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STATISTICAL MECHANICS AND THE PARTITIONS OF NUMBERS

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1. The properties of partitions of numbers extensively investigated by Hardy and Ramanujan (1) have proved to be of outstanding mathematical interest. The first physical application known to us of the Hardy-Ramanujan asymptotic expression for the number of possible ways any integer can be written as the sum of smaller positive integers is due to Bohr and Kalckar (2) for estimating the density of energy levels for a heavy nucleus. The present paper is concerned with the study of thermodynamical assemblies corresponding to the partition functions familiar in the theory of numbers. Such a discussion is not only of intrinsic interest, but it also leads to some properties of partition functions, which, we believe, have not been explicitly noticed before. Here we shall only consider an assembly of identical (Bose-Einstein, and Fermi-Dirac) linear simple-harmonic oscillators. The discussion will be extended to assemblies of non-interacting particles in a subsequent paper.

2. We shall use the following notation for partitions of a (positive) integer ν:

(i) $p(\nu)$ denotes the number of distinct ways of expressing ν as a sum of positive integers. Hardy and Ramanujan established the asymptotic expression

$$p(\nu) = \frac{1}{(4\sqrt{3})\,\nu}\exp\left\{\pi\sqrt{\frac{2\nu}{3}}\right\}. \tag{1}$$

Recently, Rademacher (3) has given an *exact* expression for $p(\nu)$.

(ii) $q(\nu)$ denotes the number of partitions of ν into summands which must be all different*. For example, for $\nu = 3$ the allowed partitions are $3, 2+1$; $q(3) = 2$; $q(4) = 2$; $q(5) = 3$; $q(6) = 4$. The asymptotic formula for $q(\nu)$ due to Hardy and Ramanujan is

$$q(\nu) = \frac{1}{4\,.\,3^{\frac{1}{4}}\nu^{\frac{3}{4}}}\exp\left\{\pi\sqrt{\frac{\nu}{3}}\right\}. \tag{2}$$

(iii) $p_k(\nu)$ denotes the number of partitions of ν into exactly k or less than k parts: for $k \geqslant \nu$, $p_k(\nu) = p(\nu)$.

We shall use $P_k(\nu)$ to denote partitions of ν into exactly k parts. We have

$$p_k(\nu) = \sum_{r=1}^{k} P_r(\nu).$$

* In representing partition functions we shall use the letter q instead of p when the summands are required to be all different.

(iv) $q_k(\nu)$ represents the number of partitions of ν into exactly k or less different parts, and $Q_k(\nu)$ the number of partitions into exactly k different parts: $q_k(\nu) = \sum_{r=1}^{k} Q_r(\nu)$.

We may note the following relations:

$$p_k(\nu) = P_k(\nu+k), \qquad P_k(\nu) = Q_k(\nu+\tfrac{1}{2}k(k-1)),$$
$$p_k(\nu) = Q_k(\nu+\tfrac{1}{2}k(k+1)), \quad Q_k(\nu+k) = Q_k(\nu)+Q_{k-1}(\nu).$$

(v) We shall use $p(\nu|s)$ to represent the number of ways of expressing ν as

$$\nu = a_1^s + a_2^s + \dots + a_r^s \quad (r = 1, 2, 3, \dots),$$

where $1 \leqslant a_1 \leqslant a_2 \dots \leqslant a_r$ are positive integers. In the case of $q(\nu|s)$ the summands must be all different. Hardy and Ramanujan have given asymptotic expressions for a positive integral s. The above definition can be extended to include non-integral (positive) values of s. We define $p(\nu|s)\,\Delta\nu$ as the number of distinct sums of the type $\sum_r a_r^s$ which lie between ν and $\nu+\Delta\nu$, a_r's being positive integers satisfying the above relation. Similarly $q(\nu|s)$, $p_k(\nu|s)$ and $q_k(\nu|s)$ can be defined*.

In the sequel we shall obtain asymptotic expressions for the partition functions defined in (iii) and (iv).

3. We contemplate an assembly of N identical (non-interacting) linear simple-harmonic oscillators. The energy levels of an oscillator will be $\epsilon_\rho = (\rho+\frac{1}{2})\hbar\omega$, where ω is the (angular) frequency and ρ is a positive integer (including zero). If E denotes the energy of the assembly, a number ν is defined by

$$\hbar\omega\nu = E - \tfrac{1}{2}N\hbar\omega, \tag{3}$$

where $\frac{1}{2}N\hbar\omega$ is the residual energy of the oscillators: ν represents, in units of $\hbar\omega$, the energy of the assembly, excluding the residual energy. Let $w(E)$ represent the number of distinct wave functions accessible to the assembly when in the energy state E. For a Bose-Einstein assembly the number of accessible wave functions is the number of ways of distributing ν energy quanta among N similar oscillators, there being no restriction as to the number of quanta assigned to an oscillator. For a Fermi-Dirac assembly the energy quanta assigned to the oscillators must be all different. Hence we have

$$\left.\begin{aligned} &w(E) = p_N(\nu) && \text{for Bose-Einstein assembly,}\\ &w(E) = Q_N(\nu)+Q_{N-1}(\nu) = Q_N(\nu+N) && \text{for Fermi-Dirac assembly,}\\ \text{and}\quad &w(E) = \frac{{}^N H_\nu}{N!} = \frac{(N+\nu-1)!}{N!(N-1)!\,\nu!} && \text{for Maxwell-Boltzmann assembly.}\end{aligned}\right\} \tag{4}$$

In the case of a 'classical' (Maxwell-Boltzmann) assembly the oscillators are considered as distinguishable from each other, and the number of wave functions is simply the number of ways of distributing ν quanta among N distinguishable oscillators which is equal to the number of ways of assigning N 'objects' to ν 'places', repetitions of any

* These functions will be required to describe the thermodynamic behaviour of an assembly to be discussed in a subsequent paper.

object being permissible. There is no valid classical reason for the inclusion of the factor $1/N!$, but it is necessary for the expression for entropy to be sensible*.

The function Z for the assembly—called hereafter as *states function*—is as usual defined by

$$Z = \sum_l w(E_l)\, e^{-E_l \mu}, \tag{5}$$

which serves to determine the thermodynamic functions according to the relations

$$U = -\frac{\partial}{\partial\mu}\log Z, \tag{6a}$$

$$S = \log Z + \mu\nu = \log Z - \mu\frac{\partial}{\partial\mu}\log Z, \tag{6b}$$

$$F = U - \frac{S}{\mu} = -\frac{1}{\mu}\log Z, \tag{6c}$$

where U is the energy, S the entropy and F the Helmholtz free energy of the assembly. The temperature measured in energy units is $1/\mu$. The application of the Mellin-Burkill inversion formula to (5) readily gives

$$w(E)\,dE = \frac{e^S}{(-2\pi\,\partial E/\partial\mu)^{\frac{1}{2}}}\,dE, \tag{7}$$

which we shall refer to as Bethe's theorem (4).

The states function Z which for the Bose-Einstein assembly of linear oscillator is defined by

$$Z = \sum_{\nu=1}^{\infty} p_N(\nu)\, e^{-(\nu+\frac{1}{2}N)\mu}, \tag{8}$$

where $1/\mu$ is the temperature measured in terms of the energy unit $\hbar\omega$ ($\mu = \hbar\omega/(kT)$, where k is the Boltzmann constant), may also be written as

$$Ze^{\frac{1}{2}N\mu} = \prod_{r=1}^{N}(1-e^{-r\mu})^{-1}. \tag{9}$$

For the Fermi-Dirac assembly we obtain, as can readily be verified,

$$\begin{aligned} Ze^{\frac{1}{2}N\mu} &= \sum_{\nu=1}^{\infty}[Q_N(\nu)+Q_{N-1}(\nu)]\,e^{-\nu\mu} \\ &= e^{-\frac{1}{2}N(N-1)\mu}\prod_{r=1}^{N}(1-e^{-r\mu})^{-1}, \end{aligned} \tag{10}$$

and for the 'classical' case we have

$$Ze^{\frac{1}{2}N\mu} = (1-e^{-\mu})^{-N}/N!. \tag{11}$$

It may be noted that for $N^2\mu \to 0$

$$\prod_{r=1}^{N}(1-e^{-r\mu})^{-1} = (1-e^{-\mu})^{-N}\prod_{r=1}^{N}\frac{1}{\{1+e^{-\mu}+\ldots+e^{-(r-1)\mu}\}} \to (1-e^{-\mu})^{-N}/N!,$$

and hence both (9) and (10) tend to the 'classical' expression (11).

* When $N = 0(\nu^{\frac{1}{2}})$, $p_N(\nu)$ and $Q_N(\nu)+Q_{N-1}(\nu)$ tend to ${}^N H_\nu/N!$ which means that for $N \ll \nu^{\frac{1}{2}}$ Bose and Fermi statistics merge into classical statistics.

Using the above expressions for the state function Z we have for the thermodynamic functions E and S,

$$\frac{E-\frac{1}{2}N\hbar\omega}{\hbar\omega}=\nu=\begin{cases}\sum_{r=1}^{N}\frac{r}{e^{r\mu}-1} & \text{B.-E. statistics,} \quad (12a)\\ \frac{N(N-1)}{2}+\sum_{r=1}^{N}\frac{r}{e^{r\mu}-1} & \text{F.-D. statistics,} \quad (12b)\\ \frac{N}{e^{\mu}-1} & \text{M.-B. statistics,} \quad (12c)\end{cases}$$

$$S=\begin{cases}\sum_{r=1}^{N}\frac{r\mu}{e^{r\mu}-1}-\sum_{1}^{N}\log(1-e^{-r\mu}) & \text{B.-E. and F.-D. statistics,} \quad (13a)\\ \frac{N\mu}{e^{\mu}-1}-\log N!-N\log(1-e^{-\mu}) & \text{M.-B. statistics.} \quad (13b)\end{cases}$$

It is remarkable that for an assembly of a given number of oscillators at an assigned temperature the entropy is the same whether the assembly obeys Fermi-Dirac or Bose-Einstein statistics.

4. We shall first discuss the Bose-Einstein assembly. We begin with the limiting case when $N\mu$ is small compared to unity. The expression ($12a$) for ν gives the power series in terms of μ

$$\nu=\frac{N}{\mu}-\tfrac{1}{2}S_1+B_1\frac{S_2}{2!}\mu-B_2\frac{S_4}{4!}\mu^3+B_3\frac{S_6}{6!}\mu^5\ldots, \tag{14}$$

where $B_1=\frac{1}{6}$, $B_2=\frac{1}{30}$, $B_3=\frac{1}{42}$, ... are the Bernoulli numbers and

$$S_r=\sum_{n=1}^{N}n^r.$$

The expansion (14) holds so long as

$$e^{N\mu}<1+2N\mu, \quad \text{or} \quad N\mu<1{\cdot}256 \tag{15}$$

(which includes $N\sim 0(\nu^{\frac{1}{2}})$). Similarly for the entropy we have the expression

$$S=N-\log N!-N\log\mu+B_1\frac{S_2}{2!}\frac{\mu^2}{2}-B_2\frac{S_4}{4!}\frac{3\mu^4}{4}+B_3\frac{S_6}{6!}\frac{5\mu^6}{6}\ldots, \tag{16}$$

and hence

$$F=\frac{1}{\mu}\log N!+\frac{N}{\mu}\log\mu-\frac{N(N-1)}{4}+B_1\frac{S_2}{2!}\frac{\mu}{2}-B_2\frac{S_4}{4!}\frac{\mu^3}{4}\ldots; \tag{17}$$

these are valid under restriction (15).

For $N\mu\to 0$ (this condition, because of (14) is equivalent to $N/\nu^{\frac{1}{2}}\to 0$) which represents the non-degenerate or 'classical' approximation, the expressions for E, S and F reduce to

$$\nu=\frac{N}{\mu} \quad \text{or} \quad E=\frac{N\hbar\omega}{2}+NkT, \tag{18a}$$

$$S=N\log\frac{e^2}{N\mu} \quad \text{or} \quad S=Nk\log\frac{e^2kT}{N\hbar\omega}, \tag{18b}$$

and

$$F=\frac{N}{\mu}\log\frac{N\mu}{e} \quad \text{or} \quad F=NkT\log\frac{N\hbar\omega}{ekT}. \tag{18c}$$

We shall now consider series expressions for ν, S and F suitable for $\mu N \gg 1$ but which also hold generally. We have for ν, using the Euler summation formula,

$$\nu = \frac{1}{\mu^2}\int_0^{N\mu}\frac{t\,dt}{e^t-1} - \frac{1}{2\mu} + \frac{N}{2(e^{N\mu}-1)} + \frac{1}{24} + \frac{1}{12}\left(\frac{1}{e^{N\mu}-1} - \frac{N\mu e^{N\mu}}{(e^{N\mu}-1)^2}\right) + O(\mu^2). \quad (19)$$

Similarly we have for the entropy and free energy the series expressions

$$S = \left(\frac{\pi^2}{3} - 2\sum_1^\infty \frac{e^{-rN\mu}}{r^2}\right)\frac{1}{\mu} - N\sum_1^\infty \frac{e^{-rN\mu}}{r}$$
$$+\tfrac{1}{2}\log\frac{\mu}{2\pi e(1-e^{-N\mu})} + \frac{N\mu}{2(e^{N\mu}-1)} - \frac{N\mu^2 e^{N\mu}}{12(e^{N\mu}-1)^2} + 0(\mu^3), \quad (20)$$

$$F = -\left(\frac{\pi^2}{6} - \sum_1^\infty \frac{e^{-rN\mu}}{r^2}\right)\frac{1}{\mu^2} - \frac{1}{2\mu}\log\frac{\mu e^{-N\mu}}{2\pi(1-e^{-N\mu})} + \frac{1}{24} + \frac{1}{12(e^{N\mu}-1)} + 0(\mu^2). \quad (21)$$

We shall utilize the above expression for entropy to derive the asymptotic formulae for the partition functions $p_N(\nu)$ and $p(\nu)$ with the help of Bethe's theorem. We have, using (14) and (16) in (7),

$$p_N(\nu) \sim \frac{1}{N!}\,{}^N H_\nu \sim \frac{e^{2N}\nu^{N-1}}{2\pi N^{2N}} \quad \text{for} \quad N \ll \nu^{\frac{1}{2}}, \quad (22)$$

and from (19), (20) and (7) we obtain

$$p_N(\nu) \sim \frac{1}{(4\sqrt{3})\,\nu}\exp\left\{\pi\sqrt{(\tfrac{2}{3}\nu)} - \frac{\sqrt{(6\nu)}}{\pi}e^{-\pi N/\sqrt{(6\nu)}}\right\} \quad \text{for} \quad N \gg \nu^{\frac{1}{2}}, \quad (23)$$

and hence

$$p(\nu) \sim \frac{1}{(4\sqrt{3})\,\nu}\exp[\pi\sqrt{(\tfrac{2}{3}\nu)}], \quad (24)$$

which is the Hardy-Ramanujan formula. In general we obtain from (19) and (20) for $p_N(\nu)$ the expression

$$p_N(\nu) \sim \frac{D^{\frac{1}{2}}\exp\left[\left\{\left(\frac{\nu}{D}\right)^{\frac{1}{2}} + \tfrac{1}{4}D\left(1 - \frac{x}{e^x-1}\right)\right\}\int_0^x\left(\frac{t}{e^t-1} - \log(1-e^{-t})\right)dt + \frac{x}{2(e^x-1)}\right]}{2\pi\nu\left\{2e(1-e^{-x})\left(1 - \frac{x^2}{2D(e^x-1)}\right)\right\}^{\frac{1}{2}}}, \quad (25)$$

where

$$D = \int_0^x \frac{t\,dt}{e^t-1},$$

and $x \equiv \mu N$ is given by (19). It may be noticed that the above expression for $p_N(\nu)$ reduces to (22) when $x \to 0$ and to (23) when $x \to \infty$*.

5. We now revert to the Fermi-Dirac assembly for which the treatment runs on essentially the same lines as for the Bose-Einstein case, and we shall quote the results. We have

$$\nu = \frac{N(N-1)}{2} + \frac{1}{\mu^2}\int_0^{N\mu}\frac{t\,dt}{e^t-1} - \frac{1}{2\mu} + \frac{N}{2(e^{N\mu}-1)} + \frac{1}{24} + \frac{1}{12}\left\{\frac{1}{e^{N\mu}-1} - \frac{N\mu e^{N\mu}}{(e^{N\mu}-1)^2}\right\} + 0(\mu^2), \quad (26)$$

$$S = \frac{1}{\mu}\left(\frac{\pi^2}{3} - 2\sum_1^\infty \frac{e^{-rN\mu}}{r^2} - N\mu\sum_1^\infty \frac{e^{-rN\mu}}{r}\right)$$
$$+\tfrac{1}{2}\log\frac{\mu}{2\pi e(1-e^{-N\mu})} + \frac{N\mu}{2(e^{N\mu}-1)} - \frac{N\mu^2 e^{N\mu}}{12(e^{N\mu}-1)^2} + 0(\mu^3), \quad (27)$$

* Erdos and Lehner (5) have discussed the functions $p_N(\nu)$ and $q_N(\nu)$, and obtained asymptotic expressions for certain ranges for N. The present simple treatment gives expressions for $p_N(\nu)$ covering the entire range for N (see also Auluck, Chowla and Gupta (6), Auluck (7)).

$$F = \frac{N(N-1)}{2} - \frac{1}{\mu^2}\left(\frac{\pi^2}{6} - \sum_1^\infty \frac{e^{-rN\mu}}{r^2}\right) - \frac{1}{2\mu}\log\frac{\mu e^{-N\mu}}{2\pi(1-e^{-N\mu})} + \frac{1}{24} + \frac{1}{12(e^{N\mu}-1)} + 0(\mu^2). \quad (28)$$

As in Bose statistics the case for $N\nu^{-\frac{1}{2}} \sim N\mu \to 0$ represents the non-degenerate or 'classical' approximation and the expressions for E, S and F reduce to (18). From (4) it follows that

$$Q_N(\nu) \sim \frac{1}{N!}{}^N H_\nu, \quad \text{when} \quad N \ll \nu^{\frac{1}{2}}, \quad (29)$$

and hence we have

$$q_N(\nu) = \sum_{r=1}^{N} Q_r(\nu) \sim \frac{1}{N!}{}^N H_\nu, \quad \text{when} \quad N \ll \nu^{\frac{1}{2}}. \quad (30)$$

When N is given by the relation*

$$\nu - \frac{N(N+1)}{2} = y\nu^{\frac{1}{4}}, \quad y \ll \nu^{\frac{1}{4}}, \quad (31)$$

we have

$$Q_N(\nu) \sim \frac{1}{4y\sqrt{(3\nu)}} \exp\{\pi\sqrt{(\tfrac{2}{3}y)}\nu^{\frac{1}{4}} - 2\nu^{\frac{1}{2}} e^{-\pi\nu^{\frac{1}{2}}/\sqrt{(3\nu)}}\}.$$

The above expression for $Q_N(\nu)$ does not appear suitable for evaluating $q_N(\nu)$. The discussion of the present paper is specially convenient for treating $p_N(\nu)$†.

It may be mentioned that a two-dimensional (two spatial coordinates) gas or non-interacting particles corresponds practically, though not exactly, to an assembly of linear-harmonic oscillators and is, therefore, describable by the partition functions $p_N(\nu)$ and $Q_N(\nu)$. It is easy to see that an assembly of non-interacting particles, where each particle requires α spatial coordinates to describe its motion, requires for its description the partition functions $p_N(\nu \mid 2/\alpha)$ and $Q_N(\nu \mid 2/\alpha)$; the notation is in accordance with § 2. The properties of $p(\nu \mid s)$ will be discussed in a subsequent paper.

* The non-degenerate case corresponds to $N\mu \ll 1$, i.e. $N \ll \nu^{\frac{1}{2}}$. For the degenerate case $N\mu \gg 1$ which in Bose-Einstein statistics reduces to $N \gg \nu^{\frac{1}{2}}$, and in Fermi-Dirac statistics to $N \to (2\nu)^{\frac{1}{2}}$.

† The general method for evaluating $p_N(\nu|s)$ and $q_N(\nu|s)$ for any s, to be described in a subsequent paper, readily lends itself to the determination of $q_N(\nu)$.

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