Chapter 1

Path integrals and superfluidity

1.1 Density matrix for many identical Bosons

For the sake of simplicity we start with two free particles. Let us suppose first that they are distinguishable. Then, since

$$H = -\frac{\hbar^2}{2m}\left(\nabla_1^2 + \nabla_2^2\right)\,, \tag{1.1}$$

and $\rho(\mathbf{x}_1\mathbf{x}_2;\mathbf{x}_1'\mathbf{x}_2';\beta)$ satisfies the equation

$$\frac{\partial\rho}{\partial\beta} = -\frac{\hbar^2}{2m}\left(\nabla_1^2 + \nabla_2^2\right)\rho\,, \tag{1.2}$$

we have (in three dimensions)

$$\rho(\mathbf{x}_1\mathbf{x}_2;\mathbf{x}_1'\mathbf{x}_2';\beta) = \left(\frac{m}{2\pi\hbar^2\beta}\right)^{\frac{3}{2}*2} e^{-\frac{m}{2\hbar^2\beta}[(\mathbf{x}_1-\mathbf{x}_1')^2+(\mathbf{x}_2-\mathbf{x}_2')^2]}\,. \tag{1.3}$$

On the other hand we have (from the general principles)

$$\rho(\mathbf{x}_1\mathbf{x}_2;\mathbf{x}_1'\mathbf{x}_2';\beta)\; = \sum_i e^{-\beta E_i}\,\psi_i(\mathbf{x}_1\mathbf{x}_2)\,\psi_i^*(\mathbf{x}_1'\mathbf{x}_2') \tag{1.4}$$

where E_i is the energy of the i'th eigenstate of H:

$$-\frac{\hbar^2}{2m}\left(\nabla_1^2 + \nabla_2^2\right)\psi_i(\mathbf{x}_1\mathbf{x}_2) = E_i\,\psi_i(\mathbf{x}_1\mathbf{x}_2)\,. \tag{1.5}$$

Let us spell out in detail (1.4) for noninteracting two particle wavefunctions, which we take in the form of plane waves satisfying this last equation. So the energy of the system is determined by the two wave vectors of these two plane waves, ($i = (\mathbf{lk})$),

$$\psi_{(\mathbf{lk})}(\mathbf{x}_1\mathbf{x}_2) = \frac{1}{\sqrt{(2\pi)^3}}\,e^{i\mathbf{l}\cdot\mathbf{x}_1}\,\frac{1}{\sqrt{(2\pi)^3}}\,e^{i\mathbf{k}\cdot\mathbf{x}_2}\,, \qquad E_{(\mathbf{lk})} = \frac{\hbar^2\mathbf{l}^2}{2m} + \frac{\hbar^2\mathbf{k}^2}{2m}\,. \tag{1.6}$$

So, we can write (1.4) in the following form

$$\rho(\mathbf{x}_1\mathbf{x}_2;\mathbf{x}_1'\mathbf{x}_2') = \int d^3\mathbf{l} \int d^3\mathbf{k}\ \exp\left\{\frac{-\beta}{2m}(\mathbf{l}^2+\mathbf{k}^2)\right\} \psi_{(\mathbf{lk})}(\mathbf{x}_1\mathbf{x}_2)\, \psi^*_{(\mathbf{lk})}(\mathbf{x}_1'\mathbf{x}_2') \tag{1.7}$$

where

$$\psi_{(\mathbf{lk})}(\mathbf{x}_1\mathbf{x}_2) = \frac{1}{(2\pi)^3}\, e^{i(\mathbf{l}\cdot\mathbf{x}_1+\mathbf{k}\cdot\mathbf{x}_2)}\,,$$

and an analogous expression for ψ^*. Note that performing integration over $d^3\mathbf{l}\, d^3\mathbf{k}$ we get back (1.3).

But ρ given in (1.3) cannot describe two identical Bose particles. This is seen from (1.7) and (1.8) because the wavefunctions $\psi_{(\mathbf{lk})}(\mathbf{x}_1\mathbf{x}_2)$ do not have the right symmetry for Bosons, i.e. they are not symmetric under exchange of $\mathbf{x}_1$ and $\mathbf{x}_2$.

We introduce the correct symmetry into ρ through the simple device of performing all permutations of the primed variables and multiplying this sum by the inverse factorial of the number of particles (just two of them in our simple example):

$$\frac{1}{2!}\sum_{\mathcal{P}} \mathcal{P}\psi_i^*(\mathbf{x}_1'\mathbf{x}_2') \;=\; \frac{1}{2!}\sum_{\mathcal{P}} \psi_i^*(\mathcal{P}\mathbf{x}_1'\mathcal{P}\mathbf{x}_2')\,. \tag{1.8}$$

This somewhat strange notation for a permutation: keeping the symbol $\mathcal{P}$ in front of each variable of a set which undergoes a permutation turns out to be quite handy (see [11.1] and the text below).

Let us check explicitly how it works on our simple example. Indeed, applying the operation (1.8) to the wavefunction $\psi^*_{(\mathbf{lk})}(\mathbf{x}_1'\mathbf{x}_2')$ and substituting the result into ρ given in (1.7) we obtain a result which is identical to the one obtained when both wavefunctions in (1.7) are symmetrized according to (1.8). Note that this identity is evident when we exchange the integration variables $\mathbf{l}$ and $\mathbf{k}$ in some terms, and the integral $d^3\mathbf{l}\, d^3\mathbf{k}$ is taken. Note also that the factor 1/2! is uniquely detrmined through this operation. *Exercise:* show it! In other words: the operation (1.8) performed on *one of the wavefunctions* appearing in ρ does effectively *the same as symmetrization of both wavefunctions.*

Our simple example is - as one may suspect - a special case of a general formula for an arbitrary number, N, of interacting Bosons. Thus to obtain a Bosonic density matrix one follows this prescription:

$$\rho_B(\mathbf{x}_1\mathbf{x}_2...\mathbf{x}_N;\mathbf{x}_1'\mathbf{x}_2'...\mathbf{x}_N';\beta) \;=\; \frac{1}{N!}\sum_{\mathcal{P}} \rho(\mathbf{x}_1\mathbf{x}_2...\mathbf{x}_N;\mathcal{P}\mathbf{x}_1'\mathcal{P}\mathbf{x}_2'...\mathcal{P}\mathbf{x}_N';\beta)$$

$$= \left(\frac{1}{N!}\right)^2 \sum_{sym\ i} e^{-\beta E_i} \sum_{\mathcal{P}} \psi_i(\mathcal{P}\mathbf{x}_1\mathcal{P}\mathbf{x}_2...\mathcal{P}\mathbf{x}_N) \sum_{\mathcal{P}'} \psi_i^*(\mathcal{P}'\mathbf{x}_1'\mathcal{P}'\mathbf{x}_2'...\mathcal{P}'\mathbf{x}_N') \tag{1.9}$$

where the summation over symmetric states i is performed. In order to prove this general formula one has to employ some group-theoretic arguments. The interested reader is referred to [...]. The last equation in (1.9) stresses the point discussed above on our simple example: symmetrization of just one set of variables leads to symmetrization of both wavefunctions.

So, we have now a well defined procedure of constructing a Bosonic density matrix from any density matrix obtained for N distinguishable particles.

Note that ρ_B constructed above can be used to define the well known measurable objects: one- and two-particle distribution functions. We have

$$n_1(\mathbf{x}_1) \;=\; N\,\frac{\int \rho_B(\mathbf{x}_1\mathbf{x}_2...\mathbf{x}_N;\mathbf{x}_1\mathbf{x}_2...\mathbf{x}_N;\beta)\,d^3\mathbf{x}_2...d^3\mathbf{x}_N}{\int \rho_B(\mathbf{x}_1\mathbf{x}_2...\mathbf{x}_N;\mathbf{x}_1\mathbf{x}_2...\mathbf{x}_N;\beta)\,d^3\mathbf{x}_1...d^3\mathbf{x}_N}\,,$$

and

$$n_2(\mathbf{x}_1\mathbf{x}_2) \;=\; N(N-1)\,\frac{\int \rho_B(\mathbf{x}_1\mathbf{x}_2\mathbf{x}_3...\mathbf{x}_N;\mathbf{x}_1\mathbf{x}_2\mathbf{x}_3...\mathbf{x}_N;\beta)\,d^3\mathbf{x}_3...d^3\mathbf{x}_N}{\int \rho_B(\mathbf{x}_1\mathbf{x}_2...\mathbf{x}_N;\mathbf{x}_1\mathbf{x}_2...\mathbf{x}_N;\beta)\,d^3\mathbf{x}_1...d^3\mathbf{x}_N}\,.$$

1.2 The system of N noninteracting Bosons

It is instructive to discuss the role of the Bose - Einstein symmetry for N identical (noninteracting - to start with) particles as a function of temperature. What we intend to argue about is that on the one hand the identity of Bose particles leads to their very lengthy paths (e.g. in the functional representation of the partition function) and, on the other hand, that only the very low temperatures can accomodate (i.e. keep their contributions important) such lenghty paths. In other words the very low temperatures emphasize the characteristics of bosonic systems, whereas the high temperatures tend to smear them out.

Let us continue discussing a system of noninteracting Bosons which exhibits most simply the role of the symmetrization. So, our starting point is the density matrix for N distinguishable particles (in three spatial dimensions)

$$\rho(\mathbf{x}_1\mathbf{x}_2...\mathbf{x}_N;\mathbf{x}'_1\mathbf{x}'_2...\mathbf{x}'_N;\beta) \;=\; \left(\frac{m}{2\pi\hbar^2\beta}\right)^{\frac{3}{2}N} e^{-\frac{m}{2\hbar^2\beta}\sum_{i=1}^{N}(\mathbf{x}_i-\mathbf{x}'_i)^2}\,. \qquad (1.10)$$

Following the prescription for construction of a bosonic density matrix discussed earlier, we write down the partition function for noninteracting Bosons

$$\begin{aligned}\mathcal{Z}_B = e^{-\beta F_B} &= \frac{1}{N!}\sum_{\mathcal{P}}\int \rho(\mathbf{x}_1\mathbf{x}_2...\mathbf{x}_N;\mathcal{P}\mathbf{x}_1\mathcal{P}\mathbf{x}_2...\mathcal{P}\mathbf{x}_N;\beta)\,d^3\mathbf{x}_1d^3\mathbf{x}_2...d^3\mathbf{x}_N\\ &= \frac{1}{N!}\left(\frac{m}{2\pi\hbar^2\beta}\right)^{\frac{3}{2}N}\sum_{\mathcal{P}}\int e^{-\frac{m}{2\hbar^2\beta}\sum_{i=1}^{N}(\mathbf{x}_i-\mathcal{P}\mathbf{x}_i)^2}\,d^3\mathbf{x}_1d^3\mathbf{x}_2...d^3\mathbf{x}_N\,. \qquad (1.11)\end{aligned}$$

We can now see that symmetrization makes $\mathcal{Z}_B$ a nontrivial multidimensional integral (without it we get after a trivially simple integration: $\mathcal{Z} = \left(m/2\pi\hbar^2\beta\right)^{\frac{3}{2}N}V^N$). From (1.11) we see that, in the Euclidean time $\hbar\beta$, the trajectories run between well separated initial and final positions of particles, and that, as long as $\beta = 1/k_BT$ is large (hence the temperature low), the spatial extension of these paths can be considerable and still their contributions to $\mathcal{Z}_B$ may be significant. Relation (1.11) suggests also that it is sensible to decompose permutations into cycles which classify quantal trajectories in (1.11).

One can evaluate $\mathcal{Z}_B$ analytically (compare [11.1]). First, we decompose each permutation into cycles. For instance

$$\mathcal{P}\begin{pmatrix}12345\\32451\end{pmatrix} = \begin{pmatrix}1345\\3451\end{pmatrix}\begin{pmatrix}2\\2\end{pmatrix} \tag{1.12}$$

has two cycles of length 4 and 1, and

$$\mathcal{P}\begin{pmatrix}12345\\21435\end{pmatrix} = \begin{pmatrix}12\\21\end{pmatrix}\begin{pmatrix}34\\43\end{pmatrix}\begin{pmatrix}5\\5\end{pmatrix} \tag{1.13}$$

has three cycles of length 2, 2 and 1.

Denoting by C_ν the number of cycles, in a given permutation, of length ν we have: in the case (1.12) $C_4 = 1, C_1 = 1$, in the case (1.13) $C_2 = 2, C_1 = 1$. Note that for each permutation we have

$$\sum_\nu C_\nu \, \nu = N \tag{1.14}$$

where N is the number of particles. The cycles factorize the integral in (1.11), and we introduce the following factor for a cycle of length ν

$$h_\nu = \left(\frac{m}{2\pi\hbar^2\beta}\right)^{\frac{3}{2}\nu} \int d^3\mathbf{x}_1 d^3\mathbf{x}_2 ... d^3\mathbf{x}_\nu \, e^{-\frac{m}{2\hbar^2\beta}[(\mathbf{x}_1-\mathbf{x}_2)^2+(\mathbf{x}_2-\mathbf{x}_3)^2+...+(\mathbf{x}_\nu-\mathbf{x}_1)^2]}, \tag{1.15}$$

for a cycle of length 1

$$h_1 = \left(\frac{m}{2\pi\hbar^2\beta}\right)^{\frac{3}{2}} \int d^3\mathbf{x}_1 = V\left(\frac{m}{2\pi\hbar^2\beta}\right)^{\frac{3}{2}}. \tag{1.16}$$

Therefore, the partition function is

$$\mathcal{Z}_B = e^{-\beta F_B} = \frac{1}{N!}\sum_{\mathcal{P}}\left(\prod_\nu (h_\nu)^{C_\nu}\right). \tag{1.17}$$

All these integrals are Gaussian, and can be evaluated with the help of

$$\int_{-\infty}^{+\infty} dy \, e^{-a(x-y)^2-b(y-z)^2} = \left(\frac{\pi}{a+b}\right)^{\frac{3}{2}} e^{-\frac{ab}{a+b}(x-z)^2}, \tag{1.18}$$

and we obtain

$$h_\nu = V\left(\frac{m}{2\pi\hbar^2\beta\nu}\right)^{\frac{3}{2}} \tag{1.19}$$

which reproduces (1.16) as a special case.

In order to compute (1.17) we must know how to handle permutations. We count permutations through performing a bookkeeping of cycles [11.1]. Let C_ν be the numbers of cycles of length ν. They have to satisfy the constraint (1.14). To a given set of C_ν satisfying the above condition we generate all possible permutations through:

- interchanging cycles of the same length (in $\prod_\nu C_\nu!$ ways)
- making cyclic permutations within cycles (in $\prod_\nu \nu^{C_\nu}$ ways).

Since there are $N!$ possible permutations, the number of permutations corresponding to a set $C_1C_2...C_q$ is

$$L(C_1C_2...C_q) \;=\; \frac{N!}{\prod_\nu C_\nu!\,\nu^{C_\nu}}\,. \tag{1.20}$$

Thus the final expression for $\mathcal{Z}_B$ is

$$\mathcal{Z}_B \;=\; e^{-\beta F_B} \;=\; \sum_{C_1C_2...C_q}\prod_\nu \frac{h_\nu^{C_\nu}}{C_\nu!\,\nu^{C_\nu}}\,, \tag{1.21}$$

with the constraint (1.14) imposed on $C_1C_2...C_q$ (otherwise they are arbitrary).

Evaluation of (1.21) for a fixed N is not easy and, to simplify matters and to recover contact with the textbook formulae, we will evaluate (1.21) with a *variable* N whose *average* value, $\langle N\rangle$, is *fixed* by a chemical potential μ (thus we employ the grand canonical ensemble formulation).

The new partition function is a superposition of partition functions (1.21) for various N's:

$$\mathcal{Z} \;=\; e^{-\beta F} \;=\; \sum_{N=1}^{\infty} e^{-\beta F_B(N)}\,e^{\beta\mu N}\,. \tag{1.22}$$

By fixing μ we fix the average number of particles, $\langle N\rangle$, the system has at a fixed temperature $k_BT = 1/\beta$. Indeed, from the general thermodynamic relation we have

$$\langle N\rangle \;=\; -\frac{\partial F}{\partial\mu} \;=\; \sum_{N=1}^{\infty} N\,p(N,\mu) \tag{1.23}$$

where $p(N,\mu)$ is the probability of occurence of N particles in our system

$$p(N,\mu) \;=\; \frac{1}{\mathcal{Z}}\,e^{-\beta F_B+\beta\mu N}\,, \qquad\qquad \sum_{N=1}^{\infty} p(N,\mu) = 1\ . \tag{1.24}$$

Denoting $e^{\mu\beta} = \alpha$, hence $e^{\mu\beta N} = \prod_\nu \alpha^{\nu C_\nu}$, we get from (1.21) and (1.22)

$$e^{-\beta F} \;=\; \sum_{C_1...C_q}\prod_\nu \frac{h_\nu^{C_\nu}}{C_\nu!\,\nu^{C_\nu}}\,\alpha^{\nu C_\nu} \;=\; \sum_{C_1...C_q}\prod_\nu \frac{[h_\nu\alpha^\nu/\nu]^{C_\nu}}{C_\nu!}\,. \tag{1.25}$$

Since N is not fixed C_q's are not restricted: $0 \le C_q \le \infty$. Therefore,

$$e^{-\beta F} \;=\; \prod_\nu \sum_{C_\nu=0}^{\infty} \frac{[h_\nu\alpha^\nu/\nu]^{C_\nu}}{C_\nu!} \;=\; \prod_\nu e^{h_\nu\alpha^\nu/\nu} \;=\; e^{\Sigma_\nu h_\nu\alpha^\nu/\nu}\,, \tag{1.26}$$

and introducing h_ν from (1.19) we get

$$\beta F \;=\; -\sum_{\nu=1}^{\infty}\frac{h_\nu\alpha^\nu}{\nu} \;=\; -\left(\frac{m}{2\pi\hbar^2\beta}\right)^{\frac{3}{2}} V\sum_{\nu=1}^{\infty}\frac{\alpha^\nu}{\nu^{5/2}} \;=\; -\left(\frac{m}{2\pi\hbar^2\beta}\right)^{\frac{3}{2}} V\,\zeta_{5/2}(\alpha)\,. \tag{1.27}$$

Note that for $\alpha > 1$ we have $\zeta_{5/2} = \infty$.

To make a contact with the texbook formulae let us calculate $\langle N \rangle$ from F given in (1.27)

$$\langle N \rangle \; = \; -\frac{\partial F}{\partial \mu} \; = \left(\frac{m}{2\pi\hbar^2\beta} \right)^{\frac{3}{2}} V \, \zeta_{3/2}(\alpha) \tag{1.28}$$

where we introduced another ζ function:

$$\frac{\partial}{\partial \mu} \left(\sum_{\nu=1}^{\infty} \frac{\alpha^\nu}{\nu^{5/2}} \right) \; = \; \beta \sum_{\nu=1}^{\infty} \frac{\alpha^\nu}{\nu^{3/2}} \; = \; \beta \, \zeta_{3/2}(\alpha) \, . \tag{1.29}$$

But (1.28) can be resolved into a sum over the energies of the system. One finds [11.1]

$$\langle N \rangle \; = \; V \left(\frac{m k_B T}{2\pi\hbar^2} \right)^{3/2} \zeta_{3/2}(\alpha) \; = \; V \int \frac{d^3 p}{(2\pi\hbar)^3} \left(e^{\beta(\frac{p^2}{2m} - \mu)} - 1 \right)^{-1} \tag{1.30}$$

where the last expression is the well known sum over the average numbers of Bosons at each energy $p^2/2m$. To prove it, it is easier to go from the right to the left in (1.30) doing an infinite series of Gaussian integrals.

Note that (1.30) tells us that for Bosons we must have $\mu \leq 0$ to keep the partial averages of particles positive and finite. For $\mu > 0$, (1.30) becomes singular. However, for $\mu = 0$, hence $\alpha = 1$, our zeta functions

$$\zeta_{3/2}(1) = \zeta(3/2) = 2.612 \, , \qquad \zeta_{5/2}(1) = \zeta(5/2) = 1.341 \tag{1.31}$$

become the Riemannn ζ-functions taken at the values when their arguments equal 3/2 and 5/2, respectively.

The temperature at which $\mu(T_c) = 0$ (hence $\alpha = 1$) is the critical temperature for Bose - Einstein condensation. The formula (1.30) is well suited to discuss the onset and the evolution of condensation as the temperature falls below T_c.

We fix the average number of particles, $\langle N \rangle$, and the volume, V (thus we fix the density of particles). The critical temperature T_c is therefore determined from (1.30):

$$\langle N \rangle \; = \; V \left(\frac{m k_B T_c}{2\pi\hbar^2} \right)^{\frac{3}{2}} 2.612 \, . \tag{1.32}$$

Formula (1.30) makes sense only for $T \geq T_c$. Indeed, as we lower the temperature towards T_c we have to increase $\zeta_{3/2}(\alpha = \exp\{\mu/k_B T\})$ in order to keep $\langle N \rangle$ constant. Since $\zeta_{3/2}(\alpha)$ is an *increasing* function of α, and is well defined only for $\alpha \leq 1$, we have to have $\mu(T)$ increasing and ≤ 0 as T drops. So, we can keep $\langle N \rangle$ constant increasing $\mu(T)$ until it reaches $\mu(T_c) = 0$.