Commun. Math. Phys. 89, 117–129 (1983)

Communications in
Mathematical
Physics
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Steepest Descent Path for the Microcanonical Ensemble-Resolution of an Ambiguity

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Abstract. The microcanonical entropy plays an essential role in the equilibrium statistical mechanics of gravitating systems. A peculiar feature of many of these systems is the existence of stable thermodynamic equilibrium configurations with negative heat capacities. Different methods have been developed for calculating the microcanonical entropy involving multivariate integrals of constraints and functional integrations. An apparent ambiguity between an approach due to Hawking and Gibbons, based on an entropy definition involving an inverse Laplace transform of the partition function, which they developed to treat quantum systems with gravity, and a different approach developed by Horwitz and Katz defining the entropy as an equal weight sum over a constant energy surface developed originally to treat Newtonian and classical GR systems is shown here to be spurious, at least at the level of quadratic fluctuations of all variables about the extremal solutions. The two approaches involve distinct contours for different orders of integration, each of which is shown to be the appropriate steepest descent path corresponding to the given order of investigation. Up to quadratic fluctuations both methods yield identical results. However, they represent different perturbation expansions for the gravitational modes of freedom with different radii of convergence. The discussion is made in terms of a particular convenient model, a system of point particles interacting via Newtonian forces, confined to a sphere, but results are quite general.

I. Introduction

Calculations using a microcanonical ensemble (MCE) involve many practical difficulties for virtually any system. On the basis of the equivalence of different ensemble which is valid for the usual uniform system, one commonly carries out calculations in the most convenient ensemble and then one obtains the entropy by means of a Legendre transformation. Thus, for classical systems, standard calculations use either the canonical ensemble (CE) or the grand canonical ensemble (GCE). The entropy is then obtained for the CE as the energy transform of the Helmholtz free energy F_N:

$$S(E, V, N) = -\beta F_N + \beta E, \tag{1}$$

where the temperature $T = \beta^{-1}$ (the Boltzmann constant $= k_B = 1$), or for the GCE from the grand potential q with an energy and particle number Legendre transform:

$$S(E, V, N) = -\beta q + \beta E - \alpha N, \tag{2}$$

with the chemical potential $\mu = \alpha/\beta$.

For quantum systems one commonly calculates with the GCE for reasons of calculational simplicity [2], carrying out the Legendre transform (2). For gravitational systems, the above is, in general inadequate. Self-bound gravitational systems are typically nonuniform in space or in time; ensemble equivalence has been shown to break down for such systems [3]. There exist stable thermodynamic equilibrium (TDE) configurations and TDE models which are found to be stable for MCE constraints (fixed E, V, N) which could not exist stably or in some cases not at all for systems in contact with a heat bath (CE) or heat and particle baths (GCE) [4]. These results have been known for some time and although there was some reluctance to accept stable negative heat capacity systems, they have been generally acknowledged. Examples include Newtonian [5] and general relativistic [6] models of spherical star clusters, quantum states for stars [7] and TDE black holes in radiation cavities [8], a FRW universe with positive cosmological constant and scalar conformal bosons [9]. In all of these cases the ensemble dependence of the stability conditions is striking: the range of parameters yielding stability is increased as one imposes more constraints, hence limiting fluctuations. For parameters corresponding to an unstable CE, but stable MCE, the heat capacity is negative; thus the physical partition function does not exist. An approximate partition function, e.g. that of the mean field approximation can exist and be real but will have unstable fluctuations.

Gravitating systems raise more basic problems in their statistical mechanics treatment than the ensemble dependence; the problem of formulating the equilibrium or nonequilibrium statistical mechanics for these systems presenting many difficulties. For a Newtonian potential or for GR only in the form of a background metric, more or less standard definition can be used, but there are serious convergence problems, spatially or temporally. However, for classical GR even more strikingly than for quantum GR, there is no obvious first principle definition for the entropy when gravity contributes to the statistical state.

In an earlier work on Newtonian systems [5], a functional integral formulation for the MCE entropy of TDE systems was derived; CE and GCE results for spherical star clusters were obtained for various models [10] and compared with those for the MCE. A phenomenological, analogous treatment was developed for classical GR systems again for various ensembles, including the MCE [6]. Subsequently, we were able to calculate the MCE for quantum fields with cosmological metrics in a formalism based on quantum gravity [9] from which a quasi-classical contribution was extracted [11]. A particular feature of this method was that the quadratic form was diagonalized in a specific order, constraint variables prior to gravitational degrees of freedom, in order to obtain the correct ensemble dependent stability conditions.

A different approach was developed for evaluating the entropy of quantum fields and quantum gravity by Hawking [12] and Gibbons and Hawking [13]. In their approach, they postulated the partition function Z_N on the Feynman formalism as a functional integral over the Euclideanized action including gravity, correcting the usual gravitational Lagrangian by a surface term. The entropy was then determined not from the thermodynamic connection of the Legendre transform (1), but instead as the inverse Laplace transform of Z_N (expressed as a Feynman integral)

$$\exp S = \int d\beta/2\pi i \exp \beta E \quad Z_N = \int [d\phi] \int d\beta/2\pi i \exp \beta E \exp - I(\beta, \{\phi\}), \quad (3)$$

the β integral being taken perpendicular to the real axis. This formulation was introduced with the awareness of the necessity of using the MCE, when the heat capacity is negative. However, precisely for such conditions the partition function is not well defined; this difficulty they resolved by rotating contours in a manner which we shall discuss in more detail below. However, they gave no real justification for the distortion of the integration contours which were introduced to make the integrals finite and real, and there was no clear statement of the conditions for stability of the results obtained. Partial answeres to these questions are given in the work of Gibbons et al. [14].

After we summarize the two formulations we shall observe that their respective bases are conceptually different, but they are, in particular cases, formally equivalent except for involving different orders of integration and correspondingly different contours when stable negative heat capacity systems occur. At the level of quadratic expansion around the extremal values in all variables, the steepest descent paths depend on the order of integration, the original contour being the appropriate steepest descent path for the order of integration used by Horwitz and Katz, and the rotated contours the appropriate ones for the order of integration used by Hawking and coworkers. Both are correct when appropriately used and lead to identical stability conditions. They, however, represent different expansions and potentially have different convergence conditions. This difference is especially noteworthy when noting that the common approximations involve treating the integrals of the statistical constraint (β) quadratically to test convergence and treating the gravitational variables by a perturbation expansion not necessarily limited to one loop. Most of these points will be illustrated in terms of a system of classical point masses interacting via Newtonian forces in a closed volume. The results obtained are, however, quite general; but for heuristic reasons, we chose to develop it in terms of a specific model.

II. Formulation of the Thermodynamic Equilibrium MCE

Let us first consider some arbitrary system which can be described in terms of a classical action; we shall assume that the system has among its constants of motion a suitable energy operator, a Hamitonian obtained as a projection of the energy-momentum tensor on a static time-like Killing vector [15] characterizing the background metric. Then we can define the Gibbs MCE entropy for thermodynamic equilibrium

$$\exp S = \mathrm{Tr}^{(N)}\,\delta(E-H) \tag{4}$$

(the Dirac deltafunction should more properly be spread over a narrow energy range small compared to E, but this difference is not significant in our analysis). The trace here is an equal weight sum over N particle states for the quantum system, and the corresponding result for classical systems is an integral over a $6N$-dimensional phase space multiplied by a factor of $(N!)^{-1}$. Introducing an integral representation of the δ-function

$$\exp S(E,V,N) = \mathrm{Tr}^{(N)} \int_{-i\infty+\beta_0}^{+i\infty=\beta_0} d\beta/2\pi i \exp(\beta E - \beta H)\,. \tag{5}$$

If the order of integration does not matter this becomes

$$\exp S(E,V,N) = \int_{\beta_0-i\infty}^{\beta_0+i\infty} d\beta/2\pi i \exp \beta E \cdot Z_N\,, \tag{6}$$

where the partition function Z_N analytically continued to complex β:

$$Z_N = \mathrm{Tr}^{(N)} \exp - \beta H = \exp - \beta F_N(\beta) \tag{7}$$

with F_N, the Helmoltz free energy; this result is the inverse Laplace transform relation (3). The partition function can be expressed as a Feynman integral

$$\mathrm{Tr}^{(N)} \exp - \beta H = \int [d\phi_a] \exp - I\{\phi_a\}\,, \tag{8}$$

where the ϕ_a represents the various field in I, $[d\phi_a]$ is a measure of the function space and $I\{\phi_a\}$ is the "Euclideanized" action corresponding to $\phi_a(0) = \pm\phi_a(\beta)$, the upper sign corresponding to boson and the lower to fermion operators.

In this way we have obtained the entropy in the form of an inverse Laplace transform of the partition function. One commonly then relates the results of steepest descent integration of β whose extremal value identified with β_0 is the Legendre transform relation

$$S_{\mathrm{ext}} = \beta_0 E - \beta_0 F_N(\beta_0, V)\,, \tag{9}$$

where β_0 is determined by

$$E = \langle H \rangle_0 \equiv \mathrm{Tr}^{(N)}(H \exp - \beta_0 H)/\mathrm{Tr}^{(N)} \exp - \beta_0 H\,, \tag{10}$$

and whose convergence is associated with positive fluctuation term in the β integral (since the path of integration is over imaginary values)

$$\left.\frac{\partial^2(-\beta F_N)}{\partial \beta^2}\right|_0 = \frac{\partial \langle H \rangle_0}{\partial \beta} = \langle H^2 \rangle_0 - \langle H \rangle_0^2 = \beta_0^{-2} C_V\,, \tag{11}$$

C_V being the heat capacity at fixed V and N. The apparent instability when C_V is negative contradicts the results found in a variety of cases involving gravitating systems where negative heat capacity domains are known to be stable thermodynamic equilibrium states. Probably the simplest example of a system showing this kind of behavior is a system of N, equal mass ($m=1$), classical particles interacting via Newtonian forces confined to a spherical volume, with the potential cut off at short distances to prevent divergences due to clustering. All the essential features of the general problem are illustrated by this simple system.

Aside from the ensemble dependence, we note that gravitating systems show a number of unusual features among which are:

1) The absence of the usual thermodynamic limit, N and V going to infinity with N/V finite; but some cases have an alternative limiting behavior [7].

2) A property related to 1) is that TDE gravitating systems are usually nonuniform spatially, or in cosmology temporally; this presents along with other problems substantial computational complexity.

3) The physical relevance of the CE or GCE becomes questionable when gravitational forces contribute to the TDE state: one can no longer treat part of a closed system as a CE or GCE due to the long range of gravitational interactions. The replica definition of these ensembles [16] may be still formally meaningful, but the applicability is uncertain; this is relevant even when C_V is positive.

4) The problems we have presented above, associated with the treatment of negative heat capacity domains for the inverse Laplace transform relations, will be seen to be associated with the technical difficulties of treating the multivariate integrals involving constraint integrals like that over β and sums over gravitational degrees of freedom of the system.

The last two points are the central issues of the present work, particularly 4).

III. The MCE for Newtonian Particles in a Spherical Volume

We shall discuss some very basic problems of functional integrals with microcanonical constraints for the specific, simple, classical model. This model calculation illustrates all of the essential problems of ensemble dependence of gravitational systems generally. Our system consists of N particles of mass $m=1$, interacting via Newtonian forces and confined to a spherical volume $V=\frac{4}{3}\pi R^3$. There is an implicitly assumed short distance cut off in the potential, but this will not be explicitly indicated, as at the level of approximation which we examine explicitly it has no consequences except to eliminate the UV divergence of our fluctuation spectrum; our concern in the present work is with the thermodynamic limit of stability which is a long wavelength instability. We use units in which $8\pi G=1$, G being the Newtonian constant. Thus we consider the Hamiltonian:

$$H=\frac{1}{2}\sum_{i=1}^{N} p_i^2+V=T-\frac{1}{2}\sum_{i,j}{}'(|x_i-x_j|)^{-1}. \tag{12}$$

The MCE entropy can then be written

$$\exp S=\int\prod_{i=1}^{N} d^3x_i d^3p_i/N!\,\delta(E-H)\equiv\int\frac{d\omega^{(N)}}{N!}\delta(E-H). \tag{13}$$

This is conveniently represented in the form

$$\exp S=\int d\omega^{(N)}/N!\int_{\beta_0-i\infty}^{\beta_0+i\infty} \mathrm{d}\beta/2\pi\mathrm{i}\exp\beta(E-H). \tag{14}$$

This can be expressed as a functional integral [5, 17] of one particle terms by noting that

$$V=-\frac{1}{2}\sum_{i\neq j=1}^{N}(|x_i-x_j|)^{-1}=\frac{1}{2}\int d^3xd^3y\varrho(\mathbf{x})v(|\mathbf{x}-\mathbf{y}|)\varrho(\mathbf{y}), \tag{15}$$

where

$$\varrho(\mathbf{x})\equiv\sum_{i=1}^{N}\delta(\mathbf{x}_i-\mathbf{x}), \tag{16}$$

and

$$v(|\mathbf{x}-\mathbf{y}|)=-(|\mathbf{x}-\mathbf{y}|)^{-1}. \tag{17}$$

Thus with V expressed as a quadratic form in ϱ:

$$\exp-\beta V=\exp-\tfrac{1}{2}\beta\int d^3xd^3y\varrho(\mathbf{x})v(\mathbf{x}-\mathbf{y})\varrho(\mathbf{y}), \tag{18}$$

one can write the functional expression:

$$\exp-\beta V=C\int[dW(x)]\exp-[\int d^3xd^3yW(\mathbf{x})v^{-1}(\mathbf{x}-\mathbf{y})W(\mathbf{y})+\beta^{1/2}\int d^3x\varrho(\mathbf{x})W(\mathbf{x})]. \tag{19}$$

Here C is an irrelevant constant (generally infinite) normalization factor, and the inverse potential v^{-1} is given by

$$\int d^3yv(\mathbf{z}-\mathbf{y})v^{-1}(\mathbf{y}-\mathbf{x})=\delta(\mathbf{x}-\mathbf{y}). \tag{20}$$

$W(\mathbf{x})$ must go asymptotically as $1/|\mathbf{x}|$ as $|\mathbf{x}|\to\infty$, and in the case of the Newtonian potential (ignoring the short distance cutoff)

$$v^{-1}(\mathbf{x}-\mathbf{y})=-2\Delta\delta_x(\mathbf{x}-\mathbf{y}), \tag{21}$$

and the contour of the integration of $W(\mathbf{x})$ is taken over real functions in order to get the convergent quadratic form since V is negative. Then

$$\begin{aligned}\exp S=\int[dW(\mathbf{x})]\int d\beta/2\pi i\prod_{i=1}^{N}\int d^3x_id^3y_i\\ \cdot\exp\left[\int d^3xW(\mathbf{x})\Delta W(\mathbf{x})+\beta E-\beta\sum_i p_{i/2}^2-\sqrt{\beta}\sum_i W(\mathbf{x}_i)\right].\end{aligned} \tag{22}$$

Due to homogeneity of the solution, we obtain (in the large N limit)

$$\exp S=\int[dW(\mathbf{x})]\int d\beta/2\pi i\exp\Psi(N,\beta,\{W(\mathbf{x})\}), \tag{23}$$

where

$$\Psi(N,\beta,\{W(\mathbf{x})\})\equiv\int d^3xW\Delta W+\beta E+N\ln N-N+N\ln\Phi(\beta,\{W\}), \tag{24}$$

with

$$\Phi(\beta,\{W(x)\})\equiv\iint d^3xd^3p\exp-[\tfrac{1}{2}\beta p^2+\sqrt{\beta}\,W(\mathbf{x})]. \tag{25}$$

This is a somewhat different form from that which we exploited in [5], where an additional constraint integral was introduced for N. In fact, it is analogous to our treatment there of the relation between the GCE and the CE involving the N

constraint integral instead of the E constraint integral. In order to deal with the question of the order of integration in the simplest and clearest way, we have preferred here to express results in a manner which involves only a single constraint integral.

We now proceed to evaluate S by expanding about the extrema in β and $W(\mathbf{x})$ respectively and then examining the quadratic fluctuations.

$$\Psi = \Psi^{(0)} + \Psi^{(2)} + \delta\Psi\,, \tag{26}$$

with the first order fluctuations vanishing:

$$\begin{aligned} 0 = \Psi^{(1)}(N, \beta, \{W_0(x)\}) &= \delta\beta\{E - \int d\omega \tfrac{1}{2} f_0(x,p)[p^2 + W_0(\mathbf{x})/\beta_0^{1/2}]\} \\ &+ \int d^3x \delta W(\mathbf{x})[2\Delta W_0 - \beta_0^{1/2} n_0(\mathbf{x})]\,, \end{aligned} \tag{27}$$

(the latter after an integration by parts since $W(x)$ asymptotically $\sim |\mathbf{x}|^{-1}$) where the resulting distribution function f_0 is:

$$f_0(\mathbf{x}, \mathbf{p}) = N \exp - \tfrac{1}{2}\beta_0 p^2 - \beta_0^{1/2} W_0(x) / \int d\omega \exp - [\tfrac{1}{2}\beta_0 p^2 + \beta_0^{1/2} W_0(\mathbf{x})]\,, \tag{28}$$

and the corresponding density

$$n_0(x) = \int d^3p f_0(\mathbf{x}, \mathbf{p}) = N \exp - \beta_0^{1/2} W_0(\mathbf{x}) / \int d^3x \exp - \beta_0^{1/2} W_0(\mathbf{x})\,. \tag{29}$$

The vanishing coefficient of δW corresponds to the Poisson equation for the mean Newtonian potential

$$U_0(\mathbf{x}) = W_0(\mathbf{x})/\beta_0^{1/2}\,, \tag{30}$$

while the vanishing of the coefficient of $\delta\beta$ determines the temperature $T_0 = \beta_0^{-1}$ as a function of the energy E of the gravitating particles in the mean field approximation of the gravitational energy.

The zero order term is then

$$\Psi^{(0)} \equiv \beta_0 \int d^3x U_0 \Delta U_0 + \beta_0 E + N \ln N - N + N \ln \Phi(\beta_0, \{W_0\})\,, \tag{31}$$

while the quadratic fluctuations can be written in the form

$$\Psi^{(2)} = \tfrac{1}{2} D(\delta\beta/\beta_0)^2 - \int d^3x B(\mathbf{x}) \delta W(\mathbf{x}) \delta\beta/\beta_0 - \tfrac{1}{2}\iint d^3x d^3y \delta W(\mathbf{x}) 0(\mathbf{x}, \mathbf{y}) \delta W(\mathbf{y})\,, \tag{32}$$

where

$$B(\mathbf{x}) = n_0(x)(1 - \beta_0 U_0(x) + \beta_0 \bar{U}_0) \equiv \beta_0^{1/2} \tilde{n}_0(\mathbf{x})\,, \tag{33}$$

and

$$D \equiv \beta_0[(2T_0 + V_0) + \tfrac{1}{2}\beta_0 N(U_0^2 - \bar{U}_0^2)]\,, \tag{34}$$

with the bar denoting the average

$$\bar{A} = N^{-1} \int d^3x A(\mathbf{x}) n_0(\mathbf{x})\,. \tag{35}$$

The mean kinetic and potential energies are respectively

$$T_0 = \tfrac{3}{2} N \beta_0^{-1}\,, \tag{36}$$

and

$$V_0 = \tfrac{1}{2} N \bar{U}_0\,, \tag{37}$$

and the binary fluctuation operator

$$O(x, y) = [-2\Delta_x - \beta_0 n_0(\mathbf{x})]\delta(\mathbf{x}-\mathbf{y}) + N^{-1}\beta_0 n_0(\mathbf{x}) n_0(\mathbf{y})] . \tag{38}$$

The central point of our analysis is now to determine what are the conditions on the quadratic form (32) such that the integrals on $\delta\beta$ and δW lead to a convergent, real result. In terms of the defining integrals for β (14) and for $W(\mathbf{x})$: (18), the contours are defined in a particular way, perpendicular to the real axis for β and for real functions $W(\mathbf{x})$. In terms of these contours, different orders of diagonalizing the quadratic form appear altogether nonequivalent, as we shall see more precisely below: If we diagonalize first with respect to $\delta W(\mathbf{x})$, we arrive at a form equivalent to the inverse Laplace transform relation (6) with the partition function evaluated as a quadratic expansion around the extremal solution in $W(\mathbf{x})$. This corresponds to the starting point of Hawking and Gibbons and would appear to lead to a breakdown of convergence according to (11), when C_V changes sign plus to minus infinity. They then proposed rotating the contour when C_V is negative. The alternative order of diagonalization which was employed by Horwitz and Katz was to diagonalize with respect to β first. Thus, in the first approach one finds

$$\Psi_I^{(2)} = \tfrac{1}{2}\tilde{D}(\delta\beta/\beta_0)^2 - \tfrac{1}{2}\iint d^3x d^3y \delta\hat{W}(x) O(\mathbf{x}, \mathbf{y}) \delta\hat{W}(y) , \tag{39}$$

where

$$\delta\tilde{W}(\mathbf{x}) = \delta W(\mathbf{x}) + \int d^3y O^{-1}(\mathbf{y}, \mathbf{x}) B(\mathbf{y}) , \tag{40}$$

with

$$\int O^{-1}(\mathbf{x}, \mathbf{y}) O(\mathbf{y}, \mathbf{z}) d^3y = \delta(x-z) , \tag{41}$$

and

$$\tilde{D} = D + \iint d^3x d^3y B(\mathbf{x}) O^{-1}(\mathbf{x}, \mathbf{y}) B(\mathbf{y}) . \tag{42}$$

It is clear that

$$\tilde{D} = C_V . \tag{43}$$

In the other order of diagonalizing, we obtain

$$\Psi_{II}^{(2)} = \tfrac{1}{2}D(\delta\tilde{\beta}/\beta_0)^2 - \tfrac{1}{2}\iint d^3x d^3y \delta W(\mathbf{x}) \tilde{O}(\mathbf{x}, \mathbf{y}) \delta W(\mathbf{y}) , \tag{44}$$

where

$$\delta\tilde{\beta}/\beta_0 = \delta\beta/\beta_0 - \int d^3x \delta W(\mathbf{x}) B(\mathbf{x}) , \tag{45}$$

and

$$\tilde{O}(\mathbf{x}, \mathbf{y}) = O(\mathbf{x}, \mathbf{y}) - \beta_0 \tilde{n}(\mathbf{x}) \tilde{n}(\mathbf{y}) / D . \tag{46}$$

In the form $\Psi_I^{(2)}$ it would appear that the condition of having a negative definite quadratic form given $(\delta\beta)^2$ is negative is that $C_V > 0$ and that the quadratic form $\iint \delta^3 x \delta^3 y \delta W_O \delta\tilde{W}$ is positive definite. As we shall see below, the spectrum of $O(\mathbf{x}, \mathbf{y})$ determines both, when the lowest eigenvalue of $O(\mathbf{x}, \mathbf{y})$ goes negative, both the $\delta\beta$ integral and one of the integrals of the functional integrals of δW go negative. This appears as a breakdown of stability, but in fact if we were to carry out the integral over the quadratic form in the regime where the eigenvalue approaches zero and go to the limit, we find a finite result, see below. These divergences are then seen to be spurious. The Hawking and Gibbon procedure was to rotate the contour; this corresponds then to going over to the appropriate steepest descent path for the order of diagonalization which they use into the region with negative heat capacity. In the other order $\tilde{D}$ does not change sign when D does, and the lowest eigenvalue of $\tilde{O}(\mathbf{x}, \mathbf{y})$ is shifted from that of $O(\mathbf{x}, \mathbf{y})$, so that it changes sign under completely different conditions. Thus, there is no problem of carrying out the quadratic integration to and beyond the point where the heat capacity goes negative; the limit of stability is then found to be where $C_V = 0$, corresponding to where the lowest eigenvalue of $\tilde{O}(\mathbf{x}, \mathbf{y})$ goes to zero. In the analysis below we will show that this same limit of stability is found by use of the first diagonalization and corresponding integration path of Hawking and Gibbons. Let us now turn to examine the matter in more detail.

IV. Eigenvalue Analysis of the Quadratic Fluctuations

It is most convenient to express the results in terms of a spectrum related to the operator $O(\mathbf{x}, \mathbf{y})$, Eq. (38), but we cannot use the ordinary eigenvalue expression $\int d^3y O(\mathbf{x}, \mathbf{y})\psi_r(\mathbf{y}) = \varepsilon_r \psi_r$, because the asymptotic properties of $W(x) \sim |\mathbf{x}|^{-1}$, $|\mathbf{x}| \to \infty$ would lead to eigenfunctions without finite norms. Instead we proceed as in [5] to consider the orthonormal solutions of

$$\int O(\mathbf{x}, \mathbf{y})\varphi_\lambda(\mathbf{y}) d^3y = \varepsilon_\lambda(-\Delta)\varphi_\lambda(x), \tag{47}$$

with normalization defined by

$$\int d^3x \varphi_\lambda(\mathbf{x})(-\Delta)\varphi_\mu(\mathbf{x}) = \delta_{\lambda\mu}. \tag{48}$$

Then expanding $\delta\tilde{W}(\mathbf{x})$ in the $\varphi_\lambda(\mathbf{x})$

$$\delta\tilde{W}(\mathbf{x}) = \sum_\lambda a_\lambda \varphi_\lambda(\mathbf{x}), \tag{49}$$

with (49) the quadratic form $\Psi_I^{(2)}$ (39) becomes

$$\Psi_I^{(2)} = -\tfrac{1}{2}\sum_\lambda \varepsilon_\lambda a_\lambda^2 - \tfrac{1}{2}\tilde{D}(\delta\beta/\beta_0)^2, \tag{50}$$

where in terms of this spectrum

$$\tilde{D} = D + \sum_\lambda A_\lambda^2/\varepsilon_\lambda = D\Sigma_0, \tag{51}$$

with

$$A_\lambda = \int d^3x B(\mathbf{x})\varphi_\lambda(\mathbf{x}). \tag{52}$$

Thus the relation between D and the heat capacity is

$$C_V = D + \sum_\lambda A_\lambda^2/\varepsilon_\lambda, \tag{53}$$

which is positive when all eigenvalues $\varepsilon_\lambda > 0$, and diverges positively when $\varepsilon_1 = 0$, and then goes negative for ε_1 going negative. If we find as was the case for various models of star clusters, that the eigenvalues decrease monotonically with a relevant parameter, then beyond the value where the lowest eigenvalue goes negative, the next eigenvalue (say ε_2) goes to zero and then negative in turn. Then when ε_2 goes to zero, C_V must again diverge positively. In between the zeroes of the first two eigenvalues there must therefore be a zero of C_V; as we shall show (cf. [5]), that corresponds to the true singularity and stability limit for the microcanonical ensemble. Here $C_V = 0$ corresponds to the unbounded fluctuations in the temperature of a microcanonical system, the physically plausible result for a system constrained to have fixed energy.

The alternative diagonalization $\Psi_{II}^{(2)}$ will also be evaluated in terms of this spectrum ε_λ. Introducing the φ_λ representation,

$$\Psi_{II}^{(2)} = \frac{1}{2} D(\delta\tilde{\beta}/\beta_0)^2 - \frac{1}{2} \sum_\lambda \varepsilon_\lambda a_\lambda^2 - \frac{1}{2}\left(\sum_\lambda A_\lambda a_\lambda\right)^2 \Big/ D - \frac{1}{2} \sum \varepsilon_\mu a_\mu^2 , \tag{54}$$

the states labelled μ refer to the unmodified nonspherical modes, $A_\mu = 0$. This is, of course, not yet diagonalized. If we now introduce the quantities

$$\begin{aligned} \Sigma_n &\equiv \sum_{\lambda > \lambda_n} A_\lambda^2 / \varepsilon_\lambda D , \\ \tilde{\varepsilon}_1 &= \varepsilon_1 + A_1^2 [(1 + \Sigma_1) D]^{-1} = \varepsilon_1 [(1 + \Sigma_0)/(1 + \Sigma_1)] , \end{aligned} \tag{55}$$

where

$$\Sigma_0 = \sum_{\lambda = \lambda_1} A_\lambda^2 / \varepsilon_\lambda D , \tag{56}$$

here λ_n denotes the n^{th} eigenvalue and

$${}^{(1)}a_\lambda = a_\lambda - a_1 A_1 A_\lambda [\varepsilon_\lambda (1 + \Sigma_1) D]^{-1} . \tag{57}$$

Then one finds

$$\Psi_{II}^{(2)} = \frac{1}{2} D(\delta\beta/\beta_0)^2 - \frac{1}{2} \tilde{\varepsilon}_1 a_1^2 - \frac{1}{2} \sum_{\lambda > \lambda_1} \varepsilon_\lambda^{(1)} \tilde{a}_\lambda^2 - \left(\sum_{\lambda > \lambda_1} {}^{(1)}a_\lambda A_\lambda\right)^2 \Big/ 2D - \frac{1}{2} \sum_\mu \varepsilon_\mu a_\mu^2 . \tag{58}$$

Since this leaves the quadratic form for terms $\lambda > \lambda_1$ in the identical form as in (54), this procedure can be trivially iterated to diagonalize completely the quadratic form:

$$\Psi_{II}^{(2)} = \tfrac{1}{2} D(\delta\beta/\beta_0)^2 - \tfrac{1}{2} \sum \tilde{\varepsilon}_{\lambda_n}^{(n-1)} a_{\lambda_n}^2 - \tfrac{1}{2} \sum \varepsilon_\mu a_\mu^2 . \tag{59}$$

Here

$$\tilde{\varepsilon}_{\lambda_n} \equiv \varepsilon_{\lambda_n} [(1 + \Sigma_n)/(1 + \Sigma_{n-1})] , \tag{60}$$

and

$${}^{(n-1)}a_{\lambda_n} = {}^{(n-2)}a_{\lambda_n} - {}^{(n-2)}a_{\lambda_{n-1}} A_{\lambda_{n-1}} A_{\lambda_n} [D \varepsilon_{\lambda_n} (1 + \Sigma_{n-1})]^{-1} . \tag{61}$$

Notice [see (53) and (55)] that $\tilde{\varepsilon}_1$ goes to zero when C_V goes to zero, and remains positive through the range of negative C_V.

V. Steepest Descent Contours and Interpretation of Quadratic Fluctuations

Let us now consider the steepest descent integration of $\Psi^{(2)}$ with the alternative orders of diagonalization of the quadratic form $\Psi_I^{(2)}$ and $\Psi_{II}^{(2)}$

$$I_{II} = \int d\delta\beta/2\pi i \int [d\delta W(\mathbf{x})] \exp \Psi_{II}^{(2)}(\delta\beta, \delta W(\mathbf{x})) = \int_{-\infty}^{\infty} d\bar{\beta}/2\pi \int \prod_{\lambda} da_{\lambda} \exp \Psi_{II}^{(2)}, \quad (62)$$

$$= \int_{-\infty}^{\infty} d\bar{\beta} \exp -\frac{1}{2} D(\delta\beta/\beta_0)^2 \prod_{\lambda} \int d\tilde{a}_{\lambda} \exp -\frac{1}{2} \sum_{n} \varepsilon_{\lambda_n} \tilde{a}_{\lambda_n}^2 [1+\Sigma_{n+1})/(1+\Sigma_n)], \quad (63)$$

where

$$i\delta\beta = \bar{\beta}, \quad (64)$$

$$I_{II} = (\pi\beta_0^2/D)^{1/2} \prod_{n=1}^{\infty} [(1+\Sigma_n)/(1+\Sigma_{n-1})]^{1/2} (\pi/\varepsilon_{\lambda})^{1/2} = \left[\frac{\pi\beta_0}{(1+\Sigma_0)D}\right]^{1/2} \prod_{\lambda} \left(\frac{\pi}{\varepsilon_{\lambda}}\right)^{1/2}, \quad (65)$$

$$= \exp -\frac{1}{2} \ln D/\pi\beta_0^2 - \frac{1}{2} \sum_{n} \ln \varepsilon_{\lambda_n} - \frac{1}{2} \ln(1+\Sigma_0), \quad (66)$$

$$= \exp -\frac{1}{2} \ln \tilde{D}/\pi\beta_0^2 - \frac{1}{2} \sum_{n} \ln \varepsilon_{\lambda_n}. \quad (67)$$

Notice this expression has no singularity at zeroes of $\bar{\varepsilon}_{\lambda}$ and is only singular at $1+\Sigma_0=0$. In [5] we have shown that there is no stable region beyond the first zero of $1+\Sigma_0$ in the star cluster problem. See a more detailed analysis of this problem by Katz [18].

If we now consider the alternative diagonalization $\Psi_I^{(2)}$, for $\varepsilon_1 > 0$, $C_V > 0$, and the given contour gives well defined results; in fact, exactly that of (66) obtained above for integration of $\Psi_{II}^{(2)}$. This remains well defined to the limit $\varepsilon_1 = 0$. The question is what to do when this point is passed and both ε_1 and D go negative. In that case the steepest descent path is distorted so that the $\bar{\beta}$ integral is taken parallel to the real axis in the neighborhood of the extremum and the a_1 integral is taken perpendicular to the real axis in the neighborhood of zero. This corresponds to the rotation of the contours proposed by Hawking and Gibbons. The two integrals are finite and real and yield for the entropy

$$\begin{aligned} S &= -\frac{1}{2} \ln D/\pi\beta_0^2 - \frac{1}{2} \sum_{\lambda > \lambda_1} \ln \varepsilon_{\lambda}/\pi - \ln[|\varepsilon_1|/|1+\varepsilon_0|] \\ &= \frac{1}{2} \ln D/\pi\beta_0^2 - \frac{1}{2} \sum_{\lambda > \lambda_1} \ln \varepsilon_{\lambda}/\pi - \ln \tilde{\varepsilon}_1, \end{aligned} \quad (67)$$

which remains identical with the previous result. However, when $\tilde{\varepsilon}_1 = 0$ and goes negative, an unstable regime has been reached. There is no rotation of the contour which will make the integral finite and real. Thus the $\tilde{\varepsilon}_{\lambda}$ are the physically relevant spectrum associated with the singularities for the thermodynamic fluctuations C_V^{-1}, the quadratic evaluation of the fluctuations around the mean field can be evaluated in whichever order of diagonalization one chooses with, however, the *appropriate* contour, which in these cases depends on the order of diagonalization.

If the quadratic evaluation were the whole story, that would be the end of the matter. But, in general, this quadratic evaluation is the basis of a more general expression based on a perturbation expansion. In that case the different orders of diagonalization represent different perturbation expansions with different domains of convergence. Furthermore, most commonly one terminates the expansion in the quadratic order of the constraint parameters $\delta\beta$, while developing a perturbation expansion in the field variables [here $\delta W(x)$]. In that case the perturbation expansion in $\delta W(x)$ will not be equivalent at all even in the domain where they are both convergent.

VI. Summary and Discussion

The central point of this work is the manner in which instability in the CE can be eliminated by the energy constraint. In the Horwitz-Katz formulation this is seen in an explicit modification of the fluctuation spectrum incorporating the constraint condition on the fluctuations. In the Hawking-Gibbons approach the unstable mode of the CE, which in other contexts might be interpreted as a bounce calculation (cf. Gross and Perry [19]), with the joint rotation of amplitude of the unstable mode and of the constraint variable yielding a finite and real value for the entropy. We have shown that these two versions appear as the corresponding steepest descent paths for different orders of diagonalizing the quadratic form of fluctuations, dynamic plus constraint, or equivalently the order of performing the integrations to the quadratic level. In a more general context where the quadratic treatment would be inadequate, the problem of what would comprise an acceptable perturbation expansion involving both types of variables remains uncertain. Beyond the level of terms quadratic in δW and $\delta\beta$, it is not at all obvious whether any kind of convergent expansion exists which does not mix $\delta\beta$ and δW fluctuations. For example, in some approximation like that which we have evaluated for the generalized random phase approximation (RPA) for a star cluster in the GCE [20], the density depends on the quadratic fluctuations in the form

$$\tilde{n}(\mathbf{x}) = \exp\Lambda \quad n(\mathbf{x}), \tag{68}$$

where

$$\Lambda = \sum_{\lambda} A_\lambda^2 / D\varepsilon_\lambda . \tag{69}$$

This diverges when ε_1 goes to zero and no distortion of the contour can rectify this. For this type of difficulty it is clear that a modified spectrum incorporating coupling to the $\delta\beta$ fluctuations would thoroughly modify the result. Thus there would appear to be some distinct advantages to the choice in which there is no singular behavior for the perturbation expansion and hence doing the constraint integrals first would appear to be a preferable way of evaluating the entropy in the presence of gravity.

Acknowledgements. I would like to thank D. Sciama for inviting me to Oxford where the stimulation to complete this work was achieved. E. Brenzin's remarks at an early stage of our work on steepest descent calculations in gravitational systems would have solved this problem long ago, if I had caught its significance. Thanks are also due to for useful conversations to D. Weil, J. Katz, and S. Elizur.

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Communicated by S. W. Hawking

Received November 10, 1982