

Fermi-Dirac statistics and the number theory

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Abstract. – We relate the Fermi-Dirac statistics of an ideal Fermi gas in a harmonic trap to partitions of given integers into distinct parts, studied in number theory. Using methods of quantum statistical physics we derive analytic expressions for cumulants of the probability distribution of the number of different partitions.

Introduction. – Standard textbooks use grand-canonical ensemble to describe *ideal* quantum gases [1]. It has been pointed out by Grossmann and Holthaus [2], and Wilkens and Weiss [3] that such an approach leads to pathological results for fluctuations of particle numbers in Bose-Einstein condensates (BEC). This has stimulated intensive studies of BEC fluctuations using canonical and microcanonical ensembles for ideal [4, 5] and interacting [6] gases. Grossmann and Holthaus [2] related the problem for an ideal Bose gas in a harmonic trap to the number-theoretical studies of partitions of an integer \mathcal{E} into M integers [7], and to the famous Hardy-Ramanujan formula [8]. In a series of beautiful papers, Weiss *et al.* (see [9] and references therein) have been able to apply methods of quantum statistics to derive non-trivial number-theoretical results. In this letter we apply the approach of ref. [9] to Fermi gases, and relate the problem of an ideal Fermi gas in a harmonic trap to studies of partitions of \mathcal{E} into M *distinct* integers. We show that the probability distribution of the number of different partitions is asymptotically Gaussian and we calculate analytically its cumulants. This physically motivated approach to the number-theoretical problem turns out to be more powerful than the earlier mathematical works based on the moments rather than cumulants (see, *e.g.*, [10]). Our results are complementary to those of Tran [11], who has calculate particle number fluctuations in the ground state (Fermi sea) for the fixed energy and number of particles.

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Ideal Fermi gas. – We consider a microcanonical ensemble of N thermally isolated, spinless, non-interacting fermions, trapped in a harmonic potential with frequency ω_0 . The discrete one-particle states have energies $\epsilon_\nu = \hbar\omega_0(\nu + 1/2)$, $\nu = 0, 1, \dots$. A microstate of the system is described by the sequence of the occupation numbers $\{n_\nu\}$, where $n_\nu = 0, 1$ and $\sum_{\nu=0}^\infty n_\nu = N$. The total energy of a microstate $\{n_\nu\}$ can be written as

$$E(\{n_\nu\}) = N\epsilon_0 + \hbar\omega_0 \mathcal{E}, \tag{1}$$

where the integer

$$\mathcal{E} = \sum_{\nu=1}^\infty n_\nu \nu \tag{2}$$

determines the contribution to E from one-particle excited states. Note that \mathcal{E} is a sum of M distinct integers, where $M = N - 1$ if $n_0 = 1$, or $M = N$ otherwise. Hence, in order to construct the microcanonical partition function $\Gamma(E, N)$, one has to calculate the number of partitions of the given integer \mathcal{E} into M distinct parts. This, in turn, is a standard problem in combinatorics [12]. If we call the number of distinct partitions $\tilde{\Phi}(\mathcal{E}, M)$, then $\Gamma(E, N) = \tilde{\Phi}(\mathcal{E}, M)$ and the physical problem of finding $\Gamma(E, N)$ is mapped to a combinatorial one.

Let us introduce the total number of distinct decompositions:

$$\tilde{\Omega}(\mathcal{E}) = \sum_{M=1}^{M_{max}} \tilde{\Phi}(\mathcal{E}, M), \tag{3}$$

and consider the probability (relative frequency):

$$p_{mc}(\mathcal{E}, M) = \frac{\tilde{\Phi}(\mathcal{E}, M)}{\tilde{\Omega}(\mathcal{E})}, \tag{4}$$

that exactly M distinct terms occur in the decomposition of \mathcal{E} . This is the central object of our study. In the case of bosons $p_{mc}(\mathcal{E}, M)$ possesses clear physical interpretation, as was explained in ref. [9]. This is the probability of finding M excited particles, when the total excitation energy is $\hbar\omega_0 \mathcal{E}$. For fermions, however, the ground state of the whole system corresponds to the filled Fermi sea. Since the number of partitions M differs at most by 1 from the number of particles N , we may regard (4) as a probability density in the fictitious Maxwell demon ensemble [5] with vanishing chemical potential. The distribution (4) describes at the same time an interesting mathematical problem, which, up to our knowledge, has never been treated using physical methods.

Using standard results from combinatorics [12], the exact expression for $\tilde{\Phi}(\mathcal{E}, M)$ can be written down,

$$\tilde{\Phi}(\mathcal{E}, M) = P\left(\mathcal{E} - \binom{M}{2}, M\right), \tag{5}$$

in terms of a recursively defined function P :

$$P(n, k) = \begin{cases} 0 & \text{for } k = 0 \text{ or } k > n, \\ P(n - 1, k - 1) + P(n - k, k), & \\ 1 & \text{for } k = n. \end{cases} \tag{6}$$

The above recursion enables straightforward, although tedious, numerical studies of the distribution (4) (see fig. 1).

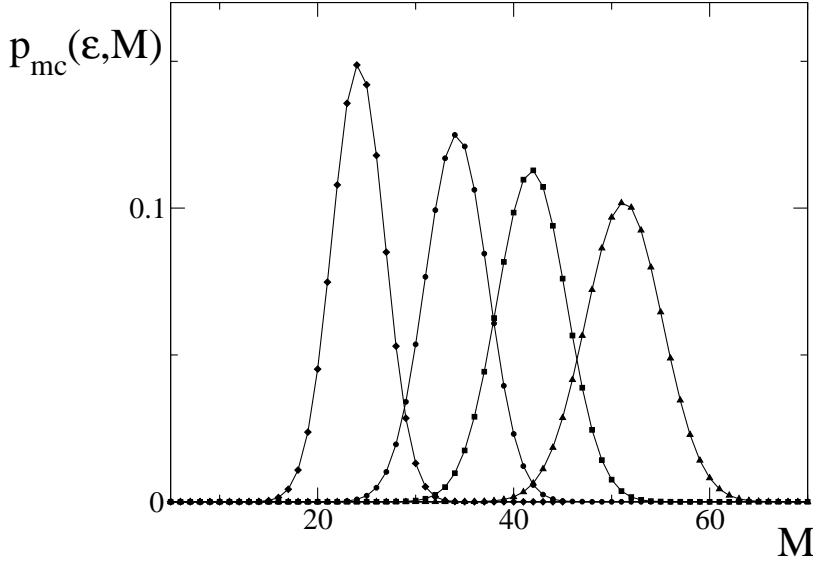


Fig. 1 – The distribution $p_{mc}(\mathcal{E}, M)$ for $\mathcal{E} = 1000, 2000, 3000,$ and 4500 .

Canonical distribution. – To proceed further with the analytical study of $p_{mc}(\mathcal{E}, M)$, we introduce the corresponding canonical description. Instead of fixing the energy E of each member of the ensemble, we consider an ensemble of systems in a thermal equilibrium with a heat bath of temperature T . The canonical partition function $Z(\beta, N)$, $\beta = 1/kT$, generating the statistical description in this case, can be written using (1) as

$$Z(\beta, N) = \sum_E e^{-\beta E} \Gamma(E, N) = e^{-\beta N \epsilon_0} \sum_{\mathcal{E}=0}^{\infty} e^{-\hbar\omega_0 \beta \mathcal{E}} \tilde{\Phi}(\mathcal{E}, M), \quad (7)$$

where $\mathcal{E} = 0$ term vanishes. Introducing $b = \hbar\omega_0 \beta$ we can define the combinatorial partition function:

$$Z_c(b, M) = \sum_{\mathcal{E}=1}^{\infty} e^{-b\mathcal{E}} \tilde{\Phi}(\mathcal{E}, M), \quad (8)$$

which can be viewed as the generating function of the microcanonical quantities $\tilde{\Phi}(\mathcal{E}, M)$. The canonical probability, corresponding to (4), is then given by

$$p_{cn}(b, M) = \frac{Z_c(b, M)}{\sum_{\mathcal{E}=1}^{\infty} e^{-b\mathcal{E}} \tilde{\Omega}(\mathcal{E})}, \quad (9)$$

A convenient and physically relevant way of an analytical description of the distribution (9) is provided by the cumulants. For a probability distribution $\{p(M), M \geq 0\}$ of an integer-valued random variable, the k -th cumulant $\kappa^{(k)}$ is defined as [13]

$$\kappa^{(k)} = \left(z \frac{d}{dz} \right)^k \ln \hat{p}(z) \Big|_{z=1}, \quad (10)$$

where $\hat{p}(z) = \sum_M e^{-Mz} p(M)$ is the (real) characteristic function of the distribution. The relation of the first few cumulants to the central moments $\mu^{(k)}$ is the following:

$$\kappa^{(1)} = \mu^{(1)} = \bar{M}, \quad \kappa^{(2)} = \mu^{(2)}, \quad \kappa^{(3)} = \mu^{(3)}, \quad \kappa^{(4)} = \mu^{(4)} - 3(\mu^{(2)})^2, \quad (11)$$

where $\bar{M} = \sum_M M p(M)$ is the mean value. Denote as $\Xi_c(b, z) = \sum_{M=0}^{\infty} z^M Z_c(b, M) = \prod_{\nu=0}^{\infty} (1 + ze^{-b\nu})$ the grand partition function, corresponding to the canonical partition function (8) with z being an analog of fugacity. We are interested in the excited part so we do not take $\Xi_c(b, z)$ but rather $\Xi_{ex}(b, z)$,

$$\Xi_{ex}(b, z) = \prod_{\nu=1}^{\infty} (1 + ze^{-b\nu}). \tag{12}$$

We substitute (9) in the definition (10) and obtain

$$\kappa_{cn}^{(k)}(b) = \left(z \frac{\partial}{\partial z} \right)^k \ln \Xi_{ex}(b, z) \Big|_{z=1}. \tag{13}$$

Now, we can apply the procedure of ref. [9] in order to obtain a compact expression for the cumulants $\kappa_{cn}^{(k)}(b)$ as well as their asymptotic behavior for $b \ll 1$. First, we note that

$$\ln \Xi_{ex}(b, z) = \sum_{\nu=1}^{\infty} \ln (1 + ze^{-b\nu}), \tag{14}$$

and we can always find such a neighborhood of $z = 1$ that $ze^{-b} < 1$. Since, according to (13), we are only interested in the behavior of Ξ_{ex} in the vicinity of $z = 1$, the logarithms in the second term can be Taylor-expanded; using then the Mellin transformation of the Euler gamma-function $\Gamma(t)$ [14], we obtain the following integral representation of $\ln \Xi_{ex}$:

$$\ln \Xi_{ex}(b, z) = \frac{1}{2\pi i} \int_{\tau-i\infty}^{\tau+i\infty} dt b^{-t} \zeta(t) \Gamma(t) f_{t+1}(z), \tag{15}$$

where $\zeta(t)$ is the Riemann zeta-function [13], and

$$f_{\alpha}(z) = \sum_{n=0}^{\infty} \frac{(-1)^n z^n}{n^{\alpha}}. \tag{16}$$

is the fermionic function [1]. The parameter $\tau > 0$ was chosen in such a way that the integration line in (15) is to the right from the last pole of the integrand.

Finally, we substitute eq. (15) into (13) and with the help of the following properties of the fermionic function f_{α} : $z df_{\alpha}(z)/dz = f_{\alpha-1}(z)$, $f_{\alpha}(1) = (1 - 2^{1-\alpha})\zeta(\alpha)$, we find that

$$\kappa_{cn}^{(k)}(b) = \kappa_{cn,boson}^{(k)}(b) - 2^k \kappa_{cn,boson}^{(k)}(2b), \tag{17}$$

where

$$\kappa_{cn,boson}^{(k)}(b) = \frac{1}{2\pi i} \int_{\tau-i\infty}^{\tau+i\infty} dt b^{-t} \Gamma(t) \zeta(t) \zeta(t+1-k) \tag{18}$$

are the canonical cumulants of the bosonic counterpart of the distribution (9).

Equation (17) is of central importance for this letter. It links the fermionic cumulants to the corresponding ones for bosons. The latter have been studied in detail in ref. [9]. In particular [9] gives the asymptotic expressions of the first few bosonic cumulants for $b \ll 1$. Using those together with (17)-(18) allows us to find the asymptotic expressions for the cumulants of the fermionic canonical distribution (9): $\kappa_{cn}^{(0)}(b) = \pi^2/12b + \ln 2/2 + b/24 + \mathcal{O}(b^{15.5})$, $\kappa_{cn}^{(1)}(b) = \ln 2/b - 1/4 + b/48 + \mathcal{O}(b^{2.5})$, $\kappa_{cn}^{(2)}(b) = 1/2b - 1/8 + \mathcal{O}(b^{14.5})$, $\kappa_{cn}^{(3)}(b) = 1/4b - b/96 + \mathcal{O}(b^{2.5})$, $\kappa_{cn}^{(4)}(b) = -1/16 + \mathcal{O}(b^{11.5})$, etc. The dependence on b in the fermionic case is of lower order than the corresponding one in the bosonic case. For example, $\kappa_{cn}^{(4)}$ is constant up to the terms of the order $b^{11.5}$.

Microcanonical distribution. – We come back to the study of the distribution (4). Our aim now is to find the cumulants $\kappa_{mc}^{(k)}(\mathcal{E})$ of this distribution. Applying the definition (10) to (4) we find that

$$\kappa_{mc}^{(k)}(\mathcal{E}) = \left(z \frac{\partial}{\partial z} \right)^k \ln \Upsilon(\mathcal{E}, z) \Big|_{z=1}, \quad (19)$$

where

$$\ln \Upsilon(\mathcal{E}, z) = \sum_{M=0}^{\infty} z^M \tilde{\Phi}(\mathcal{E}, M) \quad (20)$$

is another generating function of $\tilde{\Phi}(\mathcal{E}, M)$, complementary to $Z_c(b, M)$.

In order to calculate $\Upsilon(\mathcal{E}, z)$, we first note that

$$\Xi_{ex}(b, z) = \sum_{M=0}^{\infty} z^M \sum_{\mathcal{E}=1}^{\infty} e^{-b\mathcal{E}} \tilde{\Phi}(\mathcal{E}, M) = \sum_{\mathcal{E}=1}^{\infty} e^{-b\mathcal{E}} \Upsilon(\mathcal{E}, z). \quad (21)$$

Introducing a new variable $x = e^{-b}$ and writing $\Xi_{ex}(-\ln x, z) = \tilde{\Xi}_{ex}(x, z)$ we obtain

$$\tilde{\Xi}_{ex}(x, z) = \sum_{\mathcal{E}=1}^{\infty} x^{\mathcal{E}} \Upsilon(\mathcal{E}, z), \quad (22)$$

that is, $\Upsilon(\mathcal{E}, z)$ are the coefficients in the power series expansion of $\tilde{\Xi}_{ex}(x, z)$ with respect to x . We treat x as a complex variable and use an integral identity,

$$\Upsilon(\mathcal{E}, z) = \frac{1}{2\pi i} \oint dx \frac{\tilde{\Xi}_{ex}(x, z)}{x^{\mathcal{E}+1}}, \quad (23)$$

where the integration contour is any closed loop surrounding the origin, oriented anti-clockwise. The integral in (23) can be approximately evaluated using the saddle point method similar to that used in refs. [1, 9]. The implicit equation for the saddle point $x_0(z)$ is

$$\mathcal{E} + 1 = -\frac{\partial}{\partial b} \ln \Xi_{ex}(b_0(z), z), \quad (24)$$

with $b_0(z) = -\ln x_0(z)$. From eq. (24) we obtain in the Gaussian approximation:

$$\ln \Upsilon(\mathcal{E}, z) \approx \ln \Xi_{ex}(b_0(z), z) + \mathcal{E} b_0(z) - \frac{1}{2} \ln 2\pi - \frac{1}{2} \ln \left[\left(-\frac{\partial}{\partial b} \right)^2 \ln \Xi_{ex}(b_0(z), z) \right]. \quad (25)$$

The above solution for $\Upsilon(\mathcal{E}, z)$ is of course similar to the one obtained in a bosonic case in ref. [9], the difference being just in the form of the grand-canonical partition function Ξ_{ex} .

The microcanonical cumulants are then calculated from (25) according to eq. (19):

$$\kappa_{mc}^{(k)}(\mathcal{E}) = \left(z \frac{\partial}{\partial z} + z \frac{db_0(z)}{dz} \frac{\partial}{\partial b_0} \right)^k \ln \Upsilon(\mathcal{E}, z) \Big|_{z=1}, \quad (26)$$

where from eq. (24) $db_0(z)/dz \Big|_{z=1} = -\partial_b \kappa_{cn}^{(1)}(b_0(1)) / \partial_b^2 \kappa_{cn}^{(0)}(b_0(1))$, where in the last expression we used the definitions of the canonical cumulants (13). Generally, from (13), (25) and (26) it follows that the microcanonical cumulants $\kappa_{mc}^{(k)}(\mathcal{E})$ can be expressed in terms of the canonical

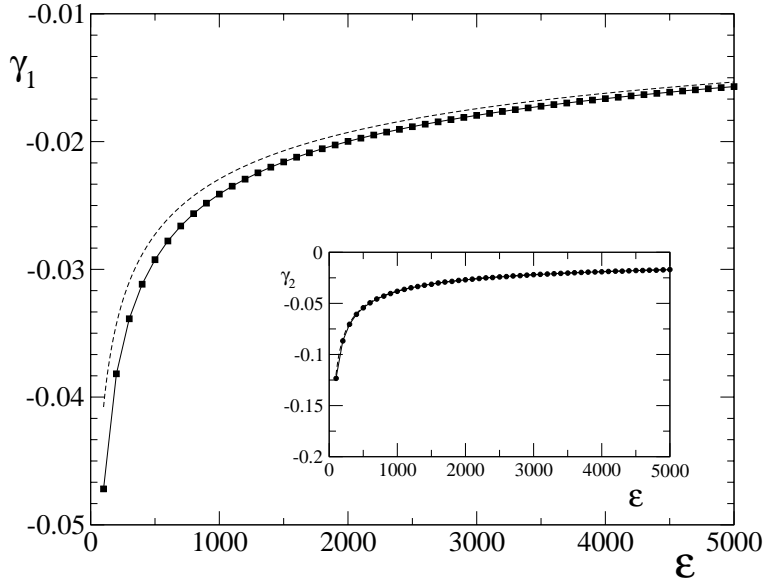


Fig. 2 – The skewness γ_1 obtained from numerically generated cumulants as compared with the asymptotic analytic prediction (dashed line). The insert shows the comparison for the excess γ_2 . Observe that the analytical asymptotics (dashed line) practically coincides with the numerical data.

cumulants $\kappa_{cn}^{(k)}(b)$ and their derivatives with respect to the temperature parameter b . For example, for the first cumulant $\kappa_{mc}^{(1)}$ one obtains

$$\kappa_{mc}^{(1)}(\mathcal{E}) = \kappa_{cn}^{(1)}(b_0(1)) - \frac{1}{2} \frac{\partial_b^2 \kappa_{cn}^{(1)}(b_0(1))}{\partial_b^2 \kappa_{cn}^{(0)}(b_0(1))} + \frac{\partial_b \kappa_{cn}^{(1)}(b_0(1))}{\partial_b \kappa_{cn}^{(0)}(b_0(1))} \left(1 + \frac{1}{2} \frac{\partial_b^3 \kappa_{cn}^{(0)}(b_0(1))}{\partial_b^2 \kappa_{cn}^{(0)}(b_0(1))} \right). \quad (27)$$

For $b \ll 1$ we can calculate the first few microcanonical cumulants explicitly:

$$\kappa_{mc}^{(1)}(\mathcal{E}) = \frac{2\sqrt{3} \ln 2}{\pi} \sqrt{\mathcal{E}} - \frac{1}{4} + \frac{3 \ln 2}{\pi^2} + \mathcal{O}(\mathcal{E}^{-\frac{1}{2}}), \quad (28)$$

$$\kappa_{mc}^{(2)}(\mathcal{E}) = -\frac{\sqrt{3}}{\pi^3} [-\pi^2 + 12(\ln 2)^2] \sqrt{\mathcal{E}} - \frac{36(\ln 2)^2 - \frac{2}{3}\pi^2}{\pi^4} - \frac{1}{8} + \mathcal{O}(\mathcal{E}^{-\frac{1}{2}}), \quad (29)$$

$$\kappa_{mc}^{(3)}(\mathcal{E}) = \frac{\sqrt{3}}{\pi^5} [-36\pi^2 \ln 2 + \pi^4 + 432(\ln 2)^3] \sqrt{\mathcal{E}} + \frac{\frac{3}{4}\pi^4 - 54\pi^2 + 864(\ln 2)^3}{\pi^6} + \mathcal{O}(\mathcal{E}^{-\frac{1}{2}}), \quad (30)$$

$$\begin{aligned} \kappa_{mc}^{(4)}(\mathcal{E}) = & -\frac{3\sqrt{3}}{\pi^7} [4\pi^4 \ln 2 + 2160(\ln 2)^4 - 216\pi^2(\ln 2)^2 + 3\pi^4] \sqrt{\mathcal{E}} + \\ & + \frac{1}{\pi^8} \left[\frac{1}{16}\pi^8 + 31104(\ln 2)^4 + 27\pi^4 - 2592\pi^2(\ln 2)^2 + 36\pi^4 \ln 2 \right] + \mathcal{O}(\mathcal{E}^{-\frac{1}{2}}). \end{aligned} \quad (31)$$

Using (28)-(31), we obtain the analytic expressions for the skewness and excess [13] of the distribution (4) $\gamma_1(\mathcal{E}) = \kappa_{mc}^{(3)}(\mathcal{E})/(\kappa_{mc}^{(2)}(\mathcal{E}))^{\frac{3}{2}}$, $\gamma_2(\mathcal{E}) = \kappa_{mc}^{(4)}(\mathcal{E})/(\kappa_{mc}^{(2)}(\mathcal{E}))^2$; these parameters measure the deviation of the distribution (4) from the Gaussian one. We obtain

$$\gamma_1(\mathcal{E}) = -\frac{0.12894}{4\sqrt{\mathcal{E}}} + \mathcal{O}(\mathcal{E}^{-\frac{3}{4}}), \quad \gamma_2(\mathcal{E}) = -\frac{1.2001}{\sqrt{\mathcal{E}}} + \mathcal{O}(\mathcal{E}^{-1}), \quad (32)$$

and hence in the limit $\mathcal{E} \rightarrow \infty$ both γ_1 and γ_2 vanish, implying that for large integers \mathcal{E} the distribution (4) approaches a Gaussian (see also a comment in [10]). This is a different situation from the bosonic case, where, as shown in ref. [9], both skewness and excess are non-zero in the limit of large integers, so that the bosonic microcanonical distribution does not approach Gaussian. In fig. 2 we compare the numerically obtained dependence of the skewness and excess with the analytical predictions of eq. (32).

Summarizing, we have studied relations between the Fermi-Dirac statistics for an ideal, harmonically trapped Fermi gas, and the theory of partitions of integers into distinct parts. Using methods of quantum statistical physics, we have described analytically the properties of the probability distribution of the number of different partitions. We anticipate that the results concerning a microcanonical ensemble for fermions can be used to characterize degeneracies of fermionic many-body states, that play an essential role in the process of laser cooling of small samples of atoms in microtraps in the so-called Lamb-Dicke limit [15].

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