

ANALYTIC RESULTS ON LEVEL DENSITIES

H. J. KRAPPE

*Hahn-Meitner Institut
 D-14091 Berlin, Germany
 krappe@hmi.de*

Received 24 September 2003

Use of the free energy in dynamical fission calculations and of the level density in simultaneous particle-evaporation yields raises the question of compatibility of these two pieces of input of quite different origin in calculations of the decay of hot compound nuclei. Seeming discrepancies between the Bethe formula for the level density and the popular assumption of a quadratic temperature dependence of the free energy are discussed in the framework of the picket-fence model, where the theory of partitions allows to calculate all thermodynamic functions analytically together with their limits for large systems and high temperature.

1. Introduction

When nuclear fission dynamics is described by Langevin equations, one derives the conservative forces from the derivatives of the free energy $F(\mathbf{q})$ with respect to the shape parameters \mathbf{q} at fixed temperature. For moderate excitation energies, corresponding to temperatures $T < 4$ MeV, the free energy is written as¹

$$F = F_0(\mathbf{q}) - a(\mathbf{q})T^2, \quad (1)$$

where F_0 is the zero-temperature liquid-drop energy. A temperature-dependent shell and pairing correction^{2,3} is to be added to F_0 for temperatures below the shell-model energy $\hbar\omega$. The emission rates of light particles from an excited compound nucleus are proportional to the ratio $\rho(E_{\text{sd}}^*)/\rho(E_0^*)$ of the level densities at the intrinsic energy E_{sd}^* at the saddle point of the emission channel to the level density at the excitation energy E_0^* of the initial state. For the level density the asymptotically valid Bethe formula⁴

$$\rho(E^*, \mathbf{q}) \simeq \frac{\exp\left(2\sqrt{a(\mathbf{q})E^*}\right)}{\sqrt{48 E^*}}, \quad aE^* \gg 1 \quad (2)$$

is mostly used, where we left out spin and isospin degrees of freedom. Consistency of fission-evaporation models requires that the level-density parameter $a(\mathbf{q})$ in Eqs. (1) and (2) should be the same quantity, moreover Eq. (1) should imply Eq. (2).

2. Two Seeming Discrepancies

From the canonical partition sum

$$Z(\beta) = \sum_i e^{-\beta E_i} \approx \int_{-\infty}^{\infty} \overline{\rho}(U) e^{-\beta U} dU \tag{3}$$

with $\beta = 1/T$ and the definition of the free energy $F = -T \ln Z$ one finds for the level density the inverse Laplace transform

$$\overline{\rho}(U) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} e^{\beta(U-F)} d\beta = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} e^{a/\beta + \beta(U-F_0)} d\beta, \tag{4}$$

where Eq. (1) has been used. This integral diverges. However, the ansatz

$$\overline{\rho}(U) = \delta(E^*) + \Theta(E^*) \rho(E^*) \tag{5}$$

with the excitation energy $E^* = U - F_0$ and $\rho(E^*) = 0$ for $E^* < 0$ leads to the convergent integral

$$\rho(E^*) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} (e^{a/\beta} - 1) e^{\beta E^*} d\beta = \sqrt{a/E^*} I_1(2\sqrt{aE^*}) \tag{6}$$

with the modified Bessel function I_1 . Using its asymptotic expansion, one finds

$$\rho(E^*) \simeq \frac{(aE^*)^{1/4}}{\sqrt{4\pi E^*}} \left(1 - \frac{3}{16} (aE^*)^{-1/2} + \dots \right) e^{2\sqrt{aE^*}} \tag{7}$$

in disagreement with Eq. (2). If the integral (4) would be evaluated in the saddle-point approximation – although it does not exist – the result (7) would also be obtained.

An alternative way to relate the free energy (naively) to the level density starts with the observation that from the definition of the entropy S as the logarithm of the phase-space volume $\Omega(E^*)$ follows

$$\rho(E^*) = \frac{\partial \Omega}{\partial E^*} = \frac{\partial S}{\partial E^*} e^{S(E^*)}. \tag{8}$$

One may use the thermodynamic relations

$$S(T) = -\partial F / \partial T \tag{9}$$

and

$$E^*(T) = F(T) - F_0 - T \partial F / \partial T, \tag{10}$$

invert the last equation, and insert $T(E^*)$ into Eq. (9) to obtain $S(E^*)$. With the form (1) for the free energy $F(T)$ the equation

$$\rho(E^*) = \sqrt{\frac{a}{E^*}} e^{2\sqrt{aE^*}} \tag{11}$$

follows, which is again different from Eq. (2) as well as from Eq. (7). Obviously something is wrong with some of the relations used above.

3. Canonical Partition Sum in the Picket-Fence Model

One of the very few model systems which allow an analytical treatment is the picket-fence model. It consists of non-interacting fermions in a one-dimensional harmonic oscillator, i.e. with an equidistant single-particle spectrum. We shall see that even this almost trivial model is sufficient to clarify the discrepancies mentioned above.

From the generating function $G(y)$ for the canonical partition sum $Z(\beta, N)$ for N non-interacting fermions at temperature $T = 1/\beta$ ⁵

$$G(y) = \prod_{n=1}^{\infty} (1 + e^{-\beta\epsilon_n} y) = \sum_{N=0}^{\infty} Z(\beta, N) y^N \quad (12)$$

with single-particle energies ϵ_n one derives for the picket-fence model $\epsilon_n = n\epsilon_0$

$$Z(\beta, N) = \frac{b^{N(N+1)/2}}{\prod_{n=1}^N (1 - b^n)} \quad (13)$$

with $b = \exp(-\beta\epsilon_0)$. This is easily seen in the following way: In the picket-fence model the product representation (12) of the generating function yields the functional relation $G(y) = (1 + by)G(by)$. Inserting the power series for G on both sides of this equation and equating coefficients of the same power in y yields the recurrence relation $Z(N) = b^N(1 - b^N)^{-1}Z(N - 1)$, from which Eq. (13) follows with the initial value $Z(\beta, 0) = 1$. The free energy is then given by

$$F(\beta, N) = -\frac{1}{\beta} \ln Z(\beta, N) = N(N+1)\frac{\epsilon_0}{2} + \frac{1}{\beta} \sum_{n=1}^N \ln(1 - e^{-n\beta\epsilon_0}) \quad (14)$$

and is seen to have an essential singularity at $T = 0$.

The denominator of the partition sum (13) is the generating function of the partition numbers $p_N(n)$. They are the number of partitions $\{n_j\}$ of n into at most N integers $n_j \geq 0$ with repetition⁶

$$n = \sum_{j=1}^N j n_j. \quad (15)$$

The partition sum becomes $Z(\beta, N) = b^{N(N+1)/2} \sum_{n=0}^{\infty} p_N(n) b^n$ in terms of the $p_N(n)$. Inverting Eq. (3) with this expression for $Z(\beta, N)$, the level density is

$$\rho(E^*) = \sum_{n=0}^{\infty} p_N(n) \delta(E^* - n\epsilon_0), \quad (16)$$

where $F_0 = N(N+1)\epsilon_0/2$ has been used. As expected, the level density has contributions at the discrete excitation energies $E_n^* = n\epsilon_0$ of the picket-fence model. In view of the relation (15) the weights $p_N(n)$ appear to describe the eigenvalue multiplicity of a system of N bosons in the picket-fence model. And in fact, starting from the generating function for bosons⁵ $G^{(B)}(y) = \prod_{n=1}^{\infty} (1 - b^n y)^{-1}$, one obtains for the bosonic partition sum $Z^{(B)}(\beta, N) = b^N \prod_{n=1}^N (1 - b^n)^{-1}$. Since in this case $F_0 = N\epsilon_0$, the expression (16) is seen to be also valid for the boson system.

To see that the $p_N(n)$ also describe the degeneracy in the picket-fence model for fermions, we represent the excitations of the fermion system as the sum of the excitation energy of n_h holes, distributed over N levels below and at the Fermi energy and n_p particles, which are allowed to occupy any states above the Fermi energy. The generating function for the holes is

$$G^{(h)}(y_h) = \prod_{n=0}^{n-1} (1 + b^n y_h) = \sum_{n_h=0}^N Z_h(\beta, n_h) y_h^{n_h},$$

where the fact has been used that the lowest hole state, the one at the Fermi energy, has zero energy. Expanding the product into a power series with respect to b and y_h gives

$$G^{(h)}(y_h) = \sum_{n_h=0}^N \sum_{n=n_{\min}}^{n_{\max}} q_{n_h}^{(N)}(n) b^n y_h^{n_h},$$

in terms of the number $q_{n_h}(n)$ of partitions of n into exactly n_h integers $\leq N$, without repetition. The boundaries of the inner sum are $n_{\min} = n_h(n_h - 1)/2$ and $n_{\max} = n_h(N - (n_h + 1)/2)$. By an argument similar to the one sketched above in connection with Eq. (13) one can prove that the partition sum for the holes is

$$Z_h(\beta, n_h) = b^{n_h(n_h-1)/2} \prod_{n=1}^{n_h} \frac{1 - b^{N+1-n}}{1 - b^n}. \tag{17}$$

Similarly the generating function for the partition function of the particle states is

$$G^{(p)}(y_p) = \prod_{n=1}^{\infty} (1 + b^n y_p) = \sum_{n_p=0}^{\infty} Z_p(n_p) y_p^{n_p}$$

with the partition sum

$$Z_p(\beta, n_p) = \frac{b^{n_p(n_p+1)/2}}{\prod_{n=1}^{n_p} (1 - b^n)}. \tag{18}$$

$Z_p(\beta, n_p) Z_h(\beta, n_p)$ is the partition function for the combined system with $n_p = n_h$. Summing over all $n_p \leq N$ represents the same system as the N -fermion system with the partition function (13), except that the energy zero-point is shifted by $F_0 = \epsilon_0 N(N + 1)/2$. One therefore expects the identity

$$\sum_{n_p=0}^N Z_p(\beta, n_p) Z_h(\beta, n_p) = b^{-N(N+1)/2} Z(\beta, N)$$

to hold. Inserting the expressions (17), (18), and (13) leads to the algebraic identity

$$\sum_{n_p=0}^N b^{n_p^2} \prod_{n=1}^{n_p} \frac{1 - b^{N+1-n}}{(1 - b^n)^2} = \prod_{n=1}^N \frac{1}{1 - b^n}, \tag{19}$$

which can also be proved directly.⁶ An expansion of Eq. (19) in powers of b leads to a sum rule for partition numbers

$$\sum_{\mu=0}^N \sum_{n'=0}^{\mu(N-\mu)} p_{\mu}(n-n'-\mu) q_{\mu}^{(N)}(n') = p_N(n).$$

4. The Thermodynamic Limit

It is instructive to consider the thermodynamic limit $N \rightarrow \infty$, $\epsilon_0 = E_f/N$, E_f fixed, for the level density and the free energy per particle $f(\beta) = F/N$. Expanding the logarithm in Eq. (14) in a power series, one obtains

$$f = \lim_{N \rightarrow \infty} F(\beta, N)/N = \frac{E_f}{2} - \frac{1}{E_f \beta^2} \left(\frac{\pi^2}{6} - \text{Li}_2(e^{-\beta E_f}) \right)$$

with the dilogarithm $\text{Li}_2(x) = \sum_{l=1}^{\infty} l^{-2} x^l = -\int_0^x t^{-1} \ln(1-t) dt$. The temperature-independent part of f is the average energy of particles in an external (one-dimensional harmonic oscillator) potential, where E_f is the highest occupied state. The temperature-dependent part has again an essential singularity for $\beta \rightarrow \infty$, i.e. $T \rightarrow 0$. However, if this limit is taken along the real axis, the dilogarithmic term vanishes exponentially. For real T the form (1) with $F = Nf$ is therefore justified and gives

$$\frac{a}{N} = \frac{\pi^2}{6E_f}. \quad (20)$$

The expression (1) must however not be extended into the complex β -plane as it was done in Eq. (4).

In order to take the thermodynamic limit of the level density, we write

$$\rho(E^*) dE^* = \sum_{n=NE^*/E_f}^{N(E^*+dE^*)/E_f} p_N(n) = p_N(NE^*/E_f) N \frac{dE^*}{E_f}. \quad (21)$$

For $E^* \geq E_f$ one has $p_N(NE^*/E_f) = p(NE^*/E_f)$, the unrestricted partition ($N \rightarrow \infty$). An asymptotic approximation for this partition is the first term of the Hardy-Ramanujan-Rademacher series⁷

$$p(n) \simeq \frac{\exp(\sqrt{2\pi^2 \bar{n}/3})}{\sqrt{48 \bar{n}}} \left[1 - \frac{1}{\sqrt{2\pi^2 \bar{n}/3}} + \mathcal{O}\left(\exp(-\sqrt{2\pi^2 \bar{n}/6})\right) \right]$$

with $\bar{n} = n - 1/24$. Putting $n = NE^*/E_f$ in this equation and introducing a instead of E_f with Eq. (20), we find – neglecting terms of order $n^{-1/2}$ – the asymptotic expansion of the level density, Eq. (21)

$$\rho(E^*) \simeq a \frac{\exp\left(2\sqrt{aE^* - (\pi/12)^2}\right)}{\sqrt{48} [aE^* - (\pi/12)^2]}. \quad (22)$$

This agrees with Bethe's result (2), apart from the term $(\pi/12)^2$, which is in general very small compared to the leading term aE^* . An alternative, asymptotic expression, this time for $p_N(n)$, was derived by Auluck and Kothari ⁸

$$p_N(n) \simeq \frac{1}{\sqrt{48n}} \exp \left(\pi \sqrt{\frac{2}{3}} n - \frac{\sqrt{6n}}{\pi} e^{-\pi N/\sqrt{6n}} \right), \qquad N \gg n^{1/2},$$

which yields

$$\rho(E^*) \simeq \frac{1}{\sqrt{48} E^*} \exp \left(2\sqrt{aE^*} \left[1 - \frac{3}{\pi^2} e^{-\sqrt{aE_f(E_f/E^*)}} \right] \right).$$

This again agrees with Eq. (2), except for the very small correction term in the exponent.

There is an alternative way to show the problems connected with a tacit extension of the ansatz (1) into the complex β -plane. Trying to evaluate integral (4) by the saddle-point method with the exact expression (14) for the free energy, yields the saddle-point condition

$$0 = \frac{\partial(\beta[U - F])}{\partial\beta} = E^* - \sum_{n=1}^{\infty} \frac{n\epsilon_0}{e^{\beta n\epsilon_0} - 1}.$$

Besides the real solution β_0 of this equation, which one would also have obtained with Eq. (1), there is an infinity of additional solutions

$$\beta_\nu = \beta_0 \pm i \frac{2\pi}{\epsilon_0} \nu, \qquad \nu = 1, \dots, \tag{23}$$

which move to infinity in the thermodynamic limit $\epsilon_0 \rightarrow 0$. The integrand in Eq. (4) should therefore not be evaluated by the saddle-point approximation.

Difficulties with the use of the saddle-point approximation to evaluate the integral (4) were noticed already by Van Lier and Uhlenbeck, ⁵ but seem to have been disregarded later.

It remains to understand why the expression (11) for the level density differs from Eq. (7) although the same ansatz (1) for $F(\beta)$ has been used in both cases. With Eq. (8) for the level density the saddle-point approximation for the canonical partition sum Eq. (3) yields

$$e^{-\beta F} = S'(E_0) e^{S(E_0) - \beta E_0} \sqrt{2\pi/(S + \ln S')''}, \tag{24}$$

where $E_0(\beta)$ follows from the saddle-point condition $\beta = S'(E_0) + (\ln S)'$. One now argues that for large N the second term on the right side of this equation is of order $1/N$ smaller than the first term and it is dropped. Taking the logarithm of Eq. (24)

$$-\beta F = S(E_0) - \beta E_0 + \frac{1}{2} \ln \frac{2\pi S'^2}{(S + \ln S')''},$$

one argues again that the last term on the right side of this equation is of order $1/N$ smaller than the other terms and drops it. Identifying in Eq. (10) E^* with E_0 , one obtains from i Eq. (1) $E^* = aT^2$ and $S(E^*) = 2\sqrt{aE^*}$ and therefore Eq. (11)

follows by insertion into Eq. (8). This derivation of the thermodynamic relations shows that the contributions from the factor $\partial S/\partial E^*$ in Eq. (8) are always neglected and in fact, taking the logarithm of this equation, $\ln \rho = S + \ln S'$, one would drop the $\ln S'$ term for large N . In this strong thermodynamic limit only the exponential term in Eq. (11) is well-defined, the rest is of the neglected order.

5. Grand Canonical Ensemble

Since Bethe's treatment of the nuclear level density, the starting point has always been the partition sum of the grand canonical ensemble

$$G(e^{-\alpha}, \beta) = \sum_{N=0}^{\infty} Z(\beta, N) e^{-N\alpha} = \prod_{n=1}^{\infty} (1 + e^{-\beta(\epsilon_n - \mu)}),$$

where $\alpha = -\mu/\beta$ with the chemical potential μ . In the picket-fence model, $\epsilon_n = n\epsilon_0$,

$$\begin{aligned} G(\alpha, \beta) &= \sum_{N=0}^{\infty} \frac{e^{-(\epsilon_0 N(N+1)/2 - N\mu)\beta}}{\prod_{n=1}^N (1 - b^n)} \\ &= \sum_{N=0}^{\infty} e^{-(\epsilon_0 N(N+1)/2 - N\mu)\beta} \sum_{n=0}^{\infty} p_N(n) e^{-\beta n \epsilon_0}. \end{aligned} \quad (25)$$

In view of the relation

$$\prod_{n=1}^{\infty} (1 + e^{-\alpha - \beta \epsilon_n}) = \sum_N \sum_{U_i} e^{-\alpha N - \beta U_i} \approx \int dN \int dU \rho(N, U) e^{-\alpha N - \beta U}$$

the level density for the N -particle system is represented by the double inverse Laplace transform

$$\rho(E^*) = \frac{1}{(2\pi i)^2} \int_{c-i\infty}^{c+i\infty} d\alpha \int_{c-i\infty}^{c+i\infty} d\beta G(\alpha, \beta) e^{-\alpha N' + \beta U}. \quad (26)$$

Inserting the expression (25) for the picket-fence model, one obtains

$$\rho(E^*) = \delta_{NN'} \sum_n p_N(n) \delta(n\epsilon_0 - E^*),$$

in agreement with Eq. (16), as it should be.

We now consider the Gibbs potential

$$\Psi(\alpha, \beta) = \ln G(\alpha, \beta) = \sum_{n=1}^{\infty} \ln(1 + b^{n-n_\mu}) \quad (27)$$

with $n_\mu = [\mu/\epsilon_0]$. Using standard manipulations, but dropping no terms, gives

$$\Psi = \frac{1}{2} \beta \epsilon_0 n_\mu (n_\mu - 1) + 2 \sum_{n=0}^{\infty} \ln(1 + b^n) - \ln 2 - \sum_{n=n_\mu}^{\infty} \ln(1 + b^n).$$

Expanding $\ln(1 + b^n) = -\sum_{l=1}^{\infty} (-b^n)^l/l$ and interchanging l and n summations,

one obtains

$$\Psi = -\frac{1}{2}\alpha\left(\frac{\mu}{\epsilon_0} - 1\right) + \frac{1}{\beta\epsilon_0}\left(\frac{\pi^2}{6} + \sum_{l=1}^{\infty} \frac{1}{l} \frac{(-b^{n_\mu})^l}{1-b^l}\right) - \ln 2.$$

In the thermodynamic limit $\epsilon_0 \rightarrow 0$, $\epsilon_0 N = E_f$ fixed, the potential per particle becomes

$$\psi(\alpha, \beta) = \lim_{n \rightarrow \infty} \frac{\Psi}{N} = \frac{1}{\beta E_f} \left(\frac{\alpha^2}{2} + \frac{\pi^2}{6} + \text{Li}_2(-e^{-\alpha}) \right).$$

For real β with $\alpha = \mu\beta \gg 1$ the dilogarithm is negligible. If the approximation $G(\alpha, \beta) \approx \exp(N\psi(\alpha, \beta))$ is inserted into Eq. (26) and the double integral is evaluated in the saddle-point approximation, Eq. (2) results, despite the fact that for the Gibbs potential (27), before the limit $N \rightarrow \infty$ is taken, the saddle-point condition $\partial_\beta \Psi = -U$ has clearly the infinitely many complex solutions (23). Similarly the second saddle condition $\partial_\alpha \Psi = -N$ has also an infinity of complex solutions.

6. Concluding Remarks

We have seen that approximations for the free energy $F(\beta)$, valid on the real β -axis, can in general not be extended into the complex β -plane, in particular since $F(\beta)$ has an essential singularity at $T = 1/\beta = 0$. When the thermodynamic limit in the derivation of asymptotic approximations for the level density is taken in several separate steps, special care is needed to ascertain the validity of all equations to the desired order of N . This has to be kept in mind when, for instance, one wants to find out which shell and pairing corrections to the Bethe formula follow from given Strutinsky-type, temperature-dependent corrections to the free energy.

It should be stressed that the above considerations do not shed light on the puzzling fact that empirical fits of the level-density parameter a yield substantially larger values than predictions on the basis of any independent fermion model, self-consistent or not.⁹

Acknowledgement

I am obliged to Dr. A. Ecker for initiating me into the theory of partitions.

References

1. M. Brack, C. Guet, and H. B. Håkansson, *Phys. Rep.* **123**, 275 (185).
2. A. S. Jensen and J. Damgaard, *Nucl. Phys.* **A203**, 578 (1973).
3. M. Bolsterli, E. O. Fiset, J. R. Nix, and J. L. Norton, *Phys. Rev.* **C5**, 1050 (1972).
4. H. Bethe, *Phys. Rev.* **50**, 332 (1936).
5. C. Van Lier and G. E. Uhlenbeck, *Physica* **4**, 531 (1937).
6. G. H. Hardy and E. M. Wright, *An Introduction into the Theory of Numbers* (Clarendon, Oxford, 5th edition, 1979) chap. XIX.
7. H. Rademacher, *Topics in Analytic Number Theory* (Springer, Berlin, 1973) sec. 121.
8. F. C. Auluck and D. S. Kothari, *Proc. Camb. Phil. Soc.* **42**, 272 (1946).
9. H. J. Krappe, *Phys. Rev.* **C59**, 2640 (1999).