

Level density of a Fermi gas and integer partitions: A Gumbel-like finite-size correction

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We investigate the many-body level density of a gas of noninteracting fermions. We determine its behavior as a function of the temperature and the number of particles. As the temperature increases, and beyond the usual Sommerfeld expansion that describes the degenerate gas behavior, corrections due to a finite number of particles lead to Gumbel-like contributions. We discuss connections with the partition problem in number theory, extreme value statistics, and differences with respect to the Bose gas.

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I. INTRODUCTION

The many-body (MB) level density ρ_{MB} is a fundamental quantity that describes basic properties of thermodynamical systems. Its behavior is of principal interest in many different fields such as nuclear decay rate [1,2], thermonuclear reactions in stellar processes, and, more recently, black hole entropy [3–5]. Unfortunately *ab initio* computations are out of reach for interacting systems and for large particle numbers. However, a statistical treatment is still possible when interactions are taken into account in a mean-field approximation. For fermions, two extreme regimes can be identified. At temperatures that are low compared to the Fermi energy μ_0 but high with respect to the mean level spacing at μ_0 (degenerate gas approximation), ρ_{MB} has a stretched exponential growth [6],

$$\rho_{\text{MB}} \propto e^{2\sqrt{\pi^2 \bar{\rho}(\mu_0) Q/6}}, \quad (1)$$

where Q is the excitation energy and $\bar{\rho}$ is the smooth single-particle (SP) level density. Nowadays Bethe's theory still remains a basic ingredient for advanced MB theories like back-shifted Fermi gas models [7] and the Gilbert-Cameron model [8]. From Eq. (1), we see ρ_{MB} is essentially sensitive to the SP level density around the Fermi energy. The second regime corresponds to high temperatures $Q \gg \mu_0$, where the classical limit is reached and where ρ_{MB} has a power-law behavior (Maxwell-Boltzmann regime). The aim of this article is to analyze, for fermions, the transition between the two regimes (see Fig. 1). To tackle this, we compute—in the degenerate gas limit—the effect of a finite number of particles when the temperature increases. For a power-law SP level density $\bar{\rho}(\mu_0)$, we find two contributions to ρ_{MB} : the first one is given by the usual Sommerfeld expansion while the second one is related to low-lying level excitations. This work is in connection with similar results obtained by Comtet *et al.* for bosons [9]. In a mean-field approximation, ρ_{MB} is also directly related to a combinatorial problem: to find the number of configurations of the SP occupied levels for a given excitation energy [10,11].

The article is organized as follows. In Sec. II we introduce basic definitions of the MB level density. We calculate the expression of the smooth part of the MB level density in the low- and high-temperature regimes. In Sec. III, we establish

a relation between the partition problem in number theory and the MB level density by using an equidistant spectrum. We compute corrections due to a finite number of particles from an exact asymptotic formula. Finally we generalize in Sec. IV the result to a power-law spectrum using a *nonlocal* Sommerfeld expansion provided by Garoni *et al.* [12].

II. GENERAL FRAMEWORK

The MB level density is a discrete quantity that, for a gas in a SP potential, is given by

$$\rho_{\text{MB}}(E, N) = \sum_{\{m_j\}} \delta\left(E - \sum_{j=0}^{\infty} m_j \epsilon_j\right) \delta\left(N - \sum_{j=0}^{\infty} m_j\right). \quad (2)$$

It is a microcanonical quantity where the particle number N and the energy of the system E are fixed (all quantities are dimensionless). ϵ_j corresponds to the energy of the j th level of the SP potential for one particle and m_j is the occupation number of the j th SP level for a given configuration $\{m_j\}$. In the case of fermions without spin degeneracy, the Pauli principle leads to m_j being either 0 or 1. We define Q as the difference $E - E_0$, where E_0 is the ground-state energy. For each configuration $\{m_j\}$, the conservation of particle number and energy yields $\sum_{j=0}^{\infty} m_j = N$ and $\sum_{j=0}^{\infty} \epsilon_j m_j = E$, respectively.

Now we write Eq. (2) in terms of an inverse Laplace transform:

$$\rho_{\text{MB}}(E, N) = \frac{1}{(2\pi i)^2} \int_{c-i\infty}^{c+i\infty} \int_{b-i\infty}^{b+i\infty} e^{S(\beta, \mu)} d\beta d\mu, \quad (3)$$

where

$$S(\beta, \mu) = \beta[-\Omega(\beta, \mu) + E - \mu N] \quad (4)$$

is the entropy. The constant b (respectively c) is chosen such that it is larger (respectively smaller) than the sum index of $\exp[-\beta\Omega(\beta, \mu)]$ with respect to the variable β (respectively μ). Both parameters β and μ correspond, respectively, to the inverse temperature and to the chemical

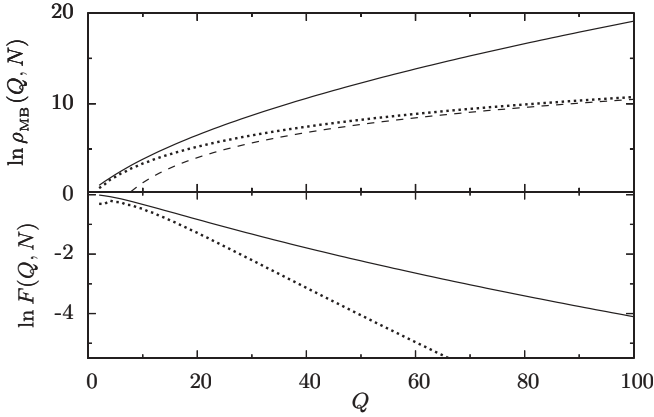


FIG. 1. (Upper panel) The MB level density for $\nu = 1$ and for five fermions as a function of the excitation energy Q . The dotted line is the exact computation. The solid line corresponds to the degenerate or low-temperature regime, Eq. (24) (with $n = Q$). The dashed line corresponds to the high-temperature regime, Eq. (23) (with $E \approx Q$; we have included the expression of the determinant $\mathcal{D} = E^2$ [see Eq. (6) and following text for discussion]). (Lower panel) The function $F(Q, N)$ for the same system. The dotted line corresponds to the exact computation and the solid line to the analytical expression, Eq. (34).

potential. $\Omega(\beta, \mu)$ is the Grand potential defined as

$$\Omega(\beta, \mu) = -\frac{1}{\beta} \int_0^\infty \rho(\epsilon) \ln[1 + e^{\beta(\mu - \epsilon)}] d\epsilon, \quad (5)$$

where $\rho(\epsilon) = \sum_{j=0}^\infty \delta(\epsilon - \epsilon_j)$ is the SP level density. The saddle point method with respect to μ and β gives the following equations:

$$\rho_{\text{MB}}(E, N) = \frac{e^{\mathcal{S}(\beta, \mu)}}{2\pi \sqrt{|\mathcal{D}(\beta, \mu)|}}, \quad (6)$$

$$N = \int_0^\infty \frac{\rho(\epsilon)}{e^{\beta(\epsilon - \mu)} + 1} d\epsilon, \quad (7)$$

$$E = \int_0^\infty \frac{\epsilon \rho(\epsilon)}{e^{\beta(\epsilon - \mu)} + 1} d\epsilon. \quad (8)$$

$\mathcal{D}(\beta, \mu)$ is the determinant of the second derivatives of $\mathcal{S}(\beta, \mu)$, which is not relevant for the following discussion. The last two equations define $\mu(E, N)$ and $\beta(E, N)$. From Eq. (7), we see that μ must decrease from positive to negative values when the temperature increases. Ignoring the discreteness of the SP level density, we now replace ρ by a smooth function:

$$\rho(\epsilon) \approx \bar{\rho}(\epsilon) = \nu \epsilon^{\nu-1}, \quad \text{for } \nu > 0. \quad (9)$$

For instance, the case $\nu = D$ is the leading order of the D -dimensional harmonic oscillator (HO). The case of billiards is given by $\nu = D/2$, where D is the dimension of space. When ρ is given by Eq. (9), Eqs. (7) and (8) become

$$N = -\frac{\Gamma(\nu + 1)}{\beta^\nu} \text{Li}_\nu(-e^{\beta\mu}), \quad (10)$$

$$E = -\frac{\nu \Gamma(\nu + 1)}{\beta^{\nu+1}} \text{Li}_{\nu+1}(-e^{\beta\mu}), \quad (11)$$

where $\text{Li}_\nu(x) = \sum_{k=1}^\infty x^k/k^\nu$ is the polylogarithm function. In this case the total energy and the Grand potential are connected by $E = -\nu \Omega(\beta, \mu)$. From Eq. (4), the entropy simplifies to

$$\mathcal{S} = \beta[(1 + 1/\nu)E - \mu N]. \quad (12)$$

For the low-temperature regime, we expand Eqs. (7) and (8) with $1/(\beta\mu)$ as a small parameter. This so-called Sommerfeld expansion [13,14] is valid for any regular function f :

$$\int_0^\infty \frac{f(\epsilon) d\epsilon}{e^{\beta(\epsilon - \mu)} + 1} = \int_0^\mu f(\epsilon) d\epsilon + 2 \sum_{j=1}^\infty C_j \beta^{-2j}, \quad (13)$$

where $C_j = \eta(2j) d^{(2j-1)} f(\epsilon)/d\epsilon^{(2j-1)}|_{\epsilon=\mu}$ and $\eta(x)$ is the Dirichlet η function. Using Eqs. (7), (8), and (13), we define the chemical potential and inverse temperature to leading order, μ_0 and β_0 , respectively, as

$$N = \int_0^{\mu_0} \rho(\epsilon) d\epsilon, \quad (14)$$

$$Q = E - E_0 = 2\eta(2)\rho(\mu_0)\beta_0^{-2}, \quad (15)$$

where $E_0 = \int_0^{\mu_0} \epsilon \rho(\epsilon) d\epsilon$. We have neglected terms in the derivatives of ρ in Eqs. (14) and (15). When ρ satisfies Eq. (9), we can easily invert (14) and (15) to obtain

$$\mu_0 = N^{1/\nu} \quad \text{and} \quad \beta_0 = \nu \sqrt{2\eta(2)/Q} N^{(\nu-1)/2\nu}. \quad (16)$$

Integrating the Grand potential, Eq. (5), by parts, we get

$$\Omega(\mu_0, \beta_0) = \Omega(0, \mu_0) - 2\eta(2)\rho(\mu_0)\beta_0^{-2}. \quad (17)$$

Using the expansions of Eqs. (14), (15), and (17) in the entropy Eq. (4), the result is

$$\mathcal{S}(\beta_0, \mu_0) = \beta_0[-\Omega(0, \mu_0) + 2\eta(2)\rho(\mu_0)\beta_0^{-2} + E - \mu_0 N]. \quad (18)$$

At zero temperature it leads to

$$-\Omega(0, \mu_0) + E_0 - \mu_0 N = 0. \quad (19)$$

We have used the latter equation in Eq. (18). Finally we obtain the leading order of the entropy for a Fermi gas at low temperature:

$$\mathcal{S}(\beta_0, \mu_0) = 2\sqrt{\frac{\pi^2}{6}} \rho(\mu_0) Q, \quad (20)$$

where we have used $\eta(2) = \pi^2/12$. This result holds for any smooth SP level density; in the case of Eq. (9) the entropy is written as $\mathcal{S}(Q, N) = 2\sqrt{\nu\pi^2 Q/6} N^{(\nu-1)/2\nu}$. Higher-order terms can be easily computed leading to a power series in Q and N . We emphasize that for fermions, the dependence of \mathcal{S} on the excitation energy does not depend on the system. In contrast, its N dependence comes through $\rho(\mu_0)$. This behavior is very different from that of the bosonic case (except for $\nu = 1$, see Sec. III) where the energy variation of the entropy strongly depends on the SP level density, that is, $\rho_{\text{MB}} \propto \exp[Q^{\nu/(\nu+1)}]$ [9,10].

When the particle number is fixed and when the temperature is sufficiently large, Eq. (7) leads to a large negative chemical potential, $e^{\beta\mu}$ tends to 0, and the Fermi-Dirac statistic

converges to the Maxwell-Boltzmann distribution. In this case Eqs. (10) and (11) become

$$N = \frac{\Gamma(\nu + 1)}{\beta^\nu} e^{\beta\mu}, \quad (21)$$

$$E = \frac{\nu\Gamma(\nu + 1)}{\beta^{\nu+1}} e^{\beta\mu}. \quad (22)$$

We invert Eqs. (21) and (22) to get μ and β as a function of N and E . Using Eqs. (6) and (12), it yields the following formulas for $E \gg N$:

$$\rho_{\text{MB}}(E, N) = \left[\frac{\Gamma(\nu + 1)E^\nu}{\nu^\nu N^{\nu+1}} \right]^N e^{(\nu+1)N} \quad (23)$$

and $\mu = \ln[\beta^\nu N / \Gamma(\nu + 1)] / \beta$. We also find the usual equation of state for perfect gases: $E = \nu NT$. In contrast to the stretched exponential growth at low temperature, we notice that the MB level density has a power-law behavior at high temperatures.

III. THE ONE-DIMENSIONAL HARMONIC OSCILLATOR

In this section we compute exactly the MB level density for a system of noninteracting particles confined by a one-dimensional harmonic potential (1DHO) with unit frequency and we make connections with number theory. We choose $\epsilon_0 = 0$ such that the spectrum is given by integers. We must compute the MB level density for a given integer excitation energy n and for a given particle number N , by counting all possible configurations of particles. A schematic way to depict this enumeration consists of using Young diagrams. They form n boxes with j nonincreasing lines such as $c_1 \geq c_2 \geq \dots \geq c_j$, $\sum_{i=1}^j c_i = n$, where c_i is the column number for the line i with $j \leq N$. Consequently, for an integer n the number of Young diagrams is the number of ways of counting n as nonzero integers when the line number is less than N . This number $p_N(n)$ is the so-called *partition function of n restricted to at most N terms*.

For each Young diagram we associate a unique configuration of particles in such a way that the horizontal axis represents the excitation energy of the particle and the vertical axis represents the index of the occupied level. Hence we have a one-to-one correspondence between each particle configuration and Young diagram; $p_N(n)$ is $\rho_{\text{MB}}(n, N)$ [10,11]. In the same way one can easily show that the result holds for particles with Bose-Einstein statistics as well.

The theory of partitions is studied in profusion by mathematicians (see [15] for an introduction). One of the most singular results comes from the works of Hardy, Ramanujan, and Rademacher, who computed an analytical expression where the number of terms into $p_N(n)$ is not restricted anymore [16,17]. In this case $p_{N \geq n}(n) = p(n)$ is called the *partition number of an integer n* . The leading asymptotic expression of $p(n)$ for large n is given by

$$p(n) \approx \frac{1}{\sqrt{48n}} e^{\sqrt{2\pi^2 n/3}}. \quad (24)$$

To leading order the exponential term in Eq. (24) is equivalent to Eq. (6) with Eq. (20) and $\nu = 1$ as expected. The correction

term for a finite number of terms to $p_N(n)$ was computed by Erdős and Lehner [18]:

$$\frac{p_N(n)}{p(n)} \approx e^{-e^{-g}}, \quad (25)$$

with $g = \sqrt{\pi^2/(6n)}N + 1/2 \ln[\pi^2/(6n)]$ and $N = o(n^{1/3})$. This distribution is the so-called Gumbel-like distribution and is one of the universal distributions in the domain of extreme values statistics [19]. It shows how the finite particle number contributes to the decrease of the number of configurations when heating the system (increases n) and determines the transition from low- to high-temperature regime. The main target of this article is to evaluate this correction when the spectrum is no longer equidistant but fulfills the more general law, Eq. (9). This is computed in the following section.

Note that in the case of fermions, the Fermi energy depends on the particle number, while this is not the case for bosons. This fundamental difference implies that the equivalence between the two statistics is only valid in the case of the 1DHO. In the context of the partition theory the generalization to a SP level density of the form Eq. (9) leads to mapping $\rho_{\text{MB}}(E, N)$ to the *partition number of an integer $n = E$ into a sum of N distinct* (due to Pauli principle) *1/ ν th powers of integers*. For bosons, a similar relation exists but without any distinction between summands [9,10].

IV. GENERAL CASE

In the degenerate gas limit the chemical potential is large with respect to the excitation energy. At low temperature, the fugacity $z = e^{\beta\mu}$ tends to infinity. To solve the equations Eqs. (10) and (11), we must find the asymptotic expansion of the polylogarithm function for a large negative argument. Garoni *et al.* give the inversion expression of $\text{Li}_\nu(-z)$ [12]:

$$\text{Li}_\nu(-z) = -2 \sum_{n=0}^{\infty} \frac{\eta(2n) \ln^{\nu-2n}(z^{-1})}{\Gamma(\nu + 1 - 2n)} - \cos(\pi\nu) \text{Li}_\nu(-z^{-1}). \quad (26)$$

Note that for the ν half-integer, the term in $\text{Li}_\nu(-z^{-1})$ vanishes. Furthermore when ν is an integer, the sum in Eq. (26) tends to the integer part of $\nu/2$. At low temperature z^{-1} tends to zero and $\lim_{x \rightarrow 0} \text{Li}_\nu(x) = x$. Equations (10) and (11) with Eq. (26) become

$$N = 2 \Gamma(\nu + 1) \sum_{n=0}^{\infty} \frac{\eta(2n) \beta^{-2n} \mu^{\nu-2n}}{\Gamma(\nu + 1 - 2n)} - \cos(\pi\nu) \frac{\Gamma(\nu + 1) e^{-\beta\mu}}{\beta^\nu} \quad (27)$$

and

$$E = 2 \nu \Gamma(\nu + 1) \sum_{n=0}^{\infty} \frac{\eta(2n) \beta^{-2n} \mu^{\nu+1-2n}}{\Gamma(\nu + 2 - 2n)} + \cos(\pi\nu) \frac{\nu \Gamma(\nu + 1) e^{-\beta\mu}}{\beta^{\nu+1}}. \quad (28)$$

Terms in the sum on the right-hand side of Eqs. (27) and (28) correspond to the Sommerfeld expansion terms. The meaning of the exponential term in Eqs. (27) and (28) emerges from the following example. With $\nu = 1$, Eqs. (27) and (28) yield

$$N = \mu + \frac{e^{-\beta\mu}}{\beta}, \quad (29)$$

$$E = \frac{\mu^2}{2} + \frac{2\eta(2)}{\beta^2} - \frac{e^{-\beta\mu}}{\beta^2}. \quad (30)$$

The computation of S to the second order is done by expanding μ and β in Eqs. (29) and (30). We have

$$\mu = \mu_0 - \sqrt{\frac{Q}{2\eta(2)}} e^{-\sqrt{2\eta(2)/Q}N} \quad (31)$$

$$\beta = \beta_0 - \frac{\left[N + \sqrt{\frac{Q}{2\eta(2)}}\right]}{2Q} e^{-\sqrt{2\eta(2)/Q}N}. \quad (32)$$

Using Eqs. (29), (30), (31), and (32) into Eq. (12), we get

$$S = 2\sqrt{2\eta(2)Q} - e^{-t}, \quad (33)$$

where $t = \sqrt{2\eta(2)/Q}N + \ln[\sqrt{2\eta(2)/Q}]$. Subtracting the leading order entropy, Eqs. (20) to (33), and using Eqs. (6) and (9), Eq. (25) is found with $n = Q$. The Gumbel law is thus recovered, as already stated in the previous section. The main contributions to ρ_{MB} are given by the Sommerfeld terms. These terms depend only on the local properties of the SP level density close to the Fermi energy and ignore the fact that the single-particle spectrum is bounded from below. The transition to the Maxwell-Boltzmann regime, where all particles contribute to a single configuration, cannot be described by this expansion. The exponentially small term $e^{-\beta\mu}$ in Eqs. (27) and (28) takes into account this effect, and this is the reason why we call it a *nonlocal* correction to the MB level density. For a given ν , we compute the nonlocal contribution to ρ_{MB} using the previous method to obtain

$$F(Q, N) = \frac{\rho_{\text{MB}}(Q, N)}{\overline{\rho_{\text{MB}}}(Q, N)} = \exp \left[\frac{\cos(\pi\nu)\Gamma(\nu+1)}{\beta_0^\nu} \exp(-\beta_0\mu_0) \right]. \quad (34)$$

$\overline{\rho_{\text{MB}}}(Q, N)$ represents the smooth MB level density computed by means of the (local) Sommerfeld expansion, Eq. (13).

Equation (34) is the main result of this article. The final correction takes the form of a modified Gumbel law. This is different with respect to the case of bosons, where, depending on the value of ν , three different functional dependencies of the correction were found [9]. They correspond to the three different distributions that appear in the theory of extreme value statistics. The difference is related, in particular, to the fact that there is no Bose-Einstein condensation for noninteracting fermions.

The qualitative behavior of $F(Q, N)$ has a strong dependence on the value of ν . For instance, $F(Q, N) = 1$ for ν half-integers. It can be larger than one for some specific values of ν . This effect is not surprising, since for $\nu \neq 1$ the Sommerfeld expansion gives the leading variation in N . In that case $F(Q, N)$ is not constrained to be less than one. The behavior of the MB level density as a function of the excitation energy is illustrated in Fig. 1 for $\nu = 1$ and for $N = 5$ fermions. This value of ν describes a 1DHO, but also, for instance, a two-dimensional billiard of arbitrary shape. A low number of particles has been chosen in order to enhance the finite N corrections. The upper panel in Fig. 1 illustrates the transition from the degenerate gas regime to the Maxwell-Boltzmann one. The lower panel shows the correction factor $F(Q, N)$. We note that the correction term is significant only in a small region around the degenerate regime, that is, for $Q \lesssim 15$. At higher excitation energies, the Maxwell-Boltzmann regime is reached.

In conclusion, we have demonstrated that in the transition from the low-temperature to the high-temperature regimes the MB level density of a Fermi gas is described by a modified law of extreme value statistics. This result is valid for a large set of systems according to Eq. (9). In the context of number theory, our results apply in particular to the partition of integers as a sum of powers of distinct integers. Our results are of interest in the computation of the level density of small nuclei for which the finite-size correction term (34) is the most important.

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