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Comparison of saddle point and exact combinatorial level densities

N C da Fonseca e Oliveira, M Dutra, B V Carlson

Technological Institute of Aeronautics

E-mail: `natalie@ita.br`

Abstract. Accurate level densities are an important ingredient in the calculation of compound nucleus emission cross sections. They are often approximated numerically using the saddle point approximation to the canonical level density obtained from the grand canonical partition function using the inverse Laplace transform. Here, we use a modified version of the saddle-point approximation proposed by Rossignoli to obtain canonical level densities and average properties of a system. However, the level density needed in nuclear reaction calculations is actually the energy-conserving microcanonical one. For simple systems, the latter can be calculated combinatorially. Here we calculate microcanonical level densities using an evenly-spaced single particle density for one type of nucleon and compare these to saddle-point canonical level densities obtained from the same single-particle density. The simplest continuous approximation to the microcanonical level density describes it well near its peak but poorly at low excitation energies. The canonical level density obtained from the partition function fares somewhat better but is still not completely successful. It tends to exceed the exact result by a few percent. We discuss the differences between the canonical and microcanonical level densities and suggest how these might be reduced.

1. Introduction

The determination of nuclear densities of states is very important for the description of nuclear reactions and decays[1]. These can be estimated using a saddle point approximation to the inverse Laplace transform of the grand canonical ensemble, as was done by Bethe many years ago[2], using Monte Carlo techniques or, in certain simple cases, calculated exactly using combinatorial methods. A direct comparison of exact combinatorial calculations with the saddle point approximation to the density of states reveals that the latter systematically overestimates the exact density.

An intermediate quantity that is also useful in nuclear decay calculations is the canonical ensemble and the associated Helmholtz free energy. Here we compare the free energy, entropy and average excitation energy obtained in two manners: from a saddle point approximation to the inverse Laplace transform in number of the grand canonical ensemble and directly from the exact combinatorial calculation. We find the agreement between these to be excellent. However, a second saddle point approximation, this time to the inverse Laplace transform of the excitation energy, still does not provide us with a good approximation to the level density.

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2. Statistical Ensembles

2.1. The Grand Canonical

The grand canonical ensemble describes a system which exchanges energy and particles with a larger reservoir [2,3]. Its partition function, in the case of a set of independent particles, is given by a product of a factor over each of the possible states E_k of the system,

$$Z_{GC}(\alpha,\beta) = \prod_K (1 + e^{\alpha - \beta E_k}), \tag{1}$$

where β is the inverse of the temperature and $\alpha = \beta\mu$, with μ being the chemical potential. In terms of this, we can determine the expectation values of the number of particles and the energy, as well as the entropy, by

$$\langle N \rangle = \frac{\partial}{\partial \alpha} \ln Z_{GC}(\alpha,\beta), \tag{2}$$

$$\langle E \rangle = -\frac{\partial}{\partial \beta} \ln Z_{GC}(\alpha,\beta), \tag{3}$$

$$S = \ln Z_{GC}(\alpha,\beta) - \alpha\langle N \rangle + \beta\langle E \rangle. \tag{4}$$

The density of states can be expressed as the inverse Laplace transform of the partition function,

$$\omega(E,N) = \frac{1}{(2\pi i)^2} \int d\alpha d\beta Z_{GC}(\alpha,\beta) e^{(-\alpha N + \beta E)}, \tag{5}$$

which, in the saddle point approximation, can be estimated as

$$\omega(E,N) = \frac{\exp[\ln Z_{GC}(\alpha_0,\beta_0) - \alpha_0 N + \beta_0 E]}{2\pi \sqrt{\left[\frac{\partial^2 \ln Z_{GC}}{\partial \beta^2} \frac{\partial^2 \ln Z_{GC}}{\partial \alpha^2} - \left(\frac{\partial^2 \ln Z_{GC}}{\partial \beta \partial \alpha}\right)^2\right]\Bigg|_{\alpha_0,\beta_0}}}, \tag{6}$$

where β_0 and α_0 are the values at the saddle point.

2.2. The Microcanonical

The microcanonical ensemble describes an isolated system with a well defined excitation energy and particle number[2,3]. For a fixed particle number, the density of states furnishes a description of the ensemble as a function of the excitation energy.

Here we will make use of a combinatorial calculation of the density of states for a fixed number of particles in a set of uniformly spaced states. In the case we show here, the density of states was calculated for 20 particles in 40 states. The density of states has 396 distinct energies and a total of 1.1×10^{11} states. This exact density of states is compared to the saddle point approximation in Fig. 1. We note that exact density of states possesses a maximum of 1.2×10^9 states at energy 198 and decreases at higher energies to a single state at energy 396. The saddle point approximation can describe the density of states only up to energy 198.

2.3. The Canonical Ensemble

The canonical ensemble describes a system with a fixed number of particles that only exchanges energy with a reservoir [2,3]. Its partition function can be defined exactly in terms of the density of states as

$$Z_C(\beta,N) = \int dE \quad \omega(E,N) e^{-\beta E}. \tag{7}$$

The partition function $Z_C(\beta, N)$ can also be obtained from the grand canonical ensemble as

$$Z_C(\beta, N) = \frac{1}{2\pi i} \int d\alpha Z_{GC}(\alpha, \beta) e^{-\alpha N} \,, \tag{8}$$

which, in the saddle point approximation, is

$$Z_C(\beta, N) = \frac{\exp[\ln Z_{GC}(\alpha_0, \beta) - \alpha_0 N]}{\sqrt{2\pi \left[\frac{\partial^2 \ln Z_{GC}}{\partial \alpha^2} \right] \Big|_{\alpha_0}}} \tag{9}$$

The Helmholtz free energy is defined as

$$F(\beta, N) = -\frac{1}{\beta} \ln Z_C(\beta, N) \,. \tag{10}$$

We can define the entropy and the expectation value of the energy in the canonical ensemble as

$$S(\beta, N) = \beta^2 \frac{\partial}{\partial \beta} F(\beta, N) \,, \tag{11}$$

$$E(\beta, N) = F(\beta, N) + \frac{1}{\beta} S(\beta, N) \,. \tag{12}$$

In Figs. 1a, 2a and 2b, we compare the Helmholtz free energy, entropy and energy obtained using the microcanonical density of states and the saddle point approximation with the grand canonical partition function for the same system of 20 particles in 40 states used in Fig. 1. We find that in this case, the saddle point approximation furnishes an excellent description of the canonical ensemble quantities.

We can also attempt an alternative approximation to the density of states, by using the fact that the latter can also be obtained as the inverse Laplace transform of the canonical partition function [8],

$$\omega(E, N) = \frac{1}{2\pi i} \int d\beta Z_C(\beta, N) e^{\beta E}. \tag{13}$$

The saddle point approximation to this expression is also displayed in Fig. 1. Unfortunately, although the Helmholtz free energy can easily be obtained from the exact combinatorial calculation of the level density, the inverse path, from the canonical partition function to the density of states through the saddle approximation, does not furnish the accuracy we would hope to obtain.

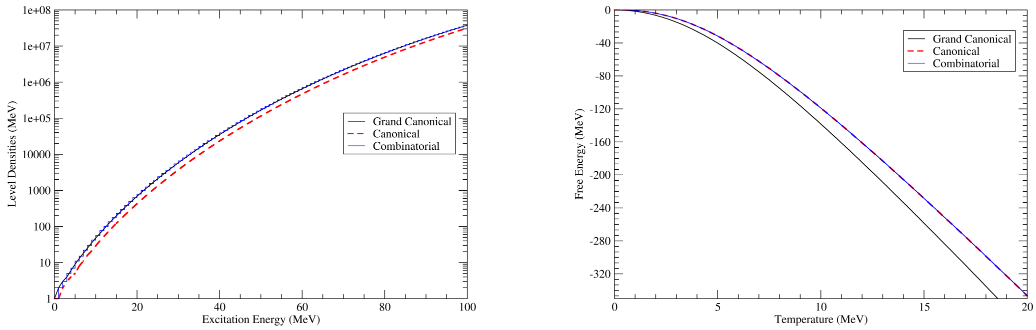

Figure 1. (Left)Density of states as a function of the excitation energy. (Right) Helmholtz free energy as a function of the temperature.

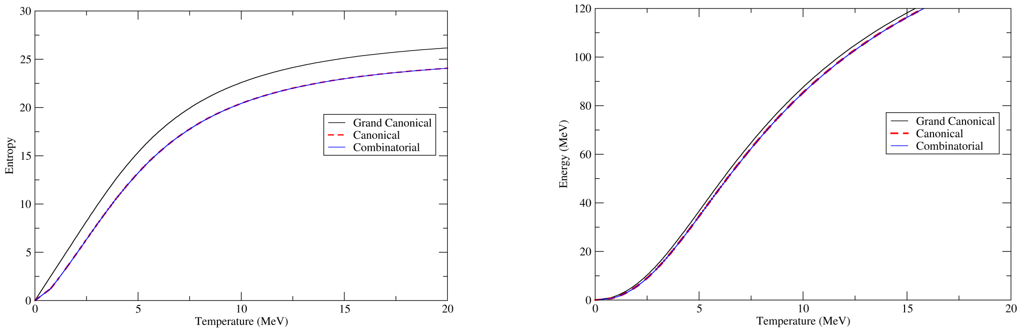

Figure 2. (Left)Entropy as a function of the temperature. (Right) Energy as a function of the temperature.

3. Conclusion

We have compared saddle point approximations to the density of states, Helmholtz free energy, entropy and excitation energy to their exact values for a system of 20 particles in 40 uniformly spaced states. We find the Helmholtz free energy and the canonical entropy and excitation energy to be in excellent agreement. However, the saddle point approximations to the density of states do not succeed in providing a similar level of agreement with the exact result.

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