Level Density of a Fermi Gas: Average Growth and Fluctuations

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We compute the level density of a two-component Fermi gas as a function of the number of particles, angular momentum, and excitation energy. The result includes smooth low-energy corrections to the leading Bethe term (connected to a generalization of the partition problem and Hardy-Ramanujan formula) plus oscillatory corrections that describe shell effects. When applied to nuclear level densities, the theory provides a unified formulation valid from low-lying states up to levels entering the continuum. The comparison with experimental data from neutron resonances gives excellent results.

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Many physical properties of interacting Fermi gases depend on the number of available states at a given energy, like, for instance, the optical and electrical response of solids, or the reaction rates in nuclear processes. The most common framework to compute the many-body (MB) density of states (DOS) is a mean-field approximation, where each (quasi)particle moves independently in an average self-consistent potential. In this case, the energy of the Fermi gas is expressed as the sum of the occupied single-particle (SP) energies. The computation of the MB DOS is thus reduced to a combinatorial problem: to count the different ways into which the energy can be distributed among the particles. A first answer to this question was given by Bethe [1], who showed that at high excitation energies Q (compared to the SP spacing at Fermi energy ϵ_F) and for two types of fermions (protons and neutrons), the MB density grows like $\rho_{MB}(Q) \sim \exp(2\sqrt{aQ})/Q^{5/4}$. The Fermi gas parameter $a = \pi^2\bar{\rho}(\epsilon_F)/6$ depends only on the average SP DOS at ϵ_F, $\bar{\rho}(\epsilon_F)$.

In practice, the parameter a is often used as a fitting parameter. For a given excitation energy Q and particle number A, $a(Q, A)$ is extracted from the available experimental data. In this way, important deviations from the independent particle model predictions are observed. Though there are certainly effects that are beyond that model, our purpose here is to show that a detailed treatment is able to describe features of individual systems with good accuracy, therefore providing a solid theoretical basis for extrapolations to unknown regions and for improvements. Generalizing the results obtained in Ref. [2] to a two-component system of given angular momentum, we show that Bethe's result can be viewed as the first (smooth) term of an expansion. The corrections to that term do not enter as corrections of the a parameter (as was often assumed in the past), but simply as additional terms in the exponential. A first series of terms are smooth in A and Q, and provide higher-order (in inverse powers of the excitation energy) corrections. Keeping only the first correction generates a uniform expression, which cancels the divergence produce by the $Q^{-5/4}$ term at low energies, and therefore make unnecessary the use of composite models (à la Gilbert-Cameron). On top of the smooth contributions are oscillatory terms, that describe density fluctuations as A varies. These are shell effects, which turn out to be related to the fluctuations of the total energy of the system. A detailed description of these fluctuations and of the relevant energy scales is provided. Finally, a comparison of the results with the nuclear level density at neutron threshold is made. With a few adjustable parameters, a very good overall agreement is obtained, with a relative error $\lesssim 10\%$ for the logarithm of the density of the 295 nuclei analyzed.

From a theoretical point of view, Ref. [2] and the present work may be viewed as a generalization to MB systems of the theory developed to describe the SP DOS [3–5]. Previous works have considered the high-energy (Mawell-Boltzmann) limit [6], while here we concentrate on the regime of a large number of particles and $Q < \epsilon_F$.

The DOS at energy E of a system composed of Z protons, N neutrons, and with projection M of the angular momentum on some given axis is defined as

$$\rho_{MB}(E, N, Z, M) = \sum_{\nu} \delta(E - E^{\nu})\delta(N - A_N^{\nu})\delta(Z - A_Z^{\nu}) \times \delta(M - M^{\nu}). \quad (1)$$

The index ν denotes all the possible neutron and proton SP configurations (of arbitrary number of particles), $A_\lambda^\nu = \sum_i n_{\lambda,i}^\nu$ are the neutron and proton number of particles, respectively ($n_{\lambda,i}^\nu = 0, 1$ are the corresponding occupation numbers of the ith SP state, and $\lambda = N$ or P); $E^\nu = \sum_\lambda \sum_i n_{\lambda,i}^\nu \epsilon_{\lambda,i}$ and $M^\nu = \sum_\lambda \sum_i n_{\lambda,i}^\nu m_{\lambda,i}$ are the energy and angular momentum projection, where $\epsilon_{\lambda,i}$ and $m_{\lambda,i}$ denote the SP energies and angular momentum projections, respectively.

The conservation of the angular momentum projection is introduced in order to deal with only a subset of states, those with given total angular momentum J. A standard treatment [7,8] of this degree of freedom leads to a DOS of angular momentum J of the form

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$$\rho_{\mathrm{MB}}(Q,N,Z,J)=\frac{2J+1}{2\sqrt{2\pi}\sigma^3}e^{-(J+1/2)^2/2\sigma^2}\rho_{\mathrm{MB}}(Q,N,Z), \tag{2}$$

where $\rho_{\mathrm{MB}}(Q,N,Z)$ is the total MB DOS, $Q=E-E_0$ is the excitation energy measured with respect to the ground-state energy of the system, and σ is the spin cutoff parameter.

For an arbitrary SP spectrum the computation of the density of excited states is a difficult combinatorial problem for which no exact solution exists. There is, however, a particular case that can be worked out explicitly: when the SP spectrum consists of equidistant levels separated by δ (we assume, for simplicity, that the neutron and proton spacings are equal). The MB excitation energies are then given by the sum of two integers corresponding to the total energy of each of the components, $Q=(j+k)\delta=K\delta$. Each MB state characterized by an integer K has a nontrivial degeneracy. The computation of the degeneracy reduces to the computation of the number of ways into which the total energy may be distributed among the two components, and of the different ways the partial energy of each component can be distributed among its elements. This leads us to compute the value of the function $p_2(K)=\sum_{j=1}^{K}p(j)p(K-j)$, where $p(j)$ is the partition of j (the number of ways into which the integer j can be decomposed as a sum of integers). We are assuming here, to avoid finite size effects, that the excitation energy is small compared to the Fermi energy of each component. Based on the work of Hardy and Ramanujan, an exact expression (written as a convergent series) for $p(j)$ was obtained by Rademacher [9]. We have adapted their method (i.e., the circle method, cf. Ref. [10]) to obtain an exact formula for $p_2(K)$. Putting back the appropriate units, the MB density can be expressed in terms of p_2 as $\rho_{\mathrm{MB}}/\bar{\rho}=2^{1/4}p_2(K=\bar{\rho}Q/2)$, where $\bar{\rho}=\bar{\rho}_P+\bar{\rho}_N=2/\delta$ is the total (proton + neutrons) SP average density. Then, expressing the exact result as an expansion in terms of $\bar{\rho}Q$ valid in the range $\bar{\rho}^{-1}\ll Q<N\delta, Z\delta$, we obtain

$$\rho_{\mathrm{MB}}(Q,N,Z)/\bar{\rho}=\frac{6^{1/4}}{12(\bar{\rho}Q)^{5/4}}\mathrm{e}^{\mathcal{S}} \tag{3}$$

where the "entropy" $\mathcal{S}=\mathcal{S}_{\mathrm{eq}}$ of the equidistant spectrum is given by

$$\mathcal{S}_{\mathrm{eq}}=2\sqrt{\frac{\pi^2}{6}\bar{\rho}Q}-\left(\frac{\pi}{36}+\frac{15}{16\pi}\right)\frac{\sqrt{6}}{\sqrt{\bar{\rho}Q}}+\left(\frac{35}{96}+\frac{\pi^2}{432}\right)\frac{1}{\bar{\rho}Q} \tag{4}$$

plus $\mathcal{O}((\bar{\rho}Q)^{-3/2})$ corrections that can be computed but are not given here. The prefactor in Eq. (3) and the first term of the expansion (4) reproduce Bethe's formula [1]. The additional terms provide further smooth corrections of higher order in inverse powers of the excitation energy. Though Eq. (4) represents an asymptotic expansion, we find that an accurate uniform approximation is obtained by keeping only up to the $1/\sqrt{\bar{\rho}Q}$ term that destroys, when $Q\to 0$, the divergence produced by the $(\bar{\rho}Q)^{-5/4}$ in the prefactor. It is also interesting to note that the correct coefficients of the correction terms in (4) are obtained through the expansion of the exact result, whereas a saddle point approximation of the sum involved in $p_2(K)$ leads to wrong coefficients.

The previous expression describes in detail the MB DOS for a SP spectrum made of equidistant levels. However, it is clearly unphysical in most situations. A generic SP spectrum contains *fluctuations*, which are manifested at the scale of the average distance between levels, but also on much larger scales (see Ref. [11] for a review). What is missing in Eq. (3) are the fluctuations in the MB density induced by the SP fluctuations. In this respect, one may consider Eq. (3) as the MB analog of the Weyl or Wigner-Kirkwood expansions.

It remains for us to compute the MB level density for an arbitrary SP spectrum, including fluctuations. The way to do it was shown, for a single-component gas, in Ref. [2]. The method uses a saddle point approximation of the inverse Laplace transform of the MB density. We have adapted that calculation, following similar lines to treat Eq. (1), which includes two components and angular momentum conservation. The result may be written under the form of Eqs. (2) and (3), but with the entropy in the latter equation given by

$$\mathcal{S}=\mathcal{S}_{\mathrm{eq}}+\frac{1}{T}[\tilde{\mathcal{E}}(N,Z,0)-\tilde{\mathcal{E}}(N,Z,T)]. \tag{5}$$

The parameter T is the temperature, connected to the excitation energy Q through the usual relation $Q=\pi^2\bar{\rho}T^2/6=aT^2$. $\tilde{\mathcal{E}}(N,Z,T)=\sum_\lambda\int d\epsilon\tilde{\rho}_\lambda(\epsilon)\epsilon f(\epsilon,\mu,T)$ is the fluctuating part of the energy of the system at temperature T and chemical potential $\mu\sim\epsilon_{\mathrm{F}}$ fixed, neglecting temperature variations, by the particle-number conditions $N\sim Z=\int^{\epsilon_{\mathrm{F}}}d\epsilon\rho_\lambda(\epsilon)$. The function $\rho_\lambda(\epsilon)=\sum_j\delta(\epsilon-\epsilon_{\lambda,j})$ is the SP density of the component λ, and $\tilde{\rho}_\lambda(\epsilon)=\rho_\lambda(\epsilon)-\bar{\rho}_\lambda(\epsilon)$ its fluctuating part. $\tilde{\mathcal{E}}(N,Z,0)$ is thus the fluctuating part of the ground-state energy of the system. Finally, $\mathcal{S}_{\mathrm{eq}}$ in Eq. (5) is given by Eq. (4), with $\bar{\rho}$ the total average SP density of the system at Fermi energy. In fact, for an arbitrary spectrum the saddle point technique does not allow to derive the terms of order $(\bar{\rho}Q)^{-1/2}$ and higher in $\mathcal{S}_{\mathrm{eq}}$. The corrections obtained from an equidistant spectrum are thus conjectured to provide a good approximation to the corrections of the smooth part of an arbitrary system, but the validity of this statement has to be confirmed. An explicit numerical verification of its validity for a two-dimensional one-component system was done in Ref. [2].

The function $\tilde{\mathcal{E}}(N,Z,T)$ presents oscillations when N or Z are varied, in contrast to the more gentle variations as a function of T (a detailed description of the fluctuations and of their T dependence is given below). The MB level density contains now two types of terms: some that vary

smoothly, and others that fluctuate as the number of particles changes. The result presented above contains the dominant smooth and oscillatory terms. In the derivation of Eqs. (2), (3), and (5), we have neglected other terms [for instance, the chemical potentials and T have small corrections that depend on J, and thus strictly speaking the factorization (2) of the angular momentum is not exact, etc.]. A detailed account of the derivation will be given elsewhere.

It is remarkable that the MB level density at excitation energy Q depends explicitly on the ground-state energy fluctuations $\tilde{\mathcal{E}}(N, Z, 0)$. A convenient way to analyze the behavior of the fluctuating part of the entropy $\tilde{\mathcal{S}} = [\tilde{\mathcal{E}}(N, Z, 0) - \tilde{\mathcal{E}}(N, Z, T)]/T$ is through a semiclassical theory. The result is an expression for $\tilde{\mathcal{S}}$ written as a sum over all the classical periodic orbits of the mean field potential. The main conclusions that can be drawn from that expression are now listed. To be specific, we consider the particular case of an atomic nucleus of Z protons and N neutrons: (a) as the mass number $A = Z + N$ varies at fixed excitation energy Q, $\tilde{\mathcal{S}}$ presents oscillations of characteristic period $\delta A \approx (\pi/3)A^{2/3}$, which are independent of Q; (b) when Q varies at fixed particle number A, $\tilde{\mathcal{S}}$ does not present similar oscillations, but rather gentle variations; (c) the typical amplitude $\sigma_{\tilde{\mathcal{S}}}$ of $\tilde{\mathcal{S}}$ at given (Q, A) depends on the dynamical properties of the classical dynamics (integrable or chaotic); (d) since the mean field dynamics of most nuclei is well approximated by a regular motion [11], then the behavior of the typical amplitude of $\tilde{\mathcal{S}}$ is given, to a first approximation, by those of a regular dynamics, that we now detail; (e) using the definition of the temperature $T = \sqrt{Q/a}$ with $a = \pi^2\bar{\rho}/6 \approx A/15$ MeV^{-1} [12], we find that there is only one relevant temperature scale in the variation of $\sigma_{\tilde{\mathcal{S}}}$ with T, given by $T_c \approx 4/A^{1/3}$ MeV (directly related to the system size—see [2]); for convenience we also introduce $T_\delta = (2\pi^2\bar{\rho})^{-1} \approx 1.3/A$ MeV (the temperature associated with the SP mean level spacing), and $g = T_c/T_\delta \approx 3A^{2/3}$; (f) at low temperatures, $\sigma_{\tilde{\mathcal{S}}} \approx \sqrt{T/T_\delta}$; the typical amplitude of shell effects in the MB DOS therefore increases from 0 at $T = 0$ up to $\sim\sqrt{g}$ at $T \sim T_c$; (g) at temperatures of order T_c the amplitude is maximal, and starts to decrease for $T > T_c$; (h) in the limit $T \gg T_c$ the typical amplitude tends to zero as $\sigma_{\tilde{\mathcal{S}}} \approx \sqrt{g/6}T_c/T$; using the previous values of T_c and g this gives $\sigma_{\tilde{\mathcal{S}}} \approx 2\sqrt{2}/T$ MeV; we thus predict a slow power-law decay of the amplitude of shell effects at high temperatures.

We now turn to a direct application of the previous results to experimental data. Though it will be important to make a systematic analysis of the validity of Eqs. (2), (3), and (5), and of their predictions at different energies and mass numbers, we restrict ourselves here to a comparison with slow neutron resonances, which have been experimentally studied for a large number of nuclei [13]. The excitation energies of neutron resonances coincide with the neutron binding energies, $Q = Q_n = S_n(N, Z)$, whose values are in the range 6–8 MeV for most nuclei. This corresponds to a temperature $T_n \approx 8/\sqrt{A}$ MeV. According to the previous results, the typical amplitude of the fluctuations depends on temperature, with a maximum at $T \approx T_c$. At neutron resonances the ratio $T_n/T_c \approx 2/A^{1/6}$. From $A = 30$ to $A = 250$, this ratio varies from 1.13 to 0.8. We thus find that at excitation energies $Q \approx Q_n$, the temperature is very close to T_c; shell effects are maximal. We expect a typical value of $\tilde{\mathcal{S}}(Q, N, Z)$ very close to its maximum $\sim\sqrt{g} \approx \sqrt{3}A^{1/3}$ (this varies from 5.4 to 11 in the previous range of A). In contrast, in the same particle-number range the first correcting term [proportional to $(\bar{\rho}Q)^{-1/2}$] in the smooth expansion (4) varies from 0.32 to 0.11. That term, and the following ones in the expansion, can thus be neglected at $Q \approx Q_n$.

To make a comparison with experiments we need the different quantities involved in the theoretical expressions. The quantity $(\tilde{\mathcal{E}}N, Z, T_n)$ is, semiclassically, written as a sum over the periodic orbits p (and repetitions) of the mean field potential [11]. The analysis of the temperature dependence of that sum and of the main contributing orbits leads to the approximation $\tilde{\mathcal{E}}(N, Z, T_n) \approx \bar{\kappa}_n\tilde{\mathcal{E}}(N, Z, 0)$, where $\bar{\kappa}_n$ is the average over the shortest periodic orbits p of the function $\kappa(x_p) = x_p/\sinh(x_p)$, where $x_p = 3\pi\ell_p A^{1/3}T_n/(4\epsilon_F)$ and ℓ_p is the length of the periodic orbit p measured in units of the nuclear radius (notice the mass number and temperature dependence of x_p). For each nucleus, A and T_n are given and the average $\bar{\kappa}_n = \bar{\kappa}(N, Z, T_n)$ is computed. In practice, the average is estimated using the shortest periodic orbits of a spherical cavity of radius $R = 1.2A^{1/3}$ fm.

The expression of the entropy $\mathcal{S}$ in Eq. (3) takes now the form

$$\mathcal{S}(Q_n, N, Z) = 2\sqrt{aQ_n} + (1 - \bar{\kappa})\tilde{\mathcal{E}}(N, Z, 0)/T_n. \quad (6)$$

Finally, a, Q_n, and $\tilde{\mathcal{E}}(N, Z, 0)$ are required. One possibility is to compute them from a particular model. In our case, however, in order to avoid model-dependent features and to make a direct test of our predictions, we prefer to extract as much information as possible from experimental data. For each nucleus, the excitation energy at neutron threshold $Q = Q_n = S_n(N, Z)$ is taken from the experimental value of $S_n(N, Z)$, and $T_n(N, Z) = \sqrt{Q_n/a}$. Analogously, $\tilde{\mathcal{E}}(N, Z, 0)$ can be obtained from the experimental value of the ground-state energy. It corresponds to the fluctuating part of the nuclear binding energy. Thus, nuclear effects that may depend on A, like deformations, are automatically incorporated. This quantity is computed by subtracting from the 1995 Audi-Wapstra compilation [14] the liquid drop expression $\bar{\mathcal{E}} = a_v A - a_s A^{2/3} - a_c Z^2/A^{1/3} - a_A(N - Z)^2/A$, using the parameters (from Ref. [15]) $a_v = 15.67$, $a_s = 17.23$, $a_A = 23.29$, and $a_c = 0.714$ (all in MeV; we have moreover excluded the pairing term). This parametrization produces a fluctuating part whose average

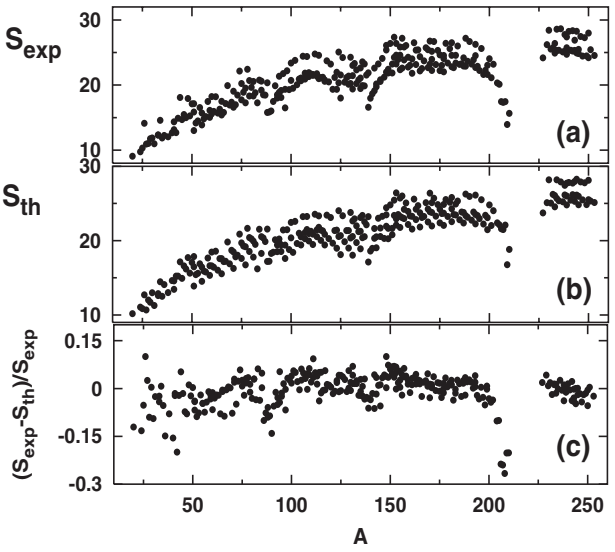

FIG. 1. Entropy $\mathcal{S}$ as a function of the mass number A for nuclear level densities at neutron threshold. (a) experimental values; (b) theoretical prediction; (c) relative error.

(over A) $\langle\tilde{\mathcal{E}}(N, Z, 0)\rangle_A \approx 0$. However, the determination of the average of the fluctuating part is a delicate question that deserves a careful discussion. Because of the discrete variation of the chemical potential as the mass number varies, one can verify that generically $\langle\tilde{\mathcal{E}}(N, Z, 0)\rangle_A$ is nonzero. We have therefore added to the fluctuating part a term $bA + c$, where b and c are two constants. Equation (6) thus depends on three constants, a, b, and c, that we fix by minimizing the root mean square error with respect to the experimental value of the density, $\mathcal{S}_{\rm exp}$ [obtained by computing $\mathcal{S}$ from Eqs. (2) and (3) when $\rho_{\rm MB}(Q, N, Z, J)$ is the experimental DOS, J the ground-state angular momentum and $\sigma^2 \approx 0.15aA^{2/3}T_n$ [13]]. The result is $a = A/10.42$ MeV^{-1}, $b = -0.019$ MeV and $c = 7.9$ MeV. The comparison is made in Fig. 1. The experimental values $\mathcal{S}_{\rm exp}$ shown on the top part are to be compared with the ''theoretical'' entropies plotted in the middle part. A clear overall agreement is observed. For most nuclei, the relative error in the lower panel is smaller than 10%, with some remaining structure as a function of A, and larger deviations for closed shells (we suspect that this is due to our very schematic estimate of $\bar{\kappa}_n$, and/or of σ^2, cf. Ref. [16]).

The precision of the present calculation, with only three adjusted parameters, is comparable to the best fits obtained nowadays. We can, in fact, make the comparison more precise by noticing that Eq. (6) can be approximated, using an effective value of a, by $\mathcal{S}(Q_n, N, Z) \approx 2\sqrt{a_{\rm ef}Q_n}$, where $a_{\rm ef} = a[1 + \tilde{\mathcal{E}}(N, Z, 0)(1 - \bar{\kappa})/Q_n]$. Under this form, Eq. (6) is quite similar to one of the best phenomenological formulas studied so far, proposed by Ignatyuk and collaborators [13,17].

To conclude, we have derived an explicit formula for the MB DOS of a two component Fermi gas of fixed angular momentum. The results were applied to the particular case of nuclear level densities, where precise predictions for the smooth dependence and shell fluctuations as a function of excitation energy and mass number were made. Different nuclear effects, like deformations, were explicitly taken into account through the function $\tilde{\mathcal{E}}(N, Z, 0)$. Good agreement between theory and experiment in the region of neutron resonances was found. Although it was derived within an independent particle model, the comparison with experiments shows that the final result is probably of more general validity and includes, through the energy fluctuations $\tilde{\mathcal{E}}$, effects like pairing. Going to high excitation energies, the main prediction is the decay of shell effects when $Q \gtrsim Q_n$ (with a power-law tail). However, that prediction is valid for closed systems. Before proceeding in that direction, the theory should be improved to include finite size effects (e.g. a finite number of nucleons) as well as the influence of the continuum.

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