\hat{H}_\omega/(N+1)}\cdots e^{-\beta\hat{H}_\omega/(N+1)}|z_a\rangle, \tag{7.356}$$

to arrive at a sliced path integral [compare (2.2)–(2.4)]

$$\langle z_b|e^{-\beta\hat{H}_\omega}|z_a\rangle = \prod_{n=1}^{N}\left[\int\frac{dz_n^*dz_n}{\pi}\right]\prod_{n=1}^{N+1}\langle z_n|e^{-\epsilon\hat{H}_\omega}|z_{n-1}\rangle,\ z_0 = z_a,\ z_{N+1} = z_b,\ \epsilon\equiv\beta/(N+1). \tag{7.357}$$

We now calculate the matrix elements $\langle z_n|e^{-\epsilon\hat{H}_\omega}|z_{n-1}\rangle$ and find

$$\langle z_n|e^{-\epsilon\hat{H}_\omega}|z_{n-1}\rangle \approx \langle z_n|1-\epsilon\hat{H}_\omega|z_{n-1}\rangle = \langle z_n|z_{n-1}\rangle - \epsilon\langle z_n|\hat{H}_\omega|z_{n-1}\rangle. \tag{7.358}$$

Using (7.350) we find

$$\langle z_n|z_{n-1}\rangle = e^{-z_n^*z_n/2 - z_{n-1}^*z_{n-1}/2 + z_n^*z_{n-1}} = e^{-(1/2)\left[z_n^*(z_n-z_{n-1}) - \left(z_n^*-z_{n-1}^*\right)z_{n-1}\right]}. \tag{7.359}$$

The matrix elements of the operator Hamiltonian (7.298) is easily found. The coherent states (7.345) are eigenstates of the annihilation operator $\hat{a}$ with eigenvalue z:

$$\hat{a}|z\rangle = e^{-z^*z/2}\sum_{n=0}^{\infty}\frac{z^n}{\sqrt{n!}}\hat{a}|n\rangle = e^{-z^*z/2}\sum_{n=1}^{\infty}\frac{z^n}{\sqrt{(n-1)!}}|n-1\rangle = z|z\rangle. \tag{7.360}$$

Thus we find immediately

$$\langle z_n|\hat{H}_\omega|z_{n-1}\rangle = \hbar\omega\langle z_n|(\hat{a}^\dagger\hat{a}+\hat{a}\,\hat{a}^\dagger)|z_{n-1}\rangle = \hbar\omega\left(z_n^\dagger z_{n-1}+\frac{1}{2}\right). \tag{7.361}$$

Inserting this together with (7.359) into (7.358), we obtain for small ϵ the path integral

$$\langle z_b|e^{-\beta\hat{H}_\omega}|z_a\rangle = \prod_{n=1}^{N}\left[\int\frac{dz_n^*dz_n}{\pi}\right]e^{-\mathcal{A}_\omega^N[z^*,z]/\hbar}, \tag{7.362}$$

with the time-sliced action

$$\mathcal{A}^N_\omega[z^*,z] = \hbar\epsilon \sum_{n=1}^{N+1} \left\{ \frac{1}{2}\left[z_n^* \overline{\nabla} z_n - (\overline{\nabla} z_n^*) z_{n-1} \right] + \omega \left(z_n^* z_{n-1} + \frac{1}{2} \right) \right\}. \tag{7.363}$$

The gradient terms can be regrouped using formula (2.35), and rewriting its right-hand side as $p_{N+1}x_{N+1} - p_0 x_0 + \sum_{n=1}^{N+1}(p_n - p_{n-1})x_{n-1}$. This leads to

$$\mathcal{A}^N_\omega[z^*,z] = \frac{\hbar}{2}(-z_b^* z_b + z_a^* z_a) + \hbar\epsilon \sum_{n=1}^{N+1} \left\{ z_n^* \overline{\nabla} z_n + \omega \left(z_n^* z_{n-1} + \frac{1}{2} \right) \right\}. \tag{7.364}$$

Except for the surface terms which disappear for periodic paths, this action agrees with the time-sliced Euclidean action (7.310), except for a trivial change of variables $a \to z$.

As a brief check of formula (7.362) we set $N = 0$ and find

$$\mathcal{A}^0_\omega[z^*,z] = \frac{\hbar}{2}(-z_b^* z_b + z_a^* z_a) + \hbar z_b^* (z_b - z_a) + \omega \left(z_b^* z_a + \frac{1}{2} \right), \tag{7.365}$$

and the short-time amplitude (7.364) becomes

$$\langle z_b | e^{-\epsilon \hat{H}_\omega} | z_a \rangle = \exp\left[-\frac{1}{2}(z_b^* z_b + z_a^* z_a) + z_b^* z_a - \epsilon\hbar\omega \left(z_b^* z_a + \frac{1}{2} \right) \right]. \tag{7.366}$$

Applying the recovery operations (7.346) we find

$$\langle 0 | e^{-\epsilon \hat{H}_\omega} | 0 \rangle = \left[e^{(z_b^* z_b + z_a^* z_a)/2} \langle z_b | e^{-\epsilon \hat{H}_\omega} | z_a \rangle \right]_{z^*=0, z=0} = e^{-\epsilon\hbar\omega/2}, \tag{7.367}$$

$$\langle 1 | e^{-\epsilon \hat{H}_\omega} | 1 \rangle = \left\{ \partial_z \left[e^{(z_b^* z_b + z_a^* z_a)/2} \langle z_b | e^{-\epsilon \hat{H}_\omega} | z_a \rangle \right] \overleftarrow{\partial}^*_z \right\}_{z^*=0, z=0} = e^{-\epsilon 3\hbar\omega/2}, \tag{7.368}$$

$$\langle 0 | e^{-\epsilon \hat{H}_\omega} | 1 \rangle = \langle 1 | e^{-\epsilon \hat{H}_\omega} | 0 \rangle = 0. \tag{7.369}$$

Thus we have shown that for fixed ends, the path integral gives the amplitude for an initial coherent state $|z_a\rangle$ to go over to a final coherent state $|z_b\rangle$. The partition function (7.337) is obtained from this amplitude by forming the diagonal integral

$$Z_\omega = \int \frac{dz^*\, dz}{\pi} \langle z | e^{-\beta \hat{H}_\omega} | z \rangle. \tag{7.370}$$

7.9 Second-Quantized Fermi Fields

The existence of the periodic system of elements is based on the fact that electrons can occupy each orbital state only once (counting spin-up and -down states separately). Particles with this statistics are called *fermions*. In the above Hilbert space in which n-particle states at a point $\mathbf{x}$ are represented by oscillator states $|n, \mathbf{x}\rangle$, this implies that the particle occupation number n can take only the values

$$\begin{aligned} n &= 0 \quad \text{(no electron)}, \\ n &= 1 \quad \text{(one electron)}. \end{aligned}$$

It is possible to construct such a restricted many-particle Hilbert space explicitly by subjecting the quantized fields $\hat{\psi}^\dagger(\mathbf{x})$, $\hat{\psi}(\mathbf{x})$ or their Fourier components $\hat{a}^\dagger_{\mathbf{p}}$, $\hat{a}_{\mathbf{p}}$ to *anticommutation relations*, instead of the commutation relations (7.282), i.e., by postulating

$$\begin{aligned} [\hat{\psi}(\mathbf{x},t),\hat{\psi}^\dagger(\mathbf{x}',t)]_+ &= \delta_{\mathbf{x}\mathbf{x}'}, \\ [\hat{\psi}^\dagger(\mathbf{x},t),\hat{\psi}^\dagger(\mathbf{x}',t)]_+ &= 0, \\ [\hat{\psi}(\mathbf{x},t),\hat{\psi}(\mathbf{x}',t)]_+ &= 0, \end{aligned} \tag{7.371}$$

or for the Fourier components

$$\begin{aligned} [\hat{a}_{\mathbf{p}}(t),\hat{a}^\dagger_{\mathbf{p}'}(t)]_+ &= \delta_{\mathbf{p}\mathbf{p}'}, \\ [\hat{a}^\dagger_{\mathbf{p}}(t),\hat{a}^\dagger_{\mathbf{p}'}(t)]_+ &= 0, \\ [\hat{a}_{\mathbf{p}}(t),\hat{a}_{\mathbf{p}'}(t)]_+ &= 0. \end{aligned} \tag{7.372}$$

Here $[\hat{A},\hat{B}]_+$ denotes the anticommutator of the operators $\hat{A}$ and $\hat{B}$

$$[\hat{A},\hat{B}]_+ \equiv \hat{A}\hat{B}+\hat{B}\hat{A}. \tag{7.373}$$

Apart from the anticommutation relations, the second-quantized description of Fermi fields is completely analogous to that of Bose fields in Section 7.6.

7.10 Fluctuating Fermi Fields

The question arises as to whether it is possible to find a path integral formulation which replaces the anticommuting operator structure. The answer is affirmative, but at the expense of a somewhat unconventional algebraic structure. The fluctuating paths can no longer be taken as c-numbers. Instead, they must be described by anticommuting variables.

7.10.1 Grassmann Variables

Mathematically, such objects are known under the name of *Grassmann variables*. They are defined by the algebraic property

$$\theta_1\theta_2 = -\theta_2\theta_1, \tag{7.374}$$

which makes them *nilpotent*:

$$\theta^2 = 0. \tag{7.375}$$

These variables have the curious consequence that an arbitrary function of them possesses only two Taylor coefficients, F_0 and F_1,

$$F(\theta) = F_0 + F_1\theta. \tag{7.376}$$

They are obtained from $F(\theta)$ as follows:

$$\begin{aligned} F_0 &= F(0), \\ F_1 &= F' \equiv \frac{\partial}{\partial\theta} F. \end{aligned} \tag{7.377}$$

The existence of only two parameters in $F(\theta)$ is the reason why such functions naturally collect amplitudes of two local fermion states, F_0 for zero occupation, F_1 for a single occupation.

It is now possible to define integrals over functions of these variables in such a way that the previous path integral formalism remains applicable without a change in the notation, leading to the same results as the second-quantized theory with anticommutators. Recall that for ordinary real functions, integrals are linear functionals. We postulate this property also for integrals with Grassmann variables. Since an arbitrary function of a Grassmann variable $F(\theta)$ is at most linear in θ, its integral is completely determined by specifying only the two fundamental integrals $\int d\theta$ and $\int d\theta\, \theta$. The values which render the correct physics with a conventional path integral notation are

$$\int \frac{d\theta}{\sqrt{2\pi}} = 0, \tag{7.378}$$

$$\int \frac{d\theta}{\sqrt{2\pi}}\, \theta = 1. \tag{7.379}$$

Using the linearity property, an arbitrary function $F(\theta)$ is found to have the integral

$$\int \frac{d\theta}{\sqrt{2\pi}} F(\theta) = F_1 = F'. \tag{7.380}$$

Thus, integration of $F(\theta)$ coincides with differentiation. This must be remembered whenever Grassmann integration variables are to be changed: The integral is transformed with the *inverse* of the usual Jacobian. The obvious equation

$$\int \frac{d\theta}{\sqrt{2\pi}} F(c\cdot\theta) = c\cdot F' = c\cdot \int \frac{d\theta'}{\sqrt{2\pi}} F(\theta') \tag{7.381}$$

for any complex number c implies the relation

$$\int \frac{d\theta}{\sqrt{2\pi}} F(\theta'(\theta)) = \int \frac{d\theta'}{\sqrt{2\pi}} \left[\frac{d\theta}{d\theta'}\right]^{-1} F(\theta'). \tag{7.382}$$

For ordinary integration variables, the Jacobian $d\theta/d\theta'$ would appear without the power -1.

When integrating over a product of two functions $F(\theta)$ and $G(\theta)$, the rule of integration by parts holds with the opposite sign with respect to that for ordinary integrals:

$$\int \frac{d\theta}{\sqrt{2\pi}} G(\theta) \frac{\partial}{\partial\theta} F(\theta) = \int \frac{d\theta}{\sqrt{2\pi}} \left[\frac{\partial}{\partial\theta} G(\theta)\right] F(\theta). \tag{7.383}$$

There exists a simple generalization of the Dirac δ-function to Grassmann variables. We shall define this function by the integral identity

$$\int \frac{d\theta'}{\sqrt{2\pi}} \delta(\theta - \theta') F(\theta') \equiv F(\theta). \tag{7.384}$$

Inserting the general form (7.376) for $F(\theta)$, we see that the function

$$\delta(\theta - \theta') = \theta' - \theta \tag{7.385}$$

satisfies (7.384). Note that the δ-function is a Grassmann variable and, in contrast to Dirac's δ-function, antisymmetric. Its derivative has the property

$$\delta'(\theta - \theta') \equiv \partial_\theta \delta(\theta - \theta') = -1. \tag{7.386}$$

It is interesting to see that δ' shares with Dirac's δ' the following property:

$$\int \frac{d\theta'}{\sqrt{2\pi}} \delta'(\theta - \theta') F(\theta') = -F'(\theta), \tag{7.387}$$

with the opposite sign of the Dirac case. This follows from the above rule of partial integration, or simpler, by inserting (7.386) and the explicit decomposition (7.376) for $F(\theta)$.

The integration may be extended to complex Grassmann variables which are combinations of two real Grassmann variables $\theta_1,\ \theta_2$:

$$a^* = \frac{1}{\sqrt{2}}(\theta_1 - i\theta_2), \qquad a = \frac{1}{\sqrt{2}}(\theta_1 + i\theta_2). \tag{7.388}$$

The measure of integration is defined by

$$\int \frac{da^* da}{\pi} \equiv \int \frac{d\theta_2 d\theta_1}{2\pi i} \equiv -\int \frac{da\, da^*}{\pi}. \tag{7.389}$$

Using (7.378) and (7.379) we see that the integration rules for complex Grassmann variables are

$$\int \frac{da^*\, da}{\pi} = 0, \ \int \frac{da^*\, da}{\pi} a = 0, \ \int \frac{da^*\, da}{\pi} a^* = 0, \tag{7.390}$$

$$\int \frac{da^*\, da}{\pi}\, a^* a = \int \frac{d\theta_2\, d\theta_1}{2\pi i}\, i\theta_1\theta_2 = 1. \tag{7.391}$$

Every function of a^*a has at most two terms:

$$F(a^*a) = F_0 + F_1\ a^*a. \tag{7.392}$$

In particular, the exponential $\exp\{-a^*Aa\}$ with a complex number A has the Taylor series expansion

$$e^{-a^*Aa} = 1 - a^*Aa. \tag{7.393}$$

Thus we find the following formula for the Gaussian integral:

$$\int \frac{da^*\,da}{\pi} e^{-a^* A a} = A. \tag{7.394}$$

The integration rule (7.390) can be used directly to calculate the Grassmann version of the product of integrals (7.315). For a matrix A which can be diagonalized by a unitary transformation, we obtain directly

$$Z^{\rm f} = \prod_n \left[\int \frac{da_n^* da_n}{\pi} \right] e^{i\Sigma_{n,n'} a_n^* A_{n,n'} a_{n'}} = \det A. \tag{7.395}$$

Remarkably, the fermion integration yields precisely the inverse of the boson result (7.315).

7.10.2 Fermionic Functional Determinant

Consider now the time-sliced path integral of the partition function written like (7.309) but with fermionic anticommuting variables. In order to find the same results as in operator quantum mechanics it is necessary to require the anticommuting Grassmann fields $a(\tau), a^*(\tau)$ to be *antiperiodic* on the interval $\tau \in (0, \hbar\beta)$, i.e.,

$$a(\hbar\beta) = -a(0), \tag{7.396}$$

or in the sliced form

$$a_{N+1} = -a_0. \tag{7.397}$$

Then the exponent of (7.395) has the same form as in (7.315), except that the matrix A of Eq. (7.318) is replaced by

$$A^{\rm f} = \epsilon(1-\epsilon\omega)\overline{\nabla}_\tau + \epsilon\omega = \begin{pmatrix} 1 & 0 & 0 & \dots & 0 & 1-\epsilon\omega \\ -1+\epsilon\omega & 1 & 0 & \dots & 0 & 0 \\ 0 & -1+\epsilon\omega & 1 & \dots & 0 & 0 \\ 0 & 0 & -1+\epsilon\omega & \dots & 0 & 0 \\ \vdots & & & & & \vdots \\ 0 & 0 & 0 & \dots & -1+\epsilon\omega & 1 \end{pmatrix}, \tag{7.398}$$

where the rows and columns are counted from 1 to $N+1$. The element in the upper right corner is positive and thus has the opposite sign of the bosonic matrix in (7.318). This makes an important difference: While for $\omega = 0$ the bosonic matrix gave

$$\det\left(-\epsilon\overline{\nabla}\right)_{\omega=0} = 0, \tag{7.399}$$

due to translational invariance in τ, we now have

$$\det\left(-\epsilon\overline{\nabla}\right)_{\omega=0} = 2. \tag{7.400}$$

The determinant of the fermionic matrix (7.398) can be calculated by a repeated expansion along the first row [recall the calculations of the determinants (2.204) and (2.418)] and is found to be

$$\det_{N+1} A = 1 + (1 - \epsilon\omega)^{N+1}. \tag{7.401}$$

Hence we obtain the time-sliced fermion partition function

$$Z_\omega^{\mathrm{f},N} = \det_{N+1}[\epsilon(1 - \epsilon\omega)\overline{\nabla} + \epsilon\omega] = 1 + (1 - \epsilon\omega)^{N+1}. \tag{7.402}$$

As in the boson case, we introduce the auxiliary frequency

$$\bar{\omega}_{\mathrm{e}} \equiv -\frac{1}{\epsilon}\log(1 - \epsilon\omega) \tag{7.403}$$

and write $Z_\omega^{\mathrm{f},N}$ in the form

$$Z_\omega^N = 1 + e^{-\beta\hbar\bar{\omega}_{\mathrm{e}}}. \tag{7.404}$$

This partition function displays the typical property of Fermi particles. There are only two terms, one for the zero-particle and one for the one-particle state at a point. Their energies are 0 and $\hbar\bar{\omega}_{\mathrm{e}}$, corresponding to the Hamiltonian operator

$$\hat{H}_\omega = \hbar\bar{\omega}_e\hat{N} = \hbar\bar{\omega}_e a^\dagger a. \tag{7.405}$$

In the continuum limit $\epsilon \to 0$, where $\bar{\omega}_{\mathrm{e}} \to \omega$, the partition function $Z\omega^N$ goes over into

$$Z_\omega = 1 + e^{-\beta\hbar\omega}. \tag{7.406}$$

Let us generalize also the fermion partition function to a system with a time-dependent frequency $\Omega(\tau)$, where it reads

$$Z_\omega^{\mathrm{f},N} = \prod_{n=0}^{N}\left[\int \frac{da_n^* da_n}{\pi}\right]\exp\left(-\frac{1}{\hbar}\mathcal{A}_\omega^N\right), \tag{7.407}$$

with the sliced action

$$\mathcal{A}_\omega^N = \hbar\sum_{n=1}^{N}\left[a_n^*(a_n - a_{n-1}) + \epsilon\Omega_n a_n^* a_{n-1}\right], \tag{7.408}$$

or, expressed in terms of the difference operator $\overline{\nabla}$,

$$\mathcal{A}_\omega^N = \hbar\epsilon\sum_{n=1}^{N} a_n^*\left[(1 - \epsilon\Omega_n)\overline{\nabla} + \Omega_n\right]a_n. \tag{7.409}$$

The result is

$$Z_\omega^{\mathrm{f},N} = \det_{N+1}[\epsilon(1 - \epsilon\Omega)\overline{\nabla} + \epsilon\omega] = 1 - \prod_{n=0}^{N}(1 - \epsilon\Omega_n). \tag{7.410}$$

As in the bosonic case, it is useful to introduce the auxiliary frequency

$$\bar{\Omega}_{\rm e} \equiv -\frac{1}{(N+1)\epsilon}\sum_{n=0}^{N}\log(1-\epsilon\Omega_n), \tag{7.411}$$

and write $Z_\omega^{{\rm f},N}$ in the form

$$Z_\omega^{{\rm f},N} = 1 + e^{-\beta\hbar\bar{\Omega}_{\rm e}}. \tag{7.412}$$

If we attempt to write down a path integral formula for fermions directly in the continuum limit, we meet the same phenomenon as in the bosonic case. The difference operator (7.318) turns into the corresponding differential operator

$$(1-\epsilon\omega)\overline{\nabla}+\omega \to \partial_\tau+\omega, \tag{7.413}$$

which now acts upon periodic complex functions $e^{-i\omega_m^{\rm f}\tau}$ with the *odd* Matsubara frequencies

$$\omega_m^{\rm f} = \pi(2m+1)k_BT/\hbar, \quad m=0,\pm1,\pm2,\dots\ . \tag{7.414}$$

The continuum partition function can be written as a path integral

$$\begin{aligned} Z_\omega^{\rm f} &= \oint\frac{\mathcal{D}a^*\mathcal{D}a}{\pi}\exp\left[-\int_0^{\hbar\beta}d\tau\,(a^*\partial_\tau a+\omega a^*a)\right] \\ &= \mathcal{N}_\omega{\rm det}\,(\partial_\tau+\omega), \end{aligned} \tag{7.415}$$

with some normalization constant $\mathcal{N}_\omega$ determined by comparison with the time-sliced result. To calculate $Z_\omega^{\rm f}$, we take the eigenvalues of the operator $\partial_\tau+\omega$, which are now $-i\omega_m^{\rm f}+\omega$, and evaluate the product of ratios

$$\prod_{m=-\infty}^{\infty}\frac{-i\omega_m^{\rm f}+\omega}{-i\omega_m^{\rm f}} = \cosh(\hbar\omega\beta/2). \tag{7.416}$$

This corresponds to the ratio of functional determinants

$$\frac{{\rm det}\,(\partial_\tau+\omega)}{{\rm det}\,(\partial_\tau)} = \cosh(\hbar\omega\beta/2). \tag{7.417}$$

In contrast to the boson case (7.336), no prime is necessary on the determinant of ∂_τ since there is no zero frequency in the product of eigenvalues (7.416). Setting $N_\omega = 1/2{\rm det}\,(\partial_\tau)$, the ratio formula produces the correct partition function

$$Z_\omega^{\rm f} = 2\cosh(\hbar\omega\beta/2). \tag{7.418}$$

Thus we may write the free-fermion path integral in the continuum form explicitly as follows:

$$\begin{aligned} Z_\omega^{\rm f} &= \oint\frac{\mathcal{D}a^*\mathcal{D}a}{\pi}\exp\left[-\int_0^{\hbar\beta}d\tau\,(a^*\partial_\tau a+\omega a^*a)\right] = 2\frac{{\rm det}\,(\partial_\tau+\omega)}{{\rm det}\,(\partial_\tau)} \\ &= 2\cosh(\hbar\omega\beta/2). \end{aligned} \tag{7.419}$$

The determinant of the operator $\partial_\tau + \omega$ can again be replaced by

$$\det(\partial_\tau + \omega) = \det(-\partial_\tau + \omega) = \sqrt{\det(-\partial_\tau^2 + \omega^2)}. \tag{7.420}$$

As in the bosonic case, this Fermi analog of the harmonic oscillator partition function agrees with the results of dimensional regularization in Subsection 2.15.4 which will ensure invariance of path integrals under a change of variables, as will be seen in Section 10.6. The proper fermionic time-sliced partition function corresponding to the dimensional regularization in Subsection 2.15.4 is obtained from a fermionic version of the time-sliced oscillator partition function by evaluating

$$\begin{aligned} Z_\omega^{\mathrm{f},N} &= \left[\det{}_{N+1}(-\epsilon^2\nabla\bar{\nabla} + \epsilon^2\omega^2)\right]^{1/2} \quad = \prod_{m=0}^{N}\left[\epsilon^2\Omega_m^{\mathrm{f}}\bar{\Omega}_m^{\mathrm{f}} + \epsilon^2\omega^2\right]^{1/2} \\ &\equiv \prod_{m=0}^{N}\left[2(1-\cos\omega_m^{\mathrm{f}}\epsilon) + \epsilon^2\omega^2\right]^{1/2} = \prod_{m=0}^{N}\left[2\sin^2\frac{\epsilon\omega_m^{\mathrm{f}}}{2} + \epsilon^2\omega^2\right]^{1/2}, \end{aligned} \tag{7.421}$$

with a product over the odd Matsubara frequencies ω_m^{f}. The result is

$$Z_\omega^{\mathrm{f},N} = 2\cosh(\hbar\tilde{\omega}_{\mathrm{e}}\beta), \tag{7.422}$$

with $\tilde{\omega}_{\mathrm{e}}$ given by

$$\sinh(\tilde{\omega}_{\mathrm{e}}/2) = \epsilon\omega/2. \tag{7.423}$$

This follows from the Fermi analogs of the product formulas (2.400), (2.402):[7] ref(2.400) lab(2.122b) est(2.271) ref(2.402) lab(2.122bc) est(2.273)

$$\prod_{m=0}^{N/2-1}\left(1 - \frac{\sin^2 x}{\sin^2\frac{(2m+1)\pi}{2(N+1)}}\right) = \frac{\cos(N+1)x}{\cos x}, \quad N = \text{even}, \tag{7.424}$$

$$\prod_{m=0}^{(N-1)/2}\left(1 - \frac{\sin^2 x}{\sin^2\frac{(2m+1)\pi}{2(N+1)}}\right) = \cos(N+1)x, \quad N = \text{odd}. \tag{7.425}$$

For odd N, where all frequencies occur twice, we find from (7.425) that

$$\prod_{m=0}^{N}\left(1 - \frac{\sin^2 x}{\sin^2\frac{(2m+1)\pi}{2(N+1)}}\right)^{1/2} = \cos(N+1)x, \tag{7.426}$$

and thus, with (7.423), directly (7.422). For even N, where the frequency with $m = N/2$ occurs only once, formula (7.424) gives once more the same answer, thus proving (7.426) for even *and* odd N.

There exists no real fermionic oscillator action since x^2 and $\dot{x}^2$ would vanish identically for fermions, due to the nilpotency (7.375) of Grassmann variables. The product of eigenvalues in Eq. (7.421) emerges naturally from a path integral in which the action (7.408) is replaced by a symmetrically sliced action.

[7] I.S. Gradshteyn and I.M. Ryzhik, op. cit., Formulas 1.391.2, 1.391.4.

An important property of the partition function (7.418) of (7.422) is that the ground-state energy is *negative*:

$$E^{(0)} = -\frac{\hbar\omega}{2}. \tag{7.427}$$

As discussed at the end of Section 7.7, such a fermionic vacuum energy is required for each bosonic vacuum energy to avoid an infinite vacuum energy of the world, which would produce an infinite cosmological constant, whose experimentally observed value is extremely small.

7.10.3 Coherent States for Fermions

For the bosonic path integral (7.304) we have studied in Section 7.8, the case that the endpoint values $a_a = a(\tau_a)$ and $a_b = a(\tau_b)$ of the paths $a(\tau)$ are held fixed. The result was found to be the matrix element of the Boltzmann operator $e^{-\beta\hat{H}_\omega}$ between coherent states $|a\rangle = e^{-a^*a/2}e^{a\hat{a}^\dagger}|0\rangle$ [recall (7.345)]. There exists a similar interpretation for the fermion path integral (7.415) if we hold the endpoint values $a_a = a(\tau_a)$ and $a_b = a(\tau_b)$ of the Grassmann paths fixed. By analogy with Eq. (7.345) we introduce coherent states [50]

$$|\zeta\rangle \equiv e^{-\zeta^*\zeta/2}e^{a^\dagger\zeta}|0\rangle = e^{-\zeta^*\zeta/2}\Big(|0\rangle - \zeta|1\rangle\Big). \tag{7.428}$$

The corresponding adjoint states read

$$\langle\zeta| \equiv e^{-\zeta^*\zeta/2}\langle 0|e^{\zeta^* a} = e^{-\zeta^*\zeta/2}\Big(\langle 0| + \zeta^*\langle 1|\Big). \tag{7.429}$$

Note that for consistency of the formalism, the Grassmann elements ζ anticommute with the fermionic operators. The states $|0\rangle$ and $\langle 1|$ and their conjugates $\langle 0|$ and $\langle 1|$ can be recovered from the coherent states $|\zeta\rangle$ and $\langle\zeta|$ by the operations:

$$|n\rangle = \Big[|\zeta\rangle e^{\zeta^*\zeta/2}\overleftarrow{\partial}_\zeta^n\Big]_{\zeta=0}\frac{1}{\sqrt{n!}}, \qquad \langle n| = \frac{1}{\sqrt{n!}}\Big[\partial_{\zeta^*}^n e^{\zeta^*\zeta/2}\langle\zeta|\Big]_{\zeta=0}. \tag{7.430}$$

These formula simplify here to

$$|0\rangle = \Big[|\zeta\rangle e^{\zeta^*\zeta/2}\Big]_{\zeta=0}, \qquad \langle 0| = \Big[e^{\zeta^*\zeta/2}\langle\zeta|\Big]_{\zeta=0}, \tag{7.431}$$

$$|1\rangle = \Big[|\zeta\rangle e^{\zeta^*\zeta/2}\overleftarrow{\partial}_\zeta\Big]_{\zeta=0}, \qquad \langle 1| = \Big[\partial_{\zeta^*}e^{\zeta^*\zeta/2}\langle\zeta|\Big]_{\zeta=0}. \tag{7.432}$$

For an operator $\hat{\mathcal{O}}$, the trace can be calculated from the integral over the *antidiagonal* elements

$$\mathrm{tr}\,\hat{\mathcal{O}} = \int\frac{d\zeta^*d\zeta}{\pi}\,\langle -\zeta|\hat{\mathcal{O}}|\zeta\rangle = \int\frac{d\zeta^*d\zeta}{\pi}\,e^{-\zeta^*\zeta}\Big(\langle 0| - \zeta^*\langle 1|\Big)\hat{\mathcal{O}}\Big(|0\rangle - \zeta|1\rangle\Big). \tag{7.433}$$

Using the integration rules (7.390) and (7.391), this becomes

$$\mathrm{tr}\,\hat{\mathcal{O}} = \langle 0|\hat{\mathcal{O}}|0\rangle + \langle 1|\hat{\mathcal{O}}|1\rangle. \tag{7.434}$$

The states $|\zeta\rangle$ form an overcomplete set in the one-fermion Hilbert space. The scalar products are [compare (7.350)]:

$$\begin{aligned}\langle\zeta_1|\zeta_2\rangle &= e^{-\zeta_1^*\zeta_1/2-\zeta_2^*\zeta_2/2+\zeta_1^*\zeta_2} \\ &= e^{-\zeta_1^*(\zeta_1-\zeta_2)/2+(\zeta_1^*-\zeta_2^*)\zeta_2/2}.\end{aligned} \tag{7.435}$$

The resolution of the identity (7.355) is now found as follows [recall (7.390)]:

$$\begin{aligned}\int \frac{d\zeta^* d\zeta}{\pi}\,|\zeta\rangle\langle\zeta| &= \int \frac{d\zeta^* d\zeta}{\pi} e^{-\zeta^*\zeta}\Big[|0\rangle\langle 0| - \zeta|1\rangle\langle 0| + \zeta^*|0\rangle\langle 1|\Big] \\ &= \int \frac{d\zeta^* d\zeta}{\pi}\Big[|0\rangle\langle 0| + |1\rangle\langle 0|\zeta + \zeta^*|0\rangle\langle 1| + \zeta\zeta^*\Big(|0\rangle\langle 0| + |1\rangle\langle 0|\Big)\Big] = 1.\end{aligned} \tag{7.436}$$

We now insert this resolution of the identity into the product of Boltzmann factors

$$\langle\zeta_b|e^{-\beta\hat{H}_\omega}|\zeta_a\rangle = \langle\zeta_b|e^{-\epsilon\hat{H}_\omega}e^{-\epsilon\hat{H}_\omega}\cdots e^{-\epsilon\hat{H}_\omega}|\zeta_a\rangle \tag{7.437}$$

where $\epsilon \equiv \beta/(N+1)$, and obtain by analogy with (7.362) the time-sliced path integral

$$\langle z_b|e^{-\beta\hat{H}_\omega}|z_a\rangle = \prod_{n=1}^{N}\left[\int \frac{dz_n^* dz_n}{\pi}\right] e^{-\mathcal{A}_{\mathrm{e}}[z^*,z]/\hbar}, \tag{7.438}$$

with the a time-sliced action similar to the bosonic one in (7.364):

$$\mathcal{A}_\omega^N[\zeta^*,\zeta] = \frac{\hbar}{2}(-\zeta_b^*\zeta_b + \zeta_a^*\zeta_a) + \hbar\epsilon\sum_{n=1}^{N+1}\left\{\zeta_n^*\overline{\nabla}\zeta_n + \omega\left(\zeta_n^*\zeta_{n-1} + \frac{1}{2}\right)\right\}. \tag{7.439}$$

Except for the surface term which disappears for antiperiodic paths, this agrees with the time-sliced Euclidean action (7.310), except for a trivial change of variables $a \to \zeta$.

We have shown that as in the Bose case the path integral with fixed ends gives the amplitude for an initial coherent state $|\zeta_a\rangle$ to go over to a final coherent state $|\zeta_b\rangle$. The fermion partition function (7.419) is obtained from this amplitude by forming the trace of the operator $e^{-\beta\hat{H}_\omega}$, which by formula (7.434) is given by the integral over the *antidiagonal* matrix elements

$$Z_\omega^{\mathrm{f}} = \int \frac{d\zeta^*\,d\zeta}{\pi}\langle -\zeta|e^{-\beta\hat{H}_\omega}|\zeta\rangle. \tag{7.440}$$

The antidiagonal matrix elements lead to antiperiodic boundary conditions of the fermionic path integral.

7.11 Hilbert Space of Quantized Grassmann Variable

To understand the Hilbert space associated with a path integral over a Grassmann variable we recall that a path integral with zero Hamiltonian serves to define the Hilbert space via all its scalar products as shown in Eq. (2.18):

$$(x_b t_b | x_a t_a) = \int \mathcal{D}x \int \frac{\mathcal{D}p}{2\pi\hbar} \exp\left[i \int dt\, p(t)\dot{x}(t) \right] = \langle x_b | x_a \rangle = \delta(x_b - x_a). \quad (7.441)$$

A momentum variable inside the integral corresponds to a derivative operator $\hat{p} \equiv -i\hbar\partial_x$ outside the amplitude, and this operator satisfies with $\hat{x} = x$ the canonical commutation relation $[\hat{p}, \hat{x}] = -i\hbar$ [see (2.19)].

By complete analogy with this it is possible to create the Hilbert space of spinor indices with the help of a path integral over anticommuting Grassmann variables. In order to understand the Hilbert space, we shall consider three different cases.

7.11.1 Single Real Grassmann Variable

First we consider the path integral of a real Grassmann field with zero Hamiltonian

$$\int \frac{\mathcal{D}\theta}{2\pi} \exp\left[\frac{i}{\hbar} \int dt\, \frac{i\hbar}{2} \theta(t)\dot{\theta}(t) \right]. \quad (7.442)$$

From the Lagrangian

$$\mathcal{L}(t) = \frac{i}{2}\hbar\theta(t)\dot{\theta}(t) \quad (7.443)$$

we obtain a canonical momentum

$$p_\theta = \frac{\partial \mathcal{L}}{\partial \dot{\theta}} = -\frac{i\hbar}{2}\theta. \quad (7.444)$$

Note the minus sign in (7.444) arising from the fact that the derivative with resect to $\dot{\theta}$ anticommutes with the variable θ on its left.

The canonical momentum is proportional to the dynamical variable. The system is therefore subject to a constraint

$$\chi = p_\theta + \frac{i\hbar}{2}\theta = 0. \quad (7.445)$$

In the Dirac classification this is a second-class constraint, in which case the quantization proceeds by forming the classical *Dirac brackets* rather than the Poisson brackets (1.20), and replacing them by $\pm i/\hbar$ times commutation or anticommutation relations, respectively. For n dynamical variables q_i and m constraints χ_p the Dirac brackets are defined by

$$\{A, B\}_D = \{A, B\} - \{A, \chi_p\} C^{pq} \{\chi_q, B\}, \quad (7.446)$$

where C^{pq} is the inverse of the matrix

$$C^{pq} = \{\chi_p, \chi_q\}. \quad (7.447)$$

For Grassmann variables p_i, q_i, the Poisson bracket (1.20) carries by definition an overall minus sign if A contains an odd product of Grassmann variables. Applying this rule to the present system we insert $A = p_\theta$ and $B = \theta$ into the Poisson bracket (1.20) we see that it vanishes. The constraint (7.445), on the other hand, satisfies

$$\{\chi, \chi\} = \left\{ p_\theta + \frac{i\hbar}{2}\theta, p_\theta + \frac{i\hbar}{2}\theta \right\} = -i\hbar\{p_\theta, \theta\} = -i\hbar. \tag{7.448}$$

Hence $C = -i\hbar$ with an inverse $i/\hbar$. The Dirac bracket is therefore

$$\{p_\theta, \theta\}_D = \{p_\theta, \theta\} - \frac{i}{\hbar}\{p_\theta, \chi\}\{\chi, \theta\} = 0 - \frac{-i}{\hbar}\left(\frac{i\hbar}{2}\right)(\hbar) = -\frac{\hbar}{2}. \tag{7.449}$$

With the substitution rule $\{A, B\}_D \to (-i/\hbar)[\hat{A}, \hat{B}]_+$, we therefore obtain the canonical equal-time anticommutation relation for this constrained system:

$$[\hat{p}(t), \hat{\theta}(t)]_+ = -\frac{i\hbar}{2}, \tag{7.450}$$

or, because of (7.444),

$$[\hat{\theta}(t), \hat{\theta}(t)]_+ = 1. \tag{7.451}$$

The proportionality of p_θ and θ has led to a factor $1/2$ on the right-hand side with respect to the usual canonical anticommutation relation.

Let $\psi(\theta)$ be an arbitrary wave function of the general form (7.376):

$$\psi(\theta) = \psi_0 + \psi_1\theta. \tag{7.452}$$

The scalar product in the space of all wave functions is defined by the integral

$$\langle\psi'|\psi\rangle \equiv \int \frac{d\theta}{2\pi}\psi'^*(\theta)\psi(\theta) = \psi_0'^*\psi_1 + \psi_1'^*\psi_0 \ . \tag{7.453}$$

In the so-defined Hilbert space, the operator $\hat{\theta}$ is diagonal, while the operator $\hat{p}$ is given by the differential operator

$$\hat{p} = i\hbar\partial_\theta, \tag{7.454}$$

to satisfy (7.450).

The matrix elements of the operator $\hat{p}$ are

$$\langle\psi'|\hat{p}|\psi\rangle \equiv \int \frac{d\theta}{2\pi}\psi'^*(\theta)i\hbar\frac{\partial}{\partial\theta}\psi(\theta) = i\hbar\psi_1'^*\psi_1. \tag{7.455}$$

By calculating

$$\langle\hat{p}\psi'|\psi\rangle \equiv \int \frac{d\theta}{2\pi}\left[i\hbar\frac{\partial}{\partial\theta}\psi'(\theta)\right]^*\psi(\theta) = -i\hbar\psi_1'^*\psi_1, \tag{7.456}$$

we see that the operator $\hat{p}$ is anti-Hermitian, this being in accordance with the opposite sign in the rule (7.383) of integration by parts.

Let $|\theta\rangle$ be the local eigenstates of which the operator $\hat{\theta}$ is diagonal:

$$\hat{\theta}|\theta\rangle = \theta|\theta\rangle. \tag{7.457}$$

The operator $\hat{\theta}$ is Hermitian, such that

$$\langle\theta|\hat{\theta} = \langle\theta|\theta = \theta\langle\theta|. \tag{7.458}$$

The scalar products satisfy therefore the usual relation

$$(\theta' - \theta)\langle\theta'|\theta\rangle = 0. \tag{7.459}$$

On the other hand, the general expansion rule (7.376) tells us that the scalar product $S = \langle\theta'|\theta\rangle$ must be a linear combination of $S_0 + S_1\theta + S_1'\theta' + S_2\theta\theta'$. Inserting this into (7.459), we find

$$\langle\theta'|\theta\rangle = -\theta' + \theta + S_2\theta\theta', \tag{7.460}$$

where the proportionality constants S_0 and S_1 are fixed by the property

$$\langle\theta'|\theta\rangle = \int \frac{d\theta''}{2\pi}\langle\theta'|\theta''\rangle\langle\theta''|\theta\rangle. \tag{7.461}$$

The constant S_2 is an arbitrary real number. Recalling (7.385) we see that Eq. (7.460) implies that the scalar product $\langle\theta'|\theta\rangle$ is equal to a δ-function:

$$\langle\theta'|\theta\rangle = \delta(\theta - \theta'), \tag{7.462}$$

just as in ordinary quantum mechanics. Note the property

$$\langle\theta'|\theta\rangle^* = -\langle\theta|\theta'\rangle = \langle-\theta| - \theta'\rangle, \tag{7.463}$$

and the fact that since the scalar product $\langle\theta'|\theta\rangle$ is a Grassmann object, a Grassmann variable anticommutes with the scalar product. Having assumed in (7.458) that the Grassmann variable θ can be taken to the left of the bra-vector $\langle\theta|$, the ket-vector $|\theta\rangle$ must be treated like a Grassmann variable, i.e.,

$$\hat{\theta}|\theta\rangle = \theta|\theta\rangle = -|\theta\rangle\theta. \tag{7.464}$$

The momentum operator has the following matrix elements

$$\langle\theta'|\hat{p}|\theta\rangle = -i\hbar\partial_{\theta'}\langle\theta'|\theta\rangle = i\hbar. \tag{7.465}$$

Let $|p\rangle$ be an eigenstate of $\hat{p}$ with eigenvalue ip, then its scalar product with $|\theta\rangle$ satisfies

$$\langle\theta|\hat{p}|p\rangle = \int \frac{d\theta'}{2\pi}\langle\theta|\hat{p}|\theta'\rangle\langle\theta'|p\rangle = i\hbar\int \frac{d\theta'}{2\pi}\langle\theta'|p\rangle = i\hbar\partial_{\theta'}\langle\theta'|p\rangle, \tag{7.466}$$

the last step following from the rule (7.380). Solving (7.466) we find

$$\langle\theta|p\rangle = e^{i\theta p/\hbar}, \tag{7.467}$$

the right-hand side being of course equal to $1 + i\theta p/\hbar$.

It is easy to find an orthonormal set of basis vectors in the space of wave functions (7.452):

$$\psi_+(\theta) \equiv \frac{1}{\sqrt{2}}(1+\theta), \quad \psi_-(\theta) \equiv \frac{1}{\sqrt{2}}(1-\theta). \tag{7.468}$$

We can easily check that these are orthogonal to each other and that they have the scalar products

$$\int \frac{d\theta}{2\pi}\psi^*_\pm(\theta)\psi_\pm(\theta) = \pm 1. \tag{7.469}$$

The Hilbert space contains states of negative norm which are referred to as *ghosts*. Because of the constraint, only half of the Hilbert space is physical. For more details on these problems see the literature on supersymmetric quantum mechanics.

7.11.2 Quantizing Harmonic Oscillator with Grassmann Variables

Let us now turn to the more important physical system containing two Grassmann variables θ_1 and θ_2, combined to complex Grassmann variables (7.388). The Lagrangian is assumed to have the same form as that of an ordinary harmonic oscillator:

$$\mathcal{L}(t) = \hbar\Big[a^*(t)i\partial_t a(t) - \omega a^*(t)a(t)\Big]. \tag{7.470}$$

We may treat $a(t)$ and $a^*(t)$ as independent variables, such that there is no constraint in the system. The classical equation of motion

$$i\dot{a}(t) = \omega a(t) \tag{7.471}$$

is solved by

$$a(t) = e^{-i\omega t}a(0), \qquad a^\dagger(t) = e^{-i\omega t}a^\dagger(0). \tag{7.472}$$

The canonical momentum reads

$$p_a(t) = \frac{\partial\mathcal{L}(t)}{\partial\dot{a}(t)} = -i\hbar a(t), \tag{7.473}$$

and the system is quantized by the equal-time anticommutation relation

$$[\hat{p}_a(t), \hat{a}(t)]_+ = -i\hbar, \tag{7.474}$$

or

$$[\hat{a}^\dagger(t), \hat{a}(t)]_+ = 1. \tag{7.475}$$

In addition we have

$$[\hat{a}(t), \hat{a}(t)]_+ = 0, \qquad [\hat{a}^\dagger(t), \hat{a}^\dagger(t)]_+ = 0. \tag{7.476}$$

Due to these anticommutation relations, the time-independent number operator

$$\hat{N} \equiv a^\dagger(t)a(t) \tag{7.477}$$

satisfies the commutation relations

$$[\hat{N}, a^\dagger(t)] = a^\dagger(t), \qquad [\hat{N}, a(t)] = -a(t). \tag{7.478}$$

We can solve the algebra defined by (7.475), (7.476), and (7.478) for any time, say $t = 0$, in the usual way, defining a ground state $|0\rangle$ by the condition

$$a|0\rangle = 0, \tag{7.479}$$

and an excited state $|1\rangle$ as

$$|1\rangle \equiv a^\dagger|0\rangle. \tag{7.480}$$

These are the only states, and the Hamiltonian operator $\hat{H} = \omega\hat{N}$ possesses the eigenvalues 0 and ω on them. Let $\psi(a)$ be wave functions in the representation where the operator a is diagonal. The canonically conjugate operator $\hat{p}_a = i\hbar\hat{a}^\dagger$ has then the form

$$\hat{p}_a \equiv -i\hbar\partial_a. \tag{7.481}$$

7.11.3 Spin System with Grassmann Variables

For the purpose of constructing path integrals of relativistic electrons later in Chapter 19 we discuss here another system with Grassmann variables.

Pauli Algebra

First we introduce three real Grassmann fields θ^i, $i = 1, 2, 3$, and consider the path integral

$$\prod_{i=1}^{3} \left[\int \mathcal{D}\theta^i\right] \exp\left[\frac{i}{\hbar}\int dt\, \frac{i\hbar}{2}\theta^i(t)\dot{\theta}^i(t)\right]. \tag{7.482}$$

The equation of motion is

$$\dot{\theta}^i(t) = 0, \tag{7.483}$$

so that $\theta^i(t)$ are time independent variables. The three momentum operators lead now to the three-dimensional version of the equal-time anticommutation relation (7.451)

$$[\hat{\theta}^i(t), \hat{\theta}^j(t)]_+ = 2\delta^{ij}, \tag{7.484}$$

where the time arguments can be omitted due to (7.483). The algebra is solved with the help of the Pauli spin matrices (1.448). The solution of (7.484) is obviously

$$\langle B|\hat{\theta}^i|A\rangle = \sigma^i_{BA}, \qquad A, B = 1, 2. \tag{7.485}$$

Let us now add in the exponent of the trivial path integral a Hamiltonian

$$H_B = -\mathbf{S}\cdot\mathbf{B}(t), \tag{7.486}$$

where

$$S^i \equiv -\frac{i}{4}\epsilon^{ijk}\theta^j\theta^k \tag{7.487}$$

plays the role of a spin vector. This can be verified by calculating the canonical commutation relations between the operators

$$[\hat{S}^i, \hat{S}^j] = i\epsilon_{ijk}\hat{S}^k, \tag{7.488}$$

and

$$[\hat{S}^i, \hat{\theta}^j] = i\epsilon_{ijk}\hat{\theta}^k. \tag{7.489}$$

Thus, the operator $\hat{H}$ describes the coupling of a spin vector to a magnetic field $\mathbf{B}(t)$. Using the commutation relation (7.488), we find the Heisenberg equation (1.283) for the Grassmann variables:

$$\dot{\boldsymbol{\theta}} = \mathbf{B} \times \boldsymbol{\theta}, \tag{7.490}$$

which goes over into a similar equation for the spin vector:

$$\dot{\mathbf{S}} = \mathbf{B} \times \mathbf{S}. \tag{7.491}$$

The important observation is now that the path integral (7.482) with the magnetic Hamiltonian (7.486) with fixed ends $\theta_b^i = \theta^i(\tau_b)$ and $\theta_a^i = \theta^i(\tau_a)$ written as

$$\int_{\theta_a^i=\theta^i(\tau_a)}^{\theta_b^i=\theta^i(\tau_b)} \mathcal{D}^3\theta \exp\left[\frac{i}{\hbar}\int dt\, \left(\frac{i\hbar}{4}\theta^i\dot{\theta}^i + B^i\frac{i}{4}\epsilon^{ijk}\theta^j\theta^k\right)\right], \tag{7.492}$$

represents the matrix

$$\hat{T}\exp\left(-\frac{i}{\hbar}\int dt\, \mathbf{B}(t)\cdot\frac{\boldsymbol{\sigma}}{2}\right), \tag{7.493}$$

where $\hat{T}$ is the time-ordering operator defined in Eq. (1.241). This operator is necessary for a time-dependent $\mathbf{B}(t)$ field since the matrices $\mathbf{B}(t)\boldsymbol{\sigma}/2$ for different times do not in general commute with each other.

The result may be expressed in a slightly different notation using the spin tensors

$$S^{ij} \equiv \epsilon^{ijk}S^k = \frac{1}{2i}\theta^i\theta^j, \tag{7.494}$$

whose matrix elements satisfy the rotation algebra

$$[\hat{S}^{ij}, \hat{S}^{kl}] = i\left(\delta^{ik}\hat{S}^{jl} - \delta^{il}\hat{S}^{jk} + \delta^{jl}\hat{S}^{ik} - \delta^{jk}\hat{S}^{il}\right), \tag{7.495}$$

and which have the matrix representation

$$\langle B|\hat{S}^{ij}|A\rangle = \frac{1}{2}\sigma_{BA}^{ij} \equiv \frac{1}{4i}[\sigma^i, \sigma^j]_{BA} = \epsilon^{ijk}\frac{\sigma^k}{2}. \tag{7.496}$$

Note the normalization

$$\sigma^{12} = \sigma^3. \tag{7.497}$$

Introducing the analogous magnetic field tensor

$$F_{ij} \equiv \epsilon^{ijk} B^k, \tag{7.498}$$

we can write the final result also in the tensorial form

$$\hat{T}\exp\Big(-\frac{i}{4\hbar}\int dt\, F_{ij}(t)\sigma^{ij}\Big) = \int_{\theta_a^i=\theta^i(\tau_a)}^{\theta_b^i=\theta^i(\tau_b)} \mathcal{D}^3\theta \exp\left[\frac{i}{\hbar}\int dt\left(\frac{i\hbar}{4}\theta^i\dot{\theta}^i + \frac{i}{4}F_{ij}\theta^i\theta^j\right)\right]. \tag{7.499}$$

The trace of the left-hand side is, of course, given by the path integral over all antiperiodic Grassmann paths on the right-hand side.

Whenever we encounter time-ordered exponentials of integrals over matrices, these can be transformed into a fluctuating path integral over Grassmann variables. If we want to find individual matrix elements, we have to make use of suitably extended recovery formulas (7.431) and (7.432).

For a constant **B**-field, the time ordering operator can be ignored and the exponential (7.493) can immediately be written down explicitly [see Eq. (1A.2)].

In the applications to come, we need only the trace of the matrix (7.493). According to Eq. (7.440), this is found from the integral over (7.492) with $\theta_b^i = -\theta_a^i$, which means performing the integral over all antiperiodic Grassmann paths $\theta^i(\tau)$. For a constant **B**-field, the trace of the operator (7.493) is immediately extracted from Eq. (1A.2):

$$\oint \mathcal{D}^3\theta \exp\left[\frac{i}{\hbar}\int dt\,\left(\frac{i\hbar}{4}\theta^i\dot{\theta}^i + B^i\frac{i}{4}\epsilon^{ijk}\theta^j\theta^k\right)\right] = 2\cos[|\mathbf{B}|(t_b-t_a)/2\hbar]. \tag{7.500}$$

This result can also be derived directly from the path integral over the Grassmann variables θ^i, which yields the square root of the functional determinant

$$2\,\mathrm{Det}^{1/2}\Big[\delta_{ij}\, i\partial_t + \frac{i}{\hbar}F_{ij}(x(t))\Big]\,. \tag{7.501}$$

Here the normalization factor 2 is determined by the path integral with $F_{ij} = 0$, which simply counts the two possible states of the matrix representation (7.496), as in the trace of the left-hand side of (7.499) for $F_{ij} = 0$. Thus

$$\int \mathcal{D}^3\theta \exp\left\{\frac{i}{\hbar}\int dt\,\left[\frac{i\hbar}{4}\,\theta^i\dot{\theta}^i\right]\right\} = 2. \tag{7.502}$$

This normalization factor and agrees with Eqs. (7.415) and (7.418), where the path integral of single complex fermion field gives the same factor 2 for $\omega = 0$

For a constant **B**-field in the z-direction, and antiperiodic boundary conditions in the time interval (t_b, t_a), the matrix in the brackets has the form

$$\begin{pmatrix} \omega_m^{\mathrm{f}} & iB & 0 \\ -iB & \omega_m^{\mathrm{f}} & 0 \\ 0 & 0 & \omega_m^{\mathrm{f}} \end{pmatrix}, \qquad \omega_m^{\mathrm{f}} = \frac{\pi(2m+1)}{t_b - t_a}, \tag{7.503}$$

where $\omega_m^{\rm f}$ are the real-time versions of the odd Matsubara frequencies (7.415). The functional determinant (7.501) is then obtained from the product [compare (7.416)]

$$\mathrm{Det}^{1/2}\Big[\delta_{ij}\, i\partial_t + \frac{i}{\hbar}F_{ij}\Big] = \left[\prod_{m=-\infty}^{\infty} |\omega_m|(\omega_m^2 - B^2/\hbar^2)\right]^{1/2} = \cos[B(t_b - t_a)/2\hbar]. \quad (7.504)$$

The determinant in the second expression is an ordinary determinant of the 4×4-dimensional matrix in the argument of the cosine, to be calculated from its Taylor expansion.

Dirac Algebra

There exists a similar path integral suitable for describing relativistic spin systems. If we introduce four Grassmann variables θ^μ, $\mu = 0, 1, 2, 3$, the path integral

$$\prod_{\mu=0}^{3}\left[\int \mathcal{D}\theta^\mu\right] \exp\left\{\frac{i}{\hbar}\int dt\, \left[-\frac{i\hbar}{4}\theta_\mu(t)\dot{\theta}^\mu(t)\right]\right\}, \quad (7.505)$$

leads to an equation of motion

$$\dot{\theta}^\mu(t) = 0, \quad (7.506)$$

and an operator algebra at equal times

$$\{\hat{\theta}^\mu(t), \hat{\theta}^\nu(t)\} = 2g^{\mu\nu}, \quad (7.507)$$

where $g_{\mu\nu}$ is the metric in Minkowski space

$$g^{\mu\nu} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}. \quad (7.508)$$

The time argument in (7.507) can again be dropped due to (7.506). The algebra (7.507) is solved by the matrix elements [recall (7.485)]

$$\langle\beta|\hat{\theta}^\mu(t)|\alpha\rangle = (\gamma^\mu)_{\beta\alpha}\,, \qquad \beta, \alpha = 1, 2, 3, 4, \quad (7.509)$$

where γ^μ, γ_5 are composed of 2×2-matrices 0, 1, and σ^i as follows:

$$\gamma^0 \equiv \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix},\ \gamma^i \equiv \begin{pmatrix} 0 & \sigma^i \\ -\sigma^i & 0 \end{pmatrix},\ \gamma_5 \equiv i\gamma^0\gamma^1\gamma^2\gamma^3 = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \equiv \gamma^5. \quad (7.510)$$

One may also introduce an additional Grassmann variable θ_5 such that the path integral

$$\prod_{\mu=0}^{3}\left[\int \mathcal{D}\theta_5\right] \exp\left[\frac{i}{\hbar}\int dt\, \frac{i\hbar}{4}\theta_5(t)\dot{\theta}_5(t)\right], \quad (7.511)$$

produces the matrix elements of $\gamma_5(t)$:

$$\langle\beta|\hat{\theta}_5(t)|\alpha\rangle = (\gamma_5)_{\beta\alpha}\,, \qquad \beta,\alpha = 1,2,3,4. \tag{7.512}$$

The Grassmann variables θ^μ and θ_5 anticommute with each other, and so do the matrices $\gamma_5\gamma^\mu$ and γ_5.

In terms of the Grassmann variables θ^μ it is possible to write down a four-dimensional version of the time-ordered 2×2 matrix integral (7.499) as a path integral without time ordering:

$$\hat{T}\exp\left(-\frac{i}{2\hbar}\int dt\, F_{\mu\nu}\Sigma^{\mu\nu}\right) = \int \mathcal{D}^4\theta \exp\left\{\frac{i}{\hbar}\int dt\left[-\frac{i\hbar}{2}\theta_\mu\dot{\theta}^\mu + \frac{i}{4}F_{\mu\nu}\theta^\mu\theta^\nu\right]\right\}, \tag{7.513}$$

where $\Sigma^{\mu\nu}$ is the Minkowski space generalization of the spin tensor matrix $\sigma^{ij}/2$ in (7.496):

$$\Sigma^{\mu\nu} \equiv \frac{i}{4}[\gamma^\mu,\gamma^\nu] = -\Sigma^{\nu\mu}. \tag{7.514}$$

As a check we use (7.510) and find

$$\Sigma^{12} = \frac{1}{2}\begin{pmatrix} \sigma^{12} & 0 \\ 0 & \sigma^{12}\end{pmatrix} = \frac{1}{2}\begin{pmatrix} \sigma^{3} & 0 \\ 0 & \sigma^{3}\end{pmatrix}, \tag{7.515}$$

in agreement with (7.497).

As remarked before, we shall need in the applications to come only the trace of the matrix (7.493), which is found, according to Eq. (7.440), from the integral over (7.492) with $\theta_b^i = -\theta_a^i$, i.e., by performing the integral over all antiperiodic Grassmann paths $\theta^i(\tau)$. If we want to find individual matrix elements, we have to make use of suitably extended recovery formulas (7.431) and (7.432).

The path integral over all antiperiodic paths for $F_{\mu\nu} = 0$ fixes the normalization. For zero fields, the trace of the left-hand side of (7.513) is equal to 4, so that we have

$$\int \mathcal{D}^4\theta \exp\left\{\frac{i}{\hbar}\int dt\left[-\frac{i\hbar}{4}\theta_\mu\dot{\theta}^\mu\right]\right\} = 4. \tag{7.516}$$

This normalization factor agrees with Eqs. (7.415) and (7.418), where we found the path integral of single complex fermion field to carry a normalization factor 2. For four real fields this corresponds to a factor 4.

In the presence of a nonzero field tensor, the result of the path integral (7.513) is therefore

$$\int \mathcal{D}^4\theta\, e^{(i/4\hbar)\int dt\left\{\left[-i\hbar\theta_\mu\dot{\theta}^\mu + iF_{\mu\nu}\theta^\mu\theta^\nu\right]\right\}} = 4\,\mathrm{Det}^{1/2}\left[-g_{\mu\nu}\,i\partial_t + \frac{i}{\hbar}F_{\mu\nu}(x(t))\right]. \tag{7.517}$$

In the presence of a constant electic and a constant magnetic field in the z-direction, then $F_{03} = E$, and

$$F_{\mu\nu} = \begin{pmatrix} 0 & 0 & 0 & E \\ 0 & 0 & -B & 0 \\ 0 & B & 0 & 0 \\ E & 0 & 0 & 0 \end{pmatrix}. \tag{7.518}$$

Thus we find

$$e^{F_{\mu\nu}t} = \begin{pmatrix} \cosh Et & 0 & 0 & \sinh Et \\ 0 & \cos Bt & -\sin Bt & 0 \\ 0 & \sin Bt & \cos Bt & 0 \\ \sinh Et & 0 & 0 & \cosh Et \end{pmatrix}, \tag{7.519}$$

so that

$$\mathrm{Det}\left(-g_{\mu\nu}\, i\partial_t + \frac{i}{\hbar}F_{\mu\nu}\right) = \det\cos\left(F_{\mu\nu}\frac{t_b - t_a}{2\hbar}\right) = \cos^2\left(B\frac{t_b - t_a}{2\hbar}\right)\cosh^2\left(E\frac{t_b - t_a}{2\hbar}\right). \tag{7.520}$$

Constant Electric and Magnetic Field in any Direction

If there are both constant electric and magnetic fields in any direction, the calculation can be reduced to the parallel case by a simple Lorentz transformation. It is always possible to find a Lorentz frame in which the fields become parallel. This special frame will be called *center-of-fields* frame, and the transformed fields in this frame will be denoted by $\mathbf{B}_{\mathrm{CF}}$ and $\mathbf{E}_{\mathrm{CF}}$. The transformation has the form

$$\mathbf{E}_{\mathrm{CF}} = \gamma\left(\mathbf{E} + \frac{\mathbf{v}}{c}\times\mathbf{B}\right) - \frac{\gamma^2}{\gamma+1}\frac{\mathbf{v}}{c}\left(\frac{\mathbf{v}}{c}\cdot\mathbf{E}\right), \tag{7.521}$$

$$\mathbf{B}_{\mathrm{CF}} = \gamma\left(\mathbf{B} - \frac{\mathbf{v}}{c}\times\mathbf{E}\right) - \frac{\gamma^2}{\gamma+1}\frac{\mathbf{v}}{c}\left(\frac{\mathbf{v}}{c}\cdot\mathbf{B}\right), \tag{7.522}$$

with a velocity of the transformation determined by

$$\frac{\mathbf{v}/c}{1+(|\mathbf{v}|/c)^2} = \frac{\mathbf{E}\times\mathbf{B}}{|\mathbf{E}|^2+|\mathbf{B}|^2}, \tag{7.523}$$

and $\gamma \equiv [1-(|\mathbf{v}|/c)^2]^{-1/2}$. The fields $|\mathbf{E}_{\mathrm{CF}}| \equiv \mathcal{E}$ and $|\mathbf{B}_{\mathrm{CF}}| \equiv \mathcal{B}$ are, of course, Lorentz-invariant quantities which can be expressed in terms of the two quadratic Lorentz invariants of the electromagnetic field: the scalar S and the pseudoscalar P defined by

$$S \equiv -\frac{1}{4}F_{\mu\nu}F^{\mu\nu} = \frac{1}{2}\left(\mathbf{E}^2 - \mathbf{B}^2\right) = \frac{1}{2}\left(\mathcal{E}^2 - \mathcal{B}^2\right), \quad P \equiv -\frac{1}{4}F_{\mu\nu}\tilde{F}^{\mu\nu} = \mathbf{E}\,\mathbf{B} = \mathcal{E}\mathcal{B}. \tag{7.524}$$

Solving these equation yields

$$\left\{\begin{matrix}\mathcal{E}\\ \mathcal{B}\end{matrix}\right\} \equiv \sqrt{\sqrt{S^2+P^2}\pm S} = \frac{1}{\sqrt{2}}\sqrt{\sqrt{(\mathbf{E}^2-\mathbf{B}^2)^2+4(\mathbf{E}\,\mathbf{B})^2}\pm(\mathbf{E}^2-\mathbf{B}^2)}. \tag{7.525}$$

After these transformations, the result (7.520) remains valid for any constant field directions if we exchange $E \to \mathcal{E}$, $B \to \mathcal{B}$.

Relation between Harmonic Oscillator, Pauli and Dirac Algebra

There exists a simple relation between the path integrals of the previous three paragraphs. We simply observe that the combinations

$$\hat{a}^\dagger = \frac{1}{2}\left(\sigma^1 + i\sigma^2\right) = \frac{1}{2}\,\sigma^+ = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix},\ \hat{a} = \frac{1}{2}\left(\sigma^1 - i\sigma^2\right) = \frac{1}{2}\,\sigma^- = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \tag{7.526}$$

satisfy the anticommutation rules

$$[\hat{a}, \hat{a}^\dagger]_+ = 1, \quad [\hat{a}^\dagger, \hat{a}^\dagger]_+ = 1, \quad [\hat{a}, \hat{a}]_+ = 0. \tag{7.527}$$

The vacuum state annihilated by a is the spin-down spinor, and the one-particle state is the spin-up spinor:

$$|0\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \qquad |1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}. \tag{7.528}$$

A similar construction can be found for the Dirac algebra. There are now two types of creation and annihilation operators

$$\hat{a}^\dagger = \frac{1}{2}\left(\gamma^1 + i\gamma^2\right) = \frac{1}{2}\begin{pmatrix} 0 & \sigma^+ \\ -\sigma^+ & 0 \end{pmatrix},\ \hat{a} = \frac{1}{2}\left(-\gamma^1 + i\gamma^2\right) = \frac{1}{2}\begin{pmatrix} 0 & -\sigma^- \\ \sigma^- & 0 \end{pmatrix}, \tag{7.529}$$

and

$$\hat{b}^\dagger = \frac{1}{2}\left(\gamma^0 + \gamma^3\right) = \frac{1}{2}\begin{pmatrix} 0 & i\sigma^2\sigma^+ \\ -i\sigma^2\sigma^+ & 0 \end{pmatrix},\ \hat{b} = \frac{1}{2}\left(\gamma^1 - \gamma^3\right) = \frac{1}{2}\begin{pmatrix} 0 & i\sigma^2\sigma^- \\ -i\sigma^2\sigma^- & 0 \end{pmatrix}. \tag{7.530}$$

The states $|n_a, a_b\rangle$ with n_a quanta a and n_b quanta b are the following:

$$|0,0\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \\ 0 \\ 1 \end{pmatrix}, \qquad |1,0\rangle = a^\dagger|0,0\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ -1 \\ 0 \end{pmatrix}, \tag{7.531}$$

$$|0,1\rangle = b^\dagger|0,0\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ -1 \\ 0 \\ 1 \end{pmatrix}, \quad |1,1\rangle = a^\dagger b^\dagger|0,0\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ 1 \\ 0 \end{pmatrix}. \tag{7.532}$$

From these relations we can easily deduce the proper recovery formulas generalizing (7.431) and (7.432).

7.12 External Sources in a^*, a -Path Integral

In Chapter 3, the path integral of the harmonic oscillator was solved in the presence of an arbitrary external current $j(\tau)$. This yielded the generating functional $Z[j]$ for the calculation of all correlation functions of $x(\tau)$. In the present context we are interested in the generating functional of correlations of $a(\tau)$ and $a^*(\tau)$. Thus we also need the path integrals quadratic in $a(\tau)$ and $a^*(\tau)$ coupled to external currents. Consider the Euclidean action

$$\mathcal{A}[a^*,a]+\mathcal{A}^{\text{source}}=\hbar\int_0^{\hbar\beta}d\tau[a^*(\tau)\partial_\tau a(\tau)+\omega a^*a(\tau)-(\eta^*(\tau)a(\tau)+\text{c.c.})], \quad (7.533)$$

with periodic boundary conditions for $a(\tau)$ and $a^*(\tau)$. For simplicity, we shall use the continuum formulation of the partition function, so that our results will correspond to the harmonic oscillator time slicing, with the energies $E_n=(n+1/2)\hbar\omega$. There is no problem in going over to the second-quantized formulation with the energies $E_n=n\hbar\omega$. The partition function is given by the path integral

$$Z_\omega[\eta^*,\eta]=\oint\frac{\mathcal{D}a^*\mathcal{D}a}{\pi}\exp\left\{-\frac{1}{\hbar}\left(\mathcal{A}[a^*,a]+\mathcal{A}^{\text{source}}\right)\right\}. \quad (7.534)$$

As in Chapter 3, we define the functional matrix between $a^*(\tau)$, $a(\tau')$ as

$$D_{\omega,\text{e}}(\tau,\tau')\equiv(\partial_\tau+\omega)\delta(\tau-\tau'),\quad \tau,\tau'\in(0,\hbar\beta). \quad (7.535)$$

The inverse is the Euclidean Green function

$$G^{\text{p}}_{\omega,\text{e}}(\tau,\tau')=D^{-1}_{\omega,\text{e}}(\tau,\tau'), \quad (7.536)$$

satisfying the periodic boundary condition. We now complete the square and rewrite the action (7.533), using the shifted fields

$$a'(\tau)=a(\tau)-\int_0^{\hbar\beta}d\tau'\,G^{\text{p}}_{\omega,\text{e}}(\tau,\tau')\eta(\tau') \quad (7.537)$$

as

$$\mathcal{A}_{\text{e}}=\hbar\int_0^{\hbar\beta}d\tau\int_0^{\hbar\beta}d\tau'[a'^*(\tau)D_{\omega,\text{e}}(\tau,\tau')a'(\tau')-\eta^*(\tau)G^{\text{p}}_{\omega,\text{e}}(\tau,\tau')\eta(\tau')]. \quad (7.538)$$

On an infinite β-interval the Green function can easily be written down in terms of the Heaviside function (1.313):

$$G_{\omega,\text{e}}(\tau,\tau')=G_{\omega,\text{e}}(\tau-\tau')=e^{-\omega(\tau-\tau')}\Theta(\tau-\tau'). \quad (7.539)$$

As we have learned in Section 3.3, the periodic Green function is obtained from this by forming a periodic sum

$$G^{\text{p}}_{\omega,\text{e}}(\tau,\tau')=G^{\text{p}}_{\omega,\text{e}}(\tau-\tau')=\sum_{n=-\infty}^{\infty}e^{-\omega(\tau-\tau'-n\hbar\beta)}\Theta(\tau-\tau'-n\hbar\beta), \quad (7.540)$$

which is equal to

$$G^{\rm p}_{\omega,{\rm e}}(\tau) = \frac{e^{-\omega(\tau-\hbar\beta/2)}}{2\sinh(\omega\hbar\beta/2)} = (1+n^{\rm b}_\omega)e^{-\omega\tau}, \tag{7.541}$$

where n_ω is the Bose-Einstein distribution function

$$n_\omega = \frac{1}{e^{\beta\hbar\omega}-1} \tag{7.542}$$

[compare (3.92) and (3.93)].

The same considerations hold for anticommuting variables with antiperiodic boundary conditions, in which case we find once more the action (7.538) with the
ref(3.112) antiperiodic Green function [compare (3.112)]
lab(3.75)
est(3.74)

$$G^a_{\omega,{\rm e}}(\tau) = \frac{e^{-\omega(\tau-\hbar\beta/2)}}{2\cosh(\omega\hbar\beta/2)} = (1-n^{\rm f}_\omega)e^{-\omega\tau}, \tag{7.543}$$

ref(3.111) where n_ω is the Fermi-Dirac distribution function [see (3.111)]:
lab(3.74)
est(3.73)

$$n^{\rm f}_\omega = \frac{1}{e^{\beta\hbar\omega}+1}. \tag{7.544}$$

In either case, we may decompose the currents in (7.538) into real and imaginary parts j and k via

$$\begin{aligned} \eta &= \sqrt{\omega/2M\hbar}(j - i\omega Mk), \\ \eta^* &= \sqrt{\omega/2M\hbar}(j + i\omega Mk), \end{aligned} \tag{7.545}$$

and write the source part of the original action (7.533) in the form

$$\mathcal{A}^{\rm source} = \hbar\int_0^{\hbar\beta} d\tau(a^*\eta + \eta^* a) = \int_0^{\hbar\beta} d\tau(jx + kp). \tag{7.546}$$

Hence, the real current $\eta = \eta^* = \sqrt{\omega/2M\hbar}\; j$ corresponds to the earlier source term
ref(3.2) (3.2). Inserting this current into the action (7.538), it yields the quadratic source
lab(3.2) term
est(3.2)

$$\mathcal{A}^{\rm s}_{\rm e} = -\frac{1}{2M\omega}\int_0^{\hbar\beta} d\tau \int_0^\tau d\tau' \frac{e^{-\omega(\tau-\tau')}}{1-e^{-\beta\hbar\omega}} j(\tau)j(\tau'). \tag{7.547}$$

This can also be rewritten as

$$\mathcal{A}^{\rm s}_{\rm e} = -\frac{1}{2M\omega}\sum_{n=0}^{\infty}\int_0^{\hbar\omega} d\tau \int_0^\tau d\tau' e^{-\omega(\tau-\tau'+n\hbar\beta)} j(\tau)j(\tau'), \tag{7.548}$$

which becomes for a current periodic in $\hbar\beta$:

$$\mathcal{A}^{\rm s}_{\rm e} = -\frac{1}{2M\omega}\int_0^{\hbar\omega} d\tau \int_{-\infty}^\tau d\tau'\; e^{-\omega(\tau-\tau')} j(\tau)j(\tau'). \tag{7.549}$$

Interchanging τ and τ', this is also equal to

$$\mathcal{A}^{\rm s}_{\rm e} = -\frac{1}{4M\omega}\int_0^{\hbar\omega} d\tau \int_{-\infty}^\infty d\tau' e^{-\omega|\tau-\tau'|} j(\tau)j(\tau'), \tag{7.550}$$

in agreement with (3.279).

7.13 Generalization to Pair Terms

There exists an important generalization of these considerations to the case of the quadratic frequency term $\hbar \int d\tau\, \Omega^2(\tau) a^*(\tau) a(\tau)$ being extended to the more general quadratic form

$$\hbar \int d\tau \left[\Omega^2(\tau) a^*(\tau) a(\tau) + \frac{1}{2} \Delta^*(\tau) a^2(\tau) + \frac{1}{2} \Delta(\tau) a^{*2}(\tau) \right]. \tag{7.551}$$

The additional off-diagonal terms in a^*, a are called *pair terms*. They play an important role in the theory of superconductivity. The basic physical mechanism for this phenomenon will be explained in Section 17.10. Here we just mention that the lattice vibrations give rise to the formation of bound states between pairs of electrons, called *Cooper pairs*. By certain manipulations of the path integral of the electron field in the second-quantized interpretation, it is possible to introduce a complex pair field $\Delta_{\mathbf{x}}(t)$ at each space point which is coupled to the electron field in an action of the type (7.551). The partition function to be studied is then of the generic form

$$Z = \oint \frac{\mathcal{D}a^*\, \mathcal{D}a}{\pi} \exp \left[- \int_0^{\hbar\beta} d\tau \, (a^* \partial_\tau a + \Omega^2 a^* a + \tfrac{1}{2} \Delta^* a^2 + \tfrac{1}{2} \Delta\, a^{*2}) \right]. \tag{7.552}$$

It is easy to calculate this partition function on the basis of the previous formulas. To this end we rewrite the action in the matrix form, using the field doublets

$$f(\tau) \equiv \begin{pmatrix} a(\tau) \\ a^*(\tau) \end{pmatrix}, \tag{7.553}$$

as

$$\mathcal{A}_{\mathrm{e}} = \frac{\hbar}{2} \int_0^{\hbar\beta} d\tau\, f^{*T}(\tau) \begin{pmatrix} \partial_\tau + \Omega(\tau) & \Delta(\tau) \\ \Delta^*(\tau) & \mp(\partial_\tau \pm \Omega(\tau)) \end{pmatrix} f(\tau), \tag{7.554}$$

where the derivative terms require a partial integration to obtain this form. The partition function can be written as

$$Z = \int \frac{\mathcal{D}f^*\, \mathcal{D}f}{\pi} e^{-\frac{1}{2} f^* M f}, \tag{7.555}$$

with the matrix

$$M = \begin{pmatrix} \partial_\tau + \Omega(\tau) & \Delta(\tau) \\ \Delta^*(\tau) & \mp(\partial_\tau \pm \Omega(\tau)) \end{pmatrix}. \tag{7.556}$$

The fields f^* and f are not independent of each other, since

$$f^* = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} f. \tag{7.557}$$

Thus, there are only half as many independent integrations as for a usual complex field. This has the consequence that the functional integration in (7.555) gives only the square root of the determinant of M,

$$Z = \mathcal{N}^{b,f} \det \begin{pmatrix} \partial_\tau + \Omega(\tau) & \Delta(\tau) \\ \Delta^*(\tau) & \mp(\partial_\tau + \Omega(\tau)) \end{pmatrix}^{\mp 1/2}, \tag{7.558}$$

with the normalization factors $\mathcal{N}^{b,f}$ being fixed by comparison with (7.337) and (7.419).

A fluctuation determinant of this type occurs in the theory of superconductivity [32], with constant parameters ω, Δ. When applied to functions oscillating like $e^{-i\omega_m^{\rm f}\tau}$, the matrix M becomes

$$M = \begin{pmatrix} -i\omega_m^{\rm f} + \omega & \Delta \\ \Delta^* & \mp(-i\omega_m^{\rm f} \pm \omega) \end{pmatrix}. \tag{7.559}$$

It is brought to diagonal form by what is called, in this context, a *Bogoliubov transformation* [33]

$$M \to M^d = \begin{pmatrix} -i\omega_m^{\rm f} + \omega_\Delta & 0 \\ 0 & \mp(-i\omega_m^{\rm f} \pm \omega_\Delta) \end{pmatrix}, \tag{7.560}$$

where ω_Δ is the frequency

$$\omega_\Delta = \sqrt{\omega^2 + \Delta^2}. \tag{7.561}$$

In a superconductor, these frequencies correspond to the energies of the quasi-particles associated with the electrons. They generalize the quasi-particles introduced in Landau's theory of Fermi liquids. The partition function (7.552) is then given by

$$\begin{aligned} Z_{\omega,\Delta} &= \mathcal{N}^{b,f} \det \begin{pmatrix} \partial_\tau + \omega & \Delta \\ \Delta^* & \mp\partial_\tau \pm \omega \end{pmatrix}^{\mp 1/2} \\ &= N^{b,f} \left[\det\left(-\partial_\tau^2 + \omega_\Delta^2\right)\right]^{\mp 1/2} = \begin{cases} \left[2\sinh(\hbar\beta\omega_\Delta/2)\right]^{-1}, \\ 2\cosh(\hbar\beta\omega_\Delta/2), \end{cases} \end{aligned} \tag{7.562}$$

for bosons and fermions, respectively. This is equal to the partition function of a symmetrized Hamilton operator

$$\hat{H} = \frac{\omega_\Delta}{2}\Delta\left(\hat{a}^\dagger\hat{a} + \hat{a}\hat{a}^\dagger\right) = \omega_\Delta\left(\hat{a}^\dagger\hat{a} \pm \frac{1}{2}\right), \tag{7.563}$$

with the eigenvalue spectrum $\omega_\Delta\left(n \pm \frac{1}{2}\right)$, where $n = 0, 1, 2, 3\ldots$ for bosons and $n = 0, 1$ for fermions:

$$Z_{\omega,\Delta} = \sum_n^{\infty,1} e^{-\hbar\omega_\Delta(n\pm 1/2)\beta}. \tag{7.564}$$

In the second-quantized interpretation where zero-point energies are omitted, this becomes

$$Z_{\omega,\Delta} = \begin{cases} (1 - e^{-\hbar\beta\omega_\Delta})^{-1}, \\ (1 + e^{-\hbar\beta\omega_\Delta}). \end{cases} \tag{7.565}$$

7.14 Spatial Degrees of Freedom

In the path integral treatment of the last sections, the particles have been restricted to a particular momentum state $\mathbf{p}$. In a three-dimensional volume, the fields $a^*(\tau)$, $\Delta(\tau)$ and their frequency ω depend on $\mathbf{p}$. With this trivial extension one obtains a free *quantum field theory*.

7.14.1 Grand-Canonical Ensemble of Particle Orbits from Free Fluctuating Field

The free particle action becomes a sum over momentum states

$$\mathcal{A}_{\rm e}[a^*,a] = \hbar \int_0^{\hbar\beta} d\tau \sum_{\mathbf{p}} \left[a^*_{\mathbf{p}} \partial_\tau a_{\mathbf{p}} + \omega(\mathbf{p}) a^*_{\mathbf{p}} a_{\mathbf{p}} \right]. \tag{7.566}$$

The time-sliced partition function is given by the product

$$\begin{aligned} Z &= \prod_{\mathbf{p}} \left\{ \det \left[\epsilon(1-\epsilon\omega)\overline{\nabla} + \epsilon\omega(\mathbf{p}) \right] \right\}^{\mp 1} \qquad (7.567) \\ &= \begin{cases} \exp\left[-\sum_{\mathbf{p}} \log\left(1 - e^{-\hbar\beta\bar{\omega}_{\rm e}(\mathbf{p})} \right) \right] & \text{for bosons,} \\ \exp\left[\sum_{\mathbf{p}} \log\left(1 + e^{-\hbar\beta\bar{\omega}_{\rm e}(\mathbf{p})} \right) \right] & \text{for fermions.} \end{cases} \end{aligned}$$

The free energy

$$F = -k_B T \log Z \tag{7.568}$$

is for bosons

$$F = k_B T \sum_{\mathbf{p}} \log\left(1 - e^{-\hbar\beta\bar{\omega}_{\rm e}(\mathbf{p})} \right), \tag{7.569}$$

and for fermions

$$F = -k_B T \sum_{\mathbf{p}} \log\left(1 + e^{-\hbar\beta\bar{\omega}_{\rm e}(\mathbf{p})} \right). \tag{7.570}$$

In a large volume, the momentum sum may be replaced by the integral

$$\sum_{\mathbf{p}} \to \int \frac{d^D p\, V}{(2\pi\hbar)^D}. \tag{7.571}$$

For infinitely thin time slices, $\epsilon \to 0$ and $\bar{\omega}_{\rm e}(\mathbf{p})$ reduces to $\omega(\mathbf{p})$ and the expressions (7.569), (7.570) turn into the usual free energies of bosons and fermions. They agree completely with the expressions (7.46) and (7.220) derived from the sum over orbits.

Next we may introduce a fluctuating field in space and imaginary time

$$\psi(\mathbf{x},\tau) = \frac{1}{\sqrt{V}} \sum_{\mathbf{p}} e^{i\mathbf{p}\mathbf{x}} a_{\mathbf{p}}(\tau), \tag{7.572}$$

and rewrite the action (7.566) in the local form

$$\mathcal{A}_{\rm e}[\psi^*,\psi] = \int_0^{\hbar\beta} d\tau \int d^D x \left[\psi^*(\mathbf{x},\tau)\hbar\partial_\tau \psi(\mathbf{x},\tau) + \frac{\hbar^2}{2M} \boldsymbol{\nabla}\psi^*(\mathbf{x},\tau) \boldsymbol{\nabla}\psi(\mathbf{x},\tau) \right]. \tag{7.573}$$

The partition function is given by the functional integral

$$Z = \oint \mathcal{D}\psi \mathcal{D}\psi^* e^{-\mathcal{A}_e[\psi^*,\psi]/\hbar}. \tag{7.574}$$

Thus we see that the functional integral over a fluctuating field yields precisely the same partition function as the sum over a grand-canonical ensemble of fluctuating orbits. Bose or Fermi statistics are naturally accounted for by using complex or Grassmann field variables with periodic or antiperiodic boundary conditions, respectively. The theory based on the action (7.573) is completely equivalent to the second-quantized theory of field operators.

In order to distinguish the second-quantized or quantum field description of many particle systems from the former path integral description of many particle orbits, the former is referred to as the *first-quantized* approach, or also the *world-line* approach.

The action (7.573) can be generalized further to include an external potential $V(\mathbf{x},\tau)$, i.e., it may contain a general Schrödinger operator $\hat{H}(\tau) = \hat{\mathbf{p}}^2 + V(\mathbf{x},\tau)$ instead of the gradient term:

$$\mathcal{A}_e[\psi^*,\psi] = \int_0^{\hbar\beta} d\tau \int d^D x \left\{ \psi^*(\mathbf{x},\tau)\hbar\partial_\tau \psi(\mathbf{x},\tau) + \psi^*(\mathbf{x},\tau)\left[\hat{H}(\tau) - \mu\right]\psi(\mathbf{x},\tau)\right\}. \tag{7.575}$$

For the sake of generality we have also added a chemical potential to enable the study of grand-canonical ensembles. This action can be used for a second-quantized description of the free Bose gas in an external magnetic trap potential $V(\mathbf{x})$, which would, of course, lead to the same results as the first-quantized approach in Section 7.2.4. The free energy associated with this action

$$F = \frac{1}{\beta}\mathrm{Tr}\log[\hbar\partial_\tau + \hat{H}(\tau) - \mu] \tag{7.576}$$

was calculated in Eq. (3.139) as an expansion

$$F = \frac{1}{2\hbar\beta}\mathrm{Tr}\left[\int_0^{\hbar\beta} d\tau\, \hat{H}(\tau)\right] - \frac{1}{\beta}\sum_{n=1}^{\infty}\frac{1}{n}\mathrm{Tr}\left\{\hat{T}e^{-n\int_0^{\hbar\beta} d\tau''\,[\hat{H}(\tau'')-\mu]/\hbar}\right\}, \tag{7.577}$$

The sum can be evaluated in the semiclassical expansion developed in Section 4.9. For simplicity, we consider here only time-independent external potentials, where we must calculate $\mathrm{Tr}\,[e^{-n\beta\,(\hat{H}-\mu)}]$. Its semiclassical limit was given in Eq. (4.258) continued to imaginary time. From this we obtain

$$F = \frac{1}{2}\mathrm{Tr}\,\hat{H} - \frac{1}{\beta}\frac{1}{\sqrt{2\pi\hbar^2\beta/M}^D}\sum_{n=1}^{\infty}\int d^D x \frac{[z(\mathbf{x})]^n}{n^{D/2+1}}, \tag{7.578}$$

where $z(\mathbf{x}) \equiv e^{-\beta[V(\mathbf{x})-\mu]}$ is the local fugacity (7.24). The sum agrees with the previous first-quantized result in (7.132) and (7.133). The first term is due to the symmetric treatment of the fields in the action (7.575) [recall the discussion after Eq. (7.340)].

One may calculate quantum corrections to this expansion by including the higher gradient terms of the semiclassical expansion (4.258). If the potential is time-dependent, the expansion (4.258) must be generalized accordingly.

7.14.2 First versus Second Quantization

There exists a simple set of formulas which illustrates nicely the difference between first and second quantization, i.e., between path and field quantization. Both may be though of as being based on two different representations of the Dirac δ-function. The first-quantized representation is

$$\delta^{(D)}(\mathbf{x}_b - \mathbf{x}_a) = \int_{\mathbf{x}(t_a)=\mathbf{x}_a}^{\mathbf{x}(t_b)=\mathbf{x}_b} \mathcal{D}^D x \oint \frac{\mathcal{D}^D p}{(2\pi\hbar)^D} e^{(i/\hbar)\int_{t_a}^{t_b} dt\, \mathbf{p}\dot{\mathbf{x}}}, \tag{7.579}$$

the second-quantized representation

$$i\hbar\delta^{(D)}(\mathbf{x}_b - \mathbf{x}_a)\delta(t_b - t_a) = \oint \mathcal{D}\psi\mathcal{D}\psi^*\, \psi(\mathbf{x}_b, t_b)\psi^*(\mathbf{x}_a, t_a) e^{(i/\hbar)\int d^D x \int_{-\infty}^{\infty} dt \psi^*(\mathbf{x},t)\psi(\mathbf{x},t)}. \tag{7.580}$$

The first representation is turned into a transition amplitude by acting upon it with the time-evolution operator $e^{-i\hat{H}(t_b-t_a)}$, which yields

$$(\mathbf{x}_b t_b|\mathbf{x}_a t_a) = e^{i\hat{H}(t_b-t_a)}\delta^{(D)}(\mathbf{x}_b - \mathbf{x}_a) = \int \mathcal{D}^D x \oint \frac{\mathcal{D}^D p}{(2\pi\hbar)^D} e^{(i/\hbar)\int_{t_a}^{t_b} dt(\mathbf{p}\dot{\mathbf{x}} - H)}. \tag{7.581}$$

By multiplying this with the Heaviside function $\Theta(t_b - t_a)$, we obtain the solution of the inhomogeneous Schrödinger equation

$$(i\hbar\partial_t - \hat{H})\Theta(t_b - t_a)(\mathbf{x}_b t_b|\mathbf{x}_a t_a) = i\hbar\delta^{(D)}(\mathbf{x}_b - \mathbf{x}_a)\delta(t_b - t_a). \tag{7.582}$$

This may be expressed as a path integral representation for the resolvent

$$\left\langle \mathbf{x}_b t_b \left| \frac{i\hbar}{i\hbar\partial_t - \hat{H}} \right| \mathbf{x}_a t_a \right\rangle = \Theta(t_b - t_a) \int_{\mathbf{x}(t_a)=\mathbf{x}_a}^{\mathbf{x}(t_b)=\mathbf{x}_b} \mathcal{D}^D x \oint \frac{\mathcal{D}^D p}{(2\pi\hbar)^D} e^{(i/\hbar)\int_{t_a}^{t_b} dt(\mathbf{p}\dot{\mathbf{x}} - H)}. \tag{7.583}$$

The same quantity is obtained from the second representation (7.580) by changing the integrand in the exponent from $\psi^*(\mathbf{x}, t)\psi(\mathbf{x}, t)$ to $\psi^*(\mathbf{x}, t)(i\hbar\partial_t - \hat{H})\psi(\mathbf{x}, t)$:

$$\left\langle \mathbf{x}_b t_b \left| \frac{i\hbar}{i\hbar\partial_t - \hat{H}} \right| \mathbf{x}_a t_a \right\rangle = \oint \mathcal{D}\psi\mathcal{D}\psi^*\, \psi(\mathbf{x}_b, t_b)\psi^*(\mathbf{x}_a, t_a) e^{(i/\hbar)\int d^D x \int_{-\infty}^{\infty} dt \psi^*(\mathbf{x},t)(i\hbar\partial_t - \hat{H})\psi(\mathbf{x},t)}. \tag{7.584}$$

This is the second-quantized functional integral representation of the resolvent.

7.14.3 Interacting Fields

The interaction between particle orbits in a grand-canonical ensemble can be accounted for by anharmonic terms in the particle fields. A pair interaction between orbits, for example, corresponds to a fourth-order self interaction. An example is the interaction in the Bose-Einstein condensate corresponding to the energy in Eq. (7.101). Expressed in terms of the fields it reads

$$\mathcal{A}_{\rm e}^{\rm int}[\psi^*,\psi]=-\int_0^{\hbar\beta}d\tau\,\Delta E=-\frac{g}{2}\int_0^{\hbar\beta}d\tau\int d^3x\,\psi^*(\mathbf{x},\tau+\eta)\psi^*(\mathbf{x},\tau+\eta)\psi(\mathbf{x},\tau)\psi(\mathbf{x},\tau), \tag{7.585}$$

where $\eta>0$ is an infinitesimal time shift. It is then possible to develop a perturbation theory in terms of Feynman diagrams by complete analogy with the treatment in Section 3.20 of the anharmonic oscillator with a fourth-order self interaction. The free correlation function is the momentum sum of oscillator correlation functions:

$$\langle\psi(\mathbf{x},\tau)\psi^*(\mathbf{x}',\tau')\rangle=\sum_{\mathbf{p},\mathbf{p}'}\langle a_{\mathbf{p}}(\tau)a^*_{\mathbf{p}'}(\tau')\rangle e^{i(\mathbf{p}\mathbf{x}-\mathbf{p}'\mathbf{x}')}=\sum_{\mathbf{p}}\langle a_{\mathbf{p}}(\tau)a^*_{\mathbf{p}}(\tau')\rangle e^{i\mathbf{p}(\mathbf{x}-\mathbf{x}')}. \tag{7.586}$$

The small $\eta>0$ in (7.585) is necessary to specify the side of the jump of the correlation functions (recall Fig. 3.2). The expectation value of ΔE is given by (7.101), with a prefactor g rather than $g/2$ due to the two possible Wick contractions. Inserting the periodic correlation function (7.541), we obtain the Fourier integral

$$\langle\psi(\mathbf{x},\tau)\psi^*(\mathbf{x}',\tau')\rangle=\sum_{\mathbf{p}}(1+n_{\omega_{\mathbf{p}}})e^{-\omega_{\mathbf{p}}(\tau-\tau')+i\mathbf{p}(\mathbf{x}-\mathbf{x}')}. \tag{7.587}$$

Recalling the representation (3.287) of the periodic Green function in terms of a sum over Matsubara frequencies, this can also be written as

$$\langle\psi(\mathbf{x},\tau)\psi^*(\mathbf{x}',\tau')\rangle=\frac{1}{\hbar\beta}\sum_{\omega_m,\mathbf{p}}\frac{-1}{i\omega_m-\omega_{\mathbf{p}}}e^{-i\omega_m(\tau-\tau')+i\mathbf{p}(\mathbf{x}-\mathbf{x}')}. \tag{7.588}$$

The terms in the free energies (7.102) and (7.107) with the two parts (7.108) and (7.109) can then be shown to arise from the Feynman diagrams in the first line of Fig. 3.7.

In a grand-canonical ensemble, the energy $\hbar\omega_{\mathbf{p}}$ in (7.588) is replaced by $\hbar\omega_{\mathbf{p}}-\mu$. The same replacement appears in $\omega_{\mathbf{p}}$ of Eq. (7.587) which brings the distribution function $n_{\omega_{\mathbf{p}}}$ to [recall (7.542)]

$$n_{\omega_{\mathbf{p}}-\mu/\hbar}=\frac{1}{z^{-1}e^{\beta\hbar\omega_{\mathbf{p}}}-1}, \tag{7.589}$$

where z is the fugacity $z=e^{\beta\mu}$. The expansion of the Feynman integrals in powers of z yields directly the expressions (7.102) and (7.107).

7.14.4 Effective Classical Field Theory

For the purpose of studying phase transitions, a functional integral over fields $\psi(\mathbf{x},\tau)$ with an interaction (7.585) must usually be performed at a finite temperature. Then is often advisable to introduce a direct three-dimensional extension of the effective classical potential $V^{\rm eff\,cl}(x_0)$ introduced in Section 3.25 and used efficiently in Chapter 5. In a field theory we can set up, by analogy, an *effective classical action* which is a functional of the three-dimensional field with zero Matsubara frequency $\phi(\mathbf{x})\equiv\psi_0(\mathbf{x})$. The advantages come from the reasons discussed in Section 3.25, that

the zero-frequency fluctuations have a linearly diverging fluctuation width at high temperature, following the Dulong-Petit law. Thus only the nonzero-modes can be treated efficiently by the perturbative methods explained in Subsection 3.25.6.

By analogy with the splitting of the measure of path integration in Eq. (3.808), we may factorize the functional integral (7.574) into zero- and nonzero-Matsubara frequency parts as follows:

$$Z = \oint \mathcal{D}\psi\mathcal{D}\psi^* e^{-\mathcal{A}_{\rm e}[\psi^*,\psi]} = \oint \mathcal{D}\psi_0\mathcal{D}\psi_0^* \oint \mathcal{D}'\psi\mathcal{D}'\psi^* e^{-\mathcal{A}_{\rm e}[\psi^*,\psi]}, \tag{7.590}$$

and introduce the Boltzmann factor [compare (3.813)] contain the effective classical action

$$B[\psi_0^*,\psi_0] \equiv e^{-\mathcal{A}^{\rm eff\ cl}[\psi_0^*,\psi_0]} \equiv \oint \mathcal{D}'\psi\mathcal{D}'\psi^*\, e^{-\mathcal{A}_{\rm e}[\psi^*,\psi]}, \tag{7.591}$$

to express the partition function as a *functional integral* over time-independent fields in three dimensions as:

$$Z = \oint \mathcal{D}\psi_0\mathcal{D}\psi_0^* e^{-\mathcal{A}^{\rm eff\ cl}[\psi_0^*,\psi_0]}. \tag{7.592}$$

In Subsection 3.25.1 we have seen that the full effective classical potential $V^{\rm eff\ cl}(x_0)$ in Eq. (3.812) reduces in the high-temperature limit to the initial potential $V(x_0)$. For the same reason, the full effective classical action in the functional integral (7.590) can be approximated at high temperature by the *bare effective classical action*, which is simply the zero-frequency part of the initial action:

$$\mathcal{A}_{\rm b}^{\rm eff\ cl}[\psi_0^*,\psi_0] = \beta \int d^3x \left\{ \psi_0^*(\mathbf{x}) \left(-\frac{1}{2m}\nabla^2 - \mu \right) \psi_0(\mathbf{x}) + \frac{2\pi a}{m} \left[\psi_0^*(\mathbf{x})\psi_0(\mathbf{x})\right]^2 \right\}. \tag{7.593}$$

This follows directly from the fact that, at high temperature, the fluctuations in the functional integral (7.591) are strongly suppressed by the large Matsubara frequencies in the kinetic terms.

Remarkably, the absence of a shift in the critical temperature in the first-order energy (7.113) deduced from Eq. (7.116) implies that the chemical potential in the effective classical action does not change at this order [34]. For this reason, the lowest-order shift in the critical temperature of a weakly interacting Bose-Einstein condensate can be calculated entirely from the three-dimensional effective classical field theory (7.590) with the bare effective classical action (7.593) in the Boltzmann factor.

The action (7.593) may be brought to a more conventional form by introducing the differently normalized two-component fields $\phi = (\phi_1, \phi_2)$ related to the original complex field ψ by $\psi(\mathbf{x}) = \sqrt{MT}[\phi_1(\mathbf{x}) + i\phi_2(\mathbf{x})]$. If we also define a square mass $m^2 \equiv -2M\mu$ and a quartic coupling $u = 48\pi aMT$, the bare effective classical action reads

$$\mathcal{A}_{\rm b}^{\rm eff\ cl}[\psi_0^*,\psi_0] = \mathcal{A}[\phi] = \int d^3x \left[\frac{1}{2}|\nabla\phi|^2 + \frac{1}{2}m^2\phi^2 + \frac{u}{4!}(\phi^2)^2 \right]. \tag{7.594}$$

In the field theory governed by the action (7.594), the relation (7.111) for the shift of the critical temperature to lowest order in the coupling constant becomes

$$\begin{aligned}\frac{\Delta T_c}{T_c^{(0)}} &\approx -\frac{2}{3}\frac{mT_c^{(0)}}{n}\left\langle\Delta\phi^2\right\rangle = -\frac{4\pi}{3}\frac{(mT_c^{(0)})^2}{n}4!\left\langle\frac{\Delta\phi^2}{u}\right\rangle a \\ &= -\frac{4\pi}{3}\frac{(2\pi)^2}{[\zeta(3/2)]^{4/3}}4!\left\langle\frac{\Delta\phi^2}{u}\right\rangle an^{1/3},\end{aligned} \tag{7.595}$$

where $\langle\Delta\phi^2\rangle$ is the shift in the expectation value of ϕ^2 caused by the interaction. Since a repulsive interaction pushes particles apart, $\langle\Delta\phi^2\rangle$ is negative, thus explaining the positive shift in the critical temperature. The evaluation of the expectation value $\langle\Delta\phi^2\rangle$ from the path integral (7.590) with the bare three-dimensional effective classical action (7.594) in the exponent can now proceed within one of the best-studied field theories in the literature [51]. The theoretical tools for calculating strong-coupling results in this theory are well developed, and this has made it possible to drive the calculations of the shift to the five-loop order [21].

Some low-order corrections to the effective classical action (7.593) have been calculated from the path integral (7.591) in Ref. [34].

7.15 Bosonization

The path integral formulation of quantum-mechanical systems is very flexible. Just as integrals can be performed in different variables of integration, so can path integrals in different path variables. This has important applications in many-body systems, which show a rich variety of so-called collective phenomena. Practically all fermion systems show collective excitations such as sound, second sound, and spin waves. These are described phenomenologically by bosonic fields. In addition, there are phase transitions whose description requires a bosonic order parameter. Superconductivity of electron systems is a famous example where a bosonic order parameter appears in a fermion system—the energy gap. In all these cases it is useful to transform the initial path variables to so-called collective path variables, in higher dimensions these become *collective fields* [32].

Let us illustrate the technique with simple a model defined by the Lagrangian

$$L(t) = a^*(t)i\partial_t a(t) - \frac{\varepsilon}{2}\left[a^*(t)a(t)\right]^2, \tag{7.596}$$

where a^*, a are commuting or anticommuting variables. All Green functions can be calculated from the generating functional

$$Z[\eta^*,\eta] = N\int \mathcal{D}a^* Da \exp\left[i\int dt\,(L+\eta^* a + a^*\eta)\right], \tag{7.597}$$

where we have omitted an irrelevant overall factor.

In operator language, the model is defined by the Hamiltonian operator

$$\hat{H} = \varepsilon(\hat{a}^\dagger\hat{a})^2/2, \tag{7.598}$$

where $\hat{a}^\dagger$, $\hat{a}$ are creation and annihilation operator of either a boson or a fermion at a point. In the boson case, the eigenstates are

$$|n\rangle = \frac{1}{\sqrt{n!}}(\hat{a}^\dagger)^n|0\rangle, \qquad n = 0, 1, 2, \dots \ , \tag{7.599}$$

with an energy spectrum

$$E_n = \varepsilon\frac{n^2}{2}. \tag{7.600}$$

In the fermion case, there are only two solutions

$$|0\rangle \qquad \text{with} \quad E_0 = 0, \tag{7.601}$$

$$|1\rangle = a^\dagger|0\rangle \quad \text{with} \quad E_1 = \frac{\varepsilon}{2}. \tag{7.602}$$

Here the Green functions are obtained from the generating functional

$$Z[\eta^\dagger, \eta] \ = \ \langle 0|\hat{T}\exp\left[i\int dt(\eta^*\hat{a} + \hat{a}^\dagger\eta)\right]|0\rangle, \tag{7.603}$$

where $\hat{T}$ is the time ordering operator (1.241). The functional derivatives with respect to the sources η^*, η generate all Green functions of the type (3.299) at $T = 0$.

7.15.1 Collective Field

At this point we introduce an additional *collective field* via the Hubbard-Stratonovich transformation [52]

$$\exp\left\{-i\frac{\varepsilon}{2}\int dt[a^*(t)a(t)]^2\right\} = N\int \mathcal{D}\rho(t)\exp\left\{i\int dt\left[\frac{\rho^2(t)}{2\varepsilon} - \rho(t)a^*(t)a(t)\right]\right\}, \tag{7.604}$$

where N is some irrelevant factor. Equivalently we multiply the partition function (7.597) with the trivial Gaussian path integral

$$1 = N\int \mathcal{D}\rho(t)\exp\left\{\int dt\,\frac{1}{2\varepsilon}\left[\rho(t) - \varepsilon a^\dagger(t)a(t)\right]^2\right\}, \tag{7.605}$$

to obtain the generating functional

$$Z[\eta^\dagger, \eta] = N\int \mathcal{D}a^*\mathcal{D}a\mathcal{D}\rho$$
$$\times\exp\left\{\int dt\left[a^*(t)i\partial_t a(t) - \varepsilon\rho(t)a^*(t)a(t) + \frac{\rho^2(t)}{2\varepsilon} + \eta^*(t)a(t) + a^*(t)\eta(t)\right]\right\}. \tag{7.606}$$

From (7.604) we see that the collective field $\rho(t)$ fluctuates harmonically around ε times particle density. By extremizing the action in (7.606) with respect to $\rho(t)$ we obtain the classical equality:

$$\rho(t) = \varepsilon a^*(t)a(t). \tag{7.607}$$

The virtue of the Hubbard-Stratonovich transformation is that the fundamental variables a^*, a appear now quadratically in the action and can be integrated out to yield a path integral involving only the collective variable $\rho(t)$:

$$Z[\eta^*,\eta] \;=\; N\int \mathcal{D}\rho \exp\left\{i\mathcal{A}[\rho] - \int dtdt'\eta^*(t)G_\rho(t,t')\eta(t')\right\}, \tag{7.608}$$

with the collective action

$$\mathcal{A}[\rho] = \pm i\mathrm{Tr}\,\log\left(iG_\rho^{-1}\right) + \int dt\frac{\rho^2(t)}{2}, \tag{7.609}$$

where G_ρ denotes the Green function of the fundamental path variables in an external $\rho(t)$ background potential, which satisfies [compare (3.75)]

$$[i\partial_t - \rho(t)]\,G_\rho(t,t') = i\delta(t-t'). \tag{7.610}$$

The Green function was found in Eq. (3.124). Here we find the solution once more in a different way which will be useful in the sequel. We introduce an auxiliary field

$$\varphi(t) = \int^t \rho(t')dt', \tag{7.611}$$

in terms of which $G_\rho(t,t')$ is simply

$$G_\rho(t,t') = e^{-i\varphi(t)}e^{i\varphi(t')}G_0(t-t'), \tag{7.612}$$

with G_0 being the free-field propagator of the fundamental particles. At this point one has to specify the boundary condition on $G_0(t-t')$. They have to be adapted to the physical situation of the system. Suppose the time interval is infinite. Then G_0 is given by Eq. (3.100), so that we obtain, as in (3.124),

$$G_\rho(t,t') = e^{-i\varphi(t)}e^{i\varphi(t')}\bar{\Theta}(t-t'). \tag{7.613}$$

The Heaviside function $\bar{\Theta}$ defined in Eq. (1.313) corresponds to $\rho(t)$ coupling to the symmetric operator combination $(\hat{a}^\dagger\hat{a}+\hat{a}\hat{a}^\dagger)/2$. The products $\hat{a}^\dagger\hat{a}$ in the Hamiltonian (7.598), however, have the creation operators left of the annihilation operators. In this case we must use the Heaviside function $\Theta(t-t')$ of Eq. (1.304). If this function is inserted into (7.613), the right-hand side of (7.613) vanishes at $t=t'$.

Using this property we see that the functional derivative of the tracelog in (7.609) vanishes:

$$\frac{\delta}{\delta\rho(t)}\left\{\pm i\mathrm{Tr}\,\log(iG_\rho^{-1})\right\} = \frac{\delta}{\delta\rho(t)}\left\{\pm i\mathrm{Tr}\,\log\left[i\partial_t - \rho(t)\right]\right\} = \mp G_\rho(t,t')|_{t'=t} = 0. \tag{7.614}$$

This makes the tracelog an irrelevant constant. The generating functional is then simply

$$Z[\eta^\dagger,\eta] = N\int \mathcal{D}\varphi(t)\exp\left\{\frac{i}{2\varepsilon}\int dt\,\dot{\varphi}(t)^2 - \int dtdt'\eta^\dagger(t)\eta(t')e^{-i\varphi(t)}e^{-i\varphi(t')}\Theta(t-t')\right\}, \tag{7.615}$$

where we have used the Jacobian

$$\mathcal{D}\rho = \mathcal{D}\varphi \,\mathrm{Det}(\partial_t) = \mathcal{D}\varphi, \tag{7.616}$$

since $\mathrm{Det}(\partial_t) = 1$ according to (2.537). Observe that the transformation (7.611) provides $\varphi(t)$ with a standard kinetic term $\dot{\varphi}^2(t)$.

The original theory has been transformed into a new theory involving the collective field φ. In a three-dimensional generalization of this theory to electron gases, the field φ describes density waves [32].

7.15.2 Bosonized versus Original Theory

The first term in the bosonized action in (7.615) is due to a Lagrangian

$$L_0(t) = \frac{1}{2\varepsilon}\dot{\varphi}(t)^2 \tag{7.617}$$

describing free particles on the infinite φ-axis. Its correlation function is divergent and needs a small frequency, say κ, to exist. Its small-κ expansion reads

$$\begin{aligned} \langle\varphi(t)\varphi(t')\rangle &= \varepsilon \int \frac{d\omega}{2\pi} \frac{i}{\omega^2 - \kappa^2 + i\epsilon} e^{-i\omega(t-t')} \\ &= \frac{\varepsilon}{2\kappa} e^{-\kappa|t-t'|} = \frac{\varepsilon}{2\kappa} - \varepsilon\,\frac{i}{2}|t-t'| + \mathcal{O}(\kappa). \end{aligned} \tag{7.618}$$

The first term plays an important role in calculating the bosonized correlation functions generated by $Z[\eta^*, \eta]$ in Eq. (7.615). Differentiating this n times with respect to η and η^* and setting them equal to zero we obtain

$$\begin{aligned} G^{(n)}(t_n, \ldots, t_1; t'_n, \ldots, t'_1) &= (-1)^n \langle e^{-i\varphi(t_n)} \cdots e^{-i\varphi(t_1)}\, e^{i\varphi(t'_n)} \cdots e^{i\varphi(t'_1)} \rangle \\ &\times \sum_p \epsilon_p \Theta(t_{p_1} - t_1) \cdots \Theta(t_{p_n} - t_1), \end{aligned} \tag{7.619}$$

where the sum runs over all permutations p of the time labels of $t_1 \ldots t_n$ making sure that these times are all later than the times $t'_1 \ldots t'_n$. The factor ϵ_p reflects the commutation properties of the sources η, η^*, being equal to 1 for all permutations if η and η^* commute. For Grassmann variables η, η^*, the factor ϵ_p is equal to -1 if the permutation p is odd. The expectation value is defined by the path integral

$$\langle \ \ldots \ \rangle \equiv \frac{1}{Z[0,0]} \int \mathcal{D}\varphi(t) \ldots \ e^{(i/2\varepsilon)\int dt\, \dot{\varphi}(t)^2}. \tag{7.620}$$

Let us calculate the expectation value of the exponentials in (7.619), writing it as

$$\left\langle \exp\left[i \sum_{i=1}^{2n} q_i \varphi(t_i) \right] \right\rangle = \left\langle \exp\left[\sum_i \int dt\, \delta(t - t_i) q_i \varphi(t) \right] \right\rangle, \tag{7.621}$$

where we have numbered the times as $t_1, t_2, \dots t_{2n}$ rather than $t_1, t'_1, t_2, t'_2, \dots t_n, t'_n$. Half of the $2n$ "charges" q_i are 1, the other half are -1. Using Wick's theorem in the form (3.310) we find

$$\begin{aligned}\left\langle e^{i\sum_{i=1}^{2n} q_i\varphi(t_i)}\right\rangle &= \exp\left[-\frac{1}{2}\int dtdt' \sum_{i=1}^{2n} q_i\delta(t-t_i)\langle\varphi(t)\varphi(t')\rangle(t')\sum_j q_j\delta(t-t_j)\right] \\ &= \exp\left[-\frac{1}{2}\sum_{i,j=1}^{2n} q_iq_j\langle\varphi(t_i)\varphi(t_j)\rangle\right]. \end{aligned} \tag{7.622}$$

Inserting here the small-κ expansion (7.618), we see that the $1/\kappa$-term gives a prefactor

$$\exp\Big[-\frac{\varepsilon}{4\kappa}\left(\sum_i q_i\right)^2\Big], \tag{7.623}$$

which vanishes since the sum of all "charges" q_i is zero. Hence we can go to the limit $\kappa \to 0$ and obtain

$$\left\langle \exp\left[i\sum_{i=1}^{2n} q_i\varphi(t_i)\right]\right\rangle = \exp\left[\varepsilon\,\frac{i}{2}\sum_{i>j} q_iq_j|t_i-t_j|\right]. \tag{7.624}$$

Note that the limit $\kappa \to 0$ makes all correlation functions vanish which do not contain an equal number of $a^*(t)$ and $a(t)$ variables. It ensures "charge conservation".

For one positive and one negative charge we obtain, after a multiplication by a Heaviside function $\Theta(t_1 - t'_1)$, the two-point function

$$G^{(2)}(t,t') = e^{-i\varepsilon(t-t')/2}\Theta(t-t'). \tag{7.625}$$

This agrees with the operator result derived from the generating functional (7.603), where

$$G^{(2)}(t,t') = \langle 0|\hat{T}\hat{a}(t)\hat{a}^\dagger(t')|0\rangle = \Theta(t-t')\langle 0|\hat{a}(t)\hat{a}^\dagger(t')|0\rangle e^{-i\varepsilon(t-t')/2}\Theta(t-t'). \tag{7.626}$$

Inserting the Heisenberg equation [recall (1.277)]

$$a(t) = e^{it\hat{H}}ae^{-it\hat{H}}, \qquad a^\dagger(t') = e^{it'\hat{H}}a^\dagger e^{-it'\hat{H}}. \tag{7.627}$$

we find

$$\begin{aligned}\langle 0|\hat{T}\hat{a}(t)\hat{a}^\dagger(t')|0\rangle &= \Theta(t-t')\langle 0|e^{i\varepsilon(\hat{a}^\dagger\hat{a})^2t/2}ae^{-\frac{i}{2}(\hat{a}^\dagger\hat{a})^2(t-t')}\hat{a}^\dagger e^{-i(\hat{a}^\dagger\hat{a})^2t'/2}|0\rangle \\ &= \Theta(t-t')\langle 1|e^{-\frac{i}{2}(\hat{a}^\dagger\hat{a})^2(t-t')}|1\rangle = \Theta(t-t')e^{-i\varepsilon(t-t')/2}. \end{aligned} \tag{7.628}$$

Let us compare the above calculations with an operator evaluation of the bosonized theory. The Hamiltonian operator associated with the Lagrangian (7.617) is $\hat{H} = \varepsilon\hat{p}^2/2$. The states in the Hilbert space are eigenstates of the momentum operator $\hat{p} = -i\partial/\partial\varphi$:

$$\{\varphi|p\} = \frac{1}{\sqrt{2\pi}}e^{ip\varphi}. \tag{7.629}$$

Here, curly brackets are a modified Dirac notation for states of the bosonized theory, which distinguishes them from the states of the original theory created by products of operators $\hat{a}^\dagger(t)$ acting on $|0\rangle$. In operator language, the generating functional of the theory (7.615) reads

$$Z[\eta^\dagger,\eta]=\frac{1}{\{0|0\}}\{0|\hat{T}\exp\left[-\int dtdt'\eta^\dagger(t)\eta(t')e^{-i\hat{\varphi}(t)}e^{i\hat{\varphi}(t')}\Theta(t-t')\right]|0\}, \quad (7.630)$$

where $\hat{\varphi}(t)$ are free-particle operators.

We obtain all Green functions of the initial operators $\hat{a}(t),\hat{a}^\dagger(t)$ by forming functional derivatives of the generating functional $Z[\eta^\dagger,\eta]$ with respect to $\eta^\dagger,\eta$. Take, for instance, the two-point function

$$\langle 0|\hat{T}\hat{a}(t)\hat{a}^\dagger(t')|0\rangle=-\frac{\delta^{(2)}Z}{\delta\eta^\dagger(t)\delta\eta(t')}\bigg|_{\eta^\dagger,\eta=0}=\frac{1}{\{0|0\}}\{0|e^{-i\hat{\varphi}(t)}e^{i\hat{\varphi}(t')}|0\}\Theta(t-t'). \quad (7.631)$$

Inserting here the Heisenberg equation (1.277),

$$\hat{\varphi}(t)=e^{i\varepsilon\frac{\hat{p}^2}{2}t}\,\hat{\varphi}(0)\,e^{-i\varepsilon\frac{\hat{p}^2}{2}t}, \quad (7.632)$$

we can evaluate the matrix element in (7.631) as follows:

$$\{0|e^{i\varepsilon\frac{\hat{p}^2}{2}t}2e^{-i\hat{\varphi}(0)}e^{-i\varepsilon\frac{\hat{p}^2}{2}(t-t')}e^{i\hat{\varphi}(0)}e^{-i\varepsilon\frac{\hat{p}^2}{2}t'}|0\}=\{0|e^{-i\hat{\varphi}(0)}e^{-i\varepsilon\frac{\hat{p}^2}{2}(t-t')}e^{i\hat{\varphi}(0)}|0\}. \quad (7.633)$$

The state $e^{i\hat{\varphi}(0)}|0\}$ is an eigenstate of $\hat{p}$ with unit momentum $|1\}$ and the same norm as $|0\}$, so that (7.633) equals

$$\frac{1}{\{0|0\}}\,\{1|1\}\,e^{-i\varepsilon(t-t')/2}=e^{-i\varepsilon(t-t')/2} \quad (7.634)$$

and the Green function (7.631) becomes, as in (7.626) and (7.628):

$$\langle 0|\hat{T}\hat{a}(t)\hat{a}^\dagger(t')|0\rangle=e^{-i\varepsilon(t-t')/2}\Theta(t-t'). \quad (7.635)$$

Observe that the Fermi and Bose statistics of the original operators $\hat{a},\hat{a}^\dagger$ enters to result only via the commutation properties of the sources.

There exists also the opposite phenomenon that a bosonic theory possesses solutions which behave like fermions. This will be discussed in Section 8.12.

Appendix 7A 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.

7A.1 Finite Box

According to Eqs. (7.83), (7.88), and (7.90), 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

$$N = N_{\rm n}(T) + N_{\rm cond}(T) = S_D(z_D) + \frac{z_D}{1-z_D}, \tag{7A.1}$$

where $S_D(z_D)$ is the subtracted infinite sum

$$S_D(z_D) \equiv \sum_{w=1}^{\infty} [Z_1^D(wb)e^{wDb/2} - 1]z_D^w, \tag{7A.2}$$

containing the Dth power of 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

$$Z_1(b) = e^{-b/2}\left[1 + e^{-3b/2}\sigma_1(b)\right], \tag{7A.3}$$

where $\sigma_1(b)$ is related to the elliptic theta function (7.85) by

$$\sigma_1(b) \equiv \sum_{k=2}^{\infty} e^{-(k^2-4)b/2} = \frac{e^{2b}}{2}\left[\vartheta_3(0, e^{-b/2}) - 1 - 2e^{-b/2}\right]. \tag{7A.4}$$

According to Eq. (7.87), this has the small-b behavior

$$\sigma_1(b) = \sqrt{\frac{\pi}{2b}}e^{2b} - e^{3b/2} - \frac{1}{2}e^{2b} + \dots\ . \tag{7A.5}$$

The omitted terms are exponentially small as long as $b < 1$ [see the sum over m in Eq. (7.86)]. For large b, these terms become important to ensure an exponentially fast falloff like $e^{-3b/2}$. Inserting (7A.3) into (7A.2), we find

$$S_D(1) \equiv D\sum_{w=1}^{\infty}\left[\sigma_1(wb)e^{-3wb/2} + \frac{D-1}{2}\sigma_1^2(wb)e^{-6wb/2} + \frac{(D-1)(D-2)}{6}\sigma_1^3(wb)e^{-9wb/2}\right]. \tag{7A.6}$$

Inserting here the small-b expression (7A.5), we obtain

$$S_2(1) \equiv \sum_{w=1}^{\infty}\left(\frac{\pi}{2wb}e^{wb} - \sqrt{\frac{\pi}{2wb}}e^{wb} + \frac{1}{4}e^{wb} - 1\right) + \dots\ , \tag{7A.7}$$

$$S_3(1) \equiv \sum_{w=1}^{\infty}\left(\sqrt{\frac{\pi}{2wb}}^3 e^{3wb/2} - \frac{3}{2}\frac{\pi}{2wb}e^{3wb/2} + \frac{3}{4}\sqrt{\frac{\pi}{2wb}}e^{3wb/2} - \frac{1}{8}e^{3wb/2} - 1\right) + \dots\ , \tag{7A.8}$$

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 (7.34), and we find, using also $\sum_{w=1}^{\infty} 1 = \zeta(0) = -1/2$ from (2.522),

$$S_2(1) = \zeta_1(e^b) - \sqrt{\frac{\pi}{2b}}\zeta_{1/2}(e^b) + \frac{1}{4}\zeta_0(e^b) - \zeta(0) + \dots\ . \tag{7A.9}$$

$$S_3(1) = \sqrt{\frac{\pi}{2b}}^3 \zeta_{3/2}(e^{3b/2}) - \frac{3}{2}\frac{\pi}{2b}\zeta_1(e^{3b/2}) + \frac{3}{4}\sqrt{\frac{\pi}{2b}}\zeta_1(e^{3b/2}) - \frac{1}{8}\zeta_0(e^{3b/2}) - \zeta(0) + \dots\ . \tag{7A.10}$$

These expressions can now be expanded in powers of b with the help of the Robinson expansion (2.581). Afterwards, b is continued analytically to positive values and we obtain

$$S_2(1) = -\frac{\pi}{2b}\log(C_2 b) - \sqrt{\frac{\pi}{2b}}\zeta(1/2) + \frac{1}{8}(3-2\pi) + \mathcal{O}(b^{1/2}), \tag{7A.11}$$

$$S_3(1) = \sqrt{\frac{\pi}{2b}}^3 \zeta(3/2) + \frac{3\pi}{4b}\log(C_3 b) + \frac{3}{4}\sqrt{\frac{\pi}{2b}}\zeta(1/2)(1+\pi) + \frac{9}{16}(1+\pi) + \mathcal{O}(b^{1/2}). \tag{7A.12}$$

The constants $C_{2,3}, C'_{2,3}$ inside the logartithms turn out to be complex, implying that the limiting expressions (7A.7) and (7A.8) cannot be used reliably. A proper way to proceed gors as follows. We subtract from $S_D(1)$ terms which remove the small-b singularties by means of modifications of (7A.7) and (7A.8) which have the same small-b expansion up to b^0:

$$\tilde{S}_2(1) \equiv \sum_{w=1}^{\infty}\left(\frac{\pi}{2wb} - \sqrt{\frac{\pi}{2wb}} + \frac{4\pi-3}{4}\right)e^{-wb} + \dots, \tag{7A.13}$$

$$\tilde{S}_3(1) \equiv \sum_{w=1}^{\infty}\left[\sqrt{\frac{\pi}{2wb}}^3 - \frac{3}{2}\frac{\pi}{2wb} + \frac{3}{4}(1+2\pi)\sqrt{\frac{\pi}{2wb}} - \frac{9}{8}(1+2\pi)\right]e^{-3wb/2} + \dots. \tag{7A.14}$$

In these expressions, the sums over w can be performed for positive b yielding

$$\tilde{S}_2(1) \equiv \frac{\pi}{2b}\zeta_1(e^{-b}) - \sqrt{\frac{\pi}{2b}}\zeta_{1/2}(e^{-b}) + \frac{4\pi-3}{4}\zeta_0(e^{-b}) + \dots, \tag{7A.15}$$

$$\tilde{S}_3(1) \equiv \sqrt{\frac{\pi}{2b}}^3 \zeta_{3/2}(e^{-3b/2}) - \frac{3}{2}\frac{\pi}{2b}\zeta_1(e^{-3b/2}) + \frac{3}{4}(1+2\pi)\sqrt{\frac{\pi}{2b}}\zeta_{1/2}(e^{-3b/2}) - \frac{9}{8}(1+2\pi)\zeta_0(e^{-3b/2}) + \dots. \tag{7A.16}$$

Inserting again the Robinson expansion (2.581), we obtain once more the above expansions (7A.11) and (7A.12), but now with the well-determined real constants

$$\tilde{C}_2 = e^{3/2\pi - 2 + \sqrt{2}} \approx 0.8973, \qquad \tilde{C}_3 = \frac{3}{2}e^{-2+1/\sqrt{3}-1/\pi} \approx 0.2630. \tag{7A.17}$$

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:

$$\int_0^\infty dw[S_2(1) - \tilde{S}_2(1)] = -\frac{1.1050938}{b}, \quad \int_0^\infty dw[S_3(1) - \tilde{S}_3(1)] = 3.0441. \tag{7A.18}$$

These modify the constants $\tilde{C}_{2,3}$ to

$$C_2 = 1.8134, \quad C_3 = 0.9574. \tag{7A.19}$$

The corrections to the sums over $S_D(1) - \tilde{S}_D(1)$ are of order b^0 an higher and already included in the expansions (7A.11) and (7A.12), which were only unreliable as far as $C_{2,3}$ os concerned.

Let us calculate from (7A.12) the finite-size correction to the critical temperature by equating $S_3(1)$ with N. Expressing this in terms of $b_c^{(0)}$ via (7.92), 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 $2b_c^{(0)}/\pi = [\zeta(3/2)/N]^{2/3}$:

$$\hat{b}_c^{3/2} = 1 + \sqrt{\frac{2b_c^{(0)}}{\pi}}\frac{3\sqrt{\hat{b}_c}}{2\zeta(3/2)}\log(C_3 b_c^{(0)}\hat{b}_c) + \frac{2b_c^{(0)}}{\pi}\frac{3}{4\zeta(3/2)}\zeta(1/2)(1+\pi)\hat{b}_c + \dots. \tag{7A.20}$$

To lowest order, the solution is simply

$$\hat{b}_c = 1 + \sqrt{\frac{2b_c^{(0)}}{\pi}}\,\frac{1}{\zeta(3/2)}\log(C_3 b_c^{(0)}) + \dots\ , \tag{7A.21}$$

yielding the would-be critical temperature to first in $1/N^{1/3}$ as stated in (7.94). To next order, we insert into the last term the zero-order solution $\hat{b}_c \approx 1$, and in the second term the first-order solution (7A.21) to find

$$\begin{aligned}\hat{b}_c^{3/2} &= 1 + \frac{3}{2}\sqrt{\frac{2b_c^{(0)}}{\pi}}\,\frac{1}{\zeta(3/2)}\log(C_3 b_c^{(0)}) \\ &+ \frac{2b_c^{(0)}}{\pi}\,\frac{3}{4\zeta(3/2)}\left\{\zeta(1/2)(1+\pi) + \frac{1}{\zeta(3/2)}\left[2\log(C_3 b_c^{(0)}) + \log^2(C_3 b_c^{(0)})\right]\right\} + \dots\ .\end{aligned} \tag{7A.22}$$

Replacing $b_c^{(0)}$ by $(2/\pi)\,[\zeta(3/2)/N]^{2/3}$, this gives us 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. 7.12, together with precise results from numeric solution of the equation $N = S_3(1)$.

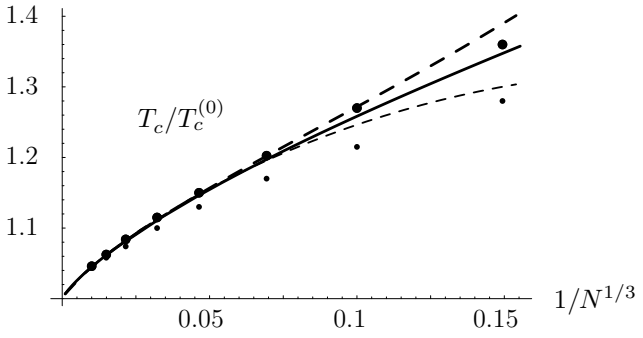

Figure 7.12 Finite-size corrections to the critical temperature for $N = 300$ to infinity calculated once from the formula $N = S_3(1)$ (solid curve) and once from the expansion (7A.22) (short-dashed up to order $[b_c^{(0)}]^{1/2} \propto 1/N^{1/3}$, long-dashed up to the order $b_c^{(0)} \propto 1/N^{2/3}$). The fat dots show the peaks in the second derivative $d^2N_{\rm cond}(T)/dT^2$. The small dots show the corresponding values for canonical ensembles, for comparison.

7A.2 Harmonic Trap

The sum relevant for the would-be phase transition in a harmonic trap is (7.138),

$$S_D(b, z_D) = \sum_{w=1}^{\infty}\left[\frac{1}{(1-e^{-wb})^D} - 1\right] z_D^w, \tag{7A.23}$$

which determines the number of normal particles in the harmonic trap via Eq. (7.139). We consider only the point $z_D = 1$ which determines the critical temperature by the condition $N_{\rm n} = N$. Restricting ourselves to the physical cases $D = 1, 2, 3$, we rewrite the sum as

$$S_D(b,1) = \sum_{w=1}^{\infty} D\left[e^{-wb} - \frac{(D-1)}{2}e^{-2wb} + \frac{(D-1)(D-2)}{6}e^{-3wb}\right]\frac{1}{(1-e^{-wb})^D}. \tag{7A.24}$$

According to the method developed in the evaluation of Eq. (2.581) 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 (7A.24) cannot be converted into an integral due to singularities at $w = 0$. These have to be first removed by subtractions. Thus we decompose $S_D(b,1)$ into a subtracted sum plus a remainder as

$$S_D(b,1) \;=\; \bar{S}_D(b,1) + \Delta_D S_D(b,1) + b\frac{D}{2}\Delta_{D-1}S_D(b,1) + b^2\frac{D(3D-1)}{24}\Delta_{D-2}S_D(b,1), \tag{7A.25}$$

where

$$\begin{aligned}\bar{S}_D(b,1) \;&=\; \sum_{w=1}^{\infty} D\left[e^{-wb} - \frac{D-1}{2}e^{-2wb} + \frac{(D-1)(D-2)}{6}e^{-3wb}\right] \\ &\times\; \left[\frac{1}{(1-e^{-wb})^D} - \frac{1}{w^D b^D} - \frac{D}{2w^{D-1}b^{D-1}} - \frac{D(3D-1)}{24w^{D-2}b^{D-2}}\right]\end{aligned} \tag{7A.26}$$

is the subtracted sum and

$$\Delta_{D'}S_D(b,1) \equiv \frac{D}{b^D}\left[\zeta_{D'}(e^{-b}) - \frac{D-1}{2}\zeta_{D'}(e^{-2b}) + \frac{(D-1)(D-2)}{6}\zeta_{D'}(e^{-3b})\right] \tag{7A.27}$$

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:

$$\int_0^\infty dx \frac{e^{-ax}}{(1-e^{-x})^b} = B(a,1-b) = \frac{\Gamma(a)\Gamma(1-b)}{\Gamma(1+a-b)}. \tag{7A.28}$$

This yields the small-b contributions to the subtracted sums

$$\begin{aligned}\bar{S}_1(b,1) \;&\underset{b\to 0}{\to}\; \frac{1}{b}\left(\gamma - \frac{7}{12}\right) \equiv s_1, \\ \bar{S}_2(b,1) \;&\underset{b\to 0}{\to}\; \frac{1}{b}\left(\gamma + \log 2 - \frac{9}{8}\right) \equiv s_2, \\ \bar{S}_3(b,1) \;&\underset{b\to 0}{\to}\; \frac{1}{b}\left(\gamma + \log 3 - \frac{19}{24}\right) \equiv s_3,\end{aligned} \tag{7A.29}$$

where $\gamma = 0.5772\ldots$ is the Euler-Mascheroni number (2.469). 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 formula (2.584). However, due to the subtractions, the corrections are all small of order $(1/b^D)\mathcal{O}(b^3)$, and will be ignored here. Thus we obtain

$$S_D(b,1) = \frac{s_D}{b^D} + \Delta S_D(b,1) + \frac{1}{b^D}\mathcal{O}(b^3). \tag{7A.30}$$

We now expand $\Delta_{D'}S_D(b,1)$ using Robinson's formula (2.583) up to b^2/b^D and find

$$\Delta_{D'}S_1(b,1) \;=\; \frac{1}{b}\zeta_{D'}(e^{-b}),$$

$$\Delta_{D'}S_2(b,1) \;=\; \frac{1}{b^2}\left[2\zeta_{D'}(e^{-b}) - \zeta_{D'}(e^{-2b})\right], \tag{7A.31}$$

$$\Delta_{D'}S_3(b,1) \;=\; \frac{1}{b^3}\left[3\zeta_{D'}(e^{-b}) - 3\zeta_{D'}(e^{-2b}) + \zeta_{D'}(e^{-3b})\right], \tag{7A.32}$$

where

$$\zeta_1(e^{-b}) \;=\; -\log\left(1-e^{-b}\right) = -\log b + \frac{b}{2} - \frac{b^2}{24} + \ldots\,,$$

$$\zeta_2(e^{-b}) = \zeta(2) + b(\log b - 1) - \frac{b^2}{4} + \dots , \tag{7A.33}$$

$$\zeta_3(e^{-b}) = \zeta(3) - \frac{b}{6}\zeta(2) - \frac{b^2}{2}\left(\log b - \frac{3}{2}\right) + \dots , \tag{7A.34}$$

The results are

$$\begin{aligned} S_1(b,1) &= \frac{1}{b}\left[(-\log b + \gamma) + \frac{b}{4} - \frac{b^2}{144} + \dots\right], \\ S_2(b,1) &= \frac{1}{b^2}\left[\zeta(2) - b\left(\log b - \gamma + \frac{1}{2}\right) + \frac{7b^2}{24} + \dots\right], \\ S_3(b,1) &= \frac{1}{b^3}\left[\zeta(3) + \frac{3b}{2}\zeta(2) - b^2\left(\log b - \gamma + \frac{19}{24}\right) + \dots\right], \end{aligned} \tag{7A.35}$$

as stated in Eqs. (7.165)–(7.167).

Note that the calculation cannot be shortened by simply expanding the factor $1/(1-e^{-wb})^D$ in the unsubtracted sum (7A.24) in powers of w, which would yield the result (7A.25) without the first term $\bar{S}_1(b,1)$, and thus without the integrals (7A.29).

Appendix 7B Experimental versus Theoretical Would-be Critical Temperature

In Fig. 7.12 we have seen that there is only a small difference between the theoretical would-be critical temperature T_c of a finite system calculated from the equation $N = S_2(1)$ and and the experimental $T_c^{\rm exp}$ determined from the maximum of the second derivative of the condensate fraction $\rho \equiv N_{\rm cond}/N$. Let us extimate the difference. The temperature T_c is found by solving the equation [recall (7.90)]

$$N = S_D(1) \equiv \sum_{w=1}^{\infty}[Z_1^D(wb_c)e^{wDb/2} - 1]. \tag{7B.1}$$

To find the latter we must solve the full equation (7A.1) and search for the maximum of $d^2N_{\rm cond}(T)/dT^2$. The last term in (7A.1) can be expressed in terms of the condensate fraction $\rho(T)$ as $N_{\rm cond}(T) = \rho(T)N$. Near the critical point, we set $\delta z_D \equiv 1 - z_D$ and see that it is equal to $\delta z_D = 1/(1+N\rho)$

In the critical regime, ρ and $1/N\rho$ are both of the same order $1/\sqrt{N}$. Thus we expand $S_D(z_D)$ to lowest order in $\delta z_D = 1/N\rho + \dots$, and replace (7A.1) by

$$N \approx [S_D(1) + \partial_b S_D(1)\delta b - \partial_{z_D} S_D(1)\,(1/N\rho - 1/N + \dots)] + \rho N, \tag{7B.2}$$

or

$$\frac{b\partial_b S_D(1)}{S_D(1)}\frac{\delta b}{b} \approx \frac{\partial_{z_D} S_D(1)}{S_D(1)}\frac{1}{N\rho} - \rho + \dots , \tag{7B.3}$$

In this leading-order discussion we may ignore the finite-size correction to $S_D(1)$, i.e., the difference between $T_c^{(0)}$ and $T_c^{(1)}$, so that $S_D(1) = (\pi/2b_c^{(0)})^{D/2}$, and we may approximate the left-hand side of (7B.3) by $(D/2)\delta T/T_c^{(0)}$. Abbreviating $\partial_{z_D} S_D(1)/S_D(1)$ by A which is of order unity, we must find $\rho(T)$ from the the equation

$$\frac{D}{2}t \approx \frac{A}{N\rho} - \rho - \frac{A}{N}, \tag{7B.4}$$

where $t \equiv \delta T/T_c^{(0)}$. This yields

$$\rho(t) = \sqrt{\frac{A}{N}} - \frac{D}{4}t + \frac{D^2}{32}\sqrt{\frac{N}{A}}t^2 - \frac{D^4}{2048}\sqrt{\frac{N}{A}}^3 t^4 + \dots . \tag{7B.5}$$

The maximum of $d^2\rho(t)/dt^2$ lies at $t = 0$, so that the experimental would-be critical coincides with the theoretical $T_c^{(1)}$ to this order.

If we carry the expansion of (7B.2) to the second order in $\rho \approx 1/N\rho \approx 1/\sqrt{N}$, we find a shift of the order $1/N$. As an example, take $D = 3$, assume $A = 1$, and use the full T-dependence rather than the lowest-order expansion in Eq. (7B.4):

$$\left(\frac{T}{T_c^{(0)}}\right)^{3/2} = (1+t)^{3/2} = \frac{1}{N\rho} - \rho. \tag{7B.6}$$

For simplicity, we ignore the $1/N$ terms in (7B.3). The resulting $\rho(t)$ and $d^2\rho/dt^2$ are plotted in Fig. 7.13. The maximum of $d^2\rho/dt^2$ lies at $t \approx 8/9N$, which can be ignored if we know T_c only up to order $\mathcal{O}(N^{-1/3})$ or $\mathcal{O}(N^{-2/3})$, as in Eqs. (7.91) and (7A.22).

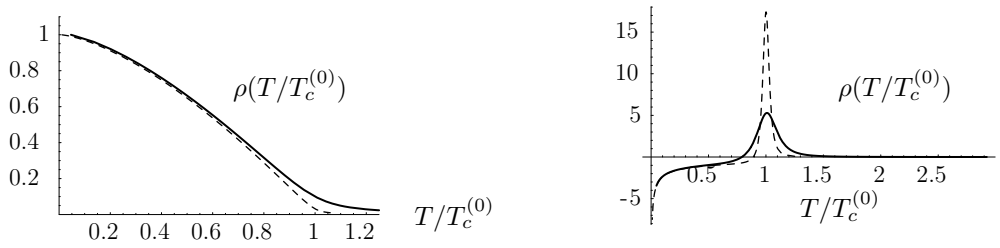

Figure 7.13 Plots of condensate fraction and its second derivative for Bose Gas in a finite box following Eq. (7B.6) for $N = 100$ and 1000.

Note that a convenient way to determine the would-be critical temperature from numerical data is via the maximal curvature of the chemical potential $\mu(T)$, i.e., from the maximum of $-d^2\mu(T)/dT^2$. Since $z_D = e^{\mu - Db/2} = 1 - \delta z_D \approx 1 + \mu - Db/2$, the second derivative of μ is related to that of δz_D by

$$-\frac{d^2\mu}{dt^2} \approx \frac{d^2\delta z_D}{dt^2} - Db_c^{(0)}. \tag{7B.7}$$

The second term is of the order $1/N^{2/D}$ and can be ignored as we shall see immediately. The equation shows that the second derivative of $-\mu$ coincides with that of δz_D, which is related to $d^2\rho/dt^2$ by

$$\frac{d^2\delta z_D}{dt^2} \approx \frac{d^2}{dt^2}\frac{1}{N\rho} = \frac{1}{N}\left[\frac{2}{\rho^3}\left(\frac{d\rho}{dt}\right)^2 - \frac{1}{\rho^2}\frac{d^2\rho}{dt^2}\right] = \frac{D^2}{16}\sqrt{\frac{N}{A^3}}\left[1 - \frac{3D^2}{32}\frac{N}{A}t^2 + \mathcal{O}(t^4)\right]. \tag{7B.8}$$

This is again maximal at $t = 0$, implying that the determination of $T_c^{(1)}$ by this procedure coincides with the previous one. The neglected term of order $1/N^{2/D}$ has a relative suppression of $1/N^{2/D+1/2}$, which can be ignored for larger N.

Notes and References

Path integrals of many identical particles are discussed in the texbook
R.P. Feynman, *Statistical Mechanics*, Benjamin, Reading, 1972.
See also the papers by
L.S. Schulman, Phys. Rev. **176**, 1558 (1968);
M.G.G. Laidlaw and C. DeWitt-Morette, Phys. Rev. D **3**, 5 (1971);
F.J. Bloore, in *Differential Geometric Methods in Math. Phys., Lecture Notes in Mathematics* **905**, Springer, Berlin, 1982;

P.A. Horvathy, G. Morandi, and E.C.G. Sudarshan, Nuovo Cimento D **11**, 201 (1989).

Path Integrals over Grassmann variables are discussed in detail in
F.A. Berezin, *The Method of Second Quantization*, Nauka, Moscow, 1965;
J. Rzewuski, *Field Theory*, Hafner, New York, 1969;
L.P. Singh and F. Steiner, Phys. Lett. B **166**, 155 (1986);
M. Henneaux and C. Teitelboim, *Quantization of Gauge Systems*, Princeton Univ. Press, 1992.

For fractional statistics see the papers by
F. Wilczek and A. Zee, Phys. Rev. Lett. **51**, 2250 (1983);
Y.S. Wu, *ibid.*, **53**, 111 (1984);
and the reprint collection by
A. Shapere and F. Wilczek and *Geometric Phases in Physics*, World Scientific, Singapore, 1989, p. 284.
The simple derivation of the statistics interaction given in this text is taken from
H. Kleinert, Phys. Lett. B **235**, 381 (1989) (`wwwK/104`, where (`wwwK` is short for `http://www.physik.fu-berlin.de/~kleinert`).
See also the notes and references in Chapter 16.

I thank Prof. Carl Wieman for his permission to publish Fig. 7.9 of the JILA BEC group.

The particular citations in this chapter refer to the publications

[1] R.P. Feynman, *Statistical Mechanics*, Benjamin, Reading, 1972.

[2] J. Flachsmeyer, *Kombinatorik*, Dtsch. Verl. der Wiss., Berlin, 1972. p. 128, Theorem 11.3. The number n_z^n of permutations of n elements consisting of z cycles satisfies the recursion relation $n_z^n = n_{z-1}^{n-1} + (n-1)\, n_z^{n-1}$, with the initial conditions $n_n^n = 1$ and $n_1^n = (n-1)!$.

[3] The Mathematica program for this can be downloaded from the internet (`wwwK/b5/pgm7`).

[4] F. Brosens, J.T. Devreese, L.F. Lemmens, Phys. Rev. E *55*, 227 (1997). See also K. Glaum, Berlin Ph.D. thesis (in preparation).

[5] P. Bormann and G. Franke, J. Chem. Phys. **98**, 2484 (1984).

[6] S. Bund and A. Schakel, Mod. Phys. Lett. B **13**, 349 (1999).

[7] See E.W. Weisstein's internet page `mathworld.wolfram.com`.

[8] See, for example, Chapter 11 in H. Kleinert, *Gauge Fields in Condensed Matter*, op. cit., Vol. I, World Scientific, Singapore, 1989 (`wwwK/b1`).

[9] The first observation was made at JILA with ^{87}Ru:
M.H. Anderson, J.R. Ensher, M.R. Matthews, C.E. Wieman, and E.A. Cornell, Science **269**, 198 (1995).
It was followed by a condensate of ^{7}Li at Rice University:
C.C. Bradley, C.A. Sackett, J.J. Tollet, and R.G. Hulet, Phys. Rev. Lett. **75**, 1687 (1995);
and in ^{30}Na at MIT:
K.B. Davis, M.-O. Mewes, M.R. Andrews, and N.J. van Druten, , D.S. Durfee, D.M. Kurn, W. Ketterle, Phys. Rev. Lett. **75**, 3969 (1995).

[10] J.R. Abo-Shaeer, C. Raman, J.M. Vogels, and W. Ketterle, Science **292**, 476 (2001).

[11] A.L. Fetter and J.D. Walecka, *Quantum Theory of Many-Particle Systems* McGraw–Hill, New York, 1971, Sec. 28.

[12] V.N. Popov, Theor. Math. Phys. **11**, 565 (1972); *Functional Integrals in Quantum Field Theory and Statistical Physics* (Reidel, Dordrecht, 1983).

[13] M. Schick, Phys. Rev. A **3**, 1067 (1971).

[14] J.O. Andersen, U. Al Khawaja, and H.T.C. Stoof, Phys. Rev. Lett. **88**, 070407 (2002).

[15] H.T.C. Stoof and M. Bijlsma, Phys. Rev. E **47**, 939 (1993);
U. Al Khawaja, J.O. Andersen, N.P. Proukakis, and H.T.C. Stoof, Phys. Rev. A **A**, 013615 (2002).

[16] D.S. Fisher and P.C. Hohenberg, Phys. Rev. B **37**, 4936 (1988).

[17] F. Nogueira and H. Kleinert, Phys. Rev. B **73**, 104515 (2006) (cond-mat/0503523).

[18] K. Huang, Phys. Rev. Lett. **83**, 3770 (1999).

[19] K. Huang, C.N. Yang, Phys. Rev. **105**, 767 (1957);
K. Huang, C.N. Yang, J.M. Luttinger, Phys. Rev. **105**, 776 (1957);
T.D. Lee, K. Huang, C.N. Yang, Phys. Rev. **106**, 1135 (1957);
K. Huang, in *Studies in Statistical Mechanics*, North-Holland, Amsterdam, 1964, Vol. II.

[20] H. Kleinert, *Strong-Coupling Behavior of Phi^4-Theories and Critical Exponents*, Phys. Rev. D **57** , 2264 (1998); Addendum: Phys. Rev. D **58**, 107702 (1998) (cond-mat/9803268); *Seven Loop Critical Exponents from Strong-Coupling ϕ^4-Theory in Three Dimensions*, Phys. Rev. D **60** , 085001 (1999) (hep-th/9812197); *Theory and Satellite Experiment on Critical Exponent alpha of Specific Heat in Superfluid Helium*, Phys. Lett. A **277**, 205 (2000) (cond-mat/9906107); *Strong-Coupling ϕ^4-Theory in $4-\epsilon$ Dimensions, and Critical Exponent*, Phys. Lett. B **434** , 74 (1998) (cond-mat/9801167); *Critical Exponents without beta-Function*, Phys. Lett. B **463**, 69 (1999) (cond-mat/9906359).
See also the textbook:
H. Kleinert and V. Schulte-Frohlinde, *Critical Properties of ϕ^4-Theories*, World Scientific, Singapore, 2001 (`wwwK/b8`).

[21] H. Kleinert, *Five-Loop Critical Temperature Shift in Weakly Interacting Homogeneous Bose-Einstein Condensate* (cond-mat/0210162).

[22] T. Toyoda, Ann. Phys. (N.Y.) **141**, 154 (1982).

[23] A. Schakel, Int. J. Mod. Phys. B **8**, 2021 (1994); *Boulevard of Broken Symmetries*, (cond-mat/9805152). The upward shift $\Delta T_c/T_c$ by a weak δ-function repulsion reported in this paper is, however, due to neglecting a two-loop contribution to the free energy. If this is added, the shift disappears. See the remarks below in [34].

[24] H.T.C. Stoof, Phys. Rev. A **45**, 8398 (1992).

[25] M. Holzmann, P. Grueter, and F. Laloe, Eur. Phys. J. B **10**, 239 (1999).

[26] G. Baym, J.-P. Blaizot, M. Holzmann, F. Laloe, and D. Vautherin, Phys. Rev. Lett. **83**, 1703 (1999).

[27] G. Baym, J.-P. Blaizot, and J. Zinn-Justin, Europhys. Lett. **49**, 150 (2000) (cond–mat/9907241)

[28] M. Holzmann, G. Baym, J.-P. Blaizot, and F. Laloe, Phys. Rev. Lett. **87**, 120403 (2001) (cond-mat/0107129).

[29] P. Grueter, D. Ceperley, and F. Laloe, Phys. Rev. Lett. **79**, 3549 (1997).

[30] M. Holzmann and W. Krauth, Phys. Rev. Lett. **83**, 2687 (1999).

[31] M. Bijlsma and H.T.C. Stoof, Phys. Rev. A **54**, 5085 (1996).

[32] H. Kleinert, *Collective Quantum Fields*, Fortschr. Phys. **26**, 565 (1978) `http://www.physik.fu-berlin.de/~kleinert/55`).

[33] N.N. Bogoliubov, Zh. Eksp. Teor. Fiz. **34**, 58 (1958).

[34] P. Arnold and B. Tomášik, Phys. Rev. A **62**, 063604 (2000).
This paper starts out from the 3+1-dimensional initial theory and derives from it the three-dimensional effective classical field theory as defined in Subsection 7.14.4. This program was initiated much earlier by
A. Schakel, Int. J. Mod. Phys. B **8**, 2021 (1994);
and explained in detail in Ref. [23]. Unfortunately, the author did not go beyond the one-loop level so that he found a positive shift $\Delta T_c/T_c$, and did not observe its cancellation at the two-loop level. See the recent paper
A. Schakel, *Zeta Function Regularization of Infrared Divergences in Bose-Einstein Condensation*, (cond-mat/0301050).

[35] F.F. de Souza Cruz, M.B. Pinto, R.O. Ramos, Phys. Rev. B **64**, 014515 (2001);
F.F. de Souza Cruz, M.B. Pinto, R.O. Ramos, P. Sena, Phys. Rev. A **65**, 053613 (2002) (cond-mat/0112306).

[36] P. Arnold, G. Moore, and B. Tomášik, Phys. Rev. A **65**, 013606 (2002) (cond-mat/0107124).

[37] G. Baym, J.-P. Blaizot, M. Holzmann, F. Laloe, and D. Vautherin (cond-mat/0107129).

[38] P. Arnold and G. Moore, Phys. Rev. Lett. **87**, 120401 (2001); V.A. Kashurnikov, N.V. Prokof´ev, and B.V. Svistunov, Phys. Rev. Lett. **87**, 120402 (2001).

[39] J.L. Kneur, M.B. Pinto, R.O. Ramos, Phys. Rev. A **68**, 43615 (2003) (cond-mat/0207295).

[40] J.D. Reppy, B.C. Crooker, B. Hebral, A.D. Corwin, J. He, and G.M. Zassenhaus, cond–mat/9910013 (1999).

[41] M. Wilkens, F. Illuminati, and M. Krämer, J. Phys. B **33**, L779 (2000) (cond-mat/0001422).

[42] E.J. Mueller, G. Baym, and M. Holzmann, J. Phys. B **34**, 4561 (2001) (cond-mat/0105359)

[43] H. Kleinert, S. Schmidt, and A. Pelster, Phys. Rev. Lett. **93**, 160402 (2004) (cond-mat/0307412).

[44] E.L. Pollock and K.J. Runge, Phys. Rev. **B 46**, 3535 (1992).

[45] J. Tempere, F. Brosens, L.F. Lemmens, and J.T. Devreese, Phys. Rev. A **61**, 043605 (2000) (cond-mat/9911210).

[46] N.N. Bogoliubov, *On the Theory of Superfluidity* , Izv. Akad. Nauk SSSR (Ser. Fiz.) **11**, 77 (1947); Sov.Phys.-JETP **7**, 41(1958).
See also
J.G. Valatin, Nuovo Cimento **7**, 843 (1958);
K. Huang, C.N. Yang, J.M. Luttinger, Phys. Rev. **105**, 767, 776 (1957).

[47] See pp. 1356–1369 in
H. Kleinert, *Gauge Fields in Condensed Matter*, op. cit., Vol. II, World Scientific, Singapore, 1989 (`wwwK/b2`);
H. Kleinert, *Gravity as Theory of Defects in a Crystal with Only Second-Gradient Elasticity*, Ann. d. Physik, **44**, 117 (1987) (`wwwK/172`);
H. Kleinert and J. Zaanen, Phys. Lett. A **324**, 361 (2004) (gr-qc/0307033).

[48] V. Bretin, V.S. Stock, Y. Seurin, F. Chevy, and J. Dalibard, *Fast Rotation of a Bose-Einstein Condensate*, Phys. Rev. Lett. **92**, 050403 (2004).

[49] For the beginnings see
J.R. Klauder, Ann. of Physics **11**, 123 (1960).
The present status is reviewed in
J.R. Klauder, *The Current State of Coherent States*, (quant-ph/0110108).

[50] G. Junker and J.R. Klauder, Eur. Phys. J. C **4**, 173 (1998) (quant-phys/9708027).

[51] See the textbook cited at the end of Ref. [20].

[52] R. Stratonovich Sov. Phys. Dokl. **2**, 416 (1958):
J. Hubbard, Phys. Rev. Lett. **3**, 77 (1959);
B. Mühlschlegel, J. Math. Phys. , **3**, 522 (1962);
J. Langer, Phys. Rev. A **134**, 553 (1964); T.M. Rice, Phys. Rev. A **140** 1889 (1965); J. Math. Phys. **8**, 1581 (1967); A.V. Svidzinskij, Teor. Mat. Fiz. **9**, 273 (1971); D. Sherrington, J. Phys. C **4**, 401 (1971).