

## Derivation and improvements of the quantum canonical ensemble from a regularized microcanonical ensemble

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

1999 J. Phys. A: Math. Gen. 32 287

(<http://iopscience.iop.org/0305-4470/32/2/005>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 171.66.16.105

The article was downloaded on 02/06/2010 at 07:31

Please note that [terms and conditions apply](#).

# Derivation and improvements of the quantum canonical ensemble from a regularized microcanonical ensemble

Jani Lukkarinen<sup>†</sup>

Helsinki Institute of Physics, PO Box 9, 00014 University of Helsinki, Finland

Received 4 September 1998

**Abstract.** We develop a regularization of the quantum microcanonical ensemble, called a Gaussian ensemble, which can be used for derivation of the canonical ensemble from microcanonical principles. The derivation differs from the usual methods by giving an explanation for the, at the first sight unreasonable, effectiveness of the canonical ensemble when applied to certain small, isolated, systems. This method also allows a direct identification between the parameters of the microcanonical and the canonical ensemble and it yields simple indicators and rigorous bounds for the effectiveness of the approximation. Finally, we derive an asymptotic expansion of the microcanonical corrections to the canonical ensemble for those systems, which are near, but not quite, at the thermodynamical limit and show how and why the canonical ensemble can be applied also for systems with an exponentially increasing density of states. The aim throughout the paper is to keep mathematical rigour intact while attempting to produce results which are both physically and practically interesting.

## 1. Introduction

The microcanonical ensemble is considered to be the fundamental ensemble of statistical physics. For example, the use of the canonical Gibbs ensemble is usually justified by showing that its expectation values coincide with the microcanonical ones in the thermodynamical limit, when the size of the system approaches infinity. However, since an application of the microcanonical ensemble requires detailed knowledge about the energy levels of the system, it is seldom possible to use it in practice. The canonical ensemble, on the other hand, has a well behaving path-integral expression easily extended to gauge field theories—therefore, it has become the standard ensemble of quantum statistics.

Nevertheless, there are situations where the easiest, canonical, alternative does not work. For instance, direct applications of the grand canonical ensemble have not been able to reproduce all the results of relativistic ion collision experiments [1]. There are two possible explanations for this shortcoming of the canonical ensemble: either the particle gas created in the collision does not reach thermal equilibrium before exploding into the final-state hadrons, or the system is too small to be handled by canonical methods. In fact, recent calculations [2] using a modified grand canonical ensemble have succeeded in describing most of the particle abundances in these experiments, but only at the cost of including finite-volume corrections to the usual ensemble. This suggests that at least the final-state hadron gas will thermalize, but it also shows that finite-volume effects are prominent in these systems.

<sup>†</sup> E-mail address: jani.lukkarinen@helsinki.fi

These results point to the fact that the microcanonical ensemble—which is optimal for describing isolated ergodic systems with small quantum numbers—should be used for obtaining quantitative information about the properties of the quark–gluon plasma possibly created in relativistic hadron collisions. There are already proposals of how this can be accomplished in the continuum path-integral formulation of field theories [3], but since the argumentation in this kind of formalism cannot be made completely mathematically rigorous, a further study of the details of the quantum microcanonical ensemble was felt to be necessary.

When trying to perform rigorous quantum microcanonical computations, one immediately encounters two practical difficulties associated with the discrete spectrum of an isolated quantum system: since the spectrum is discrete, the possible values of the spectrum have to be known in advance before any computations can be done; on the other hand, the position of the high-energy spectral levels depends on small fluctuations of the interaction potential. Consider, for example, the harmonic oscillator, for which the energy levels are  $E_n = \omega(n + \frac{1}{2})$ : for  $n = 100$ , 1% change in the oscillator frequency  $\omega$  will change the position of the level  $E_{100}$  by a whole energy unit! Therefore, the spectral levels by themselves are not very practical parameters; however, the *density* of the spectral levels is robust in fluctuations of the potential and thus a smoothed energy spectrum would offer a more stable alternative.

This paper attempts to fill the gap between the canonical and the microcanonical ensemble in quantum mechanics. The main ingredient in this is the introduction of the Gaussian ensemble, which is essentially just a regularization of the discrete spectrum of a closed quantum system. The Gaussian ensemble will be defined in section 2, where we will also show how all microcanonical results can be obtained from the Gaussian ensemble in the limit where the regularization is removed. In the following sections we will then show that in a certain range of the regularization parameter the canonical ensemble is a good approximation of the Gaussian ensemble and we will propose definite ways of estimating the difference between the two methods. These results are then employed in the derivation of an asymptotic expansion of microcanonical corrections to the canonical ensemble, which will be most useful for systems near, but not quite at, the thermodynamical limit. Finally, we will consider some implications of the present results to the thermodynamics of systems with an exponentially increasing density of states, for which the canonical ensemble is in principle not well defined.

We will not repeat standard results or definitions of the statistics of quantum systems in the thermodynamical limit here. The physical argumentation leading to the density operator formulation is explained in most textbooks on the subject, volume five of the classical series by Landau and Lifshitz [4] being a good example. More elaborate and recent analysis of the subject can be found from volume one of the series by Balian [5], while a mathematically rigorous approach is developed in volume four of ‘*A Course in Mathematical Physics*’ by Thirring [6].

## 2. Gaussian ensemble† as a regularization of the microcanonical ensemble

Consider the operator defined by

$$\hat{\rho}_\varepsilon(E) = \frac{1}{\sqrt{2\pi\varepsilon^2}} \exp\left[-\frac{1}{2}\left(\frac{\hat{H} - E}{\varepsilon}\right)^2\right] \quad (1)$$

where  $\hat{H}$  is the Hamiltonian and  $E$  and  $\varepsilon \neq 0$  are two real parameters. Since  $\hat{H}$  is self-adjoint,  $\hat{\rho}_\varepsilon(E)$  is bounded, self-adjoint and positive. For this operator to define a sensible

† On physical grounds, the idea of using a Gaussian energy distribution to define a statistical ensemble seems natural. Such a physical reasoning was adopted, for instance, in [7] to introduce a Gaussian ensemble for studying first-order phase transitions in certain lattice gauge theories.

statistical ensemble via the trace formulae, it is also necessary to require that the spectrum of the Hamiltonian is discrete and increases sufficiently fast at infinity so that  $\text{Tr} \hat{\rho}_\varepsilon(E) < \infty$ . If this is true, we will define the *Gaussian expectation values* of an observable  $\hat{A}$  by the formula

$$\langle \hat{A} \rangle_{E,\varepsilon}^{\text{gauss}} \equiv \frac{\text{Tr}(\hat{A} \hat{\rho}_\varepsilon(E))}{\text{Tr} \hat{\rho}_\varepsilon(E)}. \quad (2)$$

At this point, it will be useful to define some terminology to be used later. If the Hamiltonian of the system satisfies  $\text{Tr} \hat{\rho}_\varepsilon(E) < \infty$  for all  $E \in \mathbb{R}$  and  $\varepsilon > 0$ , we will call the system *Gaussianly bounded* and define the above trace as the Gaussian partition function  $Z_{E,\varepsilon}^{\text{gauss}}$ . Similarly, if  $\text{Tr} e^{-\beta \hat{H}} < \infty$  for all  $\beta > 0$ , we will say that the system is *canonically bounded* and the trace will give the canonical partition function  $Z_\beta^{\text{can}}$ . The terms *Gaussian* and *canonical observable*, respectively, are then used for those normal or bounded operators (i.e. observables)  $\hat{A}$  for which  $\langle |\hat{A}| \rangle_{E,\varepsilon}^{\text{gauss}} < \infty$  or  $\langle |\hat{A}| \rangle_\beta^{\text{can}} < \infty$  for all the above values of the parameters—here  $|\hat{A}|$  refers to the positive square root of  $\hat{A}^\dagger \hat{A}$ . Analogously, systems with a discrete energy spectrum with finite multiplicities are called microcanonically bounded and all normal operators having a domain which contains the domain of the Hamiltonian as well as all bounded operators are microcanonical observables. In this last case, the microcanonical partition function  $Z_E^{\text{micro}}$  is defined by the number of eigenstates with energy  $E$  and the microcanonical expectation values are the averages over these eigenstates.

Clearly, every canonically bounded system is Gaussianly bounded and every canonical observable is a Gaussian observable and the same relations also hold between the Gaussian and the microcanonical ensemble. The term bounded used here also has a direct physical interpretation in the canonical case: by the Golden–Thompson–Symanzik inequality [8], which applies for  $n$ -dimensional systems with Hamiltonians of the form  $\hat{H} = \frac{1}{2} \hat{\mathbf{p}}^2 + V(\hat{\mathbf{x}})$ , a system is canonically bounded if the potential increases fast enough at infinity so that  $\int d^n \hat{\mathbf{x}} e^{-\beta V(\hat{\mathbf{x}})} < \infty$  for all  $\beta > 0$ .

The formal relation  $\lim_{\varepsilon \rightarrow 0} \hat{\rho}_\varepsilon(E) = \delta(\hat{H} - E)$  is one obvious motivation for using this ensemble to approximate the microcanonical one. However, it can also be argued that the Gaussian ensemble is even better suited for describing typical experimental situations than the microcanonical ensemble: if a quantum system was initially prepared into, or was measured to have, an energy  $E$  and the system is almost, but not completely, isolated having interactions with the environment that lead to energy fluctuations of the order of  $\varepsilon$ , then the Gaussian ensemble using these parameters is the most natural way to predict the behaviour of a statistical average over many independent measurements of an observable. Of course, for this physical interpretation to be valid, the interactions with the environment need to be balanced in such a way as not to lead to a net flow of energy from one direction to the other—this is the essence of the requirement of ‘thermalization’ of the system in the context of the Gaussian ensemble.

Mathematically, the Gaussian ensemble is a regularization of the discrete energy spectrum by a convolution with the normal distribution. As was explained in the introduction, this is beneficial since it offers a way of removing the effect of the instability of the high-energy spectral levels. Also, its use does not require any prior knowledge about the spectrum as it is well defined for all values of  $E$ . Most important, however, is the way the Gaussian ensemble offers a natural and mathematically rigorous approximation of the microcanonical ensemble:

- (i)  $\lim_{\varepsilon \rightarrow 0} \sqrt{2\pi \varepsilon^2} Z_{E,\varepsilon}^{\text{gauss}} = Z_E^{\text{micro}}$  for all real  $E$ ;
- (ii)  $\lim_{\varepsilon \rightarrow 0} Z_{E,\varepsilon}^{\text{gauss}} = \text{Tr} \delta(\hat{H} - E)$  as distributions in  $E$ ;
- (iii)  $\lim_{\varepsilon \rightarrow 0} \langle \hat{A} \rangle_{E,\varepsilon}^{\text{gauss}} = \langle \hat{A} \rangle_{E'}^{\text{micro}}$ , where  $E'$  is the energy eigenvalue nearest to  $E$ .

We will now conclude this section by proving these three statements.

Suppose that the system is Gaussianly bounded with discrete energy levels  $E_n$ , each one having a multiplicity  $\kappa_n$  and eigenvectors  $\Omega_{n,k}$ ,  $k = 1, \dots, \kappa_n$ . Then for any Gaussian observable  $\hat{A}$ , the trace in (2) can be expressed as

$$\text{Tr}(\hat{A}\hat{\rho}_\varepsilon(E)) = \frac{1}{\sqrt{2\pi\varepsilon^2}} \sum_{n,k} \exp\left[-\frac{1}{2\varepsilon^2}(E_n - E)^2\right] \langle \Omega_{n,k} | \hat{A} | \Omega_{n,k} \rangle. \quad (3)$$

Denote  $\langle \Omega_{n,k} | \hat{A} | \Omega_{n,k} \rangle$  by  $a_{n,k}$  and note that, since  $|a_{n,k}| \leq \langle \Omega_{n,k} | \hat{A} | \Omega_{n,k} \rangle$ , the above series converges absolutely for any  $\varepsilon > 0$ .

Let us first look at the behaviour of the Gaussian partition function, i.e. use  $\hat{A} = \hat{1}$ . By (3) then

$$\sqrt{2\pi\varepsilon^2} Z_{E,\varepsilon}^{\text{gauss}} = \sum_n \kappa_n \exp\left[-\frac{1}{2\varepsilon^2}(E_n - E)^2\right].$$

Since for any  $W > 0$  the function  $e^{-W/\varepsilon^2}$  is an increasing function of  $\varepsilon$  in the region  $\varepsilon > 0$ , dominated convergence can be invoked to move the limit  $\varepsilon \rightarrow 0$  inside the sum, which then gives the result

$$\lim_{\varepsilon \rightarrow 0} \sqrt{2\pi\varepsilon^2} Z_{E,\varepsilon}^{\text{gauss}} = \begin{cases} \kappa_n & \text{if } E = E_n \text{ for some } n \\ 0 & \text{otherwise.} \end{cases}$$

Since the right-hand side equals  $Z_E^{\text{micro}}$  by definition, this proves the first statement.

Next, let  $f(E)$  be any smooth function with a compact support and let  $M > 0$  be such that  $|\text{supp } f| \leq M$ . To prove the second statement, we need to show that

$$\lim_{\varepsilon \rightarrow 0} \int_{-\infty}^{\infty} dE f(E) Z_{E,\varepsilon}^{\text{gauss}} = \sum_n \kappa_n f(E_n).$$

Since

$$\int_{-\infty}^{\infty} dE f(E) \frac{1}{\sqrt{2\pi\varepsilon^2}} \exp\left[-\frac{1}{2\varepsilon^2}(E_n - E)^2\right] \rightarrow f(E_n)$$

when  $\varepsilon \rightarrow 0$ , this is clearly true if only it were possible to move first the  $E$ -integration and then the  $\varepsilon \rightarrow 0$  limit inside the sum. In fact, both of these operations are now allowed by the dominated convergence theorem, since we have the bounds

$$\begin{aligned} & \int_{-\infty}^{\infty} dE |f(E)| \frac{\exp[-(E_n - E)^2/2\varepsilon^2]}{\sqrt{2\pi\varepsilon^2}} \\ & \leq \begin{cases} \|f\|_\infty & \text{if } |E_n| < 2M \\ \|f\|_\infty \exp[-\frac{1}{2}(|E_n| - M)^2 + \frac{1}{2}M^2] & \text{if } |E_n| \geq 2M \end{cases} \end{aligned}$$

for all  $0 < \varepsilon \leq 1$ .

Let us finally evaluate the limit of the expectation values for general  $\hat{A}$ ,

$$\langle \hat{A} \rangle_{E,\varepsilon}^{\text{gauss}} = \sum_{n,k} \frac{\exp[-(E_n - E)^2/2\varepsilon^2]}{\text{Tr } \hat{\rho}_\varepsilon \sqrt{2\pi\varepsilon^2}} \langle \Omega_{n,k} | \hat{A} | \Omega_{n,k} \rangle. \quad (4)$$

For this we will need the result

$$\begin{aligned} & \frac{1}{\sum_{n',k'} \exp[-((E_{n'} - E)^2 - (E_n - E)^2)/2\varepsilon^2]} \\ & \xrightarrow{\varepsilon \rightarrow 0} \begin{cases} 0 & \text{if } |E_{n'} - E| < |E_n - E| \text{ for some } n' \\ \left( \sum_{n'} \kappa_{n'} \delta_{|E_{n'} - E|, |E_n - E|} \right)^{-1} & \text{otherwise.} \end{cases} \quad (5) \end{aligned}$$

In other words, this limit is zero if  $E_n$  is not the eigenvalue nearest to  $E$ , it is  $(\kappa_n + \kappa_m)^{-1}$  if both  $E_n$  and  $E_m$  are nearest eigenvalues (i.e. if  $E$  lies exactly in the middle of the segment joining  $E_n$  and  $E_m$  and no other eigenvalues are on this segment) and it is  $\kappa_n^{-1}$  if  $E_n$  is a unique nearest eigenvalue. Let us use the notation  $M_n(E)$  for the sum  $\sum_{n'} \kappa_{n'} \delta_{|E_{n'}-E|, |E_n-E|}$ .

Let  $n_0$  be the index of any one of the eigenvalues nearest to  $E$ . Then for all  $n$

$$\frac{\exp[-(E_n - E)^2/2\varepsilon^2]}{\text{Tr} \hat{\rho}_\varepsilon \sqrt{2\pi\varepsilon^2}} = \frac{\exp[-(E_n - E)^2/2\varepsilon^2]}{\sum_{n'} \kappa_{n'} \exp[-(E_{n'} - E)^2/2\varepsilon^2]} < \frac{1}{\kappa_{n_0}} \exp\left[\frac{(E_{n_0} - E)^2 - (E_n - E)^2}{2\varepsilon^2}\right] \quad (6)$$

where  $(E_{n_0} - E)^2 - (E_n - E)^2 \leq 0$ . This implies that, for all  $\varepsilon$  in the range  $0 < \varepsilon \leq 1$ , the absolute value of each of the terms of the series in (4) is less than  $\exp[(E_{n_0} - E)^2/2] \exp[-(E_n - E)^2/2] |a_{n,k}|$ , which again forms an  $\varepsilon$ -independent sum that is convergent by assumption. Thus dominated convergence can be applied to move the limit inside the sum, which then by equation (5) yields the result

$$\langle \hat{A} \rangle_{E,\varepsilon}^{\text{gauss}} \xrightarrow{\varepsilon \rightarrow 0} \frac{1}{M_{n_0}(E)} \sum_{n,k} \delta_{|E_n-E|, |E_{n_0}-E|} \langle \Omega_{n,k} | \hat{A} | \Omega_{n,k} \rangle.$$

Since  $M_{n_0}(E)$  is the number of non-zero terms in the above sum, the final expression is nothing but the average of the expectation values of  $\hat{A}$  over the energy eigenstates nearest to  $E$ .

Therefore, whenever  $E$  coincides with a point in the spectrum, the limit  $\varepsilon \rightarrow 0$  will give the microcanonical expectation value. On the other hand, if  $E$  does not belong to the energy spectrum (in which case the microcanonical ensemble is in principle ill defined), then the microcanonical result corresponding to the nearest eigenvalue is obtained. The only values of  $E$  giving non-microcanonical limits are those lying exactly in the middle between two eigenvalues, but even then the result is an expectation value of a uniform distribution over two energy eigenvalues.

### 3. Canonical ensemble as an approximation to the Gaussian ensemble

We will next show how the canonical ensemble can be used for approximating the Gaussian ensemble in the region where the energy resolution  $\varepsilon$  is sufficiently large. For this we need to assume that the system is canonically bounded and that  $\hat{A}$  is a canonical observable. Since this, in particular, requires the energy spectrum to be bounded from below, we will also assume that the Hamiltonian has been normalized so that the lowest energy level  $E_0$  is non-negative.

Let us first assume that  $\beta$  is a positive parameter. Since

$$-\frac{1}{2\varepsilon^2}(E - E_n)^2 = -\frac{1}{2\varepsilon^2}(E - E_n + \beta\varepsilon^2)^2 + \beta E - \beta E_n + \frac{1}{2}\beta^2\varepsilon^2$$

we have the identity

$$\text{Tr}(\hat{A} \hat{\rho}_\varepsilon(E)) = e^{\frac{1}{2}\beta^2\varepsilon^2 + \beta E} \text{Tr}(\hat{A} \hat{\rho}_\varepsilon(E + \beta\varepsilon^2) e^{-\beta\hat{H}}). \quad (7)$$

If we integrate this multiplied by  $e^{-\beta E}$  over  $E$  and take the integration inside the trace, which is possible since  $\hat{A}$  is a canonical observable, we get the exact formula

$$\text{Tr}(\hat{A} e^{-\beta\hat{H}}) = e^{-\frac{1}{2}\beta^2\varepsilon^2} \int_{-\infty}^{\infty} dE e^{-\beta E} \text{Tr}(\hat{A} \hat{\rho}_\varepsilon(E)) \quad (8)$$

valid for all  $\varepsilon > 0$  and  $\beta > 0$ . This is a regularized form of the familiar statement that the canonical ensemble is the Laplace transform of the microcanonical one.

The result (8) has a more interesting inverse formula, which we will derive next. We will begin with the Fourier transform of the normal distribution,

$$\int_{-\infty}^{\infty} \frac{d\alpha}{2\pi} \exp\left(-\frac{1}{2}\varepsilon^2\alpha^2 + i\alpha W\right) = \frac{1}{\sqrt{2\pi\varepsilon^2}} \exp\left(-\frac{1}{2\varepsilon^2}W^2\right) \quad (9)$$

which can be applied to (7), yielding

$$\mathrm{Tr}(\hat{A}\hat{\rho}_\varepsilon(E)) = e^{\frac{1}{2}\beta^2\varepsilon^2 + \beta E} \int_{-\infty}^{\infty} \frac{d\alpha}{2\pi} e^{-\frac{1}{2}\varepsilon^2\alpha^2} \mathrm{Tr}(\hat{A} e^{-\beta\hat{H} + i\alpha(E + \beta\varepsilon^2 - \hat{H})}).$$

In changing the order of the integration and the trace we again had to use the assumption that  $\hat{A}$  is a canonical observable. Now using a new integration variable  $w = \beta + i\alpha$  we get a particularly simple form of the desired inversion formula for (8),

$$\mathrm{Tr}(\hat{A}\hat{\rho}_\varepsilon(E)) = \int_{\beta-i\infty}^{\beta+i\infty} \frac{dw}{2\pi i} e^{\frac{1}{2}\varepsilon^2 w^2 + wE} \mathrm{Tr}(\hat{A} e^{-w\hat{H}}) \quad (10)$$

valid for all  $\beta > 0$ . We can now conclude that the analytical form of the canonical trace contains all the information needed to compute the microcanonical expectation values, which are then easily extracted from the integral in (10). However, this formula also leads to a simple relation between the usual real-temperature canonical ensemble and the Gaussian ensemble which we shall inspect next.

For all canonical observables, the trace  $\mathrm{Tr}(\hat{A} e^{-w\hat{H}})$  is obviously an analytic function of  $w$  in the half-plane  $\mathrm{Re} w > 0$  and all its derivatives are given by a differentiation inside the trace, i.e.

$$\frac{d^k}{dw^k} \mathrm{Tr}(\hat{A} e^{-w\hat{H}}) = \mathrm{Tr}(\hat{A}(-\hat{H})^k e^{-w\hat{H}}).$$

Therefore, saddle-point methods can be used in evaluation of the integral in (10),

$$\int_{\beta-i\infty}^{\beta+i\infty} \frac{dw}{2\pi i} \exp\left[\frac{1}{2}\varepsilon^2 w^2 + wE + \ln \mathrm{Tr}(\hat{A} e^{-w\hat{H}})\right].$$

Here the branch of the logarithm needs to be chosen so that the logarithm is analytic on the integration contour; if the contour happens to go through a zero of the trace, then an infinitesimal deformation of the contour is necessary—note that this is always possible if we only make the trivial assumption  $\hat{A} \neq 0$ . The saddle-point equation, which is of course independent of what branch we use for the logarithm, is

$$\frac{\mathrm{Tr}(\hat{A}\hat{H} e^{-w\hat{H}})}{\mathrm{Tr}(\hat{A} e^{-w\hat{H}})} = E + \varepsilon^2 w \quad (11)$$

while the second derivative, which will determine the direction of the steepest descent path, is

$$\frac{\mathrm{Tr}(\hat{A}\hat{H}^2 e^{-w\hat{H}})}{\mathrm{Tr}(\hat{A} e^{-w\hat{H}})} - \left(\frac{\mathrm{Tr}(\hat{A}\hat{H} e^{-w\hat{H}})}{\mathrm{Tr}(\hat{A} e^{-w\hat{H}})}\right)^2 + \varepsilon^2. \quad (12)$$

So far we have only assumed that observable  $\hat{A}$  is canonical. For the following discussion we shall also assume that  $\hat{A}$  is positive, non-zero and that  $\mathrm{Tr}(\hat{A}\hat{H}) = \infty$ , keeping in mind that the special case  $\hat{A} = \hat{1}$  falls into this category. We shall also use the notation  $\overline{O}$  for  $\mathrm{Tr}(\hat{A}\hat{O} e^{-w\hat{H}})/\mathrm{Tr}(\hat{A} e^{-w\hat{H}})$ . With these definitions, the saddle-point equation becomes  $\overline{H} = E + \varepsilon^2 w$  and the second derivative is  $(H - \overline{H})^2 + \varepsilon^2$ .

If we restrict ourselves to the positive real axis, then  $\mathrm{Tr}(\hat{A} e^{-w\hat{H}})$  will always be strictly positive and both  $\overline{H}$  and  $(H - \overline{H})^2$  will be well defined and positive. From this we conclude

that on the positive real axis the logarithm  $\ln \text{Tr}(\hat{A} e^{-u\hat{H}})$  is a convex function and that the expectation value  $\overline{H}$  is strictly decreasing. Therefore, the saddle-point equation (11) has at most one positive solution for each  $E$ . On the other hand, the assumption  $\text{Tr}(\hat{A}\hat{H}) = \infty$  can be used to show that a solution exists for every  $E \in \mathbb{R}$  and  $\varepsilon > 0$ . We shall now assume that  $\beta$ , which was an arbitrary parameter of the integration contour in (10), has been chosen to equal this unique positive solution. Since the second derivative is  $(H - \overline{H})^2 + \varepsilon^2$ , it is now strictly positive and the integration contour  $\beta - i\infty \rightarrow \beta + i\infty$  in fact goes through the saddle point  $\beta$  via the path of steepest descent. Using the saddle-point approximation to evaluate the contribution of this saddle point to the integral then gives

$$\frac{1}{\sqrt{2\pi}} (\varepsilon^2 + \overline{(H - \overline{H})^2})^{-\frac{1}{2}} e^{\frac{1}{2}\beta^2\varepsilon^2 + \beta E} \text{Tr}(\hat{A} e^{-\beta\hat{H}}).$$

From this, equation (7) and the saddle-point equation we obtain the following exact result and its saddle-point approximation

$$\text{Tr}(\hat{A}\hat{\rho}_\varepsilon(E)) = e^{-\frac{1}{2}\beta^2\varepsilon^2 + \beta\overline{H}} \text{Tr}(\hat{A}\hat{\rho}_\varepsilon(\overline{H}) e^{-\beta\hat{H}}) \quad (13)$$

$$\approx \frac{1}{\sqrt{2\pi}} (\varepsilon^2 + \overline{(H - \overline{H})^2})^{-\frac{1}{2}} e^{-\frac{1}{2}\beta^2\varepsilon^2 + \beta\overline{H}} \text{Tr}(\hat{A} e^{-\beta\hat{H}}). \quad (14)$$

So far we have only inspected the saddle points on the positive real axis. However, as a simple example with, for example, a harmonic oscillator will show, there will generally be a countably infinite set of saddle points on the complex plane. Also, it is quite possible that the steepest descent path going through all the relevant saddle points will not stay on the right half-plane, which will be unfortunate unless the analytical continuation of the canonical trace over the imaginary axis is known. In addition, the values of  $\beta$  at which the traces  $\text{Tr}(\hat{A}\hat{\rho}_\varepsilon(E))$  and  $\text{Tr} \hat{\rho}_\varepsilon(E)$  need to be evaluated are typically different, which would then mean that the ratio of their saddle-point approximations does not exactly equal the canonical expectation value.

However, as we shall see in the next section, in the thermodynamical limit these considerations are not relevant and the saddle-point approximation using the positive  $\beta$  will give accurate results so long as we use a suitable  $\varepsilon$  and inspect only large enough energies  $E$ . For the partition function this saddle-point approximation reads

$$Z_{E,\varepsilon}^{\text{gauss}} \approx \frac{1}{\sqrt{2\pi(\sigma^2 + \varepsilon^2)}} e^{-\frac{1}{2}\beta^2\varepsilon^2 + \beta\overline{H}} Z_\beta^{\text{can}} \quad (15)$$

where  $\overline{H} = \langle \hat{H} \rangle_\beta^{\text{can}}$ ,  $\sigma^2 = \langle \hat{H}^2 \rangle_\beta^{\text{can}} - \overline{H}^2$  and  $\beta$  is the unique positive number satisfying  $\langle \hat{H} \rangle_\beta^{\text{can}} = E + \varepsilon^2\beta$ . Using this same  $\beta$  also for the other trace in the expectation values will give the following exact result and an approximation of the Gaussian expectation values:

$$\langle \hat{A} \rangle_{E,\varepsilon}^{\text{gauss}} = \frac{\text{Tr}(\hat{A}\hat{\rho}_\varepsilon(\overline{H}) e^{-\beta\hat{H}})}{\text{Tr}(\hat{\rho}_\varepsilon(\overline{H}) e^{-\beta\hat{H}})} \approx \langle \hat{A} \rangle_\beta^{\text{can}}. \quad (16)$$

From this formula we can already gain some idea of when the approximation will be most accurate: the contribution of the additional term  $\hat{\rho}_\varepsilon(\overline{H})$  will be small when the variance of the Gaussian peak is greater than the variance of the canonical distribution, i.e. whenever  $\varepsilon^2 > \sigma^2$ . We will derive more quantitative bounds for the accuracy of the approximation in the next section.

From the above result we can give a new interpretation of the role of the canonical ensemble in quantum statistics: *the canonical ensemble is an approximation of the regularized microcanonical ensemble from which the discrete structure of the energy levels has been smoothed out*. We have also seen that the canonical approximation works best in the limit  $\varepsilon/\sigma \rightarrow \infty$ . However, for a fixed energy  $E$  a minimum requirement for the *Gaussian* ensemble



to give meaningful results is  $\varepsilon < E - E_0$ , so that taking this limit to its extreme is not possible in practice. In the next section we will propose a procedure for inspecting how and when a suitable compromise for  $\varepsilon$  can be found.

Finally, we would like to comment on the interpretation of the canonical entropy,  $S_\beta^{\text{can}} = \beta \langle \hat{H} \rangle_\beta^{\text{can}} + \ln Z_\beta^{\text{can}}$ , in view of the previous approximation. Since the value of  $Z_{E,\varepsilon}^{\text{gauss}}$  gives the density of the energy eigenstates at energy  $E$ —the density as the number of eigenstates *per the energy interval*  $\varepsilon$ —its logarithm can be interpreted as the entropy of the system and we denote  $S_{E,\varepsilon}^{\text{gauss}} = \ln Z_{E,\varepsilon}^{\text{gauss}}$ . On the other hand, from the saddle-point approximation (15) we conclude that

$$S_{E,\varepsilon}^{\text{gauss}} \approx S_\beta^{\text{can}} - \ln \varepsilon - \frac{1}{2} \ln \left[ 2\pi \left( 1 + \frac{\sigma^2}{\varepsilon^2} \right) \right] - \frac{1}{2} \varepsilon^2 \beta^2 \quad (17)$$

which means that the canonical entropy gives a good approximation of the logarithmic density of states per energy  $\varepsilon$  *provided* the energy resolution is proportional to the canonical energy deviation, i.e.  $\varepsilon \propto \sigma$ . If the energy resolution is microscopic, then the above formula implies a correction to the canonical entropy of the form  $\ln N$ ,  $N$  being the number of particles. Thus a natural interpretation for the canonical entropy is the entropy measured from the density of states per energy  $\sigma$ , the standard deviation of the canonical ensemble—note that the relation between the density of states and the dimensionless number given by the canonical entropy is dubious in any case.

#### 4. Efficiency and improvements of the canonical ensemble

In this section we will continue working with the same set-up as in the previous one, i.e. we assume that the system is canonically bounded,  $\hat{A}$  is a canonical observable and the parameter  $\beta$  is the unique positive solution to the equation  $\langle \hat{H} \rangle_\beta^{\text{can}} = E + \varepsilon^2 \beta$ . Since we will be mainly using the canonical expectation values here, we will drop both the superscript ‘can’ and the subscript  $\beta$  from these expressions; similarly, using the ‘hats’ to signify operators will become cumbersome and we will abandon the practice at this point.

Our first aim is to derive quantitative bounds for how well the canonical ensemble approximates the Gaussian one and then to derive a method for computing corrections to the canonical ensemble when it first begins to fail. The corrections will be expressed in terms of the normalized moments of the canonical distribution and for this reason we will now adopt the notation  $\sigma^2$  for the variance  $\langle (H - \langle H \rangle)^2 \rangle$  and then define the normalized Hamiltonian  $h$  by the formula

$$h = \frac{H - \langle H \rangle}{\sigma}.$$

If  $A$  is positive and non-zero, then Jensen’s inequality [9] can be used for deriving the following bounds valid for any  $a \in \mathbb{R}$ ,

$$\exp \left( -a \frac{\langle Ah^2 \rangle}{\langle A \rangle} \right) \leq \frac{\langle A \exp(-ah^2) \rangle}{\langle A \rangle} \leq 1. \quad (18)$$

If we apply this to  $\langle A e^{-ah^2} \exp(ah^2) \rangle / \langle A e^{-ah^2} \rangle$ , we can also improve the upper bound:

$$\exp \left( -a \frac{\langle Ah^2 \rangle}{\langle A \rangle} \right) \leq \frac{\langle A \exp(-ah^2) \rangle}{\langle A \rangle} \leq \exp \left[ -a \frac{\langle Ah^2 \rangle}{\langle A \rangle} \exp \left( -a \frac{\langle Ah^4 \rangle}{\langle Ah^2 \rangle} \right) \right]. \quad (19)$$

Since  $\langle h^2 \rangle = 1$  by definition, we get for  $A = \hat{1}$

$$\exp(-a) \leq \langle \exp(-ah^2) \rangle \leq \exp[-a \exp(-a \langle h^4 \rangle)]. \quad (20)$$

Applying these bounds with  $a = \sigma^2/2\varepsilon^2$  to (16) yields the following bounds for the relative efficiency of the canonical expectation values

$$\exp\left(-\frac{\sigma^2}{2\varepsilon^2} \frac{\langle Ah^2 \rangle}{\langle A \rangle}\right) \leq \frac{\langle A \rangle_{E,\varepsilon}^{\text{gauss}}}{\langle A \rangle} \leq \exp\left(\frac{\sigma^2}{2\varepsilon^2}\right) \quad (21)$$

or by using the more accurate equation (19),

$$-\frac{\sigma^2}{2\varepsilon^2} \left[ \frac{\langle Ah^2 \rangle}{\langle A \rangle} - \exp\left(-\frac{\sigma^2}{2\varepsilon^2} \langle h^4 \rangle\right) \right] \leq \ln \frac{\langle A \rangle_{E,\varepsilon}^{\text{gauss}}}{\langle A \rangle} \leq \frac{\sigma^2}{2\varepsilon^2} \left[ 1 - \frac{\langle Ah^2 \rangle}{\langle A \rangle} \exp\left(-\frac{\sigma^2}{2\varepsilon^2} \frac{\langle Ah^4 \rangle}{\langle Ah^2 \rangle}\right) \right]. \quad (22)$$

These equations prove, for positive observables  $A$ , the earlier alluded statement that in the limit  $\varepsilon/\sigma \rightarrow \infty$  the approximation by the canonical ensemble becomes exact. On the other hand, the bounds also suggest that it is necessary to have at least  $\varepsilon^2/\sigma^2 \gtrsim \frac{1}{2}$  before the canonical expectation values give a trustworthy approximation of the Gaussian ones.

For a fixed  $E$  it is not in general possible to take the limit  $\varepsilon \rightarrow \infty$ , since then  $\beta \rightarrow 0$  and thus also  $\sigma \rightarrow \infty$ . Moreover, it is also necessary to require that  $\varepsilon \ll E$  to obtain a meaningful approximation to the microcanonical ensemble from the Gaussian one. In practice, the most interesting applications of the ongoing ideas are in the energy region in which the canonical ensemble first begins to fail. For this reason, we also need an estimate *in terms of the canonical quantities* for the region where the canonical approximation is not reliable.

Since

$$E = \langle H \rangle - \beta\varepsilon^2 = \langle H \rangle \left( 1 - \frac{\beta\sigma^2}{\langle H \rangle} \frac{\varepsilon^2}{\sigma^2} \right) \quad (23)$$

should be positive, we can now give the following rules for making an identification between the canonical and the Gaussian ensemble.

- The value of  $\beta\sigma^2/\langle H \rangle$  measures the effectiveness of the canonical ensemble with a given  $\beta$ : the smaller the value, the better the canonical ensemble works and differences are expected to arise when it gets to be of the order of one. Note that in the thermodynamical limit, we have  $\beta \propto 1/N$ ,  $\langle H \rangle \propto N$  and  $\sigma^2 \propto N$  and therefore we would expect this quantity to vanish as  $1/N$ , thus implying that the Gaussian and the canonical ensemble become equivalent in the thermodynamical limit.

- For those values of  $\beta$  with  $\beta\sigma^2/\langle H \rangle \lesssim 1$ , choosing an  $\varepsilon \propto \sigma$  will give the most reliable results. The proportionality factor need not be very large, since the relative accuracy of the canonical approximation depends on the second power of its inverse—for typical observables the accuracy can improve even more quickly as can be seen from equation (22). In any case, we get from (23) an absolute upper bound for the possible values of the proportionality factor,

$$\frac{\varepsilon}{\sigma} \leq \sqrt{\frac{\langle H \rangle}{\beta\sigma^2}} \propto \sqrt{N}.$$

Let us then derive an approximation for the Gaussian partition function in the region where the parameter  $a = \sigma^2/2\varepsilon^2$  is small. From (13) we get the following identity

$$Z_{E,\varepsilon}^{\text{gauss}} = \frac{1}{\sqrt{2\pi(\sigma^2 + \varepsilon^2)}} e^{-\frac{1}{2}\beta^2\varepsilon^2 + \beta\langle H \rangle} Z_{\beta}^{\text{can}} \sqrt{1 + 2a} (e^{-ah^2})$$

where we have extracted the saddle-point approximation that was given in (15). Let us denote the logarithm of the correction to the saddle-point approximation by  $f(a) = \frac{1}{2} \ln(1 + 2a) + \ln\langle e^{-ah^2} \rangle$ . Equation (20) immediately yields simple bounds for this correction term,

$$\frac{1}{2} \ln(1 + 2a) - a \leq f(a) \leq \frac{1}{2} \ln(1 + 2a) - a e^{-a\langle h^4 \rangle}.$$

Clearly,  $f$  is an analytic function on the right half-plane and it is infinitely many times differentiable from the right at the origin of the real axis. Thus it has a Taylor polynomial expansion at the origin,

$$f(a) = \sum_{k=0}^{K-1} \frac{a^k}{k!} f^{(k)}(0^+) + \mathcal{O}(a^K) \quad \text{for all } a > 0 \tag{24}$$

although the corresponding full Taylor series *need not* converge. This situation is the same as is often encountered in perturbation theory: the result is an asymptotic series in the perturbed coupling constant.

Since  $f(0^+) = 0$ , the constant term of the expansion vanishes and, by virtue of the saddle-point approximation, the first coefficient is also zero, since  $\langle h^2 \rangle = 1$ . The rest of the coefficients of the expansion (24) are then given by the formula

$$f^{(k)}(0^+) = (-2)^{k-1} (k-1)! + \frac{d^k}{da^k} \ln(e^{-ah^2})|_{a=0} \quad \text{for } k \geq 1$$

the first five of which are computed in table 1.

**Table 1.** The first five derivatives needed in the Taylor expansion of the Gaussian partition function. In the table,  $h_n$  refers to the canonical expectation value  $\langle h^n \rangle$ .

$k$	$f^{(k)}(0^+)$
1	0
2	$-3 + h_4$
3	$6 + 3h_4 - h_6$
4	$-54 + 12h_4 - 3h_4^2 - 4h_6 + h_8$
5	$360 + 60h_4 - 30h_4^2 - 20h_6 + 10h_4h_6 + 5h_8 - h_{10}$

With a given  $K$ , the residual term  $R_K(a)$ —denoted by  $\mathcal{O}(a^K)$  in (24)—can be written as

$$R_K(a) = \frac{a^K}{K!} f^{(K)}(\alpha)$$

where  $\alpha \in [0, a]$  depends on  $a$ . Since all derivatives are continuous, the values of the derivatives at  $0^+$  given in table 1 give an estimate for  $f^{(K)}(\alpha)$  for sufficiently small  $a$ . Therefore, these values can be used for estimating the residual term and thus for deciding the best value of  $K$  for a given, small,  $a$ .

If  $a$  is not small enough, it is possible to use other, less accurate, estimates. Now  $f^{(K)}(\alpha)$  is a polynomial of the ratios  $g_n = \langle h^n \exp(-\alpha h^2) \rangle / \langle \exp(-\alpha h^2) \rangle$ , which, on the other hand, have the exact bounds

$$\exp\left(-a \frac{h_{2k+2}}{h_{2k}}\right) \leq \frac{g_{2k}}{h_{2k}} \leq \exp(a) \quad \text{for all } k \geq 1.$$

Therefore, it is possible to use these bounds in the known form of the polynomials yielding exact bounds for the values of the derivatives. The first five of the polynomials are given in table 2 and the rest can be easily computed, if necessary.

The same Taylor polynomial approximation in  $a$  can be made equally well for expectation values of a canonical observable  $A$ . Let us define

$$g(a) = \frac{\langle A \exp(-ah^2) \rangle}{\langle \exp(-ah^2) \rangle}$$

when by (16) the function  $g(a)$  equals the Gaussian expectation value of  $A$  at energy  $E = \langle H \rangle - \varepsilon^2 \beta$  and resolution  $\varepsilon = \sigma / \sqrt{2a}$ . The Taylor expansion of  $g$  is

$$g(a) = \langle A \rangle \left( 1 + \sum_{k=1}^{K-1} \frac{a^k}{k!} G_k(0) + \frac{\langle A \exp(-\alpha h^2) \rangle}{\langle A \rangle \langle \exp(-\alpha h^2) \rangle} \frac{a^K}{K!} G_K(\alpha) \right) \tag{25}$$

**Table 2.** The first five general derivatives needed for the Taylor residuals of the Gaussian partition function. In the table,  $g_n$  refers to the  $\alpha$ -dependent ratio  $\langle h^n \exp(-\alpha h^2) \rangle / \langle \exp(-\alpha h^2) \rangle$ .

$k$	$f^{(k)}(\alpha)$
1	$\frac{1}{1+2\alpha} - g_2$
2	$-\frac{2}{(1+2\alpha)^2} - g_2^2 + g_4$
3	$\frac{8}{(1+2\alpha)^3} - 2g_2^3 + 3g_2g_4 - g_6$
4	$-\frac{48}{(1+2\alpha)^4} - 6g_2^4 + 12g_2^2g_4 - 3g_4^2 - 4g_2g_6 + g_8$
5	$\frac{384}{(1+2\alpha)^5} - 24g_2^5 + 60g_2^3g_4 - 30g_2g_4^2 - 20g_2^2g_6 + 10g_4g_6 + 5g_2g_8 - g_{10}$

**Table 3.** The first few normalized derivatives—as defined in equation (26)—needed in the Taylor expansion of the Gaussian expectation values. Here  $g_n$  and  $A_n$  refer to the  $\alpha$ -dependent ratios  $\langle h^n \exp(-\alpha h^2) \rangle / \langle \exp(-\alpha h^2) \rangle$  and  $\langle h^n A \exp(-\alpha h^2) \rangle / \langle A \exp(-\alpha h^2) \rangle$ , respectively.

$k$	$G_k(\alpha)$
1	$-A_2 + g_2$
2	$A_4 - 2A_2g_2 + 2g_2^2 - g_4$
3	$-A_6 + 3A_4g_2 - 6A_2g_2^2 + 6g_2^3 + 3A_2g_4 - 6g_2g_4 + g_6$
4	$A_8 - 4A_6g_2 + 12A_4g_2^2 - 24A_2g_2^3 + 24g_2^4 - 6A_4g_4 + 24A_2g_2g_4 - 36g_2^2g_4 + 6g_4^2 - 4A_2g_6 + 8g_2g_6 - g_8$
5	$-A_{10} + 5A_8g_2 - 20A_6g_2^2 + 60A_4g_2^3 - 120A_2g_2^4 + 120g_2^5 + 10A_6g_4 - 60A_4g_2g_4 + 180A_2g_2^2g_4 - 240g_2^3g_4 - 30A_2g_4^2 + 90g_2g_4^2 + 10A_4g_6 - 40A_2g_2g_6 + 60g_2^2g_6 - 20g_4g_6 + 5A_2g_8 - 10g_2g_8 + g_{10}$

where the coefficients  $G_k$  are normalized derivatives,

$$G_k(\alpha) = \frac{\langle \exp(-\alpha h^2) \rangle}{\langle A \exp(-\alpha h^2) \rangle} g^{(k)}(\alpha) \tag{26}$$

and we have given the first few of them in table 3. The expansion up to terms of order  $a^2$  is, therefore, given by

$$g(a) = \langle A \rangle + \langle (1 - h^2)A \rangle a + [\langle (1 - h^2)A \rangle + \frac{1}{2} \langle (h^4 - \langle h^4 \rangle)A \rangle] a^2 + \mathcal{O}(a^3).$$

### 5. Summary of the results

In the first section we have shown that when  $\varepsilon \rightarrow 0$  the Gaussian ensemble approaches the quantum microcanonical ensemble and the Gaussian expectation values pick out the nearest microcanonical expectation values. This makes the Gaussian ensemble an easy to use approximation of the microcanonical ensemble, although we have also argued that the ensemble can be given an independent physical interpretation in certain kinds of experiments.

The main results of this paper, however, consider the opposite limit, where  $\varepsilon$  is much larger than a typical distance between consecutive energy levels. We have shown how the canonical ensemble forms an accurate approximation of the Gaussian ensemble in this limit. On the other hand, since the Gaussian ensemble is a regularization of the discrete microcanonical ensemble in this limit, the canonical ensemble can also be given an interpretation as an approximation of this regularized microcanonical ensemble.

If  $E$  and  $\varepsilon$  are the Gaussian energy and energy resolution, respectively, then there always exists a unique  $\beta > 0$  defined by the equation  $\langle H \rangle_\beta^{\text{can}} = E + \beta \varepsilon^2$  and this  $\beta$  gives the best inverse

temperature for a canonical approximation of the Gaussian ensemble. This approximation is best characterized by the parameter  $a = \sigma^2/2\varepsilon^2$ , where  $\sigma^2$  is the variance of the energy in the canonical ensemble,  $\sigma^2 = \langle H^2 \rangle_\beta^{\text{can}} - (\langle H \rangle_\beta^{\text{can}})^2$ . The approximation was shown to work at least in the region where  $a \ll 1$  and, since it was necessary to have  $a \gtrsim \beta\sigma^2/\langle H \rangle_\beta^{\text{can}}$ , the latter quantity furnishes an indicator of whether or not the canonical ensemble can be used for getting reliable information about the properties of a closed system. This indicator can also be given in the form  $\beta\sigma^2/\langle H \rangle_\beta^{\text{can}} = C_V/\beta\langle H \rangle_\beta^{\text{can}}$ , where  $C_V$  is the specific heat at constant volume.

Quantitatively, we have proven the following formulae for the canonical approximation of the Gaussian ensemble

$$S_{E,\varepsilon}^{\text{gauss}} = S_\beta^{\text{can}} - \ln \varepsilon - \frac{1}{2} \ln(2\pi) - \frac{\sigma^2 \beta^2}{4a} - \frac{1}{2} \ln(1+2a) + \Delta S(a; \beta) \quad (27)$$

$$\langle A \rangle_{E,\varepsilon}^{\text{gauss}} = \langle A \rangle_\beta^{\text{can}} + \Delta A(a; \beta). \quad (28)$$

The correction terms, which become important in the region  $a \approx 1$ , can be given an asymptotic expansion in terms of the moments of the normalized canonical energy operator,  $h = (H - \langle H \rangle)/\sigma$ ,

$$\Delta S(a; \beta) = \frac{1}{2}(\langle h^4 \rangle - 3)a^2 + \frac{1}{6}(6 + 3\langle h^4 \rangle - \langle h^6 \rangle)a^3 + \mathcal{O}(a^4) \quad (29)$$

$$\Delta A(a; \beta) = \langle (1 - h^2)A \rangle a + [\langle (1 - h^2)A \rangle + \frac{1}{2}(\langle h^4 \rangle - \langle h^4 \rangle)A]a^2 + \mathcal{O}(a^3). \quad (30)$$

The entropy deviation has also the exact bounds

$$\frac{1}{2} \ln(1+2a) - a \leq \Delta S(a; \beta) \leq \frac{1}{2} \ln(1+2a) - a \exp(-a\langle h^4 \rangle) \quad (31)$$

while for *positive* observables  $A$  we have derived bounds for the logarithmic proportional deviation

$$-a \left[ \frac{\langle Ah^2 \rangle}{\langle A \rangle} - \exp(-a\langle h^4 \rangle) \right] \leq \ln \frac{\langle A \rangle_{E,\varepsilon}^{\text{gauss}}}{\langle A \rangle_\beta^{\text{can}}} \leq a \left[ 1 - \frac{\langle Ah^2 \rangle}{\langle A \rangle} \exp\left(-a \frac{\langle Ah^4 \rangle}{\langle Ah^2 \rangle}\right) \right]. \quad (32)$$

All expectation values in the above are in the canonical ensemble unless stated otherwise.

## 6. Thermodynamics of systems with exponentially increasing density of states

We will now repeat the analysis done in sections 3 and 4 on a system with exponentially increasing density of states. In this case, the canonical ensemble can be defined only up to a certain value of the inverse temperature  $\beta$  and it is not clear when and if the canonical ensemble will give meaningful results. However, since there are physically interesting systems which exhibit an exponential increase of the density of states, for example, free bosonic string theory [10], and since computations in the canonical ensemble are typically easier to perform than microcanonical ones, it is useful to know if the canonical ensemble can be applied to analysis of such a system.

We first define what is meant by an exponential increase of the density of states: if there exists a finite number

$$\beta_c = \inf\{\beta > 0 \mid \text{tr } e^{-\beta H} < \infty\}$$

then  $\beta_c$  can be identified with the speed of exponential increase of the density of states as clearly  $\text{tr } e^{-\beta H} < \infty$  for all  $\beta > \beta_c$  and  $\text{tr } e^{-\beta H} = \infty$  for  $\beta < \beta_c$ . Also, in the following we will consider only observables  $A$  with the property  $\text{tr } |A| e^{-\beta H} < \infty$  for all  $\beta > \beta_c$ . Since we have assumed that  $\beta_c < \infty$ , the system is Gaussianly bounded and  $A$  is a Gaussian observable. Note also that  $\beta_c = 0$  corresponds precisely to the canonical case.

Under these assumptions, everything stated in the beginning of section 3, especially formulae (7)–(10), still hold if we only require  $\beta > \beta_c$  instead of  $\beta > 0$ . Similarly, the analyticity of the integrand in (10) is guaranteed only in the half-plane  $\text{Re } w > \beta_c$ . In the saddle-point approximation of this integral, the uniqueness of the positive saddle point still holds with the same proof as before, but the *existence* depends crucially on the behaviour of the canonical ensemble at temperature  $1/\beta_c$  or, more specifically, on the value of  $E_c \equiv \lim_{\beta \rightarrow \beta_c^+} \langle H \rangle_\beta^{\text{can}}$ .

If  $E_c = \infty$ , then there exists for all  $E \in \mathbb{R}$  and  $\varepsilon > 0$  a unique  $\beta > \beta_c$  for which  $\langle \hat{H} \rangle_\beta^{\text{can}} = E + \beta\varepsilon^2$ . If  $E_c < \infty$ , then there is a positive saddle point  $\beta$  if and only if  $E < E_c - \beta_c\varepsilon^2$ . In these two cases everything stated in section 4 will hold for the saddle-point value of  $\beta$  and thus it is reasonable to use the canonical ensemble for those systems with  $C_V / \langle \beta H \rangle_\beta^{\text{can}} \ll 1$ .

The situation is different for those values of  $E$  for which  $E \geq E_{\text{max}} \equiv E_c - \beta_c\varepsilon^2$ . Then there are no saddle points on the positive real axis and the best one can do with the canonical ensemble is to choose  $\beta \rightarrow \beta_c$ . This approximation, however, is not good unless  $E \approx E_{\text{max}}$  as can be seen from the relation

$$\langle A \rangle_{E,\varepsilon}^{\text{gauss}} = \frac{\text{Tr}(A\rho_\varepsilon(E + \beta_c\varepsilon^2) e^{-\beta_c H})}{\text{Tr}(\rho_\varepsilon(E + \beta_c\varepsilon^2) e^{-\beta_c H})} = \frac{\langle A\rho_\varepsilon(E_c + E - E_{\text{max}}) \rangle_{\beta_c}^{\text{can}}}{\langle \rho_\varepsilon(E_c + E - E_{\text{max}}) \rangle_{\beta_c}^{\text{can}}}$$

which is a consequence of equation (7).

Thus we have found that if  $\langle H \rangle_{\beta_c}^{\text{can}} = \infty$  the system can always be approximated by the canonical ensemble in the thermodynamical limit just as has been explained in the preceding sections. In effect, as the system is ‘heated up’ by adding more and more energy to it, the temperature of the system will increase asymptotically to the limiting value  $T_c = 1/\beta_c$ . On the other hand, if  $\langle H \rangle_{\beta_c}^{\text{can}} < \infty$ , then there exists a limiting energy  $E_{\text{max}} \approx \langle H \rangle_{\beta_c}^{\text{can}}$  after which the canonical ensemble should not be used for estimating the statistical behaviour of the system but using some form of the microcanonical ensemble instead would be advisable.

## 7. Discussion

In this paper we have examined relations between the microcanonical and the canonical approach to quantum statistics. On the level of ideas, the present results are well known and well presented in most standard textbooks on statistical physics and, naturally, none of our results tells us anything new about systems fully in the thermodynamical limit. What we have aspired to do here is to develop a systematic treatment of systems, which are neither large enough to be considered thermodynamical nor simple enough to be completely solvable, but which are, nevertheless, in an energetic equilibrium with their environment.

By taking the energy fluctuations of the system as an integral part of the microcanonical formalism we have been able to show rigorously how the canonical ensemble gives an approximation of the microcanonical statistics even for systems which are not even near a thermodynamical limit and we have been able to give precise relations between canonical concepts, such as temperature, and the more fundamental concepts related directly to energy. We have also shown how and when the canonical ensemble can be stretched to aid in the analysis of these non-thermal systems.

In our analysis of regularization of the energy spectrum we have limited ourselves to the Gaussian distribution. This, however, is only a convenient choice and the analysis could be repeated by using any smooth function with a compact support instead. Using this second alternative would, in fact, be necessary for microcanonically bounded systems with the logarithm of the density of states increasing faster than quadratically in energy, but we will not redo this analysis here. Neither have we yet discussed the evaluation of the

canonical moments of the energy operator, which are required for the asymptotic expansion of the Gaussian expectation values—this will be the subject of a subsequent work, where we will also show how lattice Monte Carlo methods can be employed in evaluation of the Gaussian expectation values.

For sake of mathematical definiteness, we have in this paper inspected only quantum mechanical systems, but on the level of formal manipulation, the results given here can be equally well interpreted as statements about statistical quantum *field* theory. Since canonical quantum field theory is already a well developed part of the physicists' toolkit [11], this is not as bold a claim as it looks at first sight. In fact, the formulation of the quantum microcanonical ensemble given in [3] can also be obtained from the  $\varepsilon, \beta \rightarrow 0^+$  limit of the Gaussian formula (10), which might then lead to a more rigorous derivation of that formulation after the intricacies in the definition of four-dimensional statistical quantum field theories have been resolved.

### Acknowledgments

I would like to thank Masud Chaichian, Antti Kupiainen, Claus Montonen and Esko Suhonen for patient commentary and reading of the manuscript and Sami Virtanen and Arttu Rajantie for several useful discussions.

### References

- [1] Redlich K, Cleymans J, Satz H and Suhonen E 1994 *Nucl. Phys. A* **566** 391c
- [2] Braun-Munzinger P, Stachel J, Wessels J P and Xu N 1996 *Phys. Lett. B* **365** 1
- [3] Chaichian M and Senda I 1993 *Nucl. Phys. B* **396** 737  
Chaichian M, Satz H and Senda I 1994 *Phys. Rev. D* **49** 1566
- [4] Landau L D and Lifshitz E M 1980 *Statistical Physics (Course of Theoretical Physics vol 5)* 3rd edn (Oxford: Pergamon)
- [5] Balian R 1991 *From Microphysics to Macrophysics* vol 1 (Berlin: Springer)
- [6] Thirring W 1980 *Quantum Mechanics of Large Systems (A Course in Mathematical Physics vol 4)* (Wien: Springer)
- [7] Hetherington J H and Stump D R 1987 *Phys. Rev. D* **35** 1972
- [8] Simon B 1979 *Functional Integration and Quantum Physics* (New York: Academic). Theorem 9.2. gives a path-integral exposition of the Golden–Thompson–Symanzik formula.  
Golden S 1965 *Phys. Rev. B* **137** 1127  
Thompson C J 1965 *J. Math. Phys.* **6** 1812  
Symanzik K 1965 *J. Math. Phys.* **6** 1155
- [9] Rudin W 1987 *Real and Complex Analysis* 3rd edn (New York: McGraw-Hill) ch 3
- [10] Green M B, Schwarz J H and Witten E 1987 *Superstring theory I: Introduction* (Cambridge: Cambridge University Press) section 2.3.5.
- [11] Le Bellac M 1996 *Thermal Field Theory* (Cambridge: Cambridge University Press)