Algorithms and computations in physics (Oxford Lectures 2024)

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This is the second of two lectures on computational quantum statistical mechanics. Building on the quantum harmonic oscillator, the density matrices and the Feynman path integral introduced in the sixth lecture, we will discuss a *bona fide* quantum Monte Carlo algorithm for bosons, that illustrates the phenomenon of Bose–Einstein condensation. Before doing that, however, we must discuss quantum statistics of indistinguishable particles and set up a naive program against which to check our state-of-the-art simulation code.

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7 Quantum statistical mechanics: Bosons

7.1 Preparations

7.1.1 Counting and sampling permutations

In this section, as a preparation for our quantum statistical mechanics. The next more complicated objects, after integers, are permutations of K distinct objects, which we may take to be the integers $\{1, \dots, K\}$. A permutation P can be written as a two-row matrix[1]

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[1] Anticipating our applications of permutations to bosons, we write permutations "bottom-up" as $\left(\begin{smallmatrix} P_1 & \cdots & P_K \\ 1 & \cdots & K \end{smallmatrix}\right)$ rather than "top-down" $\left(\begin{smallmatrix} 1 & \cdots & K \\ P_1 & \cdots & P_K \end{smallmatrix}\right)$, as is more common.

$$P = \begin{pmatrix} P_1 & P_2 & P_3 & P_4 & P_5 \\ 1 & 2 & 3 & 4 & 5 \end{pmatrix}. \tag{7.1}$$

We can think of the permutation in eq. (7.1) as balls labeled $\{1, \dots, 5\}$ in the order $\{P_1, \dots, P_5\}$, on a shelf (ball P_k is at position k).

procedure `ran-perm`
$\{P_1, \dots, P_K\} \leftarrow \{1, \dots, K\}$
for $k = 1, \dots, K-1$**:**
$\left\{ \begin{array}{l} l \leftarrow \texttt{nran}\,(k, K) \\ P_l \leftrightarrow P_k \end{array} \right.$
output $\{P_1, \dots, P_K\}$

Algorithm 7.1: `ran-perm`. Generating a uniformly distributed random permutation of K elements.

For $K = 4$, this program will produce each of the 24 permutations of 4 elements with the same probability (we also notice that Alg. **??** (`ran-perm`) is almost identical to the top-to-random shuffle that we studied in an earlier lecture). Now let us modify the above program a bit, and study the cycle structure of random permutations.

Permutations can also be arranged into disjoint cycles

$$P = \left(\underbrace{\begin{matrix} P_2 & P_3 & P_4 & P_1 \\ P_1 & P_2 & P_3 & P_4 \end{matrix}}_{\text{first cycle}} \underbrace{\begin{matrix} P_6 & P_7 & P_8 & P_9 & P_5 \\ P_5 & P_6 & P_7 & P_8 & P_9 \end{matrix}}_{\text{second cycle}} \underbrace{\begin{matrix} . & . & . & . & . \\ . & . & . & . & . \end{matrix}}_{\text{other cycles}} \right), \tag{7.2}$$

which can be written in a cycle representation as

$$P = (P_1, P_2, P_3, P_4)(P_5, \dots, P_9)(\dots)(\dots). \tag{7.3}$$

where, evidently, the cycle (P_1, P_2, P_3, P_4) is identical to the cycle (P_4, P_1, P_2, P_3), etc..

Let us now study the cycle structure of random permutations. More precisely, we're interested in knowing the probability distribution of the cycle lengths for the cycle containing the element $N - 1$. A program is easily written, either from scratch or using the Python library `sympy.combinatorics`. The outcome is striking: The probability that element N is in a cycle of length k is $1/K$. This statement is a probability statement, but also an enumerative one.

7.1.2 Recursive permutation counting and sampling

Permutations play a pivotal role in the path-integral description of quantum systems, and we shall soon need to count permutations with weights, that is, compute general "partition functions" of permutations of N particles

$$Y_N = \sum_{\text{permutations } P} \text{weight}(P).$$

If the weight of each permutation is 1, then $Y_N = N!$, the number of permutations of N elements. For concreteness, we shall consider the permutations of four elements (see Fig. 7.1). For more generality, we allow arbitrary weights depending on the length of the cycles. For coherence with the later application, we denote the weight of a cycle of length k by z_k.

We now derive a crucial recursion formula for Y_N. In any permutation of N elements, the last element (in our example the element $N = 4$) is in what may be called the last-element cycle. (In permutation [5] in Fig. 7.1, the last-element cycle, of length 3, contains $\{2, 3, 4\}$. In

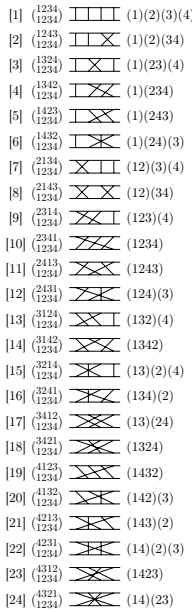

Figure 7.1: All 24 permutations of four elements.

permutation [23], the last-element cycle, of length 4, contains all elements). Generally, this last-element cycle involves k elements $\{n_1, \ldots, n_{k-1}, N\}$. Moreover, $N-k$ elements do not belong to the last-element cycle. The partition function of these elements is Y_{N-k}, because we know nothing about them, and they are unrestricted. Y_N is determined by the number of choices for k and the cycle weight z_k, the number of different sets $\{n_1, \ldots, n_{k-1}\}$ given k, the number of different cycles given the set $\{n_1, \ldots, n_{k-1}, N\}$, and the partition function Y_M of the elements not participating in the last-element cycle:

$$Y_N = \sum_{k=1}^{N} z_k \left\{ \begin{array}{c} \text{number of} \\ \text{choices for} \\ \{n_1, \ldots, n_{k-1}\} \end{array} \right\} \left\{ \begin{array}{c} \text{number of} \\ \text{cycles with} \\ \{n_1, \ldots, n_k\} \end{array} \right\} Y_{N-k}. \tag{7.4}$$

From Fig. 7.1, it follows that there are $(k-1)!$ cycles of length k with the same k elements. Likewise, the number of choices of different elements for $\{n_1, \ldots, n_{k-1}\}$ is $\binom{N-1}{k-1}$. We find

$$\underline{Y_N} = \sum_{k=1}^{N} z_k \binom{N-1}{k-1} (k-1)!\; Y_{N-k} = \underline{\sum_{k=1}^{N} \frac{1}{N} z_k \frac{N!}{(N-k)!} Y_{N-k}} \quad (\text{with } Y_0 = 1). \tag{7.5}$$

The eq. (7.5) describes a recursion because it allows us to compute Y_N from $\{Y_0, \ldots, Y_{N-1}\}$. If we take $z_k = 1\ \forall k$ in this equation, we know that $Y_{N-k} = (N-k)!$, and see that Y_N is the sum of constant terms, showing that the number of permutations with N in a cycle of length k is independent of k.

As a nontrivial application of the recursion in eq. (7.5), we now count, then sample, permutations containing only cycles of length 1 and 2. Now $\{z_1, z_2, z_3, \ldots, z_N\} = \{1, 1, 0, \ldots, 0\}$ (every permutation has, say, the same weight, under the condition that it contains no cycles of length > 2). For convenience, we set $Y_{-1} = 0$, and furthermore $Y_0 = 1$ and $Y_1 = 1$, and from eq. (7.5) obtain the recursion relation

$$Y_N = Y_{N-1} + (N-1)\; Y_{N-2}, \tag{7.6}$$

so that Y_N, the number of permutations with cycles of length at most 2, is given by:

$$\{Y_{-1}, Y_0, Y_1, Y_2, Y_3, Y_4, \dots\} = \{0, 1, 1, 2, 4, 10, \dots\}. \tag{7.7}$$

This sequence of integers is referenced in the online encyclopedia

The recursion in eq. (7.6) is implemented in Alg. 7.2 (`two-cycles`), a sampling algorithm for random permutations whose cycles only have length one or two. It is implemented in a short Python program Two-cycles.py, available on my website.

procedure `two-cycles`
input $\{Y_{-1}, Y_0, Y_1, \dots, Y_{N-1}\}$ (from eq. (7.7))
$Q \leftarrow$ `shuffle`$\{1, \dots, N\}$
$M \leftarrow N$
$P \leftarrow \{\}$
while $M > 0$**:**
$\left\{ \begin{array}{l} \Upsilon \leftarrow \texttt{ran}(0, Y_M) \\ \textbf{if } \Upsilon < Y_{M-1}\textbf{:}\ P \leftarrow P \cup \{(Q_M)\}; M \leftarrow M - 1 \\ \textbf{else:}\ P \leftarrow P \cup \{(Q_M, Q_{M-1})\}; M \leftarrow M - 2 \end{array} \right.$
output P (P in cycle representation (see eq. (7.3)))

Algorithm 7.2: `two-cycles`. Sampling a random permutation with cycles of length ≤ 2.

7.1.3 Symmetric density matrix and N-particle wave functions

In Lecture 6, the density matrix of a single-particle quantum system was shown to be

$$\rho\left(x, x', \beta\right) = \sum_n \psi_n(x) \mathrm{e}^{-\beta E_n} \psi_n^*(x'),$$

with orthonormal wave functions ψ_n ($\int \mathrm{d}x\ |\psi_n(x)|^2 = 1$ etc.). The partition function is the trace of the density matrix:

$$Z = \sum_n \mathrm{e}^{-\beta E_n} = \mathrm{Tr}\,\rho = \int \mathrm{d}x\ \rho(x, x, \beta)\,.$$

We may move from one to many particles without changing the framework simply by replacing single-particle states by N-particle states:

$$\left\{ \begin{array}{c} \text{many-particle} \\ \text{density matrix} \end{array} \right\} : \rho^{\text{dist}}\left(\{x_1, \dots, x_N\}, \{x'_1, \dots, x'_N\}, \beta\right)$$
$$= \sum_{\substack{\text{orthonormal} \\ N\text{-particle} \\ \text{states } \psi_n}} \psi_n(x_1, \dots, x_N) \mathrm{e}^{-\beta E_n} \psi_n(x'_1, \dots, x'_N). \tag{7.8}$$

For distinguishable particles, this definition is sufficient.

The bosonic density matrix is defined in analogy with eq. (7.8):

$$\rho^{\text{sym}}\left(\mathbf{x}, \mathbf{x}', \beta\right) = \sum_{\substack{\text{symmetric, orthonormal} \\ N\text{-particle wave functions } \psi_n^{\text{sym}}}} \psi_n^{\text{sym}}(\mathbf{x}) \mathrm{e}^{-\beta E_n} \psi_n^{\text{sym}}(\mathbf{x}').$$

Here, "symmetric" refers to the interchange of particles $x_k \leftrightarrow x_l$. Again, all wave functions are normalized. We remember from introductory Quantum Mechanics that symmetrized wave functions have characteristic, nontrivial normalization factors. For concreteness, we go on with two

noninteracting particles in two single-particle states, σ_1 and σ_2. The wave functions belonging to this system are the following:

$$\begin{aligned}
\psi^{\rm sym}_{\{1,1\}}(x_1,x_2) &= \psi_1(x_1)\psi_1(x_2),\\
\psi^{\rm sym}_{\{1,2\}}(x_1,x_2) &= \frac{1}{\sqrt{2}}\left[\psi_1(x_1)\psi_2(x_2)+\psi_1(x_2)\psi_2(x_1)\right],\\
\psi^{\rm sym}_{\{2,2\}}(x_1,x_2) &= \psi_2(x_1)\psi_2(x_2).
\end{aligned} \tag{7.9}$$

These three wave functions are symmetric with respect to particle exchange (for example, $\psi^{\rm sym}_{11}(x_1,x_2)=\psi^{\rm sym}_{11}(x_2,x_1)=\psi_1(x_1)\psi_1(x_2)$). They are orthonormal ($\int {\rm d}x_1\ {\rm d}x_2\ \psi^{\rm sym}_{12}(x_1,x_2)^2=1$, etc.). Hence the ideal-boson density matrix is given by

$$\begin{aligned}
\rho^{\rm sym}\big(\{x_1,x_2\},\{x_1',x_2'\},\beta\big) = {}& \psi^{\rm sym}_{11}(x_1,x_2){\rm e}^{-\beta E_{11}}\psi^{\rm sym}_{11}(x_1',x_2')\\
&+\psi^{\rm sym}_{12}(x_1,x_2){\rm e}^{-\beta E_{12}}\psi^{\rm sym}_{12}(x_1',x_2')\\
&+\psi^{\rm sym}_{22}(x_1,x_2){\rm e}^{-\beta E_{22}}\psi^{\rm sym}_{22}(x_1',x_2').
\end{aligned}$$

The various terms in this unwieldy object carry different prefactors, if we write the density matrix in terms of the symmetric wave functions in eq. (7.9). We shall, however, now express the symmetric density matrix through the many-particle density matrix of distinguishable particles without symmetry requirements, and see that the different normalization factors disappear.

We rearrange $\psi^{\rm sym}_{11}(x_1,x_2)$ as $\frac{1}{2}\left[\psi_1(x_1)\psi_1(x_2)+\psi_1(x_2)\psi_1(x_1)\right]$, and analogously for $\psi^{\rm sym}_{22}$. We also write out the part of the density matrix involving ψ_{12} twice (with a prefactor $\frac{1}{2}$). This gives the first two lines of the following expression; the third belongs to $\psi^{\rm sym}_{11}$ and the fourth to $\psi^{\rm sym}_{22}$:

$$\begin{aligned}
&\tfrac{1}{4}\left[\psi_1(x_1)\psi_1(x_2)+\psi_1(x_2)\psi_1(x_1)\right]\left[\psi_1(x_1')\psi_1(x_2')+\psi_1(x_2')\psi_1(x_1')\right]{\rm e}^{-\beta E_{11}}\\
&\tfrac{1}{4}\left[\psi_1(x_1)\psi_2(x_2)+\psi_1(x_2)\psi_2(x_1)\right]\left[\psi_1(x_1')\psi_2(x_2')+\psi_1(x_2')\psi_2(x_1')\right]{\rm e}^{-\beta E_{12}}\\
&\tfrac{1}{4}\left[\psi_2(x_1)\psi_1(x_2)+\psi_2(x_2)\psi_1(x_1)\right]\left[\psi_2(x_1')\psi_1(x_2')+\psi_2(x_2')\psi_1(x_1')\right]{\rm e}^{-\beta E_{21}}\\
&\tfrac{1}{4}\underbrace{\left[\psi_2(x_1)\psi_2(x_2)+\psi_2(x_2)\psi_2(x_1)\right]}_{\text{all permutations } Q \text{ of } \{x_1,x_2\}}\underbrace{\left[\psi_2(x_1')\psi_2(x_2')+\psi_2(x_2')\psi_2(x_1')\right]}_{\text{all permutations } P \text{ of } \{x_1',x_2'\}}{\rm e}^{-\beta E_{22}}
\end{aligned}$$

The rows of this expression correspond to a double sum over single-particle states. Each one has the same prefactor 1/4 (more generally, for N particles, we would obtain $(1/N!)^2$) and carries a double set (P and Q) of permutations of $\{x_1,x_2\}$, and of $\{x_1',x_2'\}$. More generally, for N particles and a sum over states σ, we have

$$\begin{aligned}
\rho^{\rm sym}\big(\{x_1,\dots,x_N\},\{x_1',\dots,x_N'\},\beta\big) = {}& \sum_{\{\sigma_1,\dots,\sigma_N\}}\sum_Q\sum_P\left(\frac{1}{N!}\right)^2\\
&\times\left[\psi_{\sigma_1}(x_{Q_1})\dots\psi_{\sigma_N}(x_{Q_N})\right]\left[\psi_{\sigma_1}(x'_{P_1})\dots\psi_{\sigma_N}(x'_{P_N})\right]{\rm e}^{-\beta(E_{\sigma_1}+\dots+E_{\sigma_N})}.
\end{aligned}$$

This agrees with

$$\rho^{\rm sym}\big(\{x_1,\dots,x_N\},\{x_1',\dots,x_N'\},\beta\big)=\frac{1}{N!}\sum_P\rho\big(x_1,x'_{P_1},\beta\big)\dots\rho\big(x_N,x'_{P_N},\beta\big), \tag{7.10}$$

where we were able to eliminate one set of permutations. We thus reach the bosonic density matrix in eq. (7.10) from the distinguishable density matrix by summing over permutations and dividing by $1/N!$, writing $\{x'_{P_1},\dots,x'_{P_N}\}$ instead of $\{x_1',\dots,x_N'\}$. The expression obtained for N ideal bosons—even though we strictly derived it only for two bosons in two states—carries

over to interacting systems, where we find

$$\overbrace{\rho^{\text{sym}}\big(\{x_1,\dots,x_N\},\{x'_1,\dots,x'_N\},\beta\big)}^{\text{bosonic density matrix}} = \frac{1}{N!}\sum_P \underbrace{\rho^{\text{dist}}\big(\{x_1,\dots,x_N\},\{x'_{P_1},\dots,x'_{P_N}\},\beta\big)}_{\text{distinguishable-particle density matrix}}. \quad (7.11)$$

7.2 Bosonic partition function

From the expression for the non-diagonal bosonic density matrix (eq. (7.11) we express the partition function of a bosonic system (the trace of the bosonic diagonal density matrix) as a sum over diagonal and nondiagonal density matrices for distinguishable particles:

$$Z_N = \frac{1}{N!}\sum_P Z_P \quad (7.12)$$

$$= \frac{1}{N!}\sum_P \int \mathrm{d}^N x \rho^{\text{dist}}\big(\{x_1,\dots,x_N\},\{x_{P(1)},\dots,x_{P(N)}\},\beta\big)\,. \quad (7.13)$$

For ideal particles, the distinguishable-particle density matrix separates into a product of single-particle density matrices, but the presence of permutations implies that these single-particle density matrices are not necessarily diagonal. For concreteness, we consider, for $N = 4$ particles,

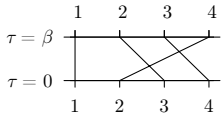

Figure 7.2: The permutation $\left(\begin{smallmatrix}1&4&2&3\\1&2&3&4\end{smallmatrix}\right)$ represented as a path.

the permutation $P = \left(\begin{smallmatrix}1&4&2&3\\1&2&3&4\end{smallmatrix}\right)$, which in cycle representation is written as $P = (1)(243)$ (see Fig. 7.2). This permutation consists of one cycle of length 1 and one cycle of length 3. The permutation-dependent partition function $Z_{(1)(243)}$ is

$$Z_{(1)(243)} = \int \mathrm{d}x_1\ \rho(x_1,x_1,\beta)\int \mathrm{d}x_2 \times \underbrace{\left[\int \mathrm{d}x_3\ \int \mathrm{d}x_4\ \rho(x_2,x_4,\beta)\,\rho(x_4,x_3,\beta)\,\rho(x_3,x_2,\beta)\right]}_{\rho(x_2,x_2,3\beta)}. \quad (7.14)$$

The last line of eq. (7.14) contains a double convolution and can be written as a diagonal single-particle density matrix at temperature $T = 1/(3\beta)$, in an elementary, yet elegant, application of the matrix squaring described in Lecture 7. After performing the last two remaining integrations, over x_1 and x_2, we find that the permutation-dependent partition function $Z_{(1)(243)}$ is the product of single-particle partition functions, one at temperature $1/\beta$ and the other at $1/(3\beta)$:

$$Z_{(1)(243)} = z(\beta)z(3\beta). \quad (7.15)$$

Here and in the following, we denote the single-particle partition functions with the symbol $z(\beta)$:

$$\left\{\begin{matrix}\text{single-particle}\\ \text{partition function}\end{matrix}\right\}:\ z(\beta) = \int \mathrm{d}x\ \rho(x,x,\beta) = \sum_\sigma \mathrm{e}^{-\beta E_\sigma}. \quad (7.16)$$

7.15 carries the essential message that—for ideal bosons— the N-particle partition function $Z(\beta)$ can be expressed as a sum of products of single-particle partition functions. However, this sum of $N!$ terms is nontrivial, unlike the one for the gas of ideal distinguishable particles. Only for small N can we think of writing out the $N!$ permutations and determining the partition function via the explicit sum in eq. (7.12). It is better to adapt the recursion formula of Sec. 7.1.2 to the ideal-boson partition functions. Now, the cycle weights are given by the single-particle density matrices at temperature $k\beta$. Taking into account that the partition functions carry a factor $1/N!$ (see eq. (7.13)), we find

$$Z_N = \frac{1}{N}\sum_{k=1}^{N} z_k Z_{N-k} \quad (\text{with } Z_0 = 1). \tag{7.17}$$

This recursion relation determines the partition function Z_N of an ideal boson system with N particles via the single-particle partition functions z_k at temperatures $\{1/\beta, \ldots, 1/(N\beta)\}$ and the partition functions $\{Z_0, \ldots, Z_{N-1}\}$ of systems with fewer particles.

The partition function $z_k(\beta)$ in the three-dimensional harmonic trap is

$$z_k(\beta) = \left(\sum_{E_x=0}^{\infty} \mathrm{e}^{-k\beta E_x}\right)\left(\sum_{E_y=0}^{\infty} \mathrm{e}^{-k\beta E_y}\right)\left(\sum_{E_z=0}^{\infty} \mathrm{e}^{-k\beta E_z}\right) = \left(\frac{1}{1-\mathrm{e}^{-k\beta}}\right)^3 \tag{7.18}$$

(we note that the ground-state energy is now $E_0 = 0$). Together with the recursion formula of eq. (7.17), it gives a general method for computing the partition function of canonical ideal bosons (see Alg. 7.3 (`canonic-recursion`)).

procedure `canonic-recursion`
input $\{z_1, \ldots, z_N\}$ ($z_k \equiv z_k(\beta)$, from eq. (7.18))
$Z_0 \leftarrow 1$
for $M = 1, \ldots, N$**:**
  $\{\ Z_M \leftarrow (z_M Z_0 + z_{M-1} Z_1 + \cdots + z_1 Z_{M-1})/M$
output Z_N

Algorithm 7.3: `canonic-recursion`. Obtaining the partition function for N ideal bosons through the recursion in eq. (7.17).

We pause for a moment to gain a better understanding of the recursion relation, and remember that each of its components relates to last-element cycles:

$$Z_N \propto \underbrace{z_N Z_0}_{\substack{\text{particle } N \\ \text{in cycle of} \\ \text{length } N}} + \cdots + \underbrace{z_k Z_{N-k}}_{\substack{\text{particle } N \\ \text{in cycle of} \\ \text{length } k}} + \cdots + \underbrace{z_1 Z_{N-1}}_{\substack{\text{particle } N \\ \text{in cycle of} \\ \text{length } 1}}. \tag{7.19}$$

It follows that the cycle probabilities satisfy

$$\left\{\begin{matrix}\text{probability of having particle} \\ N \text{ in cycle of length } k\end{matrix}\right\} : \pi_k = \frac{1}{N}\frac{z_k Z_{N-k}}{Z_N}. \tag{7.20}$$

We can compute the cycle probabilities $\{\pi_1, \ldots, \pi_N\}$ with Alg. 7.3 (`canonic-recursion`). In the zero-temperature limit, the probability of a particle to be in a cycle of length k becomes independent of k.

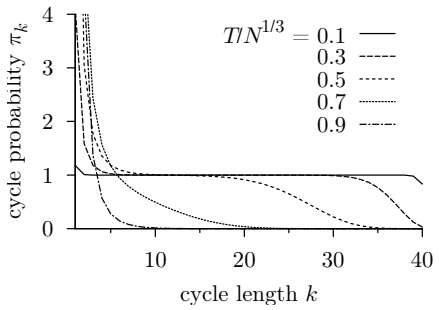

Figure 7.3: Cycle probabilities $\{\pi_1, \ldots, \pi_{40}\}$ for 40 ideal bosons in the harmonic trap (from modified Alg. 7.3 (`canonic-recursion`)).

7.2.1 Condensate fraction

Using path integrals, we have so far computed partition functions. We could also have computed internal energies (see Ref. [1] for details). It remains to be seen how Bose–Einstein condensation enters the path-integral picture. This is what we work out in two steps. In the present section, we show that the appearance of long cycles in the distribution of cycle lengths signals condensation into the ground state. In the next section, we discuss an explicit formula linking the distribution of cycle lengths to the distribution of condensed particles.

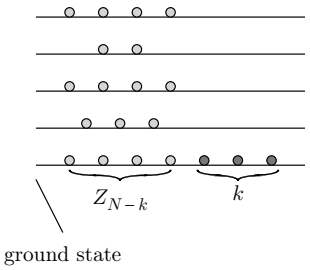

Figure 7.4: Restricted partition function $Y_{k,0}$ with at least $k = 3$ particles in the ground state.

To see the connection of condensation and cycle lengths, we consider the restricted N-particle partition function $Y_{k,0}$, where at least k particles are in the ground state. From Fig. 7.4, this partition function is

$$\left\{ \begin{array}{c} \text{partition function with} \\ \geq k \text{ bosons in ground state} \end{array} \right\} = Y_{k,0} = \mathrm{e}^{-\beta k E_0} Z_{N-k}.$$

Analogously, we may write, for $k+1$ instead of k,

$$\left\{ \begin{array}{c} \text{partition function with} \\ \geq k+1 \text{ bosons in ground state} \end{array} \right\} = Y_{k+1,0} = \mathrm{e}^{-\beta (k+1) E_0} Z_{N-k-1}.$$

Taking the difference between these two expressions, and paying attention to the special case $k = N$, we find

$$\left\{ \begin{array}{c} \text{partition function with} \\ k \text{ bosons in ground state} \end{array} \right\} = \begin{cases} Y_{k,0} - Y_{k+1,0} & \text{if } k < N \\ Y_{k,0} & \text{if } k = N \end{cases}. \tag{7.21}$$

Our choice of ground-state energy ($E_0 = 0$) implies $Y_{k,0} = Z_{N-k}$, and we may write the proba-

bility of having N_0 bosons in the ground state as

$$\pi(N_0) = \frac{1}{Z_N} \begin{cases} Z_{N-N_0} - Z_{N-(N_0+1)} & \text{if } N_0 < N \\ 1 & \text{if } N_0 = N \end{cases}. \tag{7.22}$$

The condensate fraction, the mean value of N_0, is given by

$$\langle N_0 \rangle = \sum_0^N N_0 \pi(N_0) = \frac{1}{Z_N} \left\{ \sum_{N_0=1}^{N-1} N_0 \cdot \left[Z_{N-N_0} - Z_{N-(N_0+1)} \right] + N Z_0 \right\}.$$

This is a telescopic sum, where similar terms are added and subtracted. It can be written more simply as

$$\langle N_0 \rangle = \frac{Z_{N-1} + Z_{N-2} + \cdots + Z_0}{Z_N} \quad (\text{with } E_0 = 0). \tag{7.23}$$

The calculations of the condensate fraction can be incorporated into Alg. 7.3 (`canonic-recursion`).

7.2.2 Cycle-length distribution

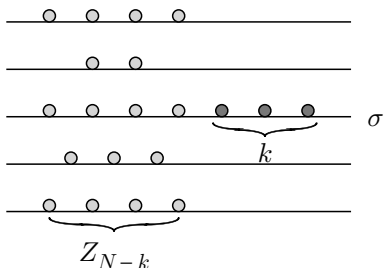

Figure 7.5: Restricted partition function $Y_{k,\sigma}$ with at least $k = 3$ particles in state σ (for $N = 20$ particles).

We continue the analysis of restricted partition functions, by simply generalizing the concept of the restricted partition functions to a state σ, rather than only the ground state (see Fig. 7.5). From eq. (7.21), we arrive at

$$\left\{ \begin{matrix} \text{partition function with} \\ \geq k \text{ bosons in state } \sigma \end{matrix} \right\} = Y_{k,\sigma} = \mathrm{e}^{-\beta k E_\sigma} Z_{N-k}.$$

This equation can be summed over all states, to arrive at a crucial expression,

$$\underbrace{\sum_\sigma \left\{ \begin{matrix} \text{partition function} \\ \text{with} \geq k \text{ bosons} \\ \text{in state } \sigma \end{matrix} \right\}}_{} = \underbrace{\sum_\sigma \mathrm{e}^{-\beta k E_\sigma}}_{z_k, \text{ see eq. (7.16)}} Z_{N-k} \propto \underbrace{\left\{ \begin{matrix} \text{cycle} \\ \text{weight} \\ \pi_k \end{matrix} \right\}}_{}, \tag{7.24}$$

because it relates the energy-level description (on the left) with the description in terms of density matrices and cycle-length distributions (on the right). Indeed, the sum over the exponential factors gives the partition function of the single-particle system at temperature $1/(k\beta)$, $z_k = z(k\beta)$, and the term $z_k Z_{N-k}$ is proportional to the cycle weight π_k. This leads to a relation between occupation probabilities of states and cycle weights:

$$\sum_\sigma \left\{ \begin{matrix} \text{partition function with} \\ k \text{ bosons in state } \sigma \end{matrix} \right\} \propto \left\{ \begin{matrix} \text{cycle weight} \\ \pi_k \end{matrix} \right\} - \left\{ \begin{matrix} \text{cycle weight} \\ \pi_{k+1} \end{matrix} \right\}. \tag{7.25}$$

To interpret this equation, we note that the probability of having $k \gg 1$ in any state other than the ground state is essentially zero. It follows that the sum in eq. (7.25) is dominated by the partition function with k particles in the ground state, and this relates the probability of having k particles in the ground state (the distribution whose mean gives the condensate fraction) to the integer derivative of the cycle-length distribution. (The difference in eq. (7.25) constitutes a negative integer derivative: $-\Delta f(k)/\Delta k = f(k) - f(k+1)$.) We arrive at the conclusion that the condensate distribution is proportional to the integer derivative of the cycle length distribution.

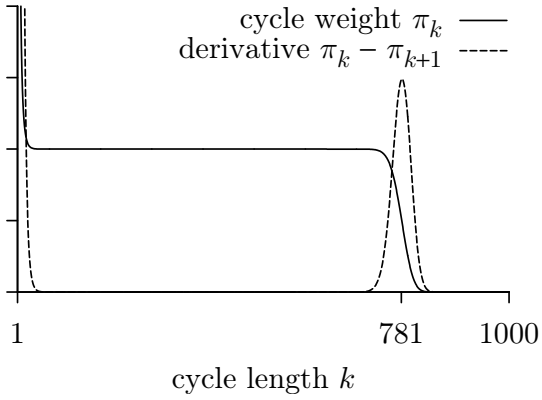

Figure 7.6: Cycle weights π_k, and derivative $\pi_k - \pi_{k+1}$, for 1000 trapped bosons at $T/N^{1/3} = 0.5$ (from Alg. 7.3 (`canonic-recursion`)).

7.2.3 Direct-sampling algorithm for ideal bosons

In the previous subsections, we computed partition functions for ideal bosons by appropriately summing over all permutations and integrating over all particle positions. We now consider sampling, the twin brother of integration, in the case of the ideal Bose gas. Specifically, we discuss a direct-sampling algorithm for ideal bosons, which lies at the heart of some path-integral Monte Carlo algorithms for interacting bosons in the same way as the children's algorithm performed in a square on the beach underlies the Markov-chain Monte Carlo algorithm for hard disks. As illustrated in eq. (7.13), a boson configuration consists of a permutation and a set of positions, that are summed and integrated over, respectively, to obtain the partition function. We sample this sum/integral in a two-step procedure.

For sampling the bosonic partition function, we start with the permutation part. We know the following from eq. (7.17):

$$Z_N = \frac{1}{N}\Big(\underbrace{z_1 Z_{N-1}}_{\substack{\text{particle } N \\ \text{in cycle of} \\ \text{length 1}}} + \underbrace{z_2 Z_{N-2}}_{\substack{\text{particle } N \\ \text{in cycle of} \\ \text{length 2}}} + \cdots + \underbrace{z_{N-1} Z_1}_{\substack{\text{particle } N \\ \text{in cycle of} \\ \text{length } N-1}} + \underbrace{z_N Z_0}_{\substack{\text{'particle } N \\ \text{in cycle of} \\ \text{length } N}}\Big).$$

Mirroring what we already did for permutations, in Alg. 7.2 (`two-cycles`), we initially set $M = N$ and sample the length k of the last-element cycle from M choices, without knowing anything about the permutations of the $N-k$ particles in other cycles. We then set $M = M-k$ and continue until we run out of bosons (see Alg. 7.4 (`direct-cycles`)). Because particles are indistinguishable, we need only remember the lengths of cycles generated, that is, the histogram of cycle lengths $\{m_1, \ldots, m_N\}$ in one permutation of N particles (m_k gives the number of cycles of length k in the sampled permutation).

After sampling the permutation, we sample the coordinates $\{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$. Particles $\{l+1, l+$

procedure `direct-cycles`
input $\{z_1, \ldots, z_N\}, \{Z_0, \ldots, Z_{N-1}\}$ (from Alg. 7.3 (`canonic-recursion`))
$\{m_1, \ldots, m_N\} \leftarrow \{0, \ldots, 0\}$
$M \leftarrow N$
while $M > 0$**:**
  $k \leftarrow$ `sample` $(\{z_1 Z_{M-1}, \ldots, z_k Z_{M-k}, \ldots, z_M Z_0\})$
  $M \leftarrow M - k$
  $m_k \leftarrow m_k + 1$
output $\{m_1, \ldots, m_N\}$ (m_k: number of cycles of length k.)

Algorithm 7.4: `direct-cycles`. Sampling a permutation, encoded in the cycle-lengths $\{m_1, \ldots, m_n\}$, for N ideal bosons.

$2, \ldots, l+k\}$ on each permutation cycle of length l form a closed path and their coordinates $\{\mathbf{x}_{l+1}(0), \ldots, \mathbf{x}_{l+k}(0)\}$ can be sampled using the Lévy construction of Lecture 6, at inverse temperature $k\beta$ and with a discretization step $\Delta_\tau = \beta$.

procedure `direct-harmonic-bosons`
input $\{z_1, \ldots, z_N\}, \{Z_0, \ldots, Z_N\}$ (for harmonic trap)
$\{m_1, \ldots, m_N\} \leftarrow$ `direct-cycles` $(\{z_1, \ldots, z_N\}, \{Z_0, \ldots, Z_{N-1}\})$
$l \leftarrow 0$
for all $m_k \neq 0$**:**
  for $i = 1, \ldots, m_k$**:**
    $\Upsilon \leftarrow$ `gauss` $(\ldots)$
    $\{x_{l+1}, \ldots, x_{l+k}\} \leftarrow$ `levy-harmonic-path` $(\Upsilon, \Upsilon, k\beta, k)$
    $l \leftarrow l + k$
output $\{x_1, \ldots, x_N\}$

Algorithm 7.5: `direct-harmonic-bosons`. Direct-sampling algorithm for ideal bosons in the harmonic trap. Only x-coordinates are shown.

The complete program for simulating ideal Bose–Einstein condensates with tens of thousands of particles in the harmonic trap takes no more than a few dozen lines of computer code (see Direct-bosons. py on my website, for a Python implementation). We may represent the spatial distribution of particles (see Fig. 7.7 for a projection in two dimensions). The wide thermal cloud at temperatures $T > T_c$ suddenly shrinks below T_c because most particles populate the single-particle ground state or, in our path-integral language, because most particles are on a few long cycles. The power of the path-integral approach resides in that interactions can be very simply introduced into the rudimentary Alg. 7.5 (`direct-harmonic-bosons`) (see Ref. [1] for more details, as well as for theoretical background on the transition temperature in a harmonic trap).

References

[1] W. Krauth, *Statistical Mechanics: Algorithms and Computations*. Oxford University Press, 2006.

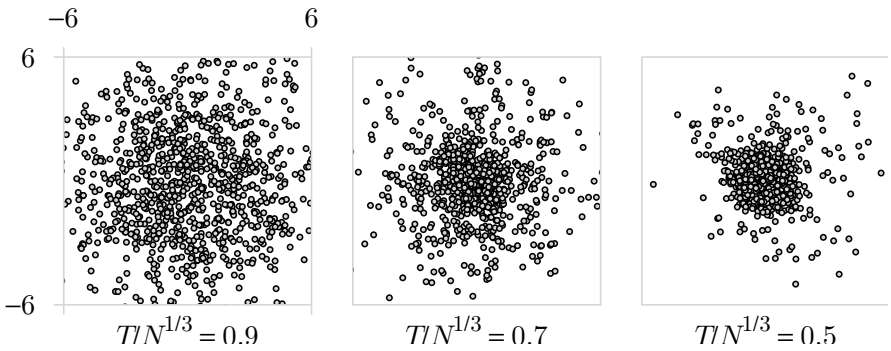

Figure 7.7: Two-dimensional snapshots of 1000 ideal bosons in a three-dimensional harmonic trap (from Alg. 7.5 (`direct-harmonic-bosons`)).